Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 09:51 am BST

PDB ID	:	7ASE
EMDB ID	:	EMD-11893
Title	:	43S preinitiation complex from Trypanosoma cruzi with the kDDX60 helicase
Authors	:	Bochler, A.; Brito Querido, J.; Prilepskaja, T.; Soufari, H.; Del Cistia, M.L.; Kuhn, L.; Rimoldi Ribeiro, A.; Valasek, L.S.; Hashem, Y.
Deposited on	:	2020-10-27
Resolution	:	3.33 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

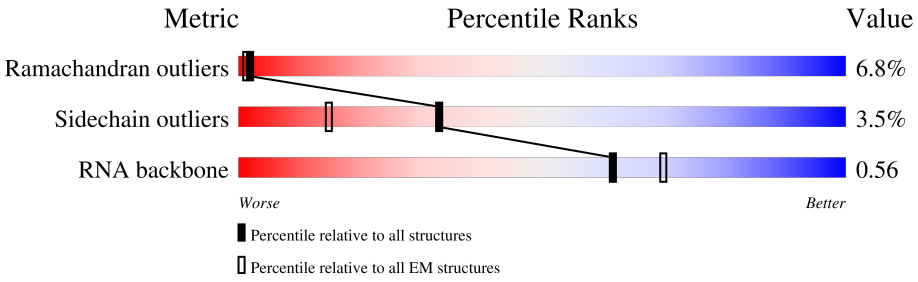
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	f	2174	54% 55% 10% 30%
2	1	75	13% 85% 15%
3	0	2319	18% 74% 17% 7%
4	y	137	9% 88% 10%
5	s	418	58% 58% 9% 29%
6	j	150	35% 46% 7% 47%
7	n	343	43% 58% 7% 34%
8	p	318	38% 93%

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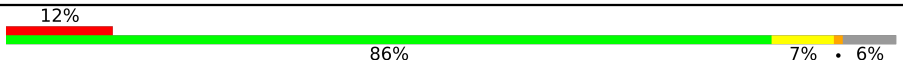
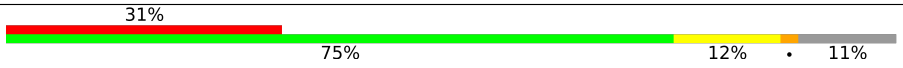
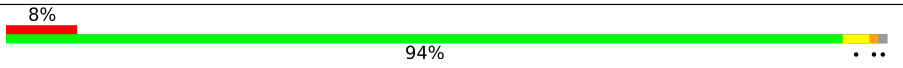
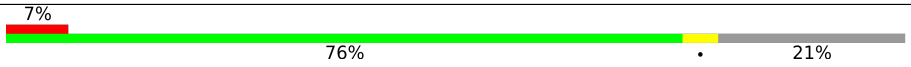
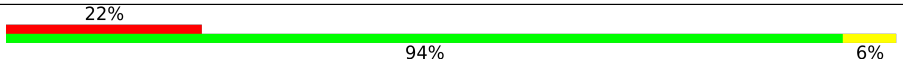
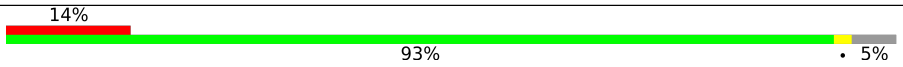
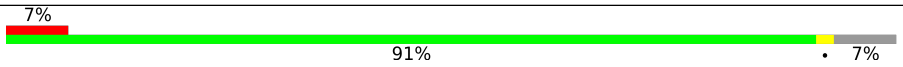
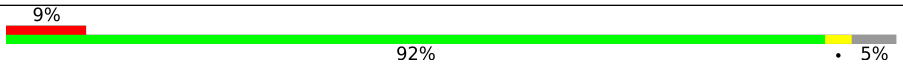
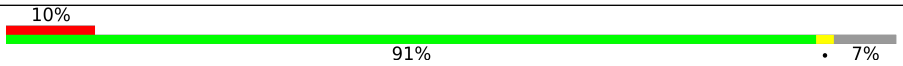
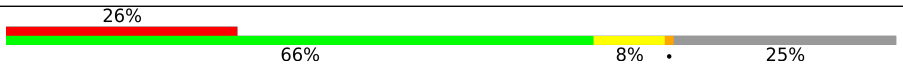
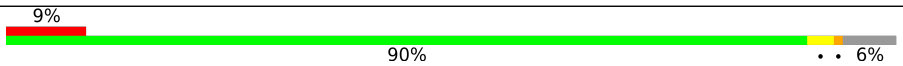
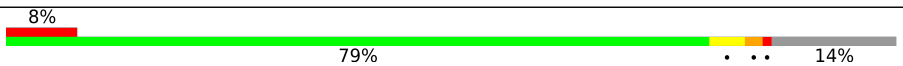
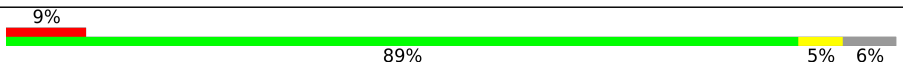
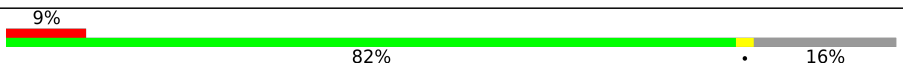
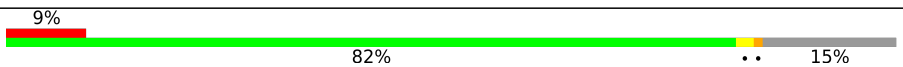
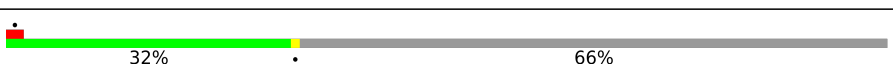
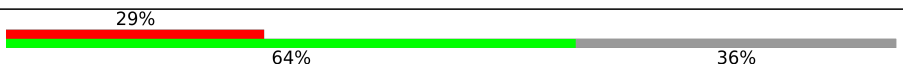
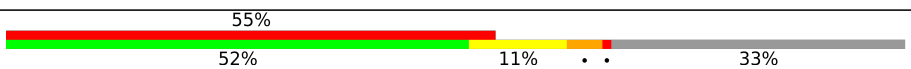
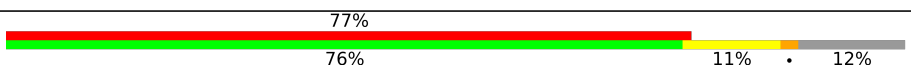
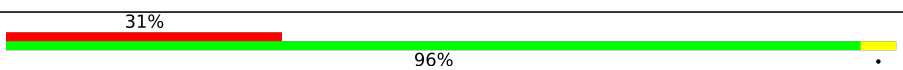
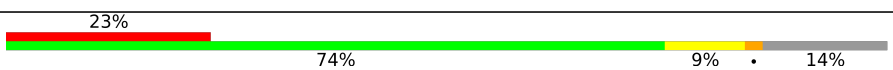
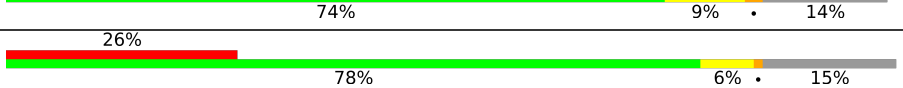
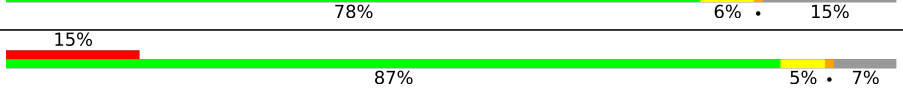
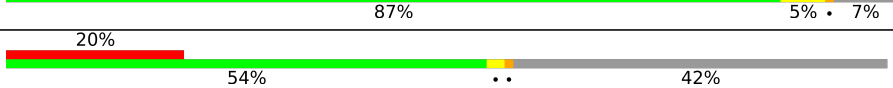
Mol	Chain	Length	Quality of chain
9	r	149	
10	u	153	
11	m	143	
12	Z	221	
13	o	190	
14	q	211	
15	R	151	
16	S	86	
17	t	112	
18	U	91	
19	v	144	
20	X	173	
21	B	190	
22	F	245	
23	d	263	
24	g	247	
25	a	110	
26	J	257	
27	h	141	
28	5	477	
29	P	250	
30	i	141	
31	L	117	
32	M	214	
33	N	161	

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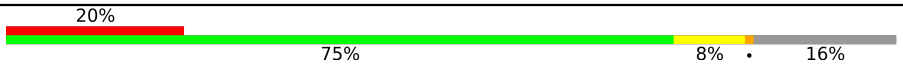
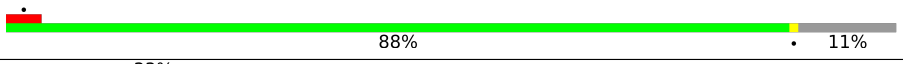
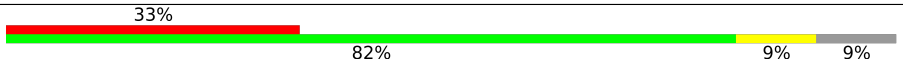
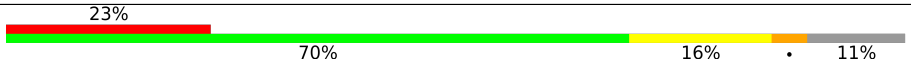
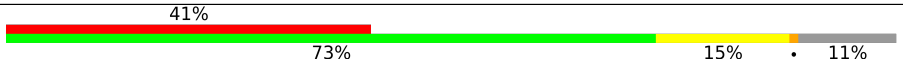
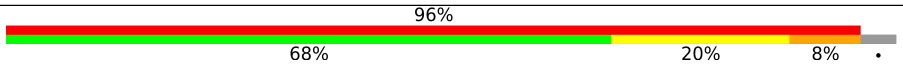
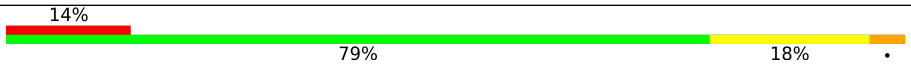
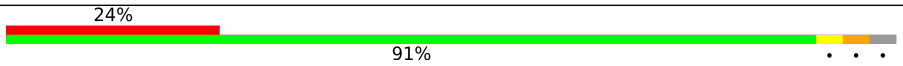
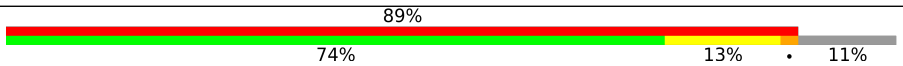
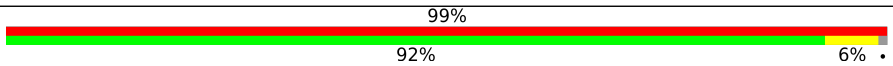
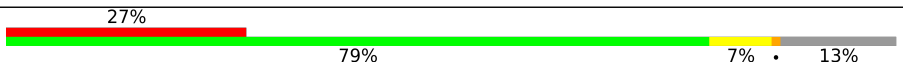
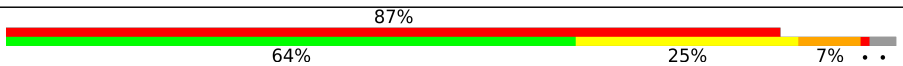
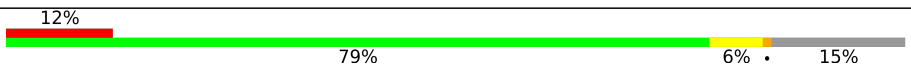
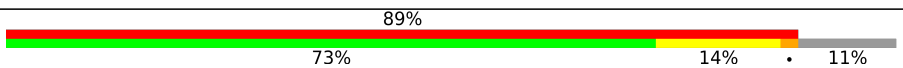
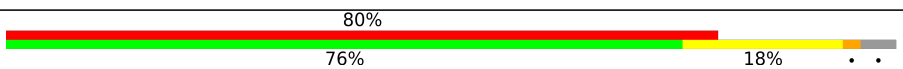
Mol	Chain	Length	Quality of chain
34	O	167	
35	b	145	
36	c	66	
37	V	109	
38	w	166	
39	E	407	
40	Y	379	
41	Q	57	
42	D	34	
43	G	345	
44	K	203	
45	T	152	
46	C	716	
47	8	762	
48	W	254	
49	I	489	
50	H	334	
51	A	502	
52	l	273	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 136847 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called kDDX60.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	1523	Total	C	N	O	S	0	0
			12257	7734	2165	2292	66		

- Molecule 2 is a RNA chain called initiator tRNA-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	75	Total	C	N	O	P	0	0
			1606	718	300	514	74		

- Molecule 3 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	2150	Total	C	N	O	P	0	0
			45795	20471	8144	15037	2143		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	143	C	A	conflict	GB 320364483
0	805	C	U	conflict	GB 320364483
0	2321	U	-	insertion	GB 320364483
0	2322	U	-	insertion	GB 320364483
0	2323	U	-	insertion	GB 320364483

- Molecule 4 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	123	Total	C	N	O	S	0	0
			989	628	194	165	2		

- Molecule 5 is a protein called Elongation initiation factor 2 alpha subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	s	295	Total	C	N	O	S	0	0
			2365	1489	436	427	13		

- Molecule 6 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	79	Total	C	N	O	S	0	0
			644	409	123	106	6		

- Molecule 7 is a protein called Translation initiation factor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	225	Total	C	N	O	S	0	0
			1796	1111	335	339	11		

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	310	Total	C	N	O	S	0	0
			2405	1505	424	463	13		

- Molecule 9 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	r	140	Total	C	N	O	S	0	0
			1113	706	212	192	3		

- Molecule 10 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	u	136	Total	C	N	O	S	0	0
			1108	689	224	190	5		

- Molecule 11 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	142	Total	C	N	O	S	0	0
			1116	706	220	188	2		

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	175	Total	C	N	O	S	0	0
			1404	885	283	233	3		

- Molecule 13 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	o	190	Total	C	N	O	S	0	0
			1493	932	286	269	6		

- Molecule 14 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	200	Total	C	N	O	S	0	0
			1670	1063	324	277	6		

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	141	Total	C	N	O	S	0	0
			1143	724	221	190	8		

- Molecule 16 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	82	Total	C	N	O	S	0	0
			630	384	121	116	9		

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	104	Total	C	N	O	S	0	0
			829	510	177	132	10		

- Molecule 18 is a protein called 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	68	Total	C	N	O	S	0	0
			526	315	107	100	4		

- Molecule 19 is a protein called 40S ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	135	Total	C	N	O	S	0	0
			1011	620	195	187	9		

- Molecule 20 is a protein called 40S ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	148	Total	C	N	O	S	0	0
			1212	760	239	207	6		

- Molecule 21 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	179	Total	C	N	O	S	0	0
			1483	935	297	243	8		

- Molecule 22 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	207	Total	C	N	O	S	0	0
			1658	1060	299	288	11		

- Molecule 23 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	223	Total	C	N	O	S	0	0
			1726	1098	304	314	10		

- Molecule 24 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	83	Total	C	N	O	S	0	0
			635	395	116	122	2		

- Molecule 25 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	70	Total	C	N	O	S	0	0
			553	356	97	97	3		

- Molecule 26 is a protein called RNA-binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	J	173	Total	C	N	O	S	0	0
			1358	862	259	234	3		

- Molecule 27 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	121	Total	C	N	O	S	0	0
			958	594	174	185	5		

- Molecule 28 is a protein called Eukaryotic translation initiation factor 2 subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	421	Total	C	N	O	S	0	0
			3245	2049	581	596	19		

- Molecule 29 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	249	Total	C	N	O	S	0	0
			1983	1244	402	333	4		

- Molecule 30 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	i	121	Total	C	N	O	S	0	0
			992	623	190	174	5		

- Molecule 31 is a protein called Ribosomal protein S20, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	99	Total	C	N	O	S	0	0
			784	497	144	140	3		

- Molecule 32 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	200	Total	C	N	O	S	0	0
			1587	995	302	279	11		

- Molecule 33 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	93	Total	C	N	O	S	0	0
			780	508	136	132	4		

- Molecule 34 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	140	Total	C	N	O	S	0	0
			1116	702	221	185	8		

- Molecule 35 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	129	Total	C	N	O	S	0	0
			1019	647	188	176	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	83	THR	ALA	conflict	UNP Q4CXX2

- Molecule 36 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	60	Total	C	N	O	S	0	0
			480	303	98	78	1		

- Molecule 37 is a protein called Protein translation factor SUI1 homolog, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V	97	Total	C	N	O	S	0	0
			789	490	152	145	2		

- Molecule 38 is a protein called Putative eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	147	Total	C	N	O	S	0	0
			1162	716	209	236	1		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	E	391	Total	C	N	O	S	0	0
			3119	1977	536	593	13		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Y	174	Total	C	N	O	S	0	0
			1387	872	243	260	12		

- Molecule 41 is a protein called Ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Q	57	Total	C	N	O	S	0	0
			462	283	96	77	6		

- Molecule 42 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	D	33	Total	C	N	O	S	0	0
			294	178	76	38	2		

- Molecule 43 is a protein called JAB_MPN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G	308	Total	C	N	O	S	0	0
			2414	1492	442	466	14		

- Molecule 44 is a protein called CSN8_PSD8_EIF3K domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	K	201	Total	C	N	O	S	0	0
			1566	1001	256	304	5		

- Molecule 45 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	132	Total	C	N	O	S	0	0
			1057	670	204	179	4		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit 8, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	C	696	Total	C	N	O	S	0	0
			5630	3542	973	1092	23		

- Molecule 47 is a protein called eIF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	8	576	Total	C	N	O	S	0	0
			4596	2882	845	847	22		

- Molecule 48 is a protein called 40S ribosomal protein S3a-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	217	Total	C	N	O	S	0	0
			1781	1124	337	313	7		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 (EIF-3) interacting protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	I	344	Total	C	N	O	S	0	0
			2770	1771	479	503	17		

- Molecule 50 is a protein called eIF3H.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	H	297	Total	C	N	O	S	0	0
			2388	1498	421	451	18		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit 7-like protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	A	483	Total	C	N	O	S	0	0
			3891	2446	691	729	25		

- Molecule 52 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	l	258	Total	C	N	O	S	0	0
			2038	1290	383	354	11		

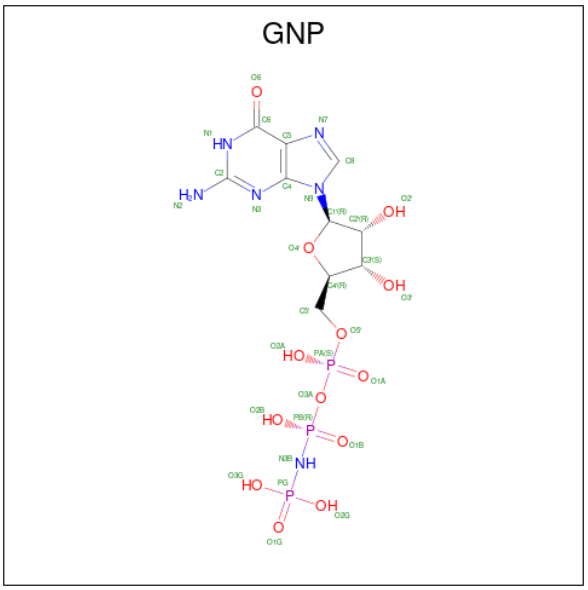
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
53	n	1	Total Zn 1 1	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
54	5	1	Total Mg 1 1	0

- Molecule 55 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



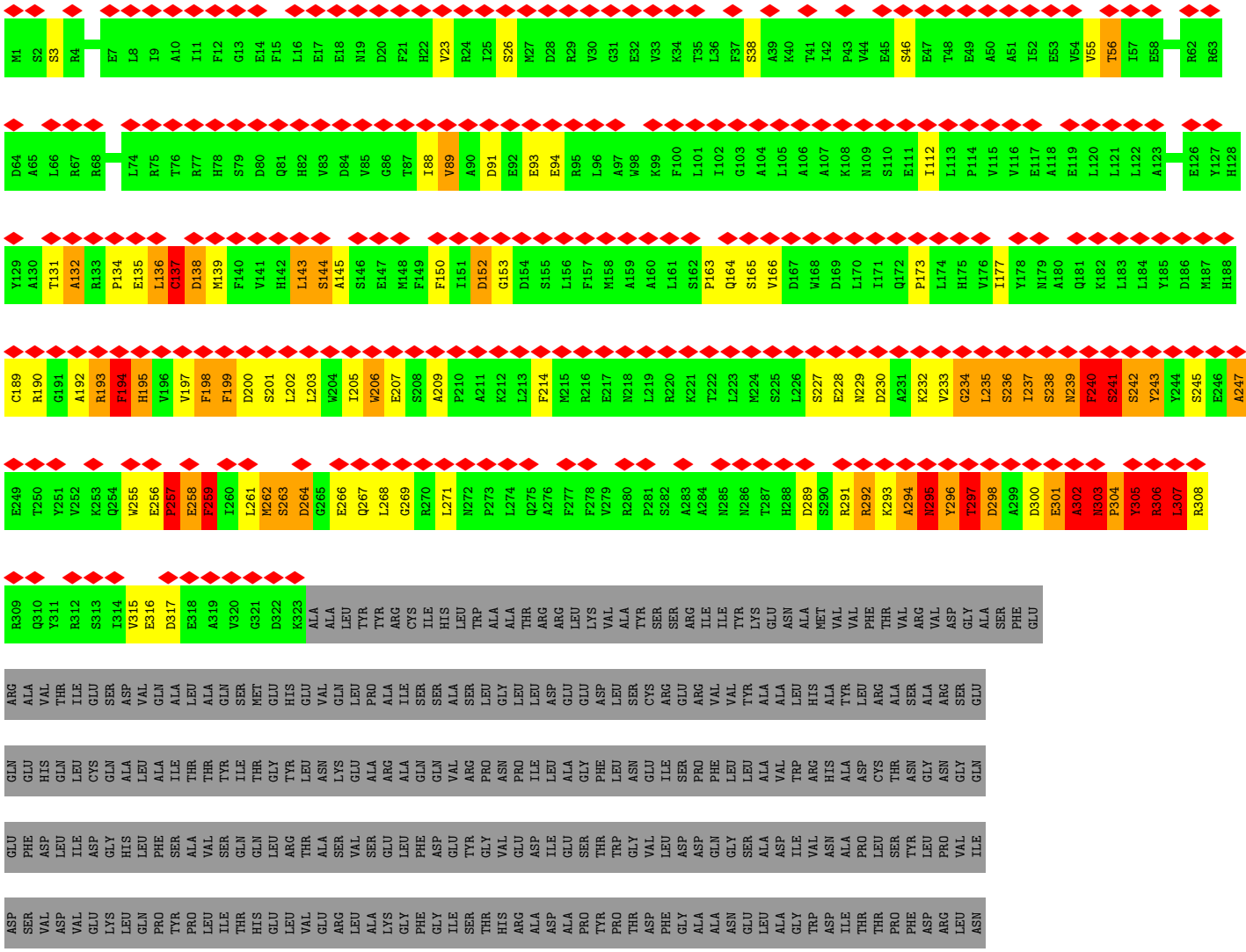
Mol	Chain	Residues	Atoms	AltConf
55	5	1	Total C N O P 32 10 6 13 3	0

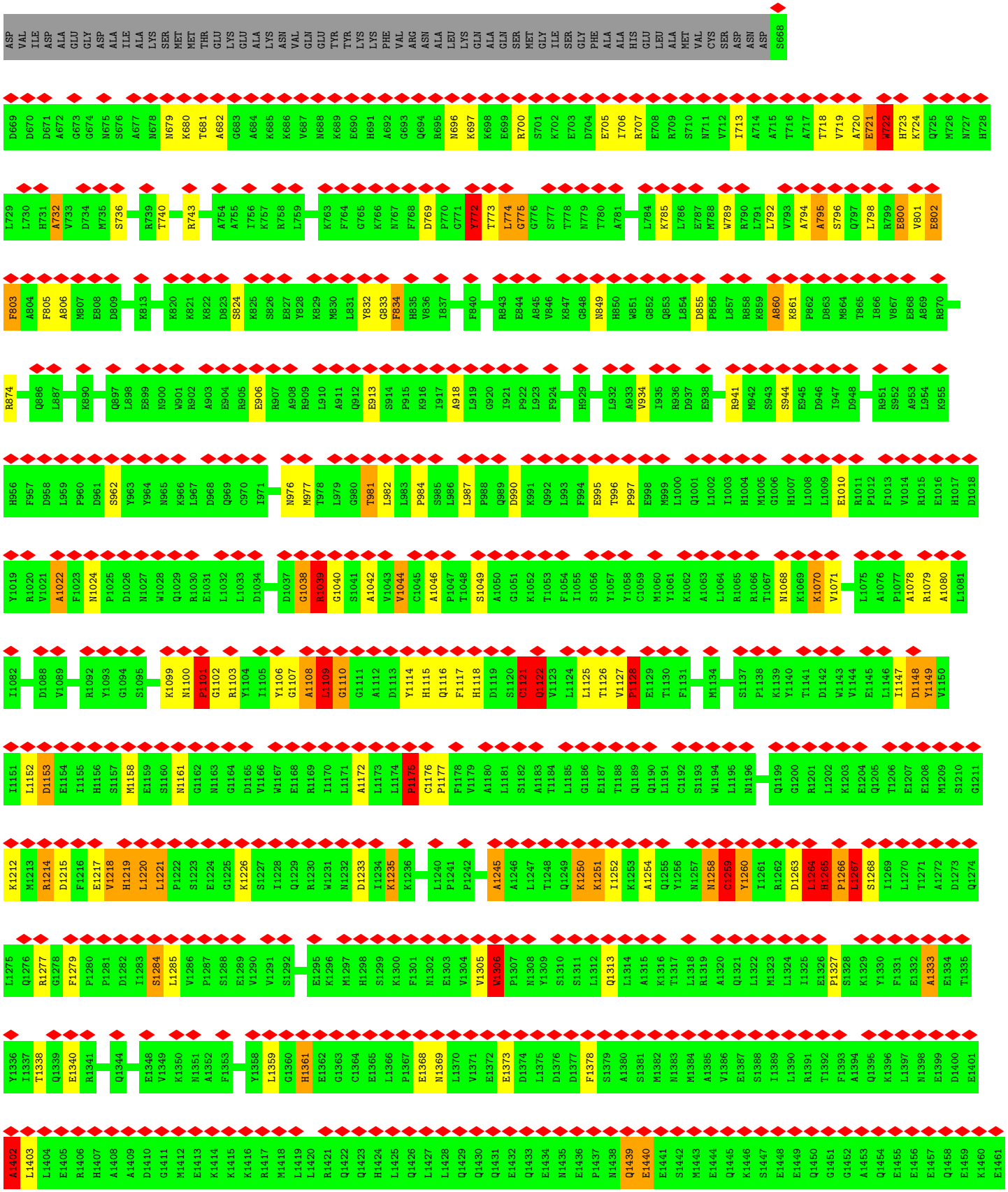
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: kDDX60

Chain f:

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D669 D670 D671 A672 G673 G674 N675 S676 A677 N678 N679 K680 T681 A682 G683 A684 K685 K686 V687 N688 K689 E690 H691 A692 G693 Q694 R695 N696 K697 K698 E699 R700 S701 K702 E703 D704 E705 I706 R707 E708 R709 S710 N711 V712 I713 A714 A715 T716 A717 T718 V719 A720 E721 W722 H723 K724 Q725 M726 N727 H728
L729 L730 H731 A732 V733 D734 M735 S736 R739 T740 R743 A754 A755 T756 K757 R758 L759 K763 F764 G765 K766 N767 F768 D769 P770 G771 Y772 T773 L774 G775 G776 S777 T778 N779 T780 A781 L784 K785 L786 E787 M788 W789 R790 L791 L792 V793 A794 A795 S796 Q797 L798 R799 E800 V801 E802
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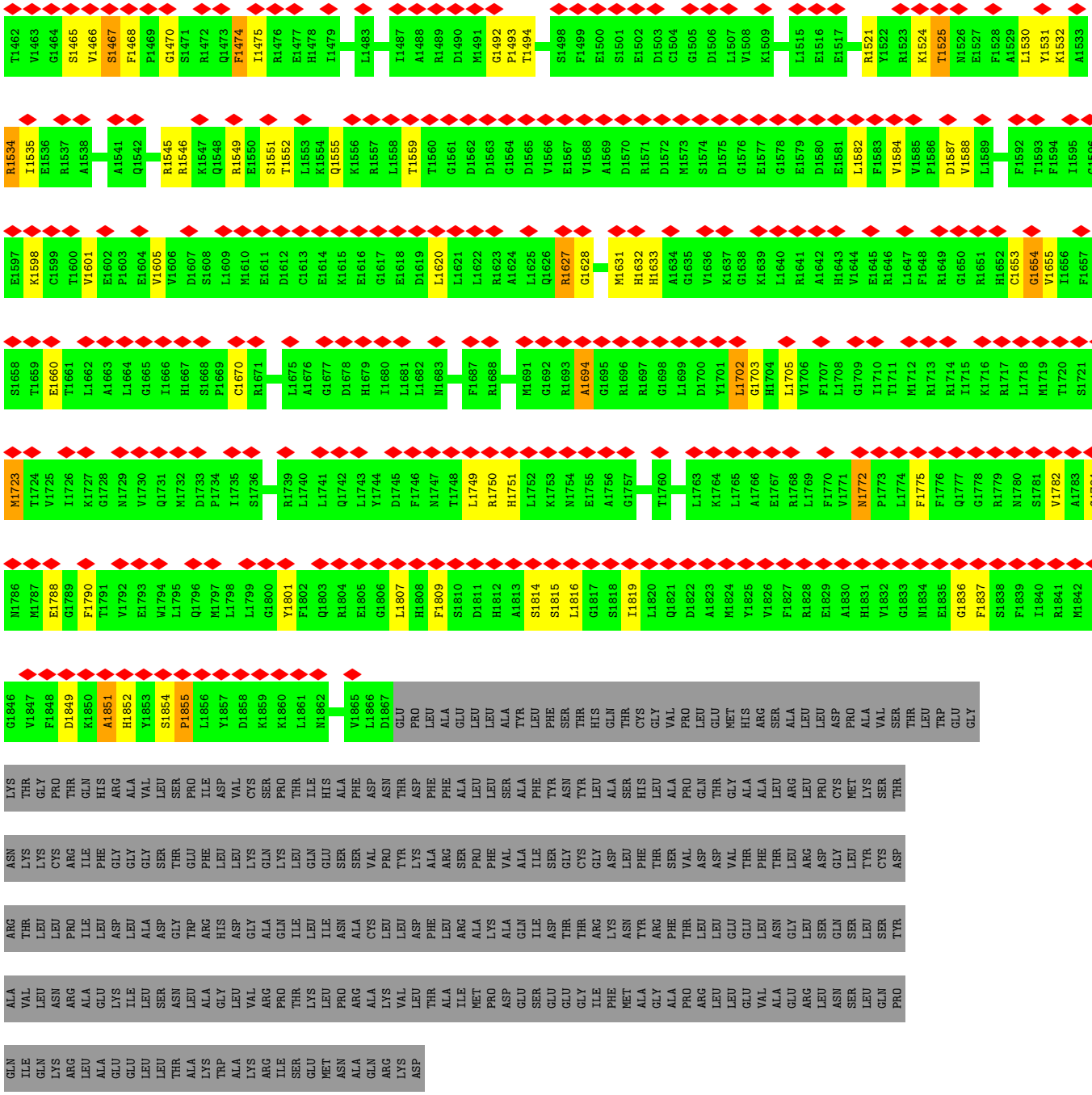
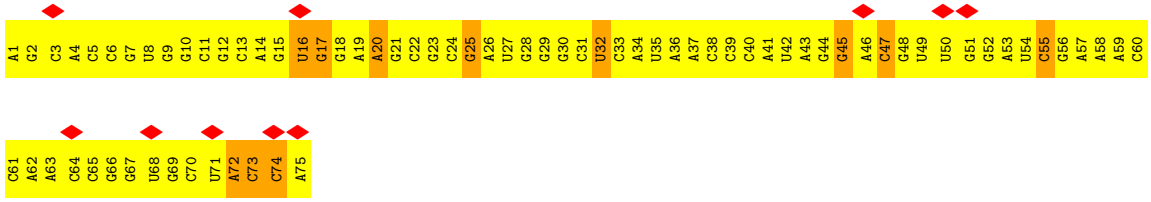
L1275 Q1276 R1277 G1278 F1279 P1280 P1281 D1282 I1283 S1284 L1285 V1286 P1287 S1288 E1289 V1290 V1291 S1292 E1295 K1296 M1297 H1298 S1299 K1300 F1301 N1302 E1303 V1304 V1305 W1306 P1307 N1308 Y1309 S1310 S1311 L1312 Q1313 L1314 A1315 K1316 T1317 L1318 R1319 A1320 Q1321 L1322 M1323 L1324 I1325 E1326 P1327 S1328 K1329 Y1330 F1331 E1332 A1333 E1334 T1335
Y1336 I1337 T1338 Q1339 E1340 R1341 Q1344 E1348 V1349 K1350 N1351 A1352 F1353 Y1358 L1359 G1360 H1361 E1362 G1363 C1364 E1365 L1366 P1367 E1368 N1369 L1370 V1371 E1372 E1373 D1374 L1375 D1376 D1377 F1378 S1379 A1380 S1381 M1382 N1383 M1384 A1385 V1386 E1387 S1388 I1389 L1390 R1391 T1392 F1393 A1394 Q1395 K1396 L1397 N1398 E1399 D1400 E1401
A1402 L1403 L1404 E1405 R1406 H1407 A1408 A1409 D1410 G1411 M1412 E1413 K1414 K1415 K1416 R1417 M1418 L1419 L1420 R1421 Q1422 Q1423 H1424 L1425 Q1426 L1427 L1428 Q1429 Q1430 Q1431 E1432 Q1433 E1434 N1435 E1436 P1437 N1438 Q1439 E1440 E1441 S1442 M1443 E1444 Q1445 K1446 S1447 E1448 E1449 Q1450 G1451 G1452 A1453 Q1454 E1455 E1456 E1457 Q1458 E1459 K1460 E1461



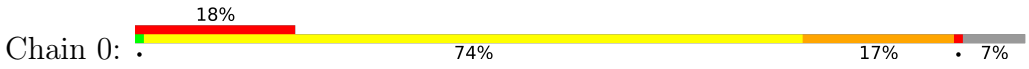
- Molecule 2: initiator tRNA-Met

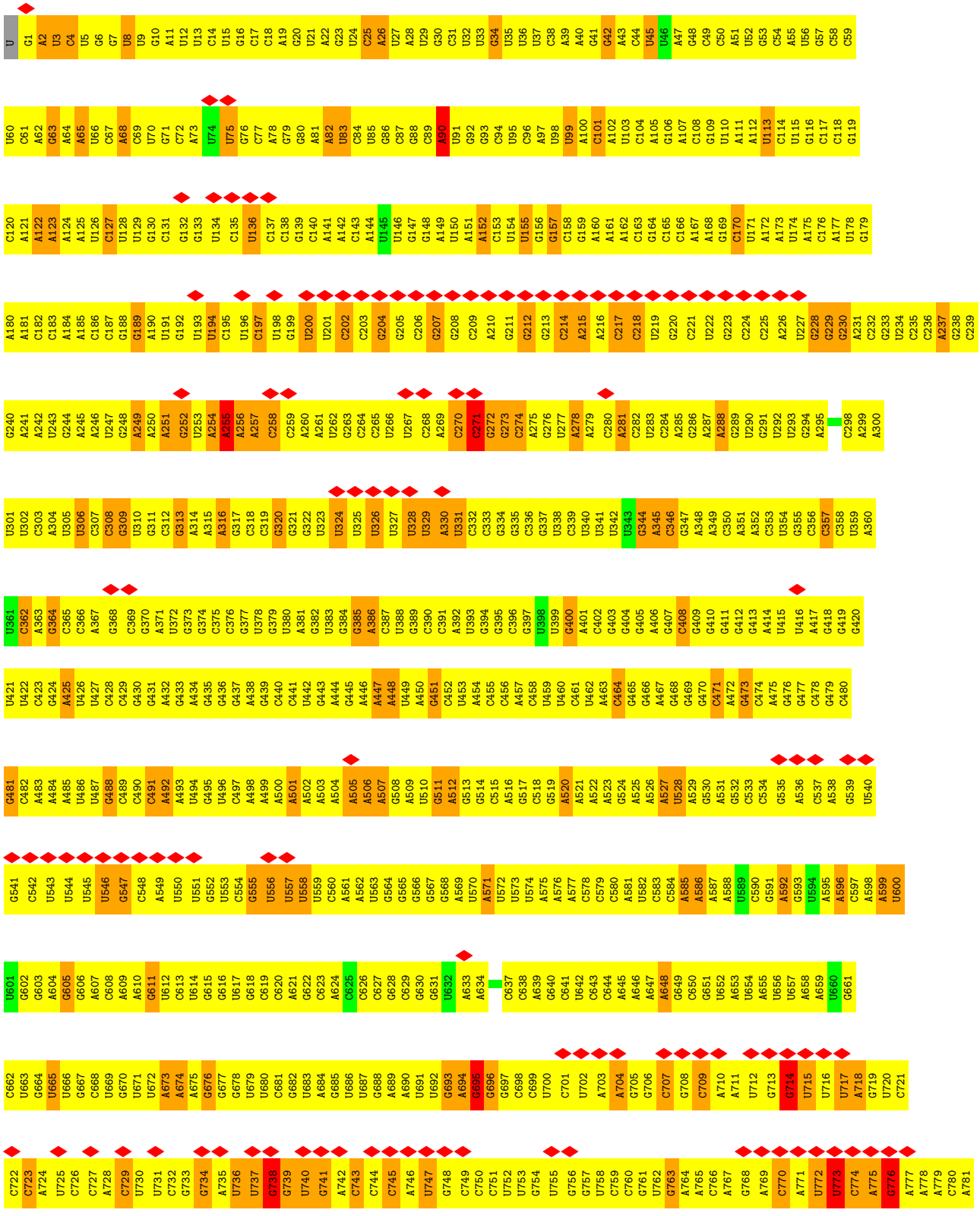
Chain 1:

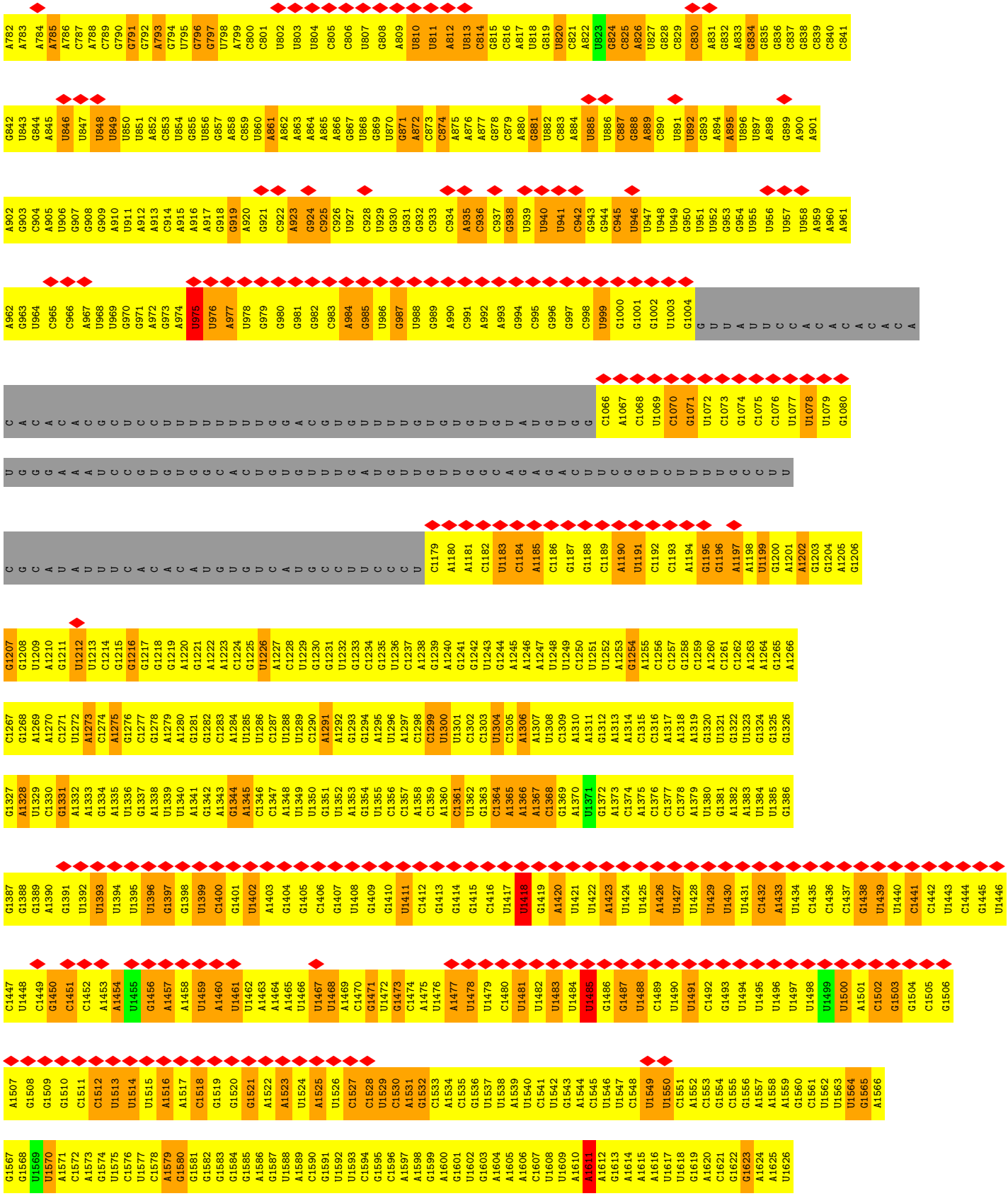


• Molecule 3: 18S

Chain 0:



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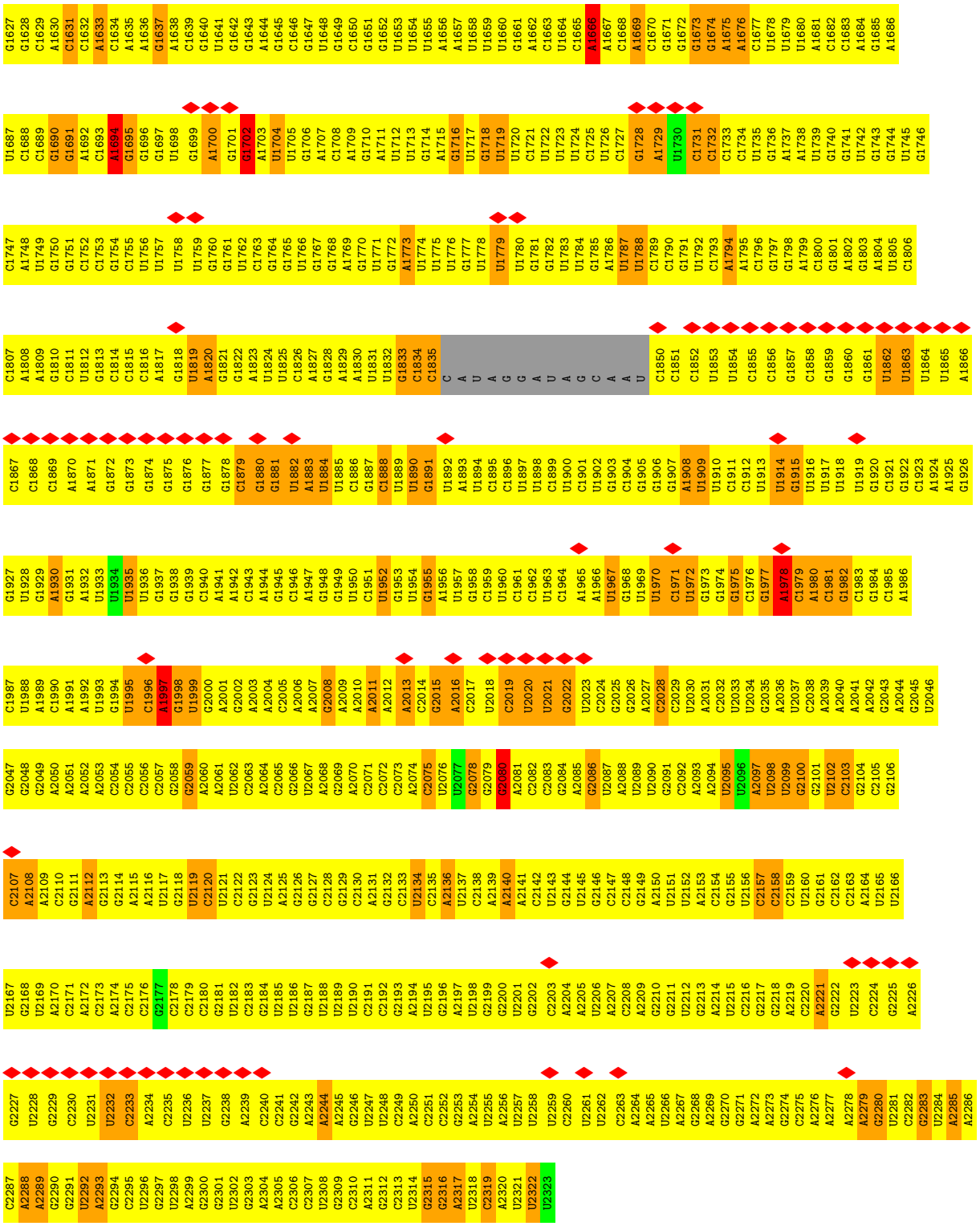
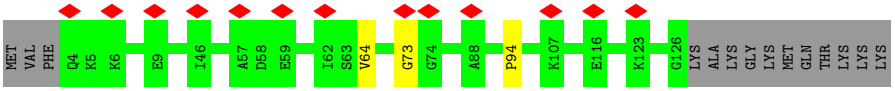
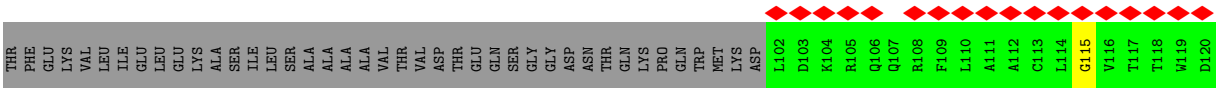


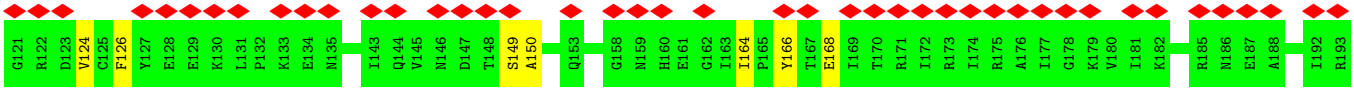
• Molecule 4: 40S ribosomal protein S24

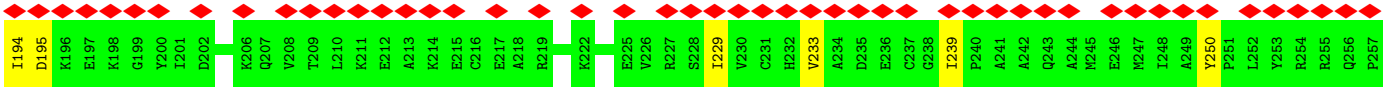
Chain y:

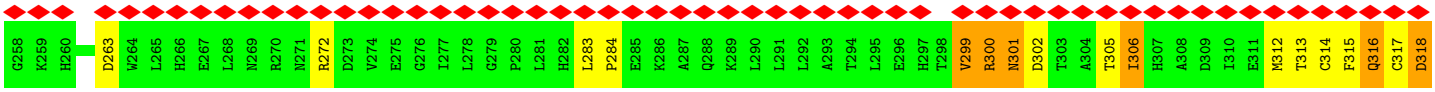


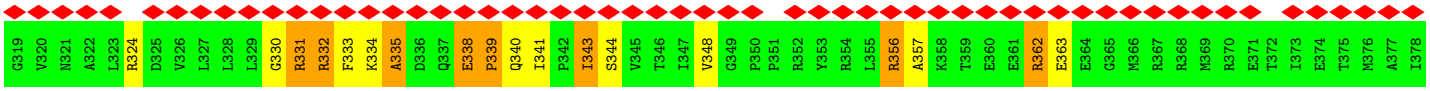
• Molecule 5: Elongation initiation factor 2 alpha subunit, putative

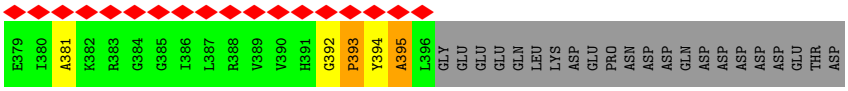




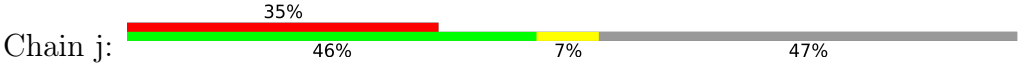


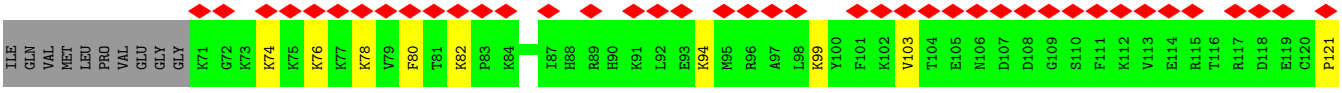


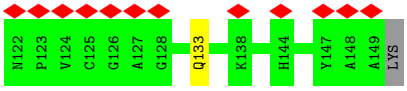




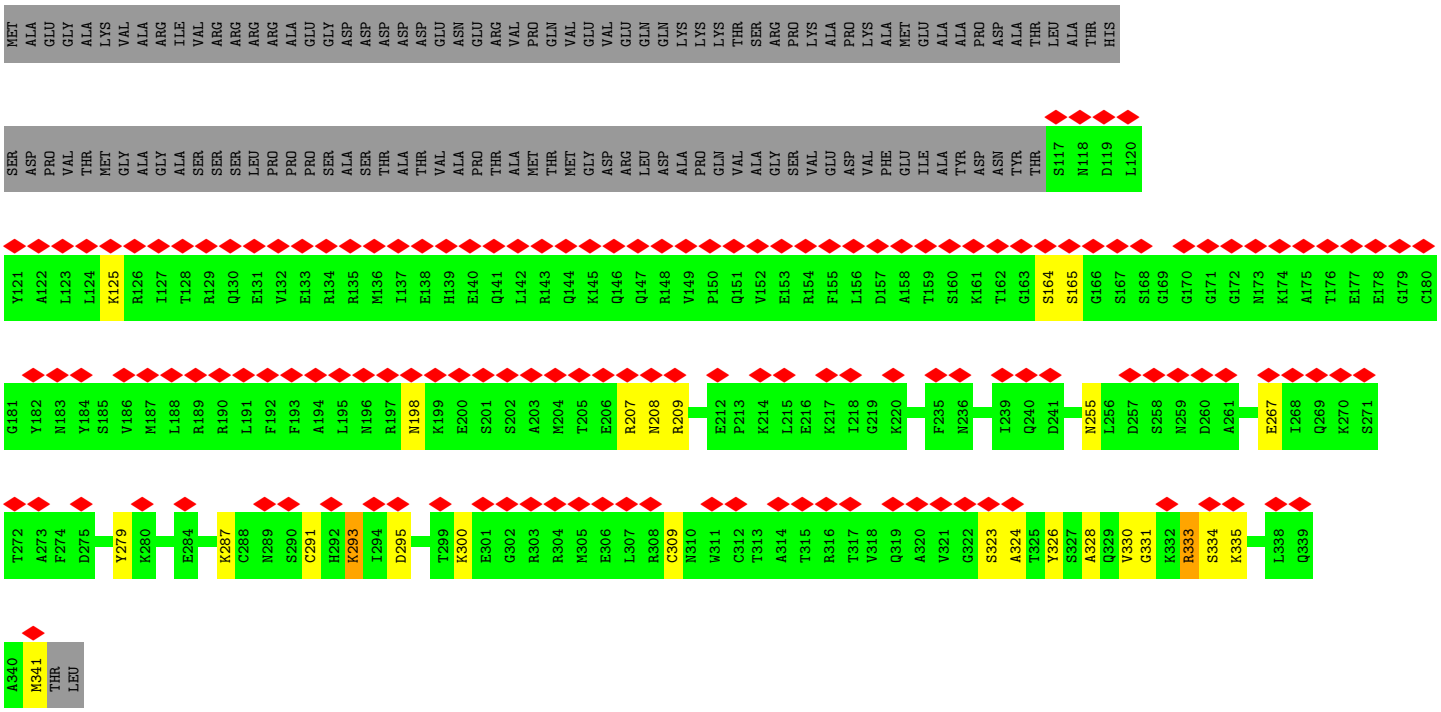
• Molecule 6: 60S ribosomal protein L40



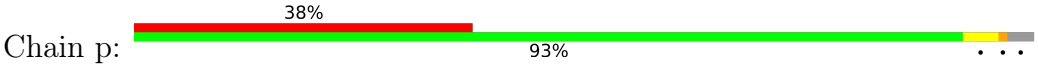


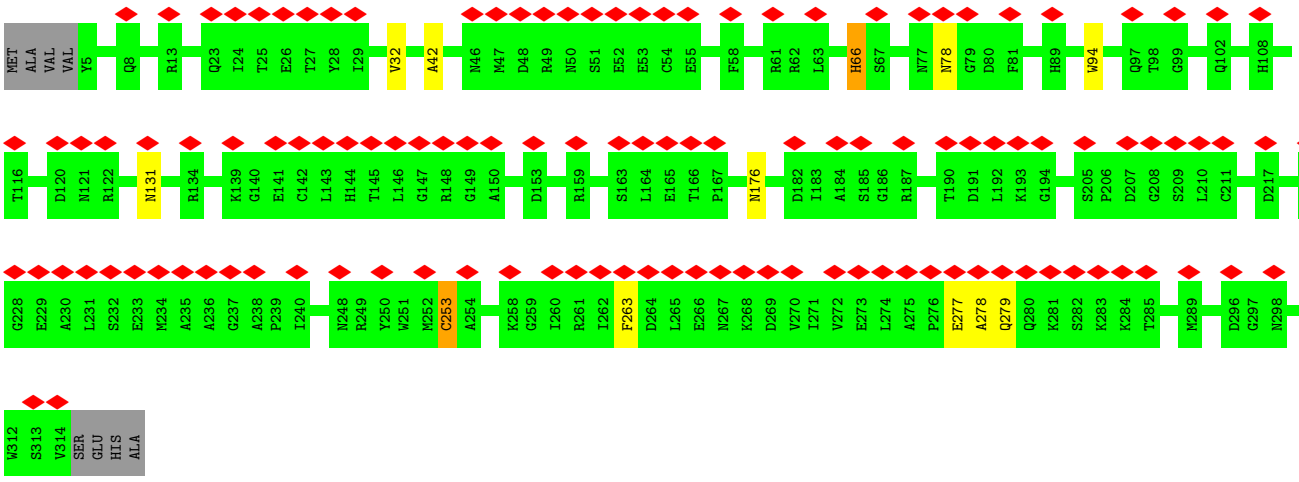


• Molecule 7: Translation initiation factor, putative

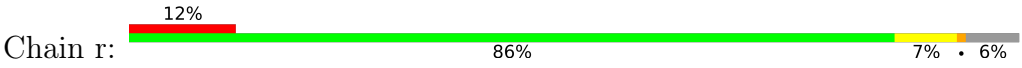


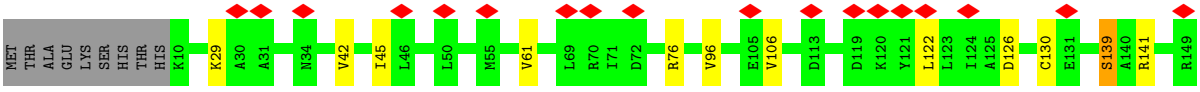
• Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein



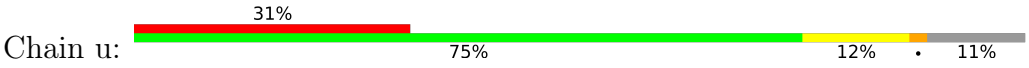


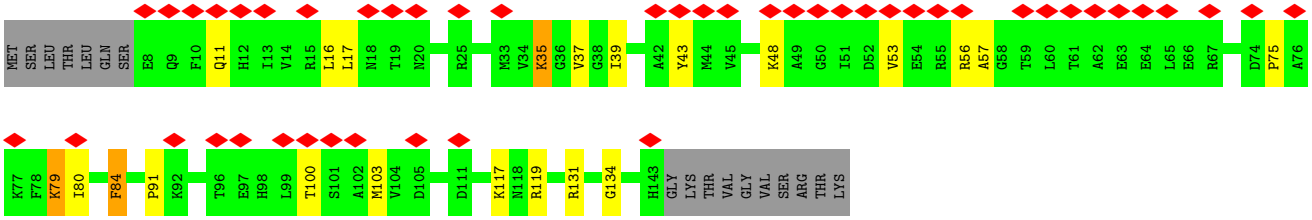
• Molecule 9: 40S ribosomal protein S16, putative



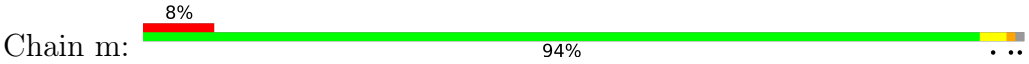


• Molecule 10: 40S ribosomal protein S18, putative

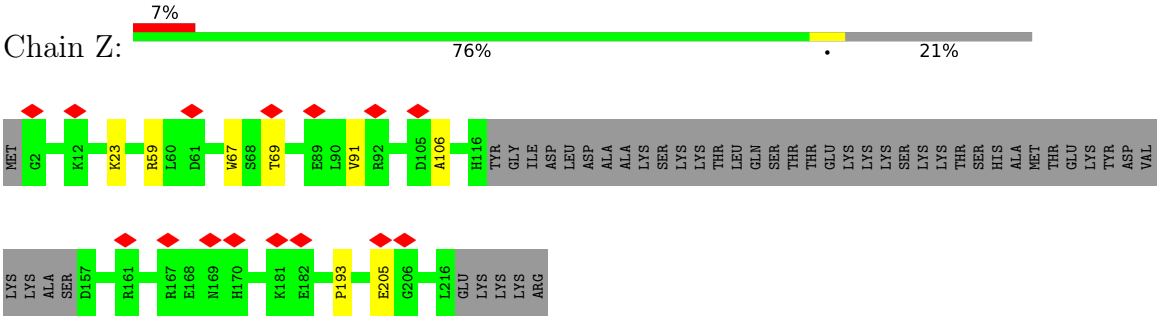




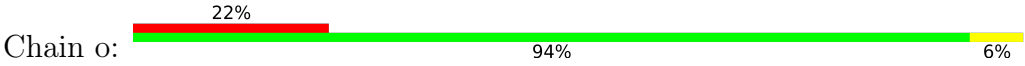
• Molecule 11: 40S ribosomal protein S23, putative

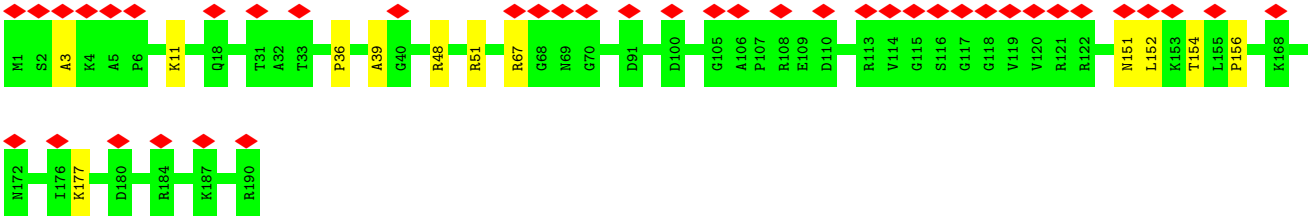


• Molecule 12: 40S ribosomal protein S8

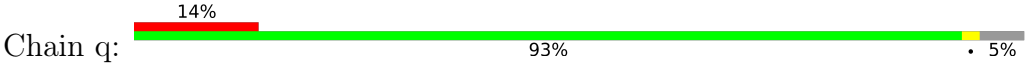


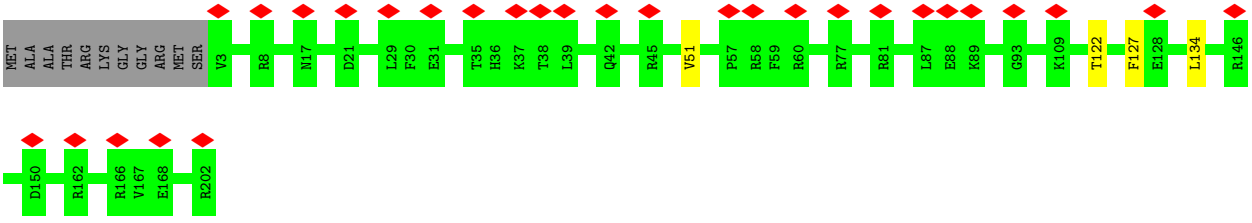
• Molecule 13: 40S ribosomal protein S5, putative





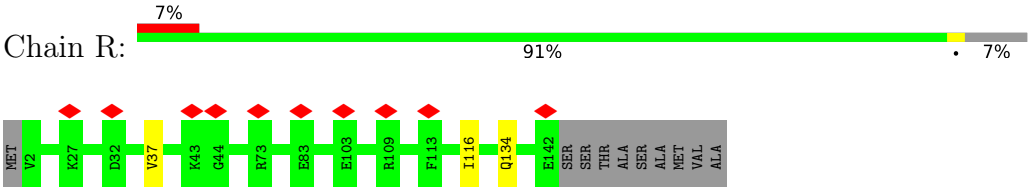
• Molecule 14: 40S ribosomal protein S7





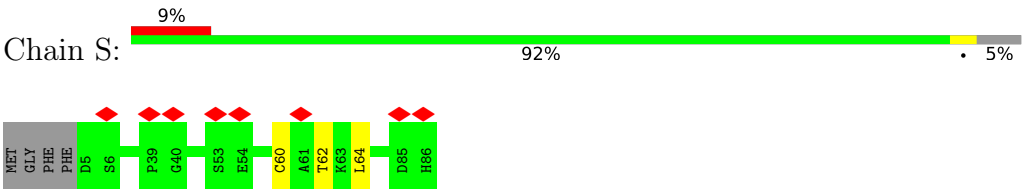
• Molecule 15: 40S ribosomal protein S13, putative

Chain R:



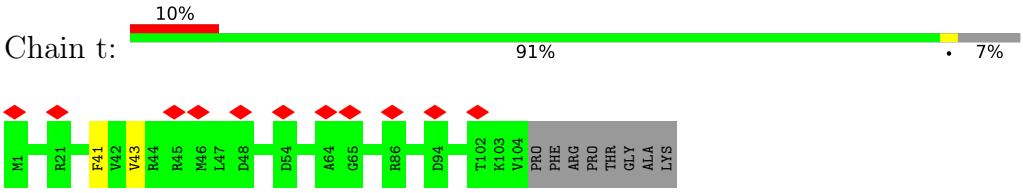
• Molecule 16: 40S ribosomal protein S27, putative

Chain S:



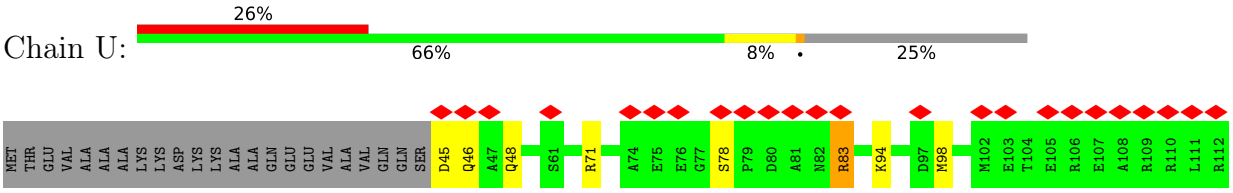
• Molecule 17: 40S ribosomal protein S26

Chain t:



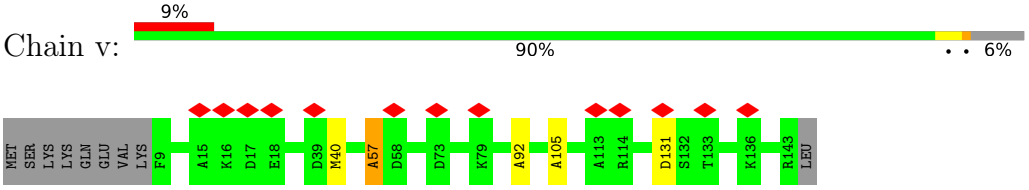
• Molecule 18: 40S ribosomal protein S33

Chain U:



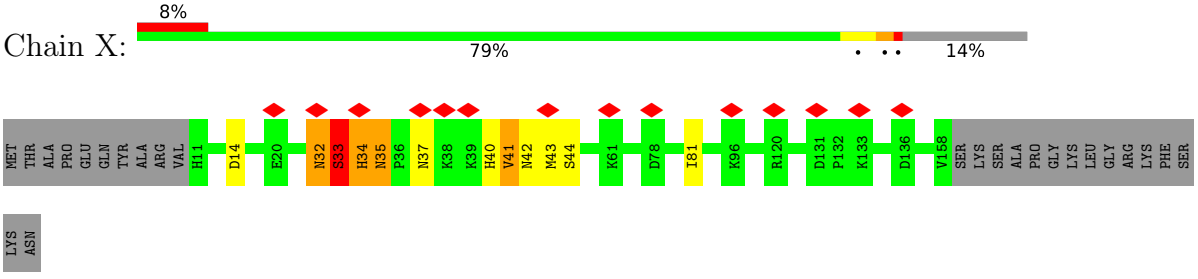
• Molecule 19: 40S ribosomal protein S14, putative

Chain v:



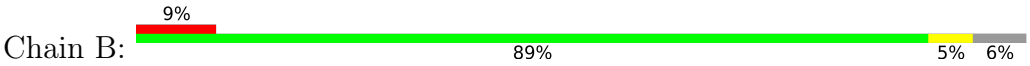
• Molecule 20: 40S ribosomal protein S11, putative

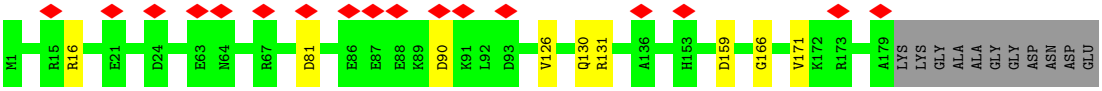
Chain X:



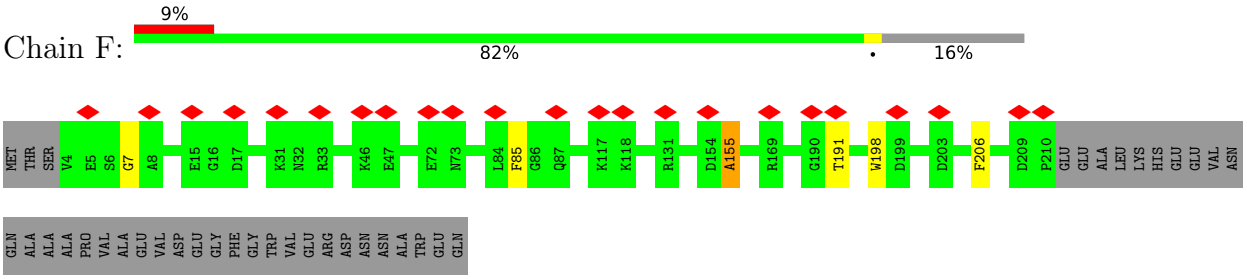
• Molecule 21: Putative 40S ribosomal protein S9

Chain B:

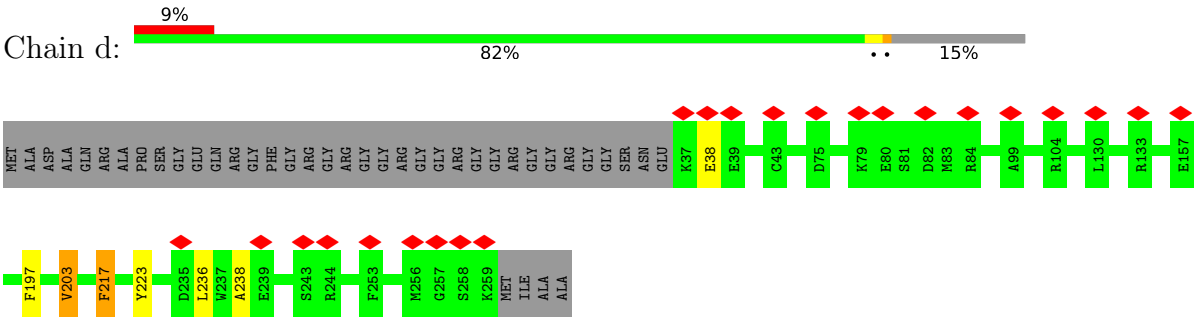




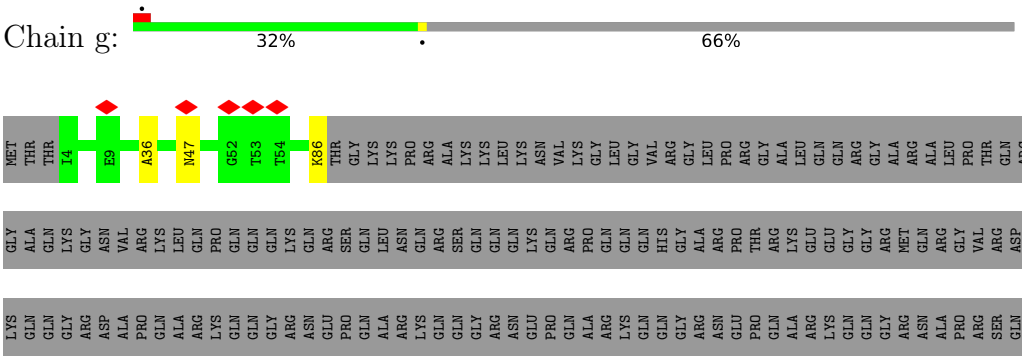
• Molecule 22: 40S ribosomal protein SA



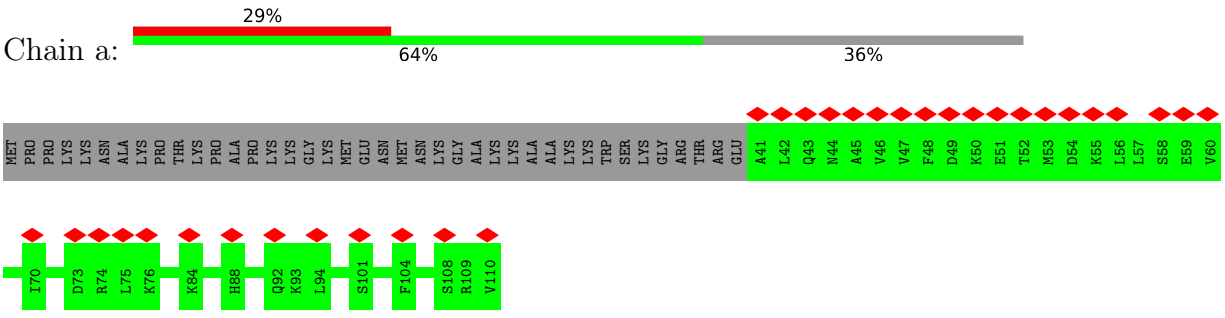
• Molecule 23: 40S ribosomal protein S2, putative



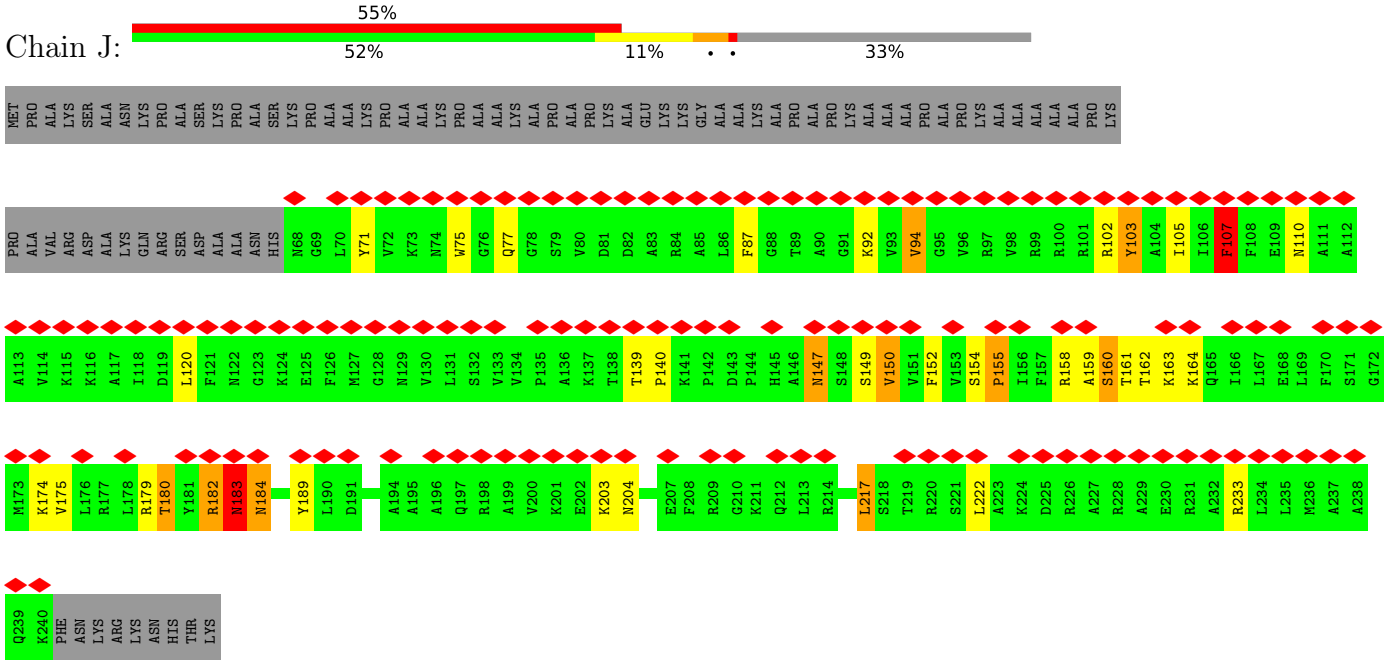
• Molecule 24: Putative 40S ribosomal protein S21



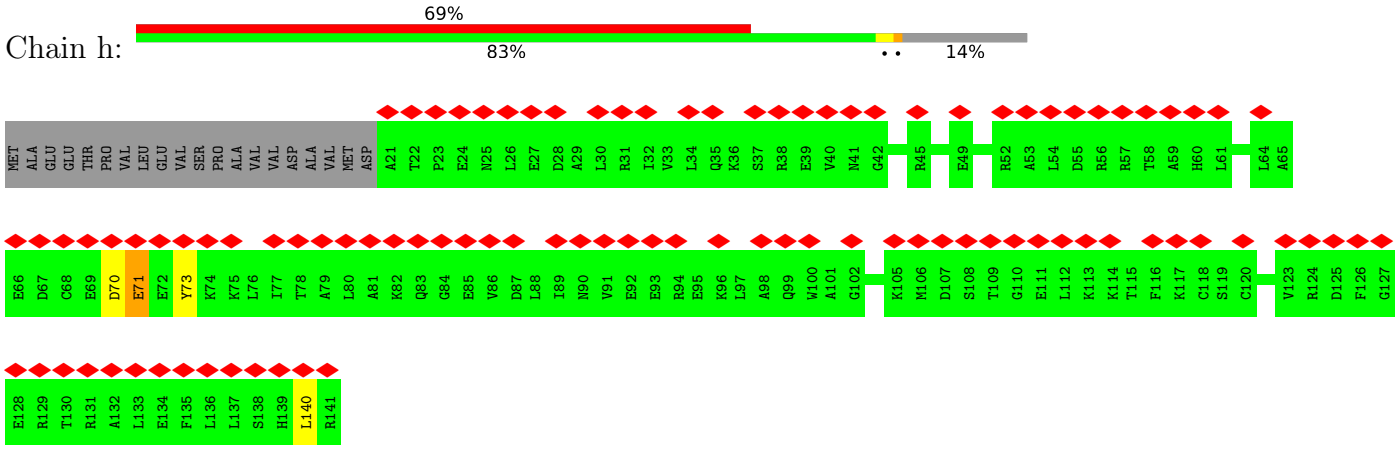
• Molecule 25: 40S ribosomal protein S25



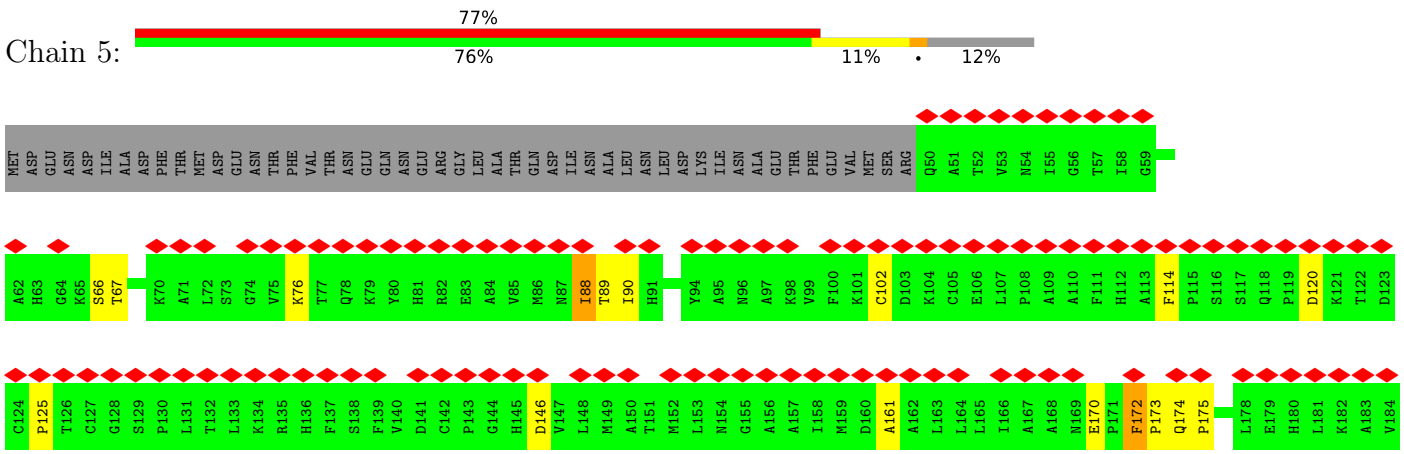
• Molecule 26: RNA-binding protein, putative

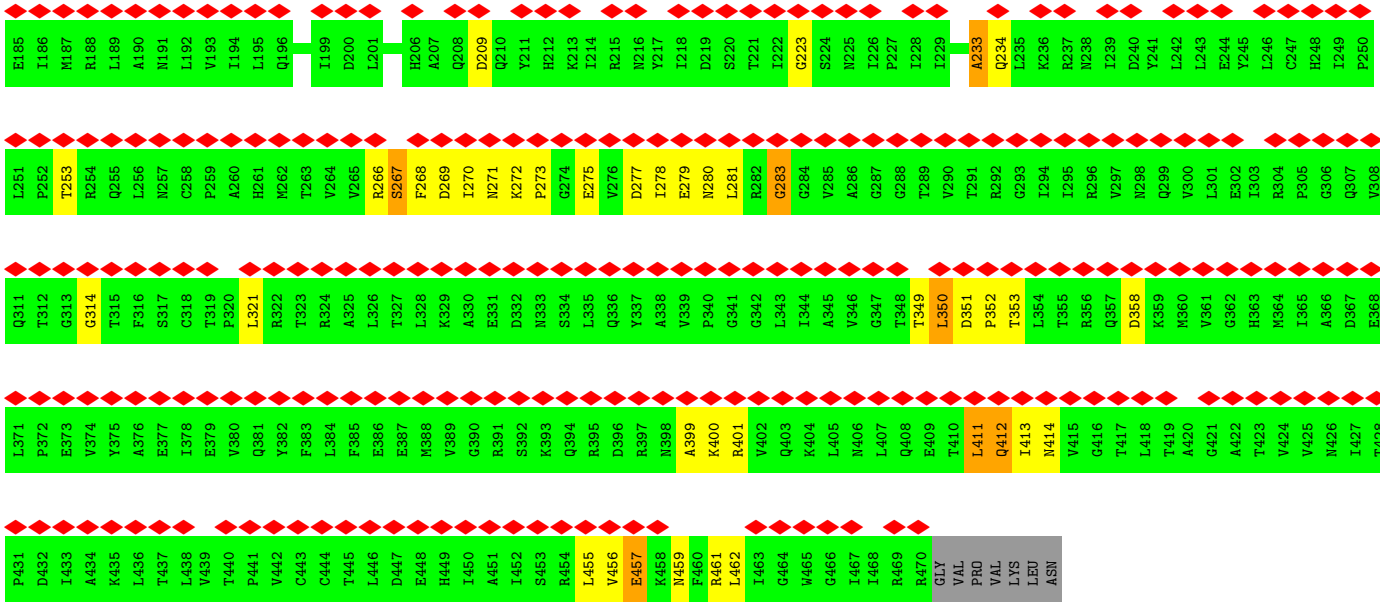


• Molecule 27: 40S ribosomal protein S12



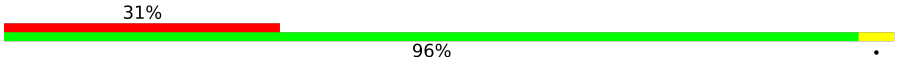
• Molecule 28: Eukaryotic translation initiation factor 2 subunit, putative

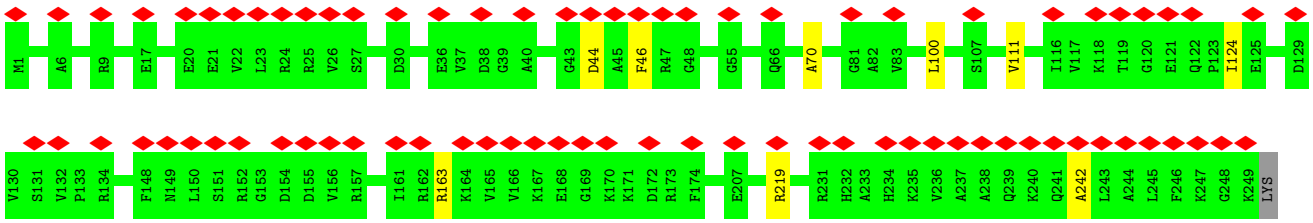




• Molecule 29: 40S ribosomal protein S6

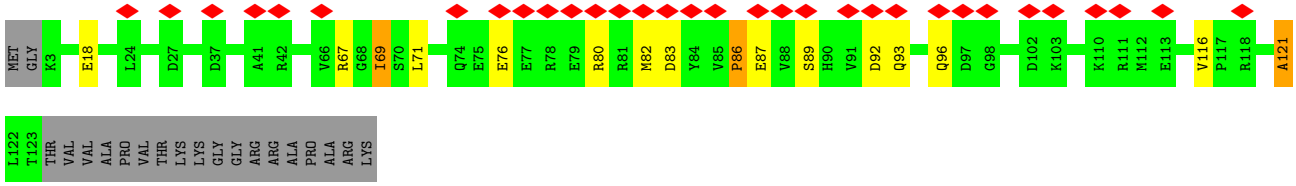
Chain P:





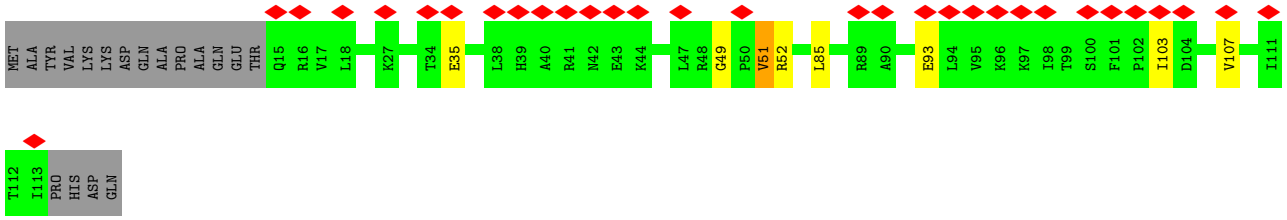
• Molecule 30: 40S ribosomal protein S17, putative

Chain i:



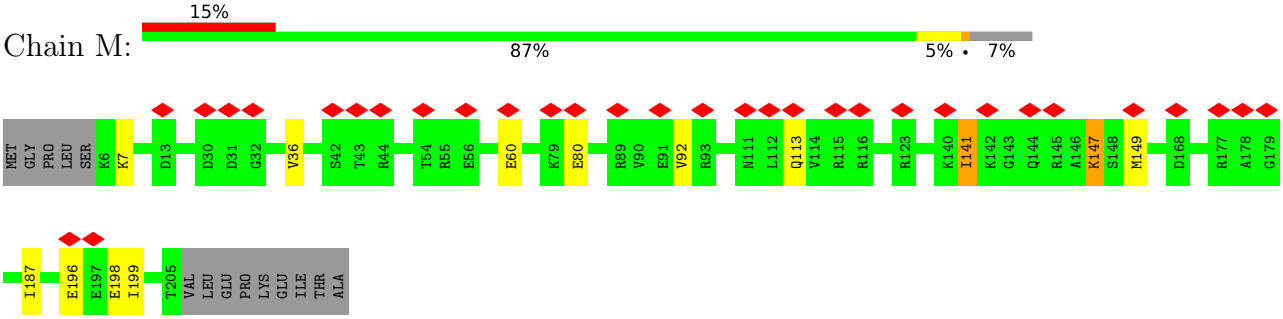
• Molecule 31: Ribosomal protein S20, putative

Chain L:



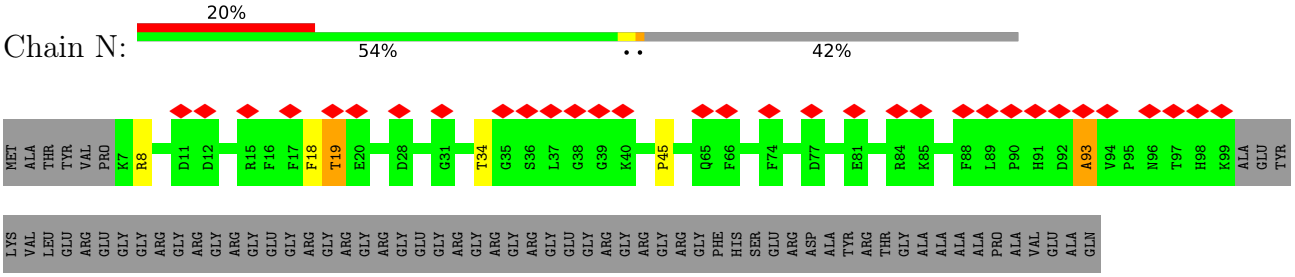
• Molecule 32: 40S ribosomal protein S3, putative

Chain M:



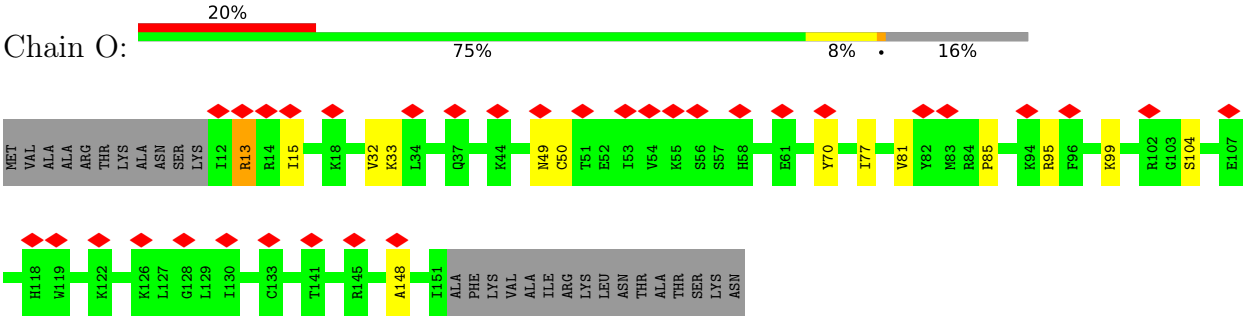
• Molecule 33: 40S ribosomal protein S10, putative

Chain N:



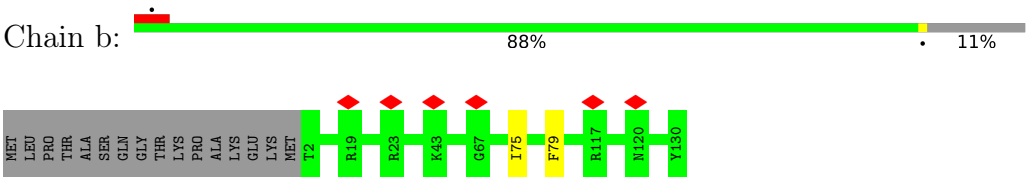
• Molecule 34: Ribosomal protein S19, putative

Chain O:



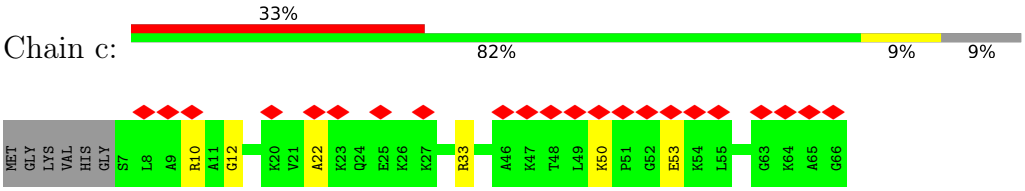
• Molecule 35: 40S ribosomal protein S15a, putative

Chain b:



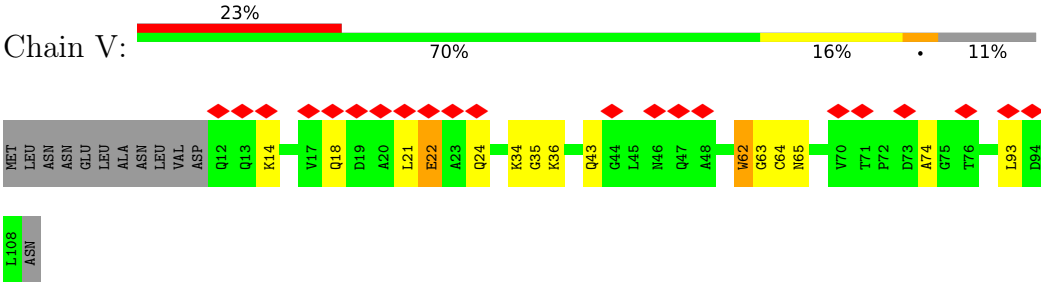
• Molecule 36: 40S ribosomal protein S30

Chain c:



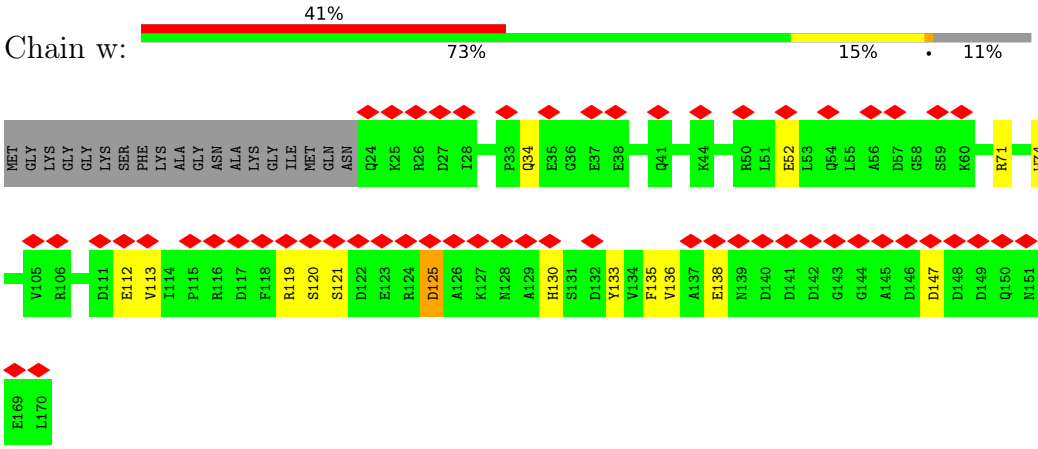
• Molecule 37: Protein translation factor SUI1 homolog, putative

Chain V:



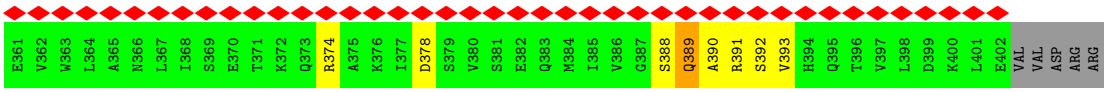
• Molecule 38: Putative eukaryotic translation initiation factor 1A

Chain w:

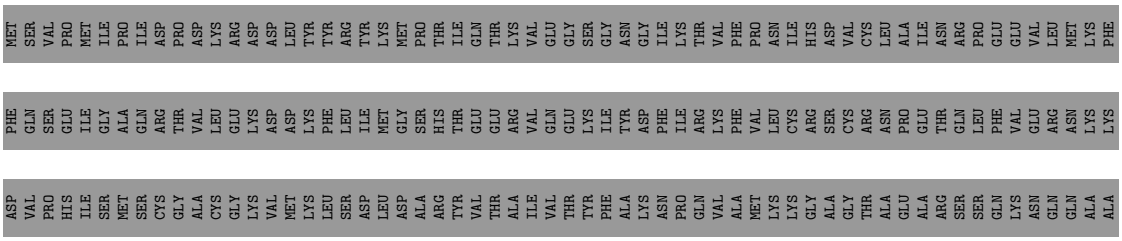


• Molecule 39: Eukaryotic translation initiation factor 3 subunit E

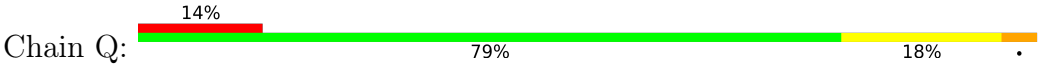
Chain E:



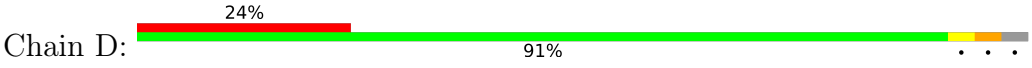
• Molecule 40: Eukaryotic translation initiation factor 5, putative

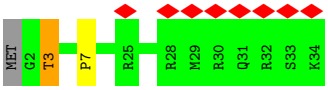


• Molecule 41: Ribosomal protein S29, putative

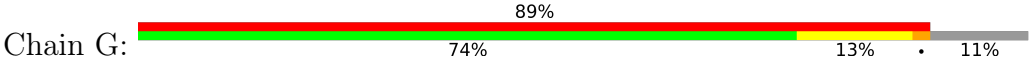


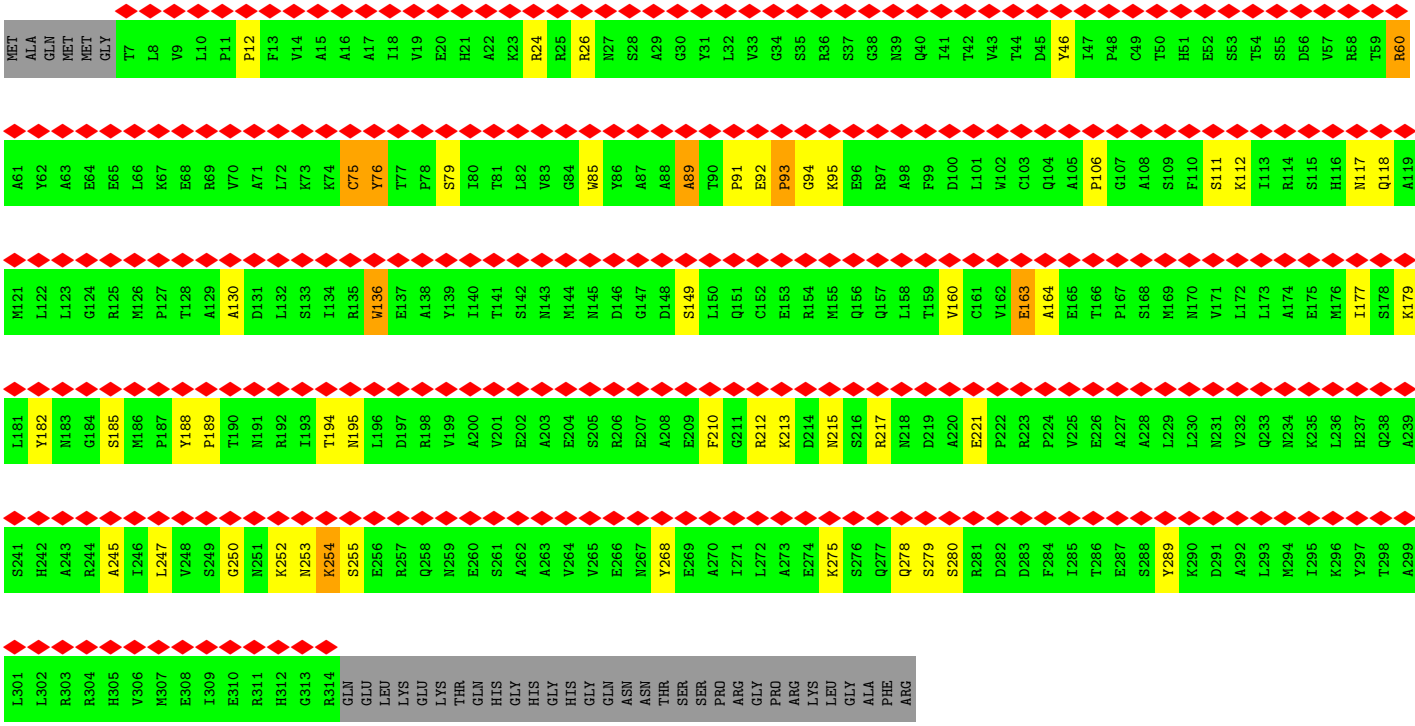
• Molecule 42: eL41





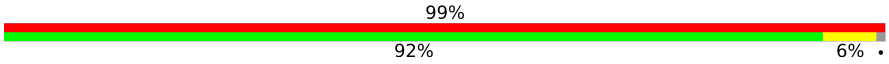
• Molecule 43: JAB_MPN domain-containing protein

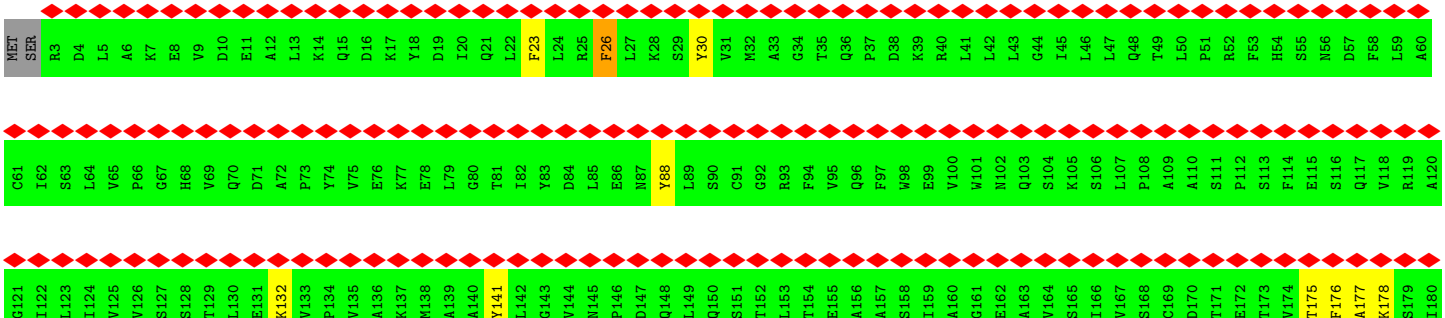




• Molecule 44: CSN8_PSD8_EIF3K domain-containing protein

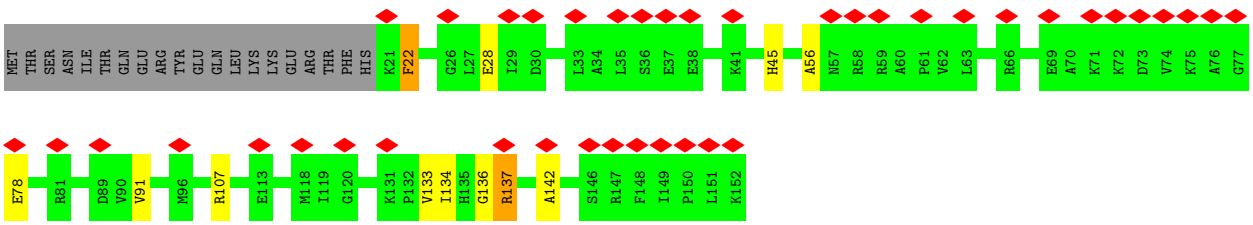
Chain K:





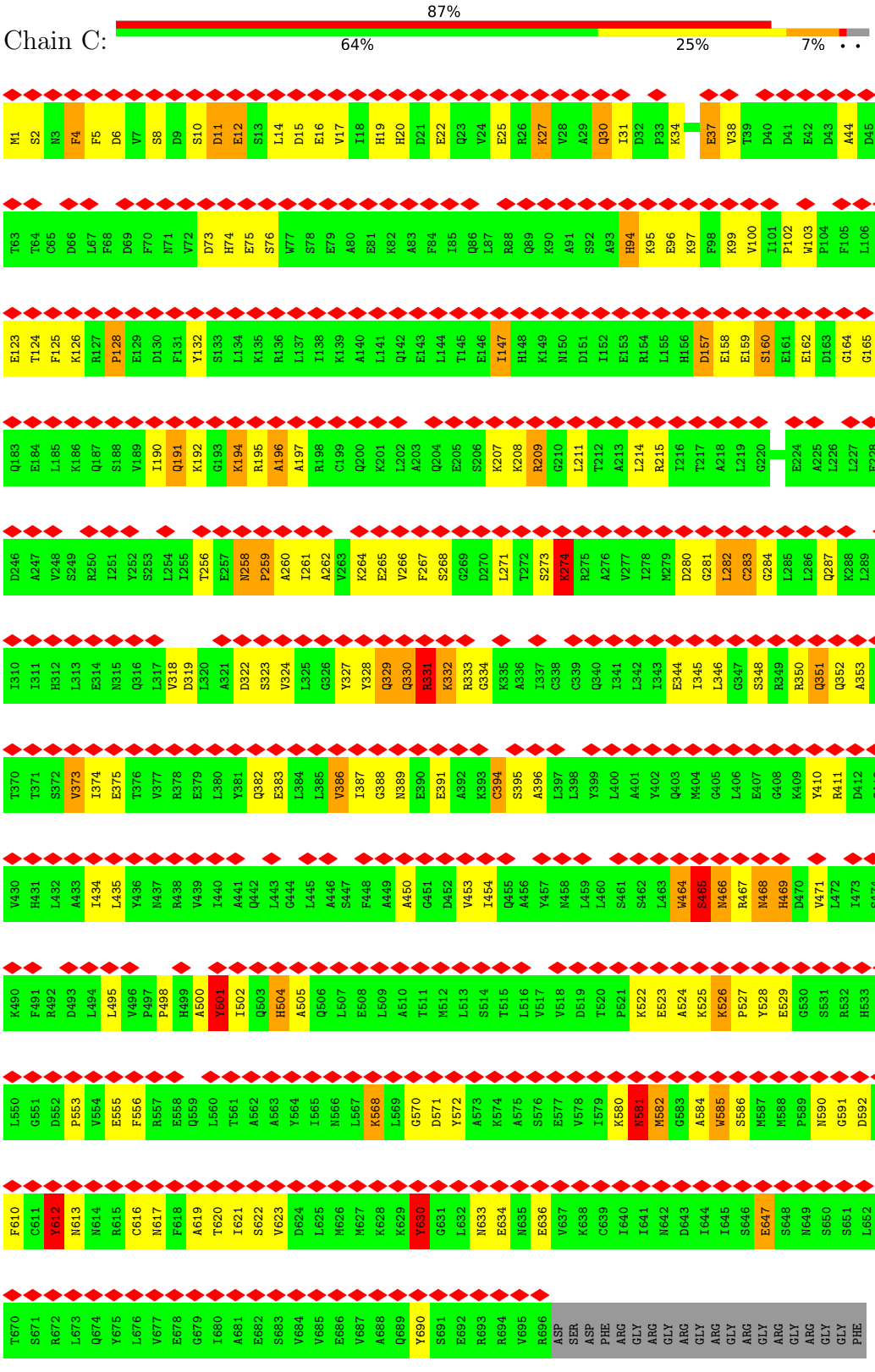
• Molecule 45: 40S ribosomal protein S15, putative

Chain T:



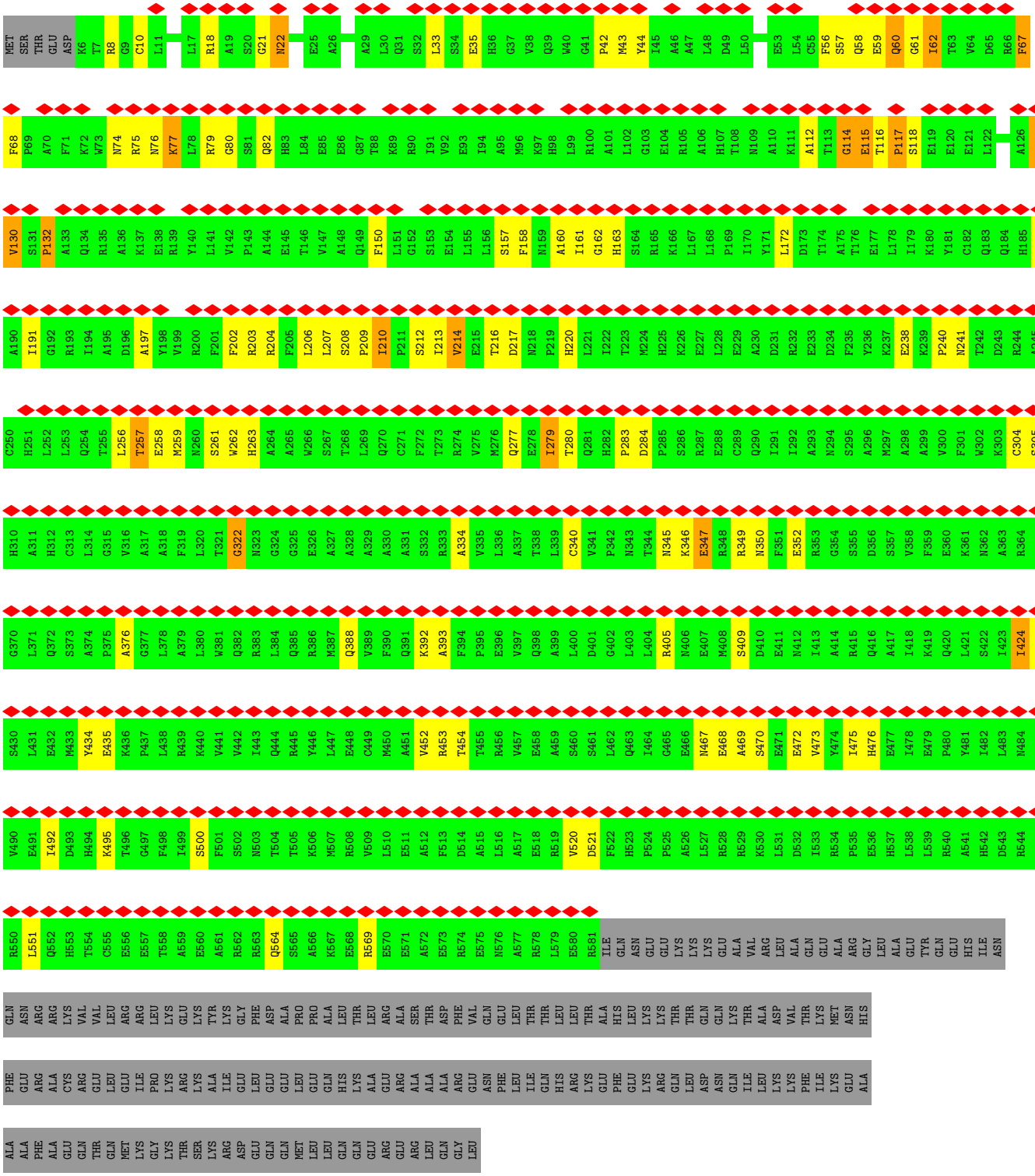
• Molecule 46: Eukaryotic translation initiation factor 3 subunit 8, putative

Chain C:



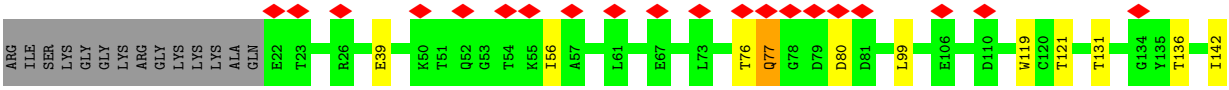
• Molecule 47: eIF3A

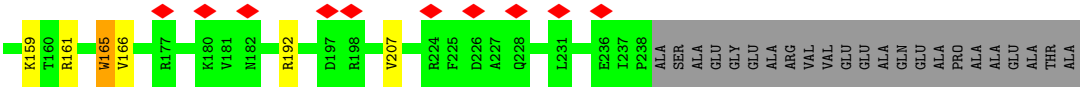
Chain 8:



• Molecule 48: 40S ribosomal protein S3a-2

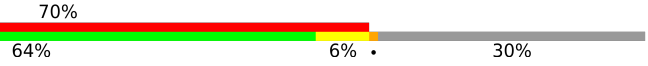
Chain W:

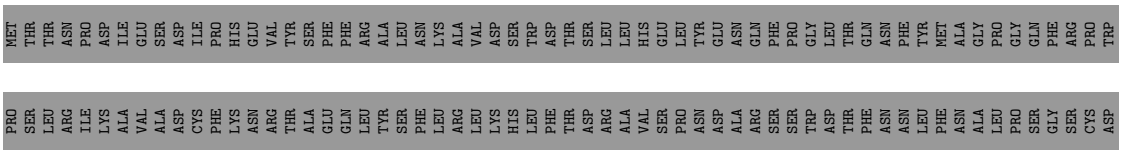


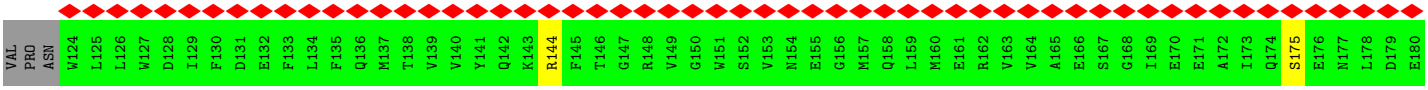


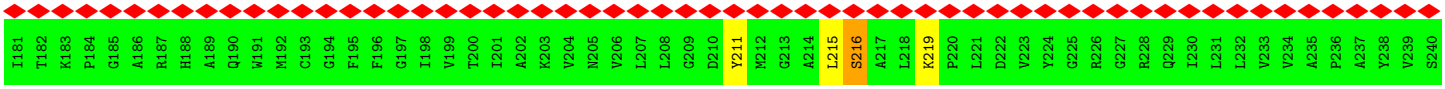
• Molecule 49: Eukaryotic translation initiation factor 3 (EIF-3) interacting protein, putative

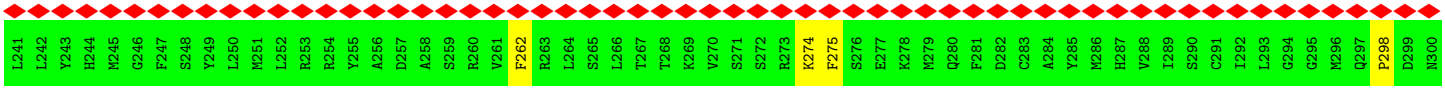
Chain I:

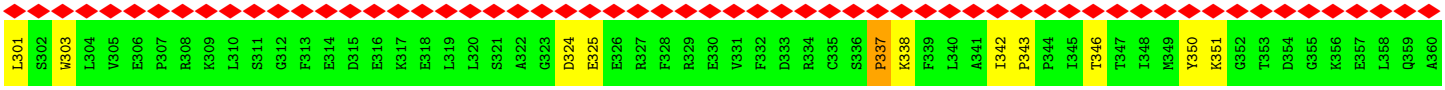


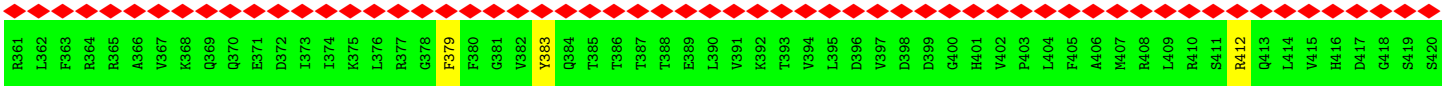


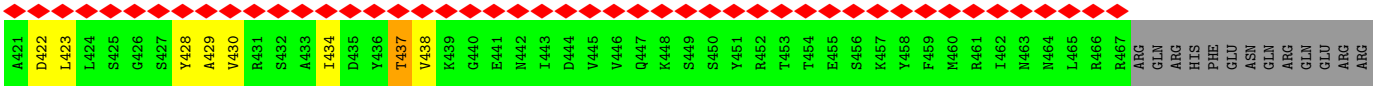






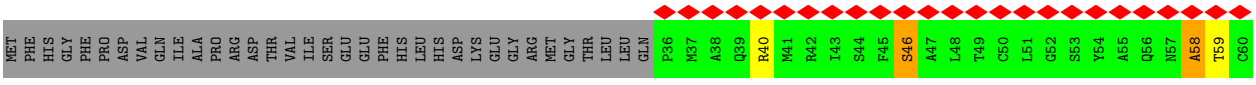


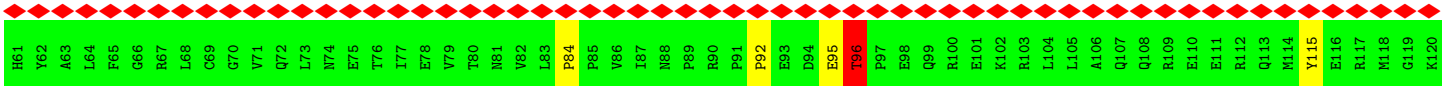


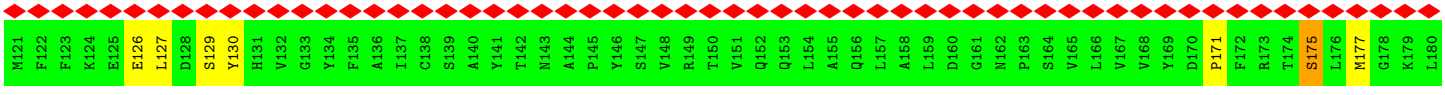


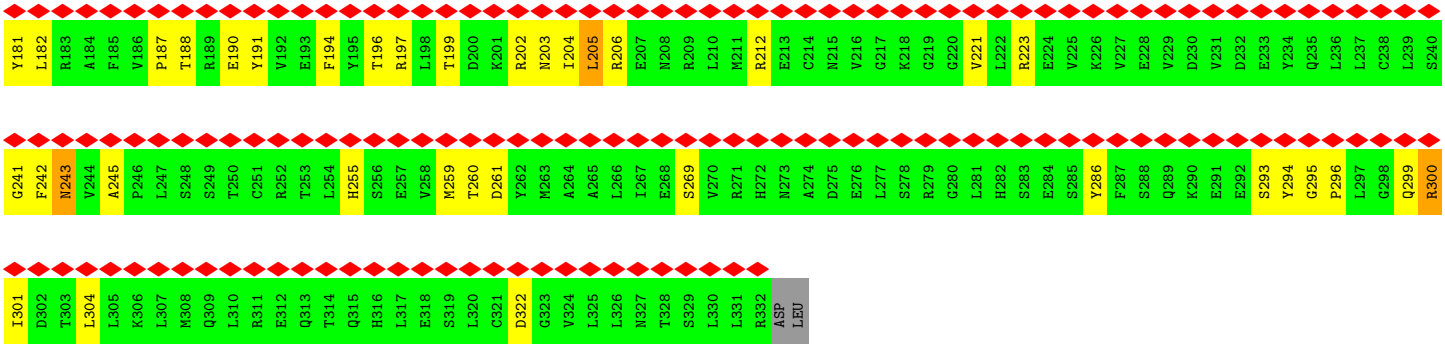
• Molecule 50: eIF3H

Chain H:

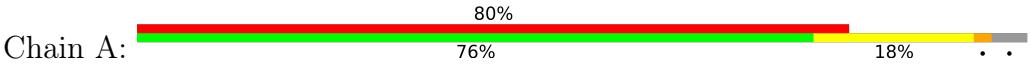


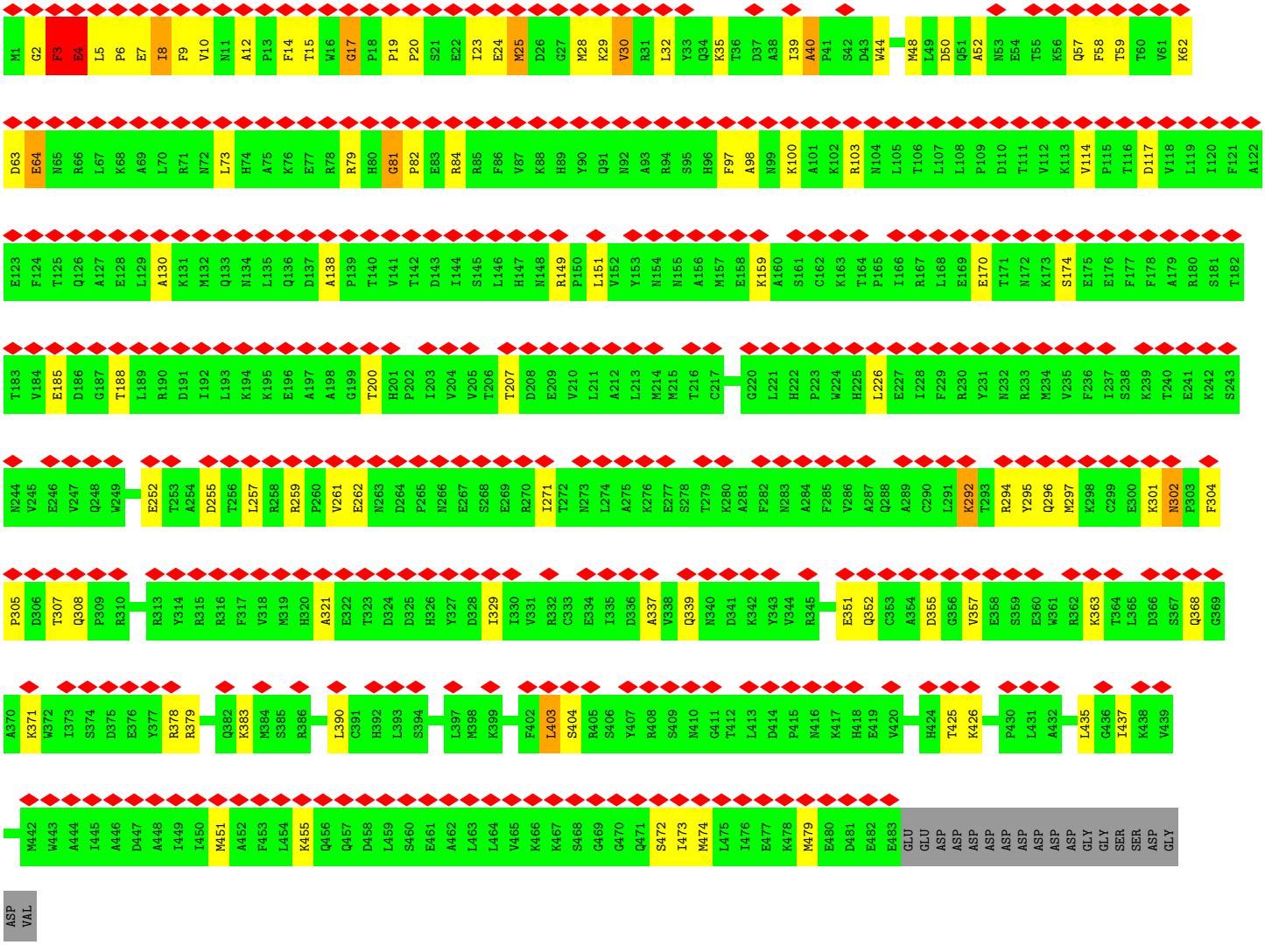




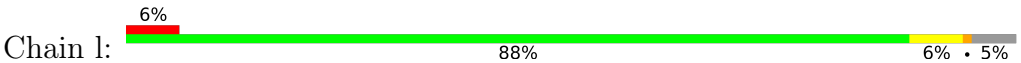


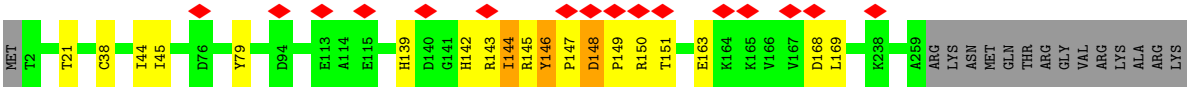
• Molecule 51: Eukaryotic translation initiation factor 3 subunit 7-like protein, putative





• Molecule 52: 40S ribosomal protein S4




MET
T2
T21
C38
I44
I45
D76
Y79
D94
E113
A114
E115
H139
D140
G141
H142
R143
I144
R145
Y146
P147
D148
P149
R150
T151
E163
K164
K165
V166
V167
D168
L169
K238
A259
ARG
LYS
ASN
MET
GLN
THR
ARG
GLY
VAL
ARG
LYS
ALA
ARG
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0193	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	f	1.28	79/12510 (0.6%)	1.48	202/16884 (1.2%)
2	1	1.61	1/1798 (0.1%)	2.50	213/2803 (7.6%)
3	0	1.59	38/51207 (0.1%)	2.44	5849/79792 (7.3%)
4	y	1.02	0/1004	1.01	0/1335
5	s	0.94	0/2405	1.09	8/3247 (0.2%)
6	j	0.94	0/658	1.04	2/871 (0.2%)
7	n	0.92	0/1818	0.93	1/2433 (0.0%)
8	p	0.94	0/2461	1.10	2/3347 (0.1%)
9	r	1.01	0/1131	1.06	1/1520 (0.1%)
10	u	1.06	0/1126	1.20	5/1508 (0.3%)
11	m	0.97	0/1137	1.02	2/1520 (0.1%)
12	Z	1.06	0/1424	1.04	0/1904
13	o	0.96	0/1515	0.97	0/2034
14	q	1.06	0/1703	1.05	2/2290 (0.1%)
15	R	1.01	0/1164	1.00	0/1559
16	S	0.97	0/641	0.95	0/858
17	t	1.14	0/845	1.05	0/1129
18	U	1.05	0/527	1.04	0/702
19	v	1.04	0/1026	1.04	1/1376 (0.1%)
20	X	1.04	1/1238 (0.1%)	1.04	1/1662 (0.1%)
21	B	1.06	0/1513	1.00	0/2030
22	F	0.98	0/1693	1.05	4/2290 (0.2%)
23	d	0.95	0/1760	1.08	5/2376 (0.2%)
24	g	0.93	0/644	1.01	0/875
25	a	0.93	0/559	0.98	0/748
26	J	1.07	0/1381	1.23	7/1857 (0.4%)
27	h	0.97	0/966	0.99	0/1295
28	5	1.02	2/3302 (0.1%)	1.27	12/4483 (0.3%)
29	P	1.09	0/2008	1.04	0/2678
30	i	1.00	0/1005	1.11	3/1341 (0.2%)
31	L	0.99	0/794	1.09	0/1076
32	M	1.04	0/1606	1.05	0/2141

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	N	0.98	0/804	1.07	2/1082 (0.2%)
34	O	1.01	0/1140	1.05	0/1524
35	b	1.00	0/1037	1.04	0/1391
36	c	0.92	0/488	1.02	0/644
37	V	0.75	0/799	0.84	0/1072
38	w	0.92	0/1177	0.94	1/1588 (0.1%)
39	E	1.49	6/3174 (0.2%)	1.15	13/4304 (0.3%)
40	Y	0.91	0/1406	1.00	2/1890 (0.1%)
41	Q	1.07	0/468	1.10	1/618 (0.2%)
42	D	1.30	0/298	1.04	0/385
43	G	1.00	0/2455	1.09	4/3323 (0.1%)
44	K	0.89	0/1597	1.06	12/2170 (0.6%)
45	T	1.00	0/1079	0.98	1/1447 (0.1%)
46	C	1.68	3/5724 (0.1%)	1.11	20/7724 (0.3%)
47	8	0.96	0/4685	1.04	6/6327 (0.1%)
48	W	1.05	4/1809 (0.2%)	1.21	7/2437 (0.3%)
49	I	0.98	0/2826	1.01	8/3809 (0.2%)
50	H	1.01	0/2431	1.11	9/3285 (0.3%)
51	A	0.95	3/3971 (0.1%)	1.04	4/5366 (0.1%)
52	l	1.01	0/2073	1.05	0/2787
All	All	1.31	137/144010 (0.1%)	1.78	6410/205137 (3.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	f	3	200
3	0	2	52
4	y	0	1
5	s	0	17
6	j	0	2
7	n	0	1
8	p	0	2
9	r	0	4
10	u	0	2
11	m	0	2
12	Z	0	2
13	o	0	1
17	t	0	1
19	v	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	X	0	10
21	B	0	4
22	F	0	3
23	d	0	3
24	g	0	1
26	J	0	21
28	5	0	12
29	P	0	4
31	L	0	7
32	M	0	2
33	N	0	1
34	O	0	6
35	b	0	1
36	c	0	3
38	w	0	6
39	E	1	73
40	Y	0	4
41	Q	0	3
42	D	0	1
43	G	0	36
44	K	0	2
45	T	0	1
46	C	1	137
47	8	0	69
48	W	0	2
49	I	2	6
50	H	0	26
51	A	0	16
52	l	0	10
All	All	9	759

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	C	411	ARG	CD-NE	105.86	3.26	1.46
39	E	279	TYR	CE1-CZ	28.41	1.75	1.38
39	E	279	TYR	CE2-CZ	28.18	1.75	1.38
39	E	279	TYR	CG-CD1	28.05	1.75	1.39
39	E	279	TYR	CG-CD2	27.28	1.74	1.39
28	5	283	GLY	N-CA	-27.21	1.05	1.46
39	E	279	TYR	CD1-CE1	22.34	1.72	1.39
39	E	279	TYR	CD2-CE2	22.10	1.72	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	301	GLU	C-O	-19.59	0.86	1.23
1	f	1221	LEU	C-N	19.32	1.71	1.34
1	f	301	GLU	CA-C	-19.29	1.02	1.52
1	f	774	LEU	C-N	18.33	1.66	1.33
1	f	1127	VAL	C-N	17.01	1.66	1.34
1	f	1149	TYR	C-N	16.88	1.72	1.34
1	f	139	MET	N-CA	-16.86	1.12	1.46
1	f	304	PRO	CA-C	-16.65	1.19	1.52
1	f	1254	ALA	C-N	15.09	1.68	1.34
1	f	1653	CYS	C-N	14.59	1.59	1.33
46	C	53	ARG	C-N	14.57	1.67	1.34
1	f	1492	GLY	C-N	14.20	1.61	1.34
1	f	307	LEU	C-N	13.64	1.65	1.34
1	f	153	GLY	N-CA	-13.50	1.25	1.46
51	A	6	PRO	N-CA	13.44	1.70	1.47
1	f	1110	GLY	N-CA	-13.42	1.25	1.46
1	f	296	TYR	N-CA	-13.41	1.19	1.46
1	f	256	GLU	N-CA	-13.39	1.19	1.46
1	f	1235	LYS	C-O	-12.88	0.98	1.23
1	f	305	TYR	CA-C	-12.42	1.20	1.52
1	f	301	GLU	C-N	12.23	1.62	1.34
1	f	772	TYR	N-CA	-12.22	1.22	1.46
1	f	234	GLY	C-N	-11.94	1.06	1.34
1	f	306	ARG	N-CA	11.48	1.69	1.46
1	f	1703	GLY	N-CA	-11.44	1.28	1.46
1	f	303	ASN	C-N	11.35	1.55	1.34
1	f	1264	LEU	C-N	11.15	1.59	1.34
1	f	259	PHE	CA-C	11.07	1.81	1.52
1	f	200	ASP	N-CA	-10.96	1.24	1.46
1	f	194	PHE	C-N	-10.92	1.08	1.34
1	f	305	TYR	C-O	10.72	1.43	1.23
1	f	1038	GLY	C-N	10.49	1.58	1.34
1	f	139	MET	C-N	-9.90	1.11	1.34
1	f	259	PHE	C-N	9.88	1.56	1.34
1	f	195	HIS	C-N	-9.24	1.12	1.34
1	f	1044	VAL	C-N	9.09	1.54	1.34
1	f	257	PRO	C-N	9.06	1.54	1.34
1	f	1149	TYR	N-CA	9.05	1.64	1.46
3	0	1531	A	O3'-P	9.00	1.72	1.61
1	f	1214	ARG	C-N	-8.99	1.13	1.34
1	f	302	ALA	N-CA	8.93	1.64	1.46
1	f	1122	GLN	C-N	8.92	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	131	THR	C-N	-8.79	1.13	1.34
1	f	199	PHE	C-N	-8.71	1.14	1.34
51	A	302	ASN	C-N	8.63	1.50	1.34
1	f	198	PHE	C-N	-8.52	1.14	1.34
1	f	1121	CYS	C-N	8.51	1.53	1.34
1	f	1108	ALA	N-CA	-8.28	1.29	1.46
48	W	165	TRP	C-N	-8.05	1.15	1.34
1	f	304	PRO	C-N	-7.88	1.16	1.34
1	f	1627	ARG	C-N	7.87	1.47	1.33
1	f	197	VAL	N-CA	7.77	1.61	1.46
1	f	264	ASP	C-N	7.75	1.47	1.33
1	f	1219	HIS	C-N	7.70	1.51	1.34
1	f	229	ASN	C-N	7.59	1.51	1.34
48	W	165	TRP	CA-CB	-7.54	1.37	1.53
1	f	1655	VAL	N-CA	-7.51	1.31	1.46
1	f	298	ASP	C-N	7.49	1.51	1.34
1	f	1153	ASP	C-N	7.43	1.51	1.34
1	f	1040	GLY	N-CA	-7.32	1.35	1.46
1	f	256	GLU	C-N	-7.18	1.20	1.34
3	0	1532	G	O3'-P	-7.05	1.52	1.61
1	f	192	ALA	C-N	7.02	1.50	1.34
1	f	292	ARG	N-CA	-7.00	1.32	1.46
1	f	263	SER	C-N	-6.92	1.18	1.34
1	f	1147	ILE	C-N	6.87	1.49	1.34
1	f	307	LEU	CA-C	-6.86	1.35	1.52
1	f	239	ASN	C-N	6.75	1.49	1.34
1	f	132	ALA	C-N	-6.56	1.19	1.34
1	f	296	TYR	C-N	-6.50	1.19	1.34
1	f	264	ASP	N-CA	-6.41	1.33	1.46
3	0	1247	A	N7-C5	-6.33	1.35	1.39
28	5	253	THR	C-N	-6.23	1.19	1.34
3	0	1598	A	N7-C5	-6.22	1.35	1.39
1	f	134	PRO	CA-C	6.09	1.65	1.52
1	f	1633	HIS	N-CA	6.09	1.58	1.46
51	A	5	LEU	C-N	6.08	1.45	1.34
3	0	1332	A	N7-C5	-6.08	1.35	1.39
3	0	1310	A	N7-C5	-6.04	1.35	1.39
1	f	199	PHE	N-CA	6.01	1.58	1.46
1	f	305	TYR	N-CA	-5.98	1.34	1.46
1	f	292	ARG	C-N	5.97	1.47	1.34
3	0	2269	A	N7-C5	-5.96	1.35	1.39
3	0	255	A	N7-C5	-5.95	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	0	1605	A	N7-C5	-5.94	1.35	1.39
1	f	303	ASN	C-O	5.72	1.34	1.23
3	0	2115	A	N7-C5	-5.71	1.35	1.39
1	f	136	LEU	C-N	5.71	1.47	1.34
3	0	2150	A	N7-C5	-5.71	1.35	1.39
1	f	294	ALA	C-N	-5.69	1.21	1.34
1	f	239	ASN	CA-C	-5.65	1.38	1.52
3	0	2194	A	N7-C5	-5.64	1.35	1.39
3	0	1353	A	N7-C5	-5.61	1.35	1.39
3	0	1773	A	N7-C5	-5.59	1.35	1.39
1	f	772	TYR	C-N	5.58	1.46	1.34
3	0	979	G	C2-N3	5.56	1.37	1.32
48	W	165	TRP	CB-CG	5.55	1.60	1.50
3	0	254	A	N7-C5	-5.52	1.35	1.39
3	0	162	A	N7-C5	-5.49	1.35	1.39
2	1	14	A	N7-C5	-5.45	1.35	1.39
3	0	761	G	C2-N3	5.44	1.37	1.32
3	0	2139	A	N7-C5	-5.43	1.35	1.39
1	f	294	ALA	N-CA	-5.33	1.35	1.46
1	f	138	ASP	C-N	-5.32	1.21	1.34
3	0	2094	A	N7-C5	-5.31	1.36	1.39
1	f	1655	VAL	C-O	5.29	1.33	1.23
3	0	275	A	N7-C5	-5.29	1.36	1.39
3	0	1559	A	N7-C5	-5.28	1.36	1.39
3	0	710	A	N7-C5	-5.27	1.36	1.39
1	f	1267	LEU	N-CA	-5.24	1.35	1.46
3	0	776	G	C2-N3	5.21	1.36	1.32
3	0	2109	A	N7-C5	-5.21	1.36	1.39
3	0	97	A	N7-C5	-5.18	1.36	1.39
3	0	1606	A	N7-C5	-5.16	1.36	1.39
3	0	1193	C	N3-C4	5.16	1.37	1.33
20	X	34	HIS	N-CA	5.14	1.56	1.46
3	0	895	A	N7-C5	-5.12	1.36	1.39
3	0	1673	G	N1-C2	5.11	1.41	1.37
3	0	2209	A	N7-C5	-5.11	1.36	1.39
48	W	166	VAL	N-CA	-5.10	1.36	1.46
3	0	2243	A	N7-C5	-5.10	1.36	1.39
3	0	712	U	C2-N3	5.08	1.41	1.37
3	0	1903	G	C2-N3	5.07	1.36	1.32
3	0	742	A	N7-C5	-5.06	1.36	1.39
46	C	411	ARG	NE-CZ	5.06	1.39	1.33
3	0	274	C	N3-C4	5.03	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	1148	ASP	C-N	-5.03	1.22	1.34
3	0	1333	A	N7-C5	-5.02	1.36	1.39
3	0	2244	A	N7-C5	-5.00	1.36	1.39

All (6410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	5	412	GLN	O-C-N	-35.37	66.11	122.70
1	f	234	GLY	O-C-N	-34.90	66.87	122.70
1	f	307	LEU	O-C-N	-26.57	80.19	122.70
1	f	1147	ILE	O-C-N	23.84	160.84	122.70
1	f	305	TYR	N-CA-CB	19.79	146.23	110.60
3	0	1531	A	O3'-P-O5'	18.80	139.71	104.00
1	f	1147	ILE	CA-C-N	-18.13	77.31	117.20
1	f	306	ARG	N-CA-CB	17.23	141.62	110.60
1	f	239	ASN	CA-C-N	16.36	153.20	117.20
1	f	308	ARG	C-N-CA	16.19	162.18	121.70
28	5	411	LEU	CA-C-N	-16.01	81.99	117.20
1	f	296	TYR	N-CA-C	15.97	154.11	111.00
3	0	1870	A	N1-C6-N6	15.83	128.10	118.60
3	0	1531	A	P-O3'-C3'	15.77	138.62	119.70
3	0	746	A	N1-C6-N6	15.74	128.04	118.60
3	0	1070	C	P-O3'-C3'	15.72	138.57	119.70
28	5	411	LEU	C-N-CA	-15.70	82.45	121.70
1	f	131	THR	O-C-N	15.24	147.09	122.70
1	f	152	ASP	O-C-N	-14.88	97.91	123.20
1	f	1070	LYS	C-N-CA	14.82	158.75	121.70
3	0	742	A	N1-C6-N6	14.51	127.30	118.60
28	5	411	LEU	O-C-N	14.42	145.78	122.70
1	f	1039	ARG	O-C-N	-14.37	98.78	123.20
46	C	411	ARG	CD-NE-CZ	14.25	143.55	123.60
1	f	1259	CYS	O-C-N	-14.22	99.94	122.70
3	0	962	A	N1-C6-N6	14.11	127.07	118.60
3	0	217	C	P-O3'-C3'	14.09	136.60	119.70
1	f	263	SER	O-C-N	-14.06	100.19	122.70
3	0	175	A	N1-C6-N6	14.03	127.02	118.60
1	f	259	PHE	N-CA-CB	-13.87	85.63	110.60
3	0	833	A	N1-C6-N6	13.84	126.91	118.60
3	0	2061	A	N1-C6-N6	13.82	126.89	118.60
3	0	1559	A	N1-C6-N6	13.77	126.86	118.60
3	0	1644	A	N1-C6-N6	13.75	126.85	118.60
1	f	1654	GLY	C-N-CA	13.65	155.83	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	710	A	N1-C6-N6	13.63	126.78	118.60
3	0	144	A	N1-C6-N6	13.57	126.74	118.60
3	0	2141	A	N1-C6-N6	13.55	126.73	118.60
1	f	296	TYR	C-N-CA	13.48	155.41	121.70
48	W	165	TRP	CB-CA-C	-13.48	83.45	110.40
1	f	1070	LYS	O-C-N	-13.45	101.18	122.70
1	f	131	THR	CA-C-N	-13.43	87.66	117.20
1	f	238	SER	CB-CA-C	-13.42	84.59	110.10
1	f	1147	ILE	C-N-CA	-13.37	88.27	121.70
3	0	2285	A	N1-C6-N6	13.31	126.58	118.60
3	0	1181	A	N1-C6-N6	13.29	126.58	118.60
1	f	132	ALA	O-C-N	13.28	143.95	122.70
3	0	2088	A	N1-C6-N6	13.24	126.54	118.60
3	0	1991	A	N1-C6-N6	13.18	126.51	118.60
2	1	37	A	N1-C6-N6	13.16	126.50	118.60
3	0	1986	A	N1-C6-N6	13.16	126.50	118.60
3	0	256	A	N1-C6-N6	13.16	126.49	118.60
3	0	2052	A	N1-C6-N6	13.15	126.49	118.60
48	W	165	TRP	CB-CG-CD2	-13.12	109.54	126.60
3	0	1636	A	N1-C6-N6	13.10	126.46	118.60
3	0	1620	A	N1-C6-N6	13.09	126.45	118.60
3	0	51	A	N1-C6-N6	13.09	126.45	118.60
3	0	831	A	N1-C6-N6	13.09	126.45	118.60
3	0	1284	A	N1-C6-N6	13.09	126.45	118.60
3	0	1460	A	N1-C6-N6	13.08	126.45	118.60
3	0	735	A	N1-C6-N6	13.08	126.45	118.60
3	0	1600	A	N1-C6-N6	13.08	126.45	118.60
48	W	165	TRP	CB-CG-CD1	13.07	144.00	127.00
2	1	43	A	N1-C6-N6	13.07	126.44	118.60
3	0	1522	A	N1-C6-N6	13.06	126.44	118.60
3	0	2085	A	N1-C6-N6	13.06	126.44	118.60
3	0	646	A	N1-C6-N6	13.05	126.43	118.60
3	0	1264	A	N1-C6-N6	13.03	126.42	118.60
48	W	165	TRP	CA-CB-CG	13.03	138.46	113.70
3	0	111	A	N1-C6-N6	13.03	126.42	118.60
3	0	1295	A	N1-C6-N6	13.02	126.41	118.60
3	0	2273	A	N1-C6-N6	13.02	126.41	118.60
3	0	2003	A	N1-C6-N6	13.02	126.41	118.60
3	0	1737	A	N1-C6-N6	13.02	126.41	118.60
3	0	864	A	N1-C6-N6	12.99	126.40	118.60
3	0	984	A	N1-C6-N6	12.99	126.39	118.60
3	0	2250	A	N1-C6-N6	12.98	126.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1360	A	N1-C6-N6	12.97	126.38	118.60
2	1	62	A	N1-C6-N6	12.96	126.38	118.60
3	0	2013	A	N1-C6-N6	12.94	126.36	118.60
3	0	1715	A	N1-C6-N6	12.93	126.36	118.60
5	s	300	ARG	N-CA-C	12.93	145.91	111.00
3	0	1403	A	N1-C6-N6	12.91	126.35	118.60
3	0	392	A	N1-C6-N6	12.88	126.33	118.60
3	0	1700	A	N1-C6-N6	12.86	126.32	118.60
3	0	2031	A	N1-C6-N6	12.83	126.30	118.60
3	0	255	A	N1-C6-N6	12.83	126.30	118.60
3	0	1534	A	N1-C6-N6	12.81	126.29	118.60
3	0	1684	A	N1-C6-N6	12.81	126.28	118.60
3	0	1930	A	N1-C6-N6	12.80	126.28	118.60
2	1	26	A	N1-C6-N6	12.80	126.28	118.60
3	0	1314	A	N1-C6-N6	12.79	126.28	118.60
3	0	718	A	N1-C6-N6	12.78	126.27	118.60
3	0	2311	A	N1-C6-N6	12.78	126.27	118.60
3	0	1223	A	N1-C6-N6	12.76	126.26	118.60
3	0	434	A	N1-C6-N6	12.76	126.26	118.60
3	0	260	A	N1-C6-N6	12.76	126.25	118.60
3	0	581	A	N1-C6-N6	12.76	126.25	118.60
3	0	1997	A	N1-C6-N6	12.75	126.25	118.60
3	0	261	A	N1-C6-N6	12.75	126.25	118.60
3	0	923	A	N1-C6-N6	12.74	126.24	118.60
3	0	249	A	N1-C6-N6	12.72	126.23	118.60
3	0	1709	A	N1-C6-N6	12.71	126.23	118.60
3	0	1307	A	N1-C6-N6	12.71	126.22	118.60
3	0	509	A	N1-C6-N6	12.71	126.22	118.60
3	0	645	A	N1-C6-N6	12.69	126.21	118.60
3	0	210	A	N1-C6-N6	12.68	126.21	118.60
3	0	141	A	N1-C6-N6	12.68	126.21	118.60
3	0	492	A	N1-C6-N6	12.68	126.21	118.60
3	0	1420	A	N1-C6-N6	12.68	126.21	118.60
3	0	1795	A	N1-C6-N6	12.68	126.21	118.60
3	0	254	A	N1-C6-N6	12.67	126.20	118.60
3	0	522	A	N1-C6-N6	12.66	126.20	118.60
3	0	2234	A	N1-C6-N6	12.66	126.19	118.60
3	0	1292	A	N1-C6-N6	12.65	126.19	118.60
3	0	73	A	N1-C6-N6	12.65	126.19	118.60
3	0	826	A	N1-C6-N6	12.63	126.18	118.60
3	0	2239	A	N1-C6-N6	12.64	126.18	118.60
3	0	884	A	N1-C6-N6	12.63	126.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	852	A	N1-C6-N6	12.62	126.17	118.60
3	0	2293	A	N1-C6-N6	12.62	126.17	118.60
1	f	772	TYR	N-CA-CB	12.61	133.29	110.60
3	0	1638	A	N1-C6-N6	12.60	126.16	118.60
3	0	858	A	N1-C6-N6	12.60	126.16	118.60
3	0	168	A	N1-C6-N6	12.59	126.15	118.60
1	f	1121	CYS	C-N-CA	12.58	153.14	121.70
3	0	1579	A	P-O3'-C3'	12.55	134.77	119.70
3	0	1925	A	N1-C6-N6	12.55	126.13	118.60
3	0	1978	A	N1-C6-N6	12.55	126.13	118.60
3	0	2279	A	N1-C6-N6	12.55	126.13	118.60
3	0	526	A	N1-C6-N6	12.54	126.12	118.60
3	0	22	A	N1-C6-N6	12.53	126.12	118.60
3	0	569	A	N1-C6-N6	12.52	126.11	118.60
3	0	1820	A	N1-C6-N6	12.52	126.11	118.60
3	0	1313	A	N1-C6-N6	12.52	126.11	118.60
3	0	257	A	N1-C6-N6	12.51	126.11	118.60
3	0	576	A	N1-C6-N6	12.51	126.11	118.60
3	0	711	A	N1-C6-N6	12.51	126.11	118.60
3	0	245	A	N1-C6-N6	12.50	126.10	118.60
3	0	2016	A	N1-C6-N6	12.49	126.10	118.60
3	0	1624	A	N1-C6-N6	12.49	126.09	118.60
3	0	1227	A	N1-C6-N6	12.49	126.09	118.60
3	0	1992	A	N1-C6-N6	12.47	126.08	118.60
3	0	2064	A	N1-C6-N6	12.46	126.08	118.60
3	0	1681	A	N1-C6-N6	12.45	126.07	118.60
3	0	1246	A	N1-C6-N6	12.45	126.07	118.60
3	0	1932	A	N1-C6-N6	12.45	126.07	118.60
3	0	2286	A	N1-C6-N6	12.45	126.07	118.60
3	0	862	A	N1-C6-N6	12.45	126.07	118.60
3	0	920	A	N1-C6-N6	12.44	126.06	118.60
3	0	2221	A	N1-C6-N6	12.44	126.06	118.60
3	0	1507	A	N1-C6-N6	12.43	126.06	118.60
3	0	1829	A	N1-C6-N6	12.43	126.06	118.60
3	0	2081	A	N1-C6-N6	12.43	126.06	118.60
3	0	78	A	N1-C6-N6	12.42	126.05	118.60
3	0	1273	A	N1-C6-N6	12.41	126.05	118.60
3	0	2172	A	N1-C6-N6	12.41	126.05	118.60
3	0	190	A	N1-C6-N6	12.40	126.04	118.60
3	0	1598	A	N1-C6-N6	12.40	126.04	118.60
3	0	1291	A	N1-C6-N6	12.40	126.04	118.60
3	0	1373	A	N1-C6-N6	12.40	126.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2226	A	N1-C6-N6	12.40	126.04	118.60
3	0	1579	A	N1-C6-N6	12.40	126.04	118.60
3	0	1205	A	N1-C6-N6	12.38	126.03	118.60
3	0	1335	A	N1-C6-N6	12.38	126.03	118.60
3	0	1240	A	N1-C6-N6	12.38	126.03	118.60
1	f	262	MET	O-C-N	-12.37	102.91	122.70
3	0	604	A	N1-C6-N6	12.37	126.02	118.60
3	0	658	A	N1-C6-N6	12.37	126.02	118.60
3	0	1319	A	N1-C6-N6	12.36	126.02	118.60
3	0	467	A	N1-C6-N6	12.36	126.02	118.60
3	0	2205	A	N1-C6-N6	12.36	126.01	118.60
3	0	142	A	N1-C6-N6	12.35	126.01	118.60
3	0	2051	A	N1-C6-N6	12.35	126.01	118.60
3	0	863	A	N1-C6-N6	12.34	126.00	118.60
3	0	414	A	N1-C6-N6	12.34	126.00	118.60
3	0	525	A	N1-C6-N6	12.33	126.00	118.60
3	0	2299	A	N1-C6-N6	12.33	126.00	118.60
3	0	639	A	N1-C6-N6	12.33	126.00	118.60
3	0	2256	A	N1-C6-N6	12.32	126.00	118.60
3	0	2320	A	N1-C6-N6	12.32	126.00	118.60
3	0	1180	A	N1-C6-N6	12.32	125.99	118.60
3	0	1365	A	N1-C6-N6	12.32	125.99	118.60
3	0	1222	A	N1-C6-N6	12.32	125.99	118.60
3	0	330	A	N1-C6-N6	12.32	125.99	118.60
3	0	2116	A	N1-C6-N6	12.31	125.99	118.60
2	1	19	A	N1-C6-N6	12.31	125.99	118.60
3	0	1610	A	N1-C6-N6	12.31	125.99	118.60
3	0	1883	A	N1-C6-N6	12.31	125.99	118.60
1	f	198	PHE	O-C-N	-12.31	103.01	122.70
3	0	788	A	N1-C6-N6	12.31	125.98	118.60
3	0	28	A	N1-C6-N6	12.30	125.98	118.60
3	0	450	A	N1-C6-N6	12.30	125.98	118.60
2	1	4	A	N1-C6-N6	12.30	125.98	118.60
3	0	592	A	N1-C6-N6	12.30	125.98	118.60
3	0	1597	A	N1-C6-N6	12.29	125.97	118.60
3	0	2108	A	N1-C6-N6	12.29	125.97	118.60
3	0	105	A	N1-C6-N6	12.29	125.97	118.60
3	0	2267	A	N1-C6-N6	12.28	125.97	118.60
3	0	1275	A	N1-C6-N6	12.28	125.97	118.60
3	0	2214	A	N1-C6-N6	12.28	125.97	118.60
3	0	43	A	N1-C6-N6	12.28	125.97	118.60
3	0	1306	A	N1-C6-N6	12.27	125.96	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1773	A	N1-C6-N6	12.27	125.96	118.60
3	0	1263	A	N1-C6-N6	12.27	125.96	118.60
3	0	314	A	N1-C6-N6	12.26	125.96	118.60
3	0	523	A	N1-C6-N6	12.26	125.95	118.60
3	0	2244	A	N1-C6-N6	12.25	125.95	118.60
3	0	499	A	N1-C6-N6	12.25	125.95	118.60
3	0	1686	A	N1-C6-N6	12.24	125.94	118.60
3	0	122	A	N1-C6-N6	12.23	125.94	118.60
3	0	123	A	N1-C6-N6	12.23	125.94	118.60
3	0	1809	A	N1-C6-N6	12.22	125.93	118.60
3	0	386	A	N1-C6-N6	12.22	125.93	118.60
3	0	889	A	N1-C6-N6	12.21	125.92	118.60
3	0	149	A	N1-C6-N6	12.21	125.92	118.60
3	0	498	A	N1-C6-N6	12.21	125.92	118.60
3	0	2207	A	N1-C6-N6	12.21	125.92	118.60
3	0	107	A	N1-C6-N6	12.20	125.92	118.60
3	0	783	A	N1-C6-N6	12.20	125.92	118.60
3	0	160	A	N1-C6-N6	12.19	125.92	118.60
3	0	586	A	N1-C6-N6	12.19	125.91	118.60
3	0	1804	A	N1-C6-N6	12.19	125.91	118.60
3	0	1823	A	N1-C6-N6	12.19	125.91	118.60
3	0	2041	A	N1-C6-N6	12.19	125.91	118.60
3	0	279	A	N1-C6-N6	12.18	125.91	118.60
3	0	894	A	N1-C6-N6	12.18	125.91	118.60
3	0	784	A	N1-C6-N6	12.18	125.91	118.60
3	0	1220	A	N1-C6-N6	12.18	125.91	118.60
3	0	11	A	N1-C6-N6	12.17	125.91	118.60
3	0	1924	A	N1-C6-N6	12.17	125.90	118.60
3	0	1379	A	N1-C6-N6	12.17	125.90	118.60
2	1	63	A	N1-C6-N6	12.16	125.90	118.60
3	0	585	A	N1-C6-N6	12.16	125.90	118.60
3	0	64	A	N1-C6-N6	12.16	125.90	118.60
3	0	588	A	N1-C6-N6	12.16	125.90	118.60
2	1	1	A	N1-C6-N6	12.16	125.89	118.60
3	0	1201	A	N1-C6-N6	12.16	125.89	118.60
3	0	2264	A	N1-C6-N6	12.15	125.89	118.60
3	0	304	A	N1-C6-N6	12.15	125.89	118.60
3	0	1297	A	N1-C6-N6	12.15	125.89	118.60
3	0	704	A	N1-C6-N6	12.15	125.89	118.60
3	0	1786	A	N1-C6-N6	12.15	125.89	118.60
3	0	1893	A	N1-C6-N6	12.15	125.89	118.60
3	0	2243	A	N1-C6-N6	12.15	125.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	531	A	N1-C6-N6	12.14	125.89	118.60
3	0	1516	A	N1-C6-N6	12.14	125.89	118.60
3	0	483	A	N1-C6-N6	12.14	125.89	118.60
3	0	2074	A	N1-C6-N6	12.14	125.89	118.60
3	0	974	A	N1-C6-N6	12.14	125.88	118.60
3	0	1454	A	N1-C6-N6	12.14	125.88	118.60
3	0	457	A	N1-C6-N6	12.14	125.88	118.60
3	0	777	A	N1-C6-N6	12.13	125.88	118.60
3	0	438	A	N1-C6-N6	12.13	125.88	118.60
3	0	1871	A	N1-C6-N6	12.13	125.88	118.60
3	0	779	A	N1-C6-N6	12.13	125.88	118.60
3	0	765	A	N1-C6-N6	12.12	125.87	118.60
3	0	561	A	N1-C6-N6	12.12	125.87	118.60
3	0	898	A	N1-C6-N6	12.12	125.87	118.60
1	f	192	ALA	C-N-CA	-12.11	91.42	121.70
3	0	1794	A	N1-C6-N6	12.11	125.87	118.60
3	0	1662	A	N1-C6-N6	12.11	125.86	118.60
3	0	295	A	N1-C6-N6	12.11	125.86	118.60
3	0	916	A	N1-C6-N6	12.10	125.86	118.60
3	0	352	A	N1-C6-N6	12.10	125.86	118.60
3	0	538	A	N1-C6-N6	12.10	125.86	118.60
3	0	689	A	N1-C6-N6	12.10	125.86	118.60
3	0	112	A	N1-C6-N6	12.09	125.86	118.60
3	0	1539	A	N1-C6-N6	12.09	125.86	118.60
3	0	177	A	N1-C6-N6	12.09	125.86	118.60
3	0	1908	A	N1-C6-N6	12.09	125.86	118.60
3	0	406	A	N1-C6-N6	12.09	125.85	118.60
3	0	1260	A	N1-C6-N6	12.08	125.85	118.60
3	0	767	A	N1-C6-N6	12.08	125.85	118.60
3	0	817	A	N1-C6-N6	12.08	125.85	118.60
3	0	1194	A	N1-C6-N6	12.07	125.84	118.60
3	0	1544	A	N1-C6-N6	12.07	125.84	118.60
3	0	2304	A	N1-C6-N6	12.07	125.84	118.60
3	0	242	A	N1-C6-N6	12.07	125.84	118.60
2	1	41	A	N1-C6-N6	12.06	125.84	118.60
3	0	348	A	N1-C6-N6	12.06	125.84	118.60
3	0	653	A	N1-C6-N6	12.06	125.84	118.60
3	0	484	A	N1-C6-N6	12.06	125.83	118.60
3	0	910	A	N1-C6-N6	12.05	125.83	118.60
3	0	1657	A	N1-C6-N6	12.05	125.83	118.60
3	0	674	A	N1-C6-N6	12.05	125.83	118.60
3	0	1808	A	N1-C6-N6	12.05	125.83	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	775	A	N1-C6-N6	12.05	125.83	118.60
3	0	1571	A	N1-C6-N6	12.05	125.83	118.60
1	f	152	ASP	C-N-CA	12.04	147.58	122.30
3	0	454	A	N1-C6-N6	12.04	125.82	118.60
3	0	269	A	N1-C6-N6	12.04	125.82	118.60
3	0	529	A	N1-C6-N6	12.04	125.82	118.60
3	0	595	A	N1-C6-N6	12.03	125.82	118.60
3	0	505	A	N1-C6-N6	12.03	125.82	118.60
3	0	659	A	N1-C6-N6	12.03	125.82	118.60
3	0	1625	A	N1-C6-N6	12.03	125.82	118.60
3	0	913	A	N1-C6-N6	12.03	125.82	118.60
3	0	1694	A	N1-C6-N6	12.03	125.82	118.60
1	f	1266	PRO	C-N-CA	12.03	151.77	121.70
3	0	504	A	N1-C6-N6	12.03	125.81	118.60
3	0	571	A	N1-C6-N6	12.02	125.81	118.60
3	0	587	A	N1-C6-N6	12.02	125.81	118.60
3	0	769	A	N1-C6-N6	12.02	125.81	118.60
3	0	231	A	N1-C6-N6	12.02	125.81	118.60
3	0	1345	A	N1-C6-N6	12.02	125.81	118.60
3	0	1358	A	N1-C6-N6	12.02	125.81	118.60
3	0	2	A	N1-C6-N6	12.01	125.81	118.60
3	0	917	A	N1-C6-N6	12.01	125.81	118.60
3	0	2276	A	N1-C6-N6	12.01	125.81	118.60
3	0	675	A	N1-C6-N6	12.01	125.81	118.60
3	0	1270	A	N1-C6-N6	12.01	125.81	118.60
3	0	1348	A	N1-C6-N6	12.01	125.80	118.60
3	0	1453	A	N1-C6-N6	12.01	125.80	118.60
3	0	607	A	N1-C6-N6	12.00	125.80	118.60
3	0	1827	A	N1-C6-N6	12.00	125.80	118.60
3	0	2131	A	N1-C6-N6	12.00	125.80	118.60
3	0	1370	A	N1-C6-N6	12.00	125.80	118.60
3	0	912	A	N1-C6-N6	12.00	125.80	118.60
3	0	2007	A	N1-C6-N6	12.00	125.80	118.60
3	0	778	A	N1-C6-N6	12.00	125.80	118.60
3	0	1210	A	N1-C6-N6	12.00	125.80	118.60
3	0	2150	A	N1-C6-N6	11.99	125.80	118.60
3	0	872	A	N1-C6-N6	11.99	125.80	118.60
3	0	2197	A	N1-C6-N6	11.99	125.80	118.60
3	0	1558	A	N1-C6-N6	11.99	125.79	118.60
3	0	65	A	N1-C6-N6	11.99	125.79	118.60
3	0	990	A	N1-C6-N6	11.99	125.79	118.60
2	1	34	A	N1-C6-N6	11.98	125.79	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	124	A	N1-C6-N6	11.98	125.79	118.60
3	0	599	A	N1-C6-N6	11.98	125.79	118.60
2	1	58	A	N1-C6-N6	11.98	125.79	118.60
3	0	172	A	N1-C6-N6	11.98	125.79	118.60
3	0	935	A	N1-C6-N6	11.98	125.79	118.60
3	0	2204	A	N1-C6-N6	11.98	125.79	118.60
3	0	771	A	N1-C6-N6	11.98	125.79	118.60
3	0	2265	A	N1-C6-N6	11.98	125.79	118.60
3	0	1067	A	N1-C6-N6	11.98	125.79	118.60
3	0	432	A	N1-C6-N6	11.97	125.78	118.60
3	0	1457	A	N1-C6-N6	11.97	125.78	118.60
3	0	349	A	N1-C6-N6	11.97	125.78	118.60
3	0	472	A	N1-C6-N6	11.97	125.78	118.60
3	0	1341	A	N1-C6-N6	11.97	125.78	118.60
3	0	181	A	N1-C6-N6	11.97	125.78	118.60
3	0	506	A	N1-C6-N6	11.97	125.78	118.60
3	0	624	A	N1-C6-N6	11.97	125.78	118.60
3	0	633	A	N1-C6-N6	11.97	125.78	118.60
3	0	1866	A	N1-C6-N6	11.97	125.78	118.60
2	1	46	A	N1-C6-N6	11.97	125.78	118.60
3	0	1604	A	N1-C6-N6	11.96	125.78	118.60
3	0	2027	A	N1-C6-N6	11.96	125.78	118.60
2	1	72	A	N1-C6-N6	11.96	125.78	118.60
3	0	764	A	N1-C6-N6	11.96	125.78	118.60
3	0	215	A	N1-C6-N6	11.95	125.77	118.60
3	0	1966	A	N1-C6-N6	11.95	125.77	118.60
3	0	610	A	N1-C6-N6	11.95	125.77	118.60
28	5	267	SER	O-C-N	-11.95	103.58	122.70
3	0	180	A	N1-C6-N6	11.95	125.77	118.60
3	0	1501	A	N1-C6-N6	11.95	125.77	118.60
3	0	1390	A	N1-C6-N6	11.94	125.77	118.60
3	0	1738	A	N1-C6-N6	11.95	125.77	118.60
3	0	902	A	N1-C6-N6	11.94	125.77	118.60
3	0	1245	A	N1-C6-N6	11.94	125.77	118.60
3	0	901	A	N1-C6-N6	11.94	125.76	118.60
3	0	250	A	N1-C6-N6	11.94	125.76	118.60
3	0	1198	A	N1-C6-N6	11.94	125.76	118.60
3	0	226	A	N1-C6-N6	11.94	125.76	118.60
3	0	447	A	N1-C6-N6	11.94	125.76	118.60
3	0	82	A	N1-C6-N6	11.93	125.76	118.60
3	0	596	A	N1-C6-N6	11.93	125.76	118.60
3	0	371	A	N1-C6-N6	11.93	125.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	961	A	N1-C6-N6	11.93	125.75	118.60
3	0	536	A	N1-C6-N6	11.92	125.75	118.60
3	0	1523	A	N1-C6-N6	11.92	125.75	118.60
3	0	905	A	N1-C6-N6	11.92	125.75	118.60
3	0	1566	A	N1-C6-N6	11.92	125.75	118.60
3	0	2272	A	N1-C6-N6	11.91	125.75	118.60
3	0	1266	A	N1-C6-N6	11.91	125.75	118.60
3	0	2040	A	N1-C6-N6	11.91	125.75	118.60
3	0	728	A	N1-C6-N6	11.91	125.75	118.60
3	0	2277	A	N1-C6-N6	11.91	125.75	118.60
3	0	502	A	N1-C6-N6	11.90	125.74	118.60
3	0	812	A	N1-C6-N6	11.90	125.74	118.60
3	0	527	A	N1-C6-N6	11.90	125.74	118.60
3	0	300	A	N1-C6-N6	11.89	125.74	118.60
3	0	2140	A	N1-C6-N6	11.89	125.74	118.60
2	1	20	A	N1-C6-N6	11.89	125.73	118.60
3	0	724	A	N1-C6-N6	11.89	125.73	118.60
3	0	993	A	N1-C6-N6	11.88	125.73	118.60
3	0	1944	A	N1-C6-N6	11.88	125.73	118.60
3	0	125	A	N1-C6-N6	11.88	125.73	118.60
3	0	1423	A	N1-C6-N6	11.88	125.73	118.60
3	0	1711	A	N1-C6-N6	11.88	125.73	118.60
3	0	1669	A	N1-C6-N6	11.88	125.72	118.60
3	0	278	A	N1-C6-N6	11.87	125.72	118.60
3	0	1667	A	N1-C6-N6	11.87	125.72	118.60
3	0	875	A	N1-C6-N6	11.87	125.72	118.60
3	0	241	A	N1-C6-N6	11.87	125.72	118.60
3	0	845	A	N1-C6-N6	11.87	125.72	118.60
3	0	1799	A	N1-C6-N6	11.87	125.72	118.60
3	0	287	A	N1-C6-N6	11.87	125.72	118.60
3	0	62	A	N1-C6-N6	11.86	125.72	118.60
3	0	1375	A	N1-C6-N6	11.87	125.72	118.60
3	0	1475	A	N1-C6-N6	11.86	125.72	118.60
3	0	316	A	N1-C6-N6	11.86	125.72	118.60
3	0	2068	A	N1-C6-N6	11.86	125.72	118.60
3	0	1318	A	N1-C6-N6	11.86	125.72	118.60
3	0	2254	A	N1-C6-N6	11.86	125.71	118.60
3	0	2039	A	N1-C6-N6	11.86	125.71	118.60
3	0	690	A	N1-C6-N6	11.85	125.71	118.60
3	0	786	A	N1-C6-N6	11.85	125.71	118.60
3	0	809	A	N1-C6-N6	11.85	125.71	118.60
3	0	1465	A	N1-C6-N6	11.85	125.71	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	503	A	N1-C6-N6	11.84	125.70	118.60
3	0	2278	A	N1-C6-N6	11.84	125.71	118.60
3	0	161	A	N1-C6-N6	11.84	125.70	118.60
3	0	516	A	N1-C6-N6	11.84	125.70	118.60
3	0	782	A	N1-C6-N6	11.84	125.70	118.60
3	0	793	A	N1-C6-N6	11.84	125.70	118.60
3	0	866	A	N1-C6-N6	11.84	125.70	118.60
3	0	900	A	N1-C6-N6	11.84	125.70	118.60
3	0	1942	A	N1-C6-N6	11.84	125.70	118.60
3	0	549	A	N1-C6-N6	11.83	125.70	118.60
3	0	915	A	N1-C6-N6	11.83	125.70	118.60
3	0	463	A	N1-C6-N6	11.83	125.70	118.60
3	0	959	A	N1-C6-N6	11.83	125.70	118.60
3	0	822	A	N1-C6-N6	11.82	125.69	118.60
3	0	865	A	N1-C6-N6	11.82	125.69	118.60
3	0	598	A	N1-C6-N6	11.82	125.69	118.60
3	0	2011	A	N1-C6-N6	11.82	125.69	118.60
3	0	577	A	N1-C6-N6	11.81	125.69	118.60
3	0	1458	A	N1-C6-N6	11.81	125.69	118.60
3	0	1956	A	N1-C6-N6	11.81	125.69	118.60
3	0	1989	A	N1-C6-N6	11.81	125.69	118.60
3	0	2050	A	N1-C6-N6	11.81	125.69	118.60
3	0	1332	A	N1-C6-N6	11.80	125.68	118.60
3	0	1464	A	N1-C6-N6	11.80	125.68	118.60
3	0	2060	A	N1-C6-N6	11.80	125.68	118.60
3	0	648	A	N1-C6-N6	11.80	125.68	118.60
3	0	246	A	N1-C6-N6	11.79	125.68	118.60
3	0	1269	A	N1-C6-N6	11.79	125.68	118.60
3	0	1253	A	N1-C6-N6	11.79	125.67	118.60
3	0	2288	A	N1-C6-N6	11.79	125.67	118.60
3	0	694	A	N1-C6-N6	11.79	125.67	118.60
3	0	1769	A	N1-C6-N6	11.79	125.67	118.60
3	0	1802	A	N1-C6-N6	11.79	125.67	118.60
3	0	1517	A	N1-C6-N6	11.78	125.67	118.60
3	0	381	A	N1-C6-N6	11.78	125.67	118.60
3	0	1947	A	N1-C6-N6	11.78	125.67	118.60
3	0	1615	A	N1-C6-N6	11.77	125.66	118.60
2	1	59	A	N1-C6-N6	11.77	125.66	118.60
3	0	55	A	N1-C6-N6	11.77	125.66	118.60
3	0	1616	A	N1-C6-N6	11.77	125.66	118.60
3	0	2009	A	N1-C6-N6	11.77	125.66	118.60
2	1	53	A	N1-C6-N6	11.77	125.66	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1190	A	N1-C6-N6	11.77	125.66	118.60
3	0	1980	A	N1-C6-N6	11.76	125.66	118.60
3	0	562	A	N1-C6-N6	11.76	125.66	118.60
3	0	1426	A	N1-C6-N6	11.76	125.65	118.60
3	0	1830	A	N1-C6-N6	11.75	125.65	118.60
3	0	446	A	N1-C6-N6	11.75	125.65	118.60
3	0	167	A	N1-C6-N6	11.75	125.65	118.60
3	0	185	A	N1-C6-N6	11.75	125.65	118.60
3	0	367	A	N1-C6-N6	11.75	125.65	118.60
3	0	1328	A	N1-C6-N6	11.75	125.65	118.60
3	0	39	A	N1-C6-N6	11.74	125.65	118.60
3	0	121	A	N1-C6-N6	11.74	125.65	118.60
3	0	1656	A	N1-C6-N6	11.74	125.64	118.60
3	0	2269	A	N1-C6-N6	11.74	125.64	118.60
3	0	501	A	N1-C6-N6	11.73	125.64	118.60
3	0	1707	A	N1-C6-N6	11.73	125.64	118.60
3	0	2170	A	N1-C6-N6	11.73	125.64	118.60
1	f	772	TYR	O-C-N	-11.72	103.95	122.70
3	0	500	A	N1-C6-N6	11.72	125.63	118.60
3	0	1367	A	N1-C6-N6	11.72	125.63	118.60
1	f	305	TYR	O-C-N	-11.72	103.95	122.70
3	0	1383	A	N1-C6-N6	11.71	125.63	118.60
3	0	2139	A	N1-C6-N6	11.71	125.62	118.60
3	0	520	A	N1-C6-N6	11.71	125.62	118.60
2	1	36	A	N1-C6-N6	11.70	125.62	118.60
3	0	102	A	N1-C6-N6	11.70	125.62	118.60
3	0	1573	A	N1-C6-N6	11.70	125.62	118.60
3	0	1637	G	N1-C6-O6	11.69	126.92	119.90
3	0	1382	A	N1-C6-N6	11.69	125.62	118.60
3	0	2305	A	N1-C6-N6	11.69	125.61	118.60
3	0	967	A	N1-C6-N6	11.69	125.61	118.60
3	0	1633	A	N1-C6-N6	11.69	125.61	118.60
3	0	2053	A	N1-C6-N6	11.68	125.61	118.60
3	0	1280	A	N1-C6-N6	11.68	125.61	118.60
3	0	2036	A	N1-C6-N6	11.67	125.60	118.60
3	0	47	A	N1-C6-N6	11.67	125.60	118.60
3	0	1965	A	N1-C6-N6	11.67	125.60	118.60
3	0	97	A	N1-C6-N6	11.66	125.60	118.60
3	0	184	A	N1-C6-N6	11.66	125.60	118.60
3	0	2006	A	N1-C6-N6	11.66	125.59	118.60
3	0	351	A	N1-C6-N6	11.66	125.59	118.60
3	0	785	A	N1-C6-N6	11.65	125.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1317	A	N1-C6-N6	11.65	125.59	118.60
3	0	2153	A	N1-C6-N6	11.65	125.59	118.60
3	0	2164	A	N1-C6-N6	11.65	125.59	118.60
3	0	781	A	N1-C6-N6	11.65	125.59	118.60
3	0	2289	A	N1-C6-N6	11.65	125.59	118.60
3	0	68	A	N1-C6-N6	11.64	125.58	118.60
3	0	281	A	N1-C6-N6	11.63	125.58	118.60
3	0	345	A	N1-C6-N6	11.63	125.58	118.60
3	0	960	A	N1-C6-N6	11.63	125.58	118.60
3	0	2044	A	N1-C6-N6	11.63	125.58	118.60
3	0	1477	A	N1-C6-N6	11.63	125.58	118.60
3	0	972	A	N1-C6-N6	11.63	125.58	118.60
3	0	2097	A	N1-C6-N6	11.63	125.58	118.60
3	0	861	A	N1-C6-N6	11.62	125.57	118.60
3	0	1606	A	N1-C6-N6	11.61	125.56	118.60
3	0	1748	A	N1-C6-N6	11.61	125.56	118.60
3	0	19	A	N1-C6-N6	11.60	125.56	118.60
3	0	673	A	N1-C6-N6	11.60	125.56	118.60
3	0	425	A	N1-C6-N6	11.60	125.56	118.60
3	0	1310	A	N1-C6-N6	11.59	125.56	118.60
3	0	1941	A	N1-C6-N6	11.59	125.56	118.60
3	0	417	A	N1-C6-N6	11.59	125.55	118.60
3	0	1338	A	N1-C6-N6	11.58	125.55	118.60
3	0	475	A	N1-C6-N6	11.58	125.55	118.60
1	f	239	ASN	O-C-N	-11.58	104.18	122.70
3	0	2010	A	N1-C6-N6	11.58	125.55	118.60
3	0	2093	A	N1-C6-N6	11.57	125.54	118.60
3	0	444	A	N1-C6-N6	11.56	125.54	118.60
3	0	1525	A	N1-C6-N6	11.56	125.54	118.60
46	C	411	ARG	NE-CZ-NH2	11.56	126.08	120.30
3	0	1817	A	N1-C6-N6	11.55	125.53	118.60
3	0	877	A	N1-C6-N6	11.55	125.53	118.60
3	0	1557	A	N1-C6-N6	11.54	125.52	118.60
3	0	647	A	N1-C6-N6	11.52	125.51	118.60
3	0	2174	A	N1-C6-N6	11.52	125.51	118.60
3	0	2136	A	N1-C6-N6	11.51	125.51	118.60
3	0	2094	A	N1-C6-N6	11.51	125.51	118.60
3	0	26	A	N1-C6-N6	11.50	125.50	118.60
3	0	992	A	N1-C6-N6	11.49	125.50	118.60
3	0	977	A	N1-C6-N6	11.49	125.49	118.60
3	0	1614	A	N1-C6-N6	11.48	125.49	118.60
3	0	2070	A	N1-C6-N6	11.48	125.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1197	A	N1-C6-N6	11.48	125.49	118.60
3	0	1552	A	N1-C6-N6	11.47	125.48	118.60
1	f	1220	LEU	O-C-N	11.47	141.05	122.70
3	0	1463	A	N1-C6-N6	11.47	125.48	118.60
3	0	2115	A	N1-C6-N6	11.47	125.48	118.60
2	1	73	C	P-O3'-C3'	11.46	133.46	119.70
3	0	315	A	N1-C6-N6	11.46	125.48	118.60
3	0	288	A	N1-C6-N6	11.46	125.48	118.60
3	0	655	A	N1-C6-N6	11.46	125.47	118.60
3	0	1469	A	N1-C6-N6	11.45	125.47	118.60
3	0	575	A	N1-C6-N6	11.44	125.47	118.60
3	0	485	A	N1-C6-N6	11.43	125.46	118.60
3	0	2157	C	P-O3'-C3'	11.43	133.42	119.70
3	0	2112	A	N1-C6-N6	11.43	125.46	118.60
3	0	1729	A	N1-C6-N6	11.42	125.45	118.60
3	0	2001	A	N1-C6-N6	11.42	125.45	118.60
3	0	880	A	N1-C6-N6	11.42	125.45	118.60
3	0	799	A	N1-C6-N6	11.42	125.45	118.60
3	0	216	A	N1-C6-N6	11.41	125.44	118.60
3	0	2317	A	N1-C6-N6	11.41	125.44	118.60
3	0	493	A	N1-C6-N6	11.40	125.44	118.60
2	1	14	A	N1-C6-N6	11.40	125.44	118.60
3	0	1247	A	N1-C6-N6	11.39	125.44	118.60
3	0	237	A	N1-C6-N6	11.39	125.43	118.60
3	0	1202	A	N1-C6-N6	11.37	125.42	118.60
3	0	2194	A	N1-C6-N6	11.34	125.40	118.60
3	0	1311	A	N1-C6-N6	11.34	125.40	118.60
3	0	703	A	N1-C6-N6	11.33	125.40	118.60
3	0	1343	A	N1-C6-N6	11.32	125.39	118.60
3	0	1635	A	N1-C6-N6	11.32	125.39	118.60
3	0	2042	A	N1-C6-N6	11.32	125.39	118.60
3	0	1980	A	P-O3'-C3'	11.31	133.27	119.70
3	0	1666	A	N1-C6-N6	11.23	125.34	118.60
3	0	2004	A	N1-C6-N6	11.22	125.33	118.60
3	0	507	A	N1-C6-N6	11.22	125.33	118.60
3	0	2012	A	N1-C6-N6	11.21	125.33	118.60
3	0	1828	G	N1-C6-O6	11.21	126.63	119.90
48	W	165	TRP	N-CA-CB	11.20	130.76	110.60
3	0	360	A	N1-C6-N6	11.20	125.32	118.60
3	0	162	A	N1-C6-N6	11.17	125.30	118.60
3	0	251	A	N1-C6-N6	11.13	125.28	118.60
3	0	1353	A	N1-C6-N6	11.12	125.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1531	A	N1-C6-N6	11.09	125.25	118.60
3	0	1859	G	N1-C6-O6	11.07	126.54	119.90
1	f	792	LEU	C-N-CA	11.02	149.24	121.70
5	s	300	ARG	CB-CA-C	-11.00	88.40	110.40
3	0	1433	A	N1-C6-N6	11.00	125.20	118.60
3	0	1255	A	N1-C6-N6	10.97	125.19	118.60
3	0	1333	A	N1-C6-N6	10.97	125.18	118.60
3	0	1530	C	OP2-P-O3'	-10.95	81.12	105.20
1	f	132	ALA	CA-C-N	-10.93	93.15	117.20
3	0	285	A	N1-C6-N6	10.93	125.16	118.60
3	0	924	G	O4'-C1'-N9	10.93	116.95	108.20
3	0	512	A	N1-C6-N6	10.92	125.15	118.60
3	0	2245	A	N1-C6-N6	10.86	125.11	118.60
3	0	609	A	N1-C6-N6	10.84	125.11	118.60
3	0	634	A	N1-C6-N6	10.84	125.10	118.60
1	f	1175	PRO	O-C-N	-10.81	105.41	122.70
3	0	1589	A	N1-C6-N6	10.79	125.08	118.60
3	0	1860	G	N1-C6-O6	10.79	126.37	119.90
2	1	75	A	N1-C6-N6	10.75	125.05	118.60
3	0	1692	A	N1-C6-N6	10.73	125.03	118.60
3	0	40	A	N1-C6-N6	10.72	125.03	118.60
3	0	122	A	P-O3'-C3'	10.72	132.56	119.70
3	0	567	G	N1-C6-O6	10.72	126.33	119.90
1	f	259	PHE	CB-CA-C	-10.71	88.98	110.40
3	0	684	A	N1-C6-N6	10.70	125.02	118.60
1	f	1122	GLN	CA-C-O	-10.70	97.63	120.10
1	f	1264	LEU	O-C-N	-10.69	105.59	122.70
3	0	151	A	N1-C6-N6	10.62	124.97	118.60
3	0	1622	G	N1-C6-O6	10.60	126.26	119.90
3	0	2309	G	N1-C6-O6	10.59	126.25	119.90
3	0	90	A	N1-C6-N6	10.55	124.93	118.60
3	0	299	A	N1-C6-N6	10.54	124.92	118.60
3	0	1873	G	N1-C6-O6	10.54	126.23	119.90
3	0	1982	G	P-O5'-C5'	10.54	137.76	120.90
3	0	953	G	N1-C6-O6	10.53	126.22	119.90
3	0	2125	A	N1-C6-N6	10.51	124.91	118.60
3	0	1521	G	N1-C6-O6	10.47	126.18	119.90
3	0	2045	G	N1-C6-O6	10.46	126.17	119.90
3	0	1282	G	N1-C6-O6	10.45	126.17	119.90
3	0	152	A	N1-C6-N6	10.44	124.87	118.60
3	0	621	A	N1-C6-N6	10.44	124.86	118.60
3	0	363	A	N1-C6-N6	10.44	124.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	989	G	N1-C6-O6	10.44	126.16	119.90
3	0	2084	G	N1-C6-O6	10.42	126.15	119.90
3	0	1874	G	N1-C6-O6	10.41	126.14	119.90
3	0	521	A	N1-C6-N6	10.36	124.82	118.60
3	0	1279	A	N1-C6-N6	10.36	124.82	118.60
3	0	1450	G	P-O3'-C3'	10.36	132.13	119.70
3	0	2109	A	N1-C6-N6	10.34	124.81	118.60
3	0	1751	G	N1-C6-O6	10.34	126.10	119.90
3	0	950	G	N1-C6-O6	10.32	126.09	119.90
3	0	1630	A	N1-C6-N6	10.31	124.79	118.60
3	0	132	G	N1-C6-O6	10.30	126.08	119.90
3	0	2113	G	N1-C6-O6	10.29	126.08	119.90
3	0	734	G	N1-C6-O6	10.29	126.07	119.90
3	0	173	A	N1-C6-N6	10.29	124.77	118.60
3	0	541	G	N1-C6-O6	10.28	126.07	119.90
1	f	243	TYR	C-N-CA	10.28	147.40	121.70
3	0	189	G	N1-C6-O6	10.28	126.07	119.90
3	0	394	G	N1-C6-O6	10.27	126.06	119.90
3	0	1903	G	N1-C6-O6	10.27	126.06	119.90
3	0	979	G	N1-C6-O6	10.27	126.06	119.90
3	0	994	G	N1-C6-O6	10.26	126.06	119.90
3	0	1531	A	C2'-C3'-O3'	10.26	132.07	109.50
1	f	1670	CYS	O-C-N	-10.26	106.29	122.70
3	0	1813	G	N1-C6-O6	10.26	126.06	119.90
1	f	1125	LEU	CB-CA-C	-10.25	90.72	110.20
3	0	273	G	N1-C6-O6	10.24	126.04	119.90
3	0	532	G	N1-C6-O6	10.23	126.04	119.90
3	0	651	G	N1-C6-O6	10.23	126.04	119.90
2	1	25	G	N1-C6-O6	10.22	126.03	119.90
3	0	678	G	N1-C6-O6	10.22	126.03	119.90
3	0	229	G	N1-C6-O6	10.22	126.03	119.90
3	0	106	G	N1-C6-O6	10.20	126.02	119.90
3	0	53	G	N1-C6-O6	10.19	126.01	119.90
3	0	2144	G	N1-C6-O6	10.18	126.01	119.90
3	0	148	G	N1-C6-O6	10.17	126.00	119.90
3	0	1294	G	N1-C6-O6	10.16	126.00	119.90
3	0	1754	G	N1-C6-O6	10.16	126.00	119.90
3	0	1906	G	N1-C6-O6	10.15	125.99	119.90
1	f	262	MET	CA-C-N	10.15	139.52	117.20
3	0	1398	G	N1-C6-O6	10.15	125.99	119.90
3	0	2127	G	N1-C6-O6	10.14	125.98	119.90
3	0	2209	A	N1-C6-N6	10.14	124.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	272	G	N1-C6-O6	10.13	125.98	119.90
3	0	1637	G	C5-C6-O6	-10.13	122.52	128.60
2	1	52	G	N1-C6-O6	10.12	125.97	119.90
3	0	1185	A	N1-C6-N6	10.12	124.67	118.60
3	0	263	G	N1-C6-O6	10.12	125.97	119.90
51	A	6	PRO	CA-N-CD	-10.12	97.34	111.50
1	f	152	ASP	CA-C-N	10.11	136.42	116.20
3	0	1977	G	N1-C6-O6	10.11	125.97	119.90
3	0	2200	G	N1-C6-O6	10.08	125.95	119.90
3	0	2149	G	N1-C6-O6	10.07	125.94	119.90
3	0	1409	G	N1-C6-O6	10.07	125.94	119.90
3	0	792	G	N1-C6-O6	10.06	125.94	119.90
3	0	1605	A	N1-C6-N6	10.06	124.64	118.60
3	0	81	A	N1-C6-N6	10.05	124.63	118.60
3	0	405	G	N1-C6-O6	10.03	125.92	119.90
3	0	1445	G	N1-C6-O6	10.03	125.92	119.90
3	0	2202	G	N1-C6-O6	10.03	125.92	119.90
3	0	1703	A	N1-C6-N6	10.02	124.61	118.60
3	0	1603	G	N1-C6-O6	10.02	125.91	119.90
3	0	2168	G	N1-C6-O6	10.01	125.91	119.90
3	0	30	G	N1-C6-O6	10.00	125.90	119.90
3	0	1905	G	N1-C6-O6	10.00	125.90	119.90
3	0	2238	G	N1-C6-O6	10.00	125.90	119.90
3	0	555	G	N1-C6-O6	9.98	125.89	119.90
3	0	1467	U	P-O3'-C3'	9.96	131.66	119.70
3	0	1768	G	N1-C6-O6	9.96	125.87	119.90
3	0	2106	G	N1-C6-O6	9.93	125.86	119.90
3	0	508	G	N1-C6-O6	9.93	125.86	119.90
1	f	1254	ALA	C-N-CA	-9.92	96.91	121.70
3	0	7	G	N1-C6-O6	9.92	125.85	119.90
3	0	71	G	N1-C6-O6	9.92	125.85	119.90
3	0	907	G	N1-C6-O6	9.91	125.85	119.90
3	0	291	G	N1-C6-O6	9.91	125.84	119.90
3	0	1857	G	N1-C6-O6	9.91	125.84	119.90
1	f	1221	LEU	O-C-N	-9.90	102.29	121.10
3	0	987	G	N1-C6-O6	9.90	125.84	119.90
3	0	836	G	N1-C6-O6	9.89	125.83	119.90
3	0	996	G	N1-C6-O6	9.89	125.83	119.90
3	0	1968	G	N1-C6-O6	9.89	125.83	119.90
3	0	86	G	N1-C6-O6	9.88	125.83	119.90
3	0	1225	G	N1-C6-O6	9.88	125.83	119.90
3	0	2274	G	N1-C6-O6	9.88	125.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2294	G	N1-C6-O6	9.87	125.82	119.90
3	0	204	G	N1-C6-O6	9.87	125.82	119.90
3	0	980	G	N1-C6-O6	9.87	125.82	119.90
3	0	2283	G	N1-C6-O6	9.87	125.82	119.90
3	0	1958	G	N1-C6-O6	9.87	125.82	119.90
3	0	706	G	N1-C6-O6	9.85	125.81	119.90
3	0	1071	G	N1-C6-O6	9.85	125.81	119.90
3	0	649	G	N1-C6-O6	9.85	125.81	119.90
3	0	1675	A	N1-C6-N6	9.85	124.51	118.60
3	0	344	G	N1-C6-O6	9.84	125.80	119.90
3	0	1970	U	O4'-C1'-N1	9.84	116.07	108.20
3	0	2271	G	N1-C6-O6	9.84	125.80	119.90
3	0	1676	A	N1-C6-N6	9.83	124.50	118.60
3	0	395	G	N1-C6-O6	9.83	125.80	119.90
3	0	834	G	N1-C6-O6	9.83	125.80	119.90
3	0	1312	G	N1-C6-O6	9.83	125.80	119.90
3	0	76	G	N1-C6-O6	9.82	125.80	119.90
3	0	697	G	N1-C6-O6	9.82	125.79	119.90
3	0	1401	G	N1-C6-O6	9.82	125.80	119.90
3	0	57	G	N1-C6-O6	9.81	125.79	119.90
3	0	2008	G	N1-C6-O6	9.81	125.79	119.90
3	0	530	G	N1-C6-O6	9.80	125.78	119.90
3	0	468	G	N1-C6-O6	9.80	125.78	119.90
3	0	1337	G	N1-C6-O6	9.79	125.77	119.90
3	0	1736	G	N1-C6-O6	9.79	125.77	119.90
3	0	1973	G	N1-C6-O6	9.79	125.77	119.90
3	0	347	G	N1-C6-O6	9.79	125.77	119.90
3	0	1413	G	N1-C6-O6	9.79	125.77	119.90
2	1	51	G	N1-C6-O6	9.78	125.77	119.90
3	0	2199	G	N1-C6-O6	9.78	125.77	119.90
3	0	2301	G	N1-C6-O6	9.78	125.77	119.90
3	0	156	G	N1-C6-O6	9.77	125.76	119.90
3	0	1640	G	N1-C6-O6	9.77	125.76	119.90
3	0	470	G	N1-C6-O6	9.77	125.76	119.90
3	0	2181	G	N1-C6-O6	9.77	125.76	119.90
3	0	1554	G	N1-C6-O6	9.76	125.76	119.90
3	0	2078	G	N1-C6-O6	9.76	125.76	119.90
3	0	412	G	N1-C6-O6	9.76	125.75	119.90
3	0	708	G	N1-C6-O6	9.75	125.75	119.90
2	1	69	G	N1-C6-O6	9.74	125.75	119.90
1	f	1121	CYS	O-C-N	9.74	138.28	122.70
3	0	1761	G	N1-C6-O6	9.73	125.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2242	G	N1-C6-O6	9.72	125.73	119.90
3	0	2002	G	N1-C6-O6	9.71	125.73	119.90
3	0	1218	G	N1-C6-O6	9.71	125.73	119.90
3	0	2100	G	N1-C6-O6	9.71	125.72	119.90
3	0	978	U	O4'-C1'-N1	9.70	115.96	108.20
3	0	869	G	N1-C6-O6	9.70	125.72	119.90
3	0	1235	G	N1-C6-O6	9.69	125.72	119.90
3	0	1535	C	O4'-C1'-N1	9.69	115.95	108.20
1	f	258	GLU	O-C-N	-9.69	107.20	122.70
2	1	2	G	N1-C6-O6	9.68	125.71	119.90
3	0	566	G	N1-C6-O6	9.68	125.71	119.90
3	0	748	G	N1-C6-O6	9.68	125.71	119.90
3	0	1211	G	N1-C6-O6	9.68	125.71	119.90
3	0	1372	G	N1-C6-O6	9.68	125.71	119.90
3	0	1397	G	N1-C6-O6	9.68	125.71	119.90
3	0	514	G	N1-C6-O6	9.68	125.71	119.90
3	0	1612	A	N1-C6-N6	9.68	124.41	118.60
3	0	435	G	N1-C6-O6	9.67	125.70	119.90
3	0	2227	G	N1-C6-O6	9.67	125.70	119.90
3	0	6	G	N1-C6-O6	9.67	125.70	119.90
3	0	476	G	N1-C6-O6	9.67	125.70	119.90
3	0	2025	G	N1-C6-O6	9.67	125.70	119.90
3	0	1074	G	N1-C6-O6	9.67	125.70	119.90
3	0	2213	G	N1-C6-O6	9.67	125.70	119.90
3	0	238	G	N1-C6-O6	9.66	125.69	119.90
3	0	320	G	N1-C6-O6	9.66	125.69	119.90
3	0	1859	G	C5-C6-O6	-9.65	122.81	128.60
3	0	1000	G	N1-C6-O6	9.65	125.69	119.90
3	0	139	G	N1-C6-O6	9.65	125.69	119.90
3	0	1070	C	O4'-C1'-N1	9.64	115.92	108.20
3	0	1404	G	N1-C6-O6	9.64	125.68	119.90
3	0	1652	G	N1-C6-O6	9.64	125.68	119.90
3	0	517	G	N1-C6-O6	9.63	125.68	119.90
3	0	622	G	N1-C6-O6	9.63	125.68	119.90
1	f	1122	GLN	CA-C-N	9.62	138.37	117.20
3	0	230	G	N1-C6-O6	9.62	125.67	119.90
3	0	971	G	N1-C6-O6	9.62	125.67	119.90
3	0	756	G	N1-C6-O6	9.62	125.67	119.90
3	0	317	G	N1-C6-O6	9.62	125.67	119.90
1	f	138	ASP	C-N-CA	-9.62	97.66	121.70
3	0	1821	G	N1-C6-O6	9.62	125.67	119.90
3	0	1984	G	N1-C6-O6	9.61	125.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	239	ASN	CA-C-O	-9.61	99.92	120.10
3	0	547	G	N1-C6-O6	9.61	125.67	119.90
3	0	1506	G	N1-C6-O6	9.61	125.67	119.90
3	0	2280	G	N1-C6-O6	9.61	125.66	119.90
3	0	311	G	N1-C6-O6	9.60	125.66	119.90
3	0	157	G	N1-C6-O6	9.59	125.65	119.90
3	0	430	G	N1-C6-O6	9.59	125.65	119.90
3	0	2118	G	N1-C6-O6	9.59	125.65	119.90
3	0	413	G	N1-C6-O6	9.58	125.65	119.90
3	0	1764	G	N1-C6-O6	9.58	125.65	119.90
3	0	79	G	N1-C6-O6	9.58	125.65	119.90
3	0	93	G	N1-C6-O6	9.57	125.64	119.90
3	0	466	G	N1-C6-O6	9.57	125.64	119.90
3	0	42	G	N1-C6-O6	9.57	125.64	119.90
3	0	733	G	N1-C6-O6	9.57	125.64	119.90
3	0	835	G	N1-C6-O6	9.56	125.64	119.90
3	0	2297	G	N1-C6-O6	9.56	125.64	119.90
3	0	524	G	N1-C6-O6	9.56	125.64	119.90
3	0	606	G	N1-C6-O6	9.56	125.64	119.90
3	0	2048	G	N1-C6-O6	9.56	125.63	119.90
3	0	488	G	N1-C6-O6	9.55	125.63	119.90
3	0	1387	G	N1-C6-O6	9.55	125.63	119.90
3	0	192	G	N1-C6-O6	9.55	125.63	119.90
3	0	2300	G	N1-C6-O6	9.55	125.63	119.90
3	0	1219	G	N1-C6-O6	9.54	125.63	119.90
3	0	1414	G	N1-C6-O6	9.54	125.63	119.90
3	0	23	G	N1-C6-O6	9.54	125.62	119.90
3	0	244	G	N1-C6-O6	9.54	125.62	119.90
3	0	385	G	N1-C6-O6	9.54	125.62	119.90
3	0	389	G	N1-C6-O6	9.54	125.62	119.90
3	0	763	G	N1-C6-O6	9.54	125.62	119.90
3	0	322	G	N1-C6-O6	9.53	125.62	119.90
3	0	796	G	N1-C6-O6	9.53	125.62	119.90
3	0	1861	G	N1-C6-O6	9.53	125.61	119.90
3	0	2049	G	N1-C6-O6	9.52	125.61	119.90
3	0	696	G	N1-C6-O6	9.52	125.61	119.90
2	1	67	G	N1-C6-O6	9.51	125.61	119.90
3	0	1242	G	N1-C6-O6	9.51	125.60	119.90
3	0	1891	G	N1-C6-O6	9.51	125.60	119.90
3	0	931	G	N1-C6-O6	9.50	125.60	119.90
3	0	2222	G	N1-C6-O6	9.50	125.60	119.90
3	0	401	A	N1-C6-N6	9.49	124.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1691	G	N1-C6-O6	9.49	125.60	119.90
3	0	1876	G	N1-C6-O6	9.49	125.60	119.90
3	0	404	G	N1-C6-O6	9.49	125.59	119.90
3	0	705	G	N1-C6-O6	9.49	125.59	119.90
3	0	790	G	N1-C6-O6	9.49	125.59	119.90
3	0	970	G	N1-C6-O6	9.49	125.59	119.90
3	0	2086	G	N1-C6-O6	9.49	125.59	119.90
3	0	164	G	N1-C6-O6	9.48	125.59	119.90
3	0	954	G	N1-C6-O6	9.48	125.59	119.90
3	0	313	G	N1-C6-O6	9.48	125.59	119.90
3	0	431	G	N1-C6-O6	9.48	125.59	119.90
3	0	2210	G	N1-C6-O6	9.48	125.59	119.90
3	0	207	G	N1-C6-O6	9.48	125.59	119.90
3	0	2211	G	N1-C6-O6	9.48	125.59	119.90
3	0	695	G	N1-C6-O6	9.47	125.58	119.90
3	0	448	A	N1-C6-N6	9.47	124.28	118.60
3	0	2132	G	N1-C6-O6	9.47	125.58	119.90
3	0	275	A	N1-C6-N6	9.46	124.28	118.60
3	0	1560	G	N1-C6-O6	9.46	125.58	119.90
3	0	1574	G	N1-C6-O6	9.46	125.58	119.90
3	0	1334	G	N1-C6-O6	9.46	125.57	119.90
3	0	2126	G	N1-C6-O6	9.46	125.57	119.90
2	1	7	G	N1-C6-O6	9.45	125.57	119.90
1	f	134	PRO	CA-C-O	-9.45	97.53	120.20
3	0	979	G	C5-C6-O6	-9.45	122.93	128.60
3	0	1354	G	N1-C6-O6	9.45	125.57	119.90
3	0	828	G	N1-C6-O6	9.44	125.57	119.90
3	0	409	G	N1-C6-O6	9.44	125.56	119.90
3	0	1239	G	N1-C6-O6	9.44	125.56	119.90
3	0	1080	G	N1-C6-O6	9.44	125.56	119.90
1	f	1109	LEU	N-CA-C	9.43	136.47	111.00
3	0	738	G	N1-C6-O6	9.43	125.56	119.90
3	0	2315	G	N1-C6-O6	9.43	125.56	119.90
3	0	63	G	N1-C6-O6	9.43	125.56	119.90
3	0	1782	G	N1-C6-O6	9.43	125.56	119.90
3	0	1915	G	N1-C6-O6	9.43	125.56	119.90
3	0	228	G	N1-C6-O6	9.43	125.56	119.90
3	0	1599	G	N1-C6-O6	9.43	125.56	119.90
3	0	410	G	N1-C6-O6	9.42	125.55	119.90
3	0	842	G	N1-C6-O6	9.41	125.55	119.90
3	0	1767	G	N1-C6-O6	9.41	125.55	119.90
3	0	1798	G	N1-C6-O6	9.41	125.55	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1584	G	N1-C6-O6	9.41	125.54	119.90
39	E	279	TYR	CB-CG-CD2	-9.41	115.36	121.00
3	0	1582	G	N1-C6-O6	9.40	125.54	119.90
3	0	1822	G	N1-C6-O6	9.40	125.54	119.90
3	0	321	G	N1-C6-O6	9.39	125.54	119.90
3	0	1215	G	N1-C6-O6	9.39	125.53	119.90
3	0	1649	G	N1-C6-O6	9.39	125.53	119.90
3	0	1877	G	N1-C6-O6	9.39	125.53	119.90
3	0	535	G	N1-C6-O6	9.39	125.53	119.90
3	0	403	G	N1-C6-O6	9.38	125.53	119.90
3	0	2161	G	N1-C6-O6	9.38	125.53	119.90
3	0	364	G	N1-C6-O6	9.38	125.53	119.90
3	0	1217	G	N1-C6-O6	9.38	125.53	119.90
3	0	2043	G	N1-C6-O6	9.38	125.53	119.90
3	0	133	G	N1-C6-O6	9.38	125.53	119.90
3	0	465	G	N1-C6-O6	9.38	125.53	119.90
2	1	23	G	N1-C6-O6	9.36	125.52	119.90
3	0	1580	G	N1-C6-O6	9.36	125.52	119.90
3	0	2219	A	N1-C6-N6	9.36	124.22	118.60
3	0	888	G	N1-C6-O6	9.36	125.51	119.90
3	0	1706	G	N1-C6-O6	9.36	125.51	119.90
1	f	263	SER	CA-C-N	9.35	137.78	117.20
3	0	477	G	N1-C6-O6	9.35	125.51	119.90
3	0	605	G	N1-C6-O6	9.35	125.51	119.90
3	0	1324	G	N1-C6-O6	9.35	125.51	119.90
3	0	513	G	N1-C6-O6	9.35	125.51	119.90
3	0	370	G	N1-C6-O6	9.34	125.51	119.90
3	0	1342	G	N1-C6-O6	9.34	125.51	119.90
3	0	1611	A	N1-C6-N6	9.34	124.20	118.60
3	0	1221	G	N1-C6-O6	9.34	125.50	119.90
3	0	1872	G	N1-C6-O6	9.34	125.50	119.90
1	f	305	TYR	CA-C-N	9.34	137.74	117.20
1	f	307	LEU	CA-C-N	9.34	137.74	117.20
3	0	2187	G	N1-C6-O6	9.34	125.50	119.90
1	f	198	PHE	N-CA-C	-9.33	85.80	111.00
3	0	1673	G	N1-C6-O6	9.33	125.50	119.90
3	0	2152	U	O4'-C1'-N1	9.33	115.67	108.20
3	0	334	G	N1-C6-O6	9.33	125.50	119.90
3	0	1937	G	N1-C6-O6	9.33	125.50	119.90
3	0	2155	G	N1-C6-O6	9.33	125.50	119.90
3	0	1471	G	N1-C6-O6	9.32	125.50	119.90
3	0	611	G	N1-C6-O6	9.32	125.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1325	G	N1-C6-O6	9.32	125.49	119.90
3	0	1781	G	N1-C6-O6	9.32	125.49	119.90
3	0	1744	G	N1-C6-O6	9.31	125.49	119.90
3	0	2246	G	N1-C6-O6	9.31	125.49	119.90
3	0	824	G	N1-C6-O6	9.31	125.48	119.90
3	0	1828	G	C5-C6-O6	-9.30	123.02	128.60
3	0	420	G	N1-C6-O6	9.30	125.48	119.90
3	0	844	G	N1-C6-O6	9.30	125.48	119.90
3	0	815	G	N1-C6-O6	9.29	125.48	119.90
3	0	963	G	N1-C6-O6	9.29	125.47	119.90
3	0	1204	G	N1-C6-O6	9.29	125.47	119.90
3	0	100	A	N1-C6-N6	9.29	124.17	118.60
3	0	791	G	N1-C6-O6	9.28	125.47	119.90
3	0	555	G	C5-C6-O6	-9.28	123.03	128.60
3	0	1206	G	N1-C6-O6	9.28	125.47	119.90
3	0	903	G	N1-C6-O6	9.27	125.46	119.90
3	0	1955	G	N1-C6-O6	9.27	125.46	119.90
3	0	240	G	N1-C6-O6	9.27	125.46	119.90
3	0	1493	G	N1-C6-O6	9.26	125.46	119.90
3	0	1878	G	N1-C6-O6	9.26	125.46	119.90
3	0	495	G	N1-C6-O6	9.26	125.45	119.90
3	0	997	G	N1-C6-O6	9.26	125.45	119.90
3	0	377	G	N1-C6-O6	9.25	125.45	119.90
3	0	1230	G	N1-C6-O6	9.25	125.45	119.90
2	1	29	G	N1-C6-O6	9.25	125.45	119.90
3	0	895	A	N1-C6-N6	9.25	124.15	118.60
3	0	2229	G	N1-C6-O6	9.25	125.45	119.90
2	1	12	G	N1-C6-O6	9.24	125.45	119.90
3	0	223	G	N1-C6-O6	9.24	125.45	119.90
3	0	908	G	N1-C6-O6	9.24	125.45	119.90
3	0	1628	G	N1-C6-O6	9.24	125.44	119.90
3	0	981	G	N1-C6-O6	9.24	125.44	119.90
3	0	1945	G	N1-C6-O6	9.24	125.44	119.90
3	0	2270	G	N1-C6-O6	9.24	125.44	119.90
3	0	1265	G	N1-C6-O6	9.23	125.44	119.90
3	0	1791	G	N1-C6-O6	9.23	125.44	119.90
3	0	1922	G	N1-C6-O6	9.23	125.44	119.90
1	f	136	LEU	N-CA-CB	-9.23	91.94	110.40
3	0	335	G	N1-C6-O6	9.23	125.44	119.90
2	1	21	G	N1-C6-O6	9.22	125.44	119.90
3	0	568	G	N1-C6-O6	9.22	125.43	119.90
3	0	1743	G	N1-C6-O6	9.22	125.43	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1473	G	N1-C6-O6	9.22	125.43	119.90
3	0	1004	G	N1-C6-O6	9.21	125.43	119.90
3	0	1188	G	N1-C6-O6	9.21	125.43	119.90
3	0	1661	G	N1-C6-O6	9.21	125.43	119.90
3	0	932	G	N1-C6-O6	9.21	125.42	119.90
3	0	930	G	N1-C6-O6	9.20	125.42	119.90
3	0	1975	G	N1-C6-O6	9.20	125.42	119.90
3	0	1233	G	N1-C6-O6	9.19	125.42	119.90
3	0	211	G	N1-C6-O6	9.19	125.41	119.90
3	0	757	G	N1-C6-O6	9.19	125.41	119.90
3	0	436	G	N1-C6-O6	9.18	125.41	119.90
3	0	1208	G	N1-C6-O6	9.18	125.41	119.90
3	0	2079	G	N1-C6-O6	9.18	125.41	119.90
2	1	28	G	N1-C6-O6	9.18	125.41	119.90
3	0	473	G	N1-C6-O6	9.18	125.41	119.90
3	0	640	G	N1-C6-O6	9.18	125.41	119.90
3	0	1567	G	N1-C6-O6	9.18	125.41	119.90
2	1	48	G	N1-C6-O6	9.17	125.40	119.90
3	0	855	G	N1-C6-O6	9.17	125.40	119.90
3	0	1258	G	N1-C6-O6	9.17	125.40	119.90
2	1	30	G	N1-C6-O6	9.17	125.40	119.90
3	0	1002	G	N1-C6-O6	9.17	125.40	119.90
3	0	944	G	N1-C6-O6	9.17	125.40	119.90
3	0	1238	A	N1-C6-N6	9.16	124.10	118.60
3	0	469	G	N1-C6-O6	9.16	125.40	119.90
3	0	1320	G	N1-C6-O6	9.16	125.40	119.90
3	0	1974	G	N1-C6-O6	9.16	125.40	119.90
3	0	2146	G	N1-C6-O6	9.15	125.39	119.90
3	0	1504	G	N1-C6-O6	9.15	125.39	119.90
3	0	616	G	N1-C6-O6	9.14	125.39	119.90
26	J	107	PHE	CA-CB-CG	9.14	135.84	113.90
1	f	1254	ALA	CA-C-N	-9.14	97.10	117.20
3	0	1419	G	N1-C6-O6	9.14	125.38	119.90
3	0	1938	G	N1-C6-O6	9.13	125.38	119.90
3	0	1583	G	N1-C6-O6	9.13	125.38	119.90
2	1	18	G	N1-C6-O6	9.12	125.38	119.90
3	0	670	G	N1-C6-O6	9.13	125.38	119.90
1	f	1259	CYS	CA-C-N	9.12	137.27	117.20
3	0	973	G	N1-C6-O6	9.12	125.37	119.90
3	0	169	G	N1-C6-O6	9.12	125.37	119.90
3	0	881	G	N1-C6-O6	9.11	125.37	119.90
3	0	233	G	N1-C6-O6	9.11	125.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	567	G	C5-C6-O6	-9.11	123.14	128.60
3	0	1710	G	N1-C6-O6	9.11	125.36	119.90
3	0	252	G	N1-C6-O6	9.10	125.36	119.90
3	0	564	G	N1-C6-O6	9.10	125.36	119.90
3	0	1410	G	N1-C6-O6	9.10	125.36	119.90
3	0	602	G	N1-C6-O6	9.09	125.36	119.90
3	0	1487	G	N1-C6-O6	9.09	125.35	119.90
3	0	1536	G	N1-C6-O6	9.09	125.35	119.90
3	0	552	G	N1-C6-O6	9.08	125.35	119.90
3	0	48	G	N1-C6-O6	9.08	125.35	119.90
3	0	832	G	N1-C6-O6	9.08	125.35	119.90
3	0	1509	G	N1-C6-O6	9.08	125.35	119.90
3	0	1651	G	N1-C6-O6	9.07	125.34	119.90
3	0	451	G	N1-C6-O6	9.07	125.34	119.90
3	0	1407	G	N1-C6-O6	9.06	125.34	119.90
1	f	134	PRO	CA-C-N	9.06	137.13	117.20
1	f	1128	PRO	O-C-N	-9.06	108.21	122.70
3	0	2069	G	N1-C6-O6	9.05	125.33	119.90
1	f	137	CYS	O-C-N	-9.04	108.23	122.70
3	0	439	G	N1-C6-O6	9.04	125.33	119.90
3	0	685	G	N1-C6-O6	9.04	125.32	119.90
3	0	119	G	N1-C6-O6	9.04	125.32	119.90
3	0	1694	A	P-O3'-C3'	9.04	130.55	119.70
3	0	982	G	N1-C6-O6	9.04	125.32	119.90
3	0	1903	G	C5-C6-O6	-9.04	123.18	128.60
3	0	1510	G	N1-C6-O6	9.04	125.32	119.90
3	0	41	G	N1-C6-O6	9.03	125.32	119.90
3	0	433	G	N1-C6-O6	9.03	125.32	119.90
3	0	631	G	N1-C6-O6	9.03	125.32	119.90
3	0	676	G	N1-C6-O6	9.03	125.31	119.90
2	1	66	G	N1-C6-O6	9.02	125.31	119.90
3	0	1281	G	N1-C6-O6	9.01	125.31	119.90
3	0	1810	G	N1-C6-O6	9.01	125.31	119.90
3	0	276	G	N1-C6-O6	9.01	125.31	119.90
3	0	443	G	N1-C6-O6	9.00	125.30	119.90
3	0	2312	G	N1-C6-O6	9.00	125.30	119.90
3	0	271	C	O4'-C1'-N1	9.00	115.40	108.20
1	f	136	LEU	CA-C-N	9.00	136.99	117.20
3	0	137	C	O4'-C1'-N1	8.99	115.40	108.20
3	0	355	G	N1-C6-O6	8.99	125.30	119.90
3	0	893	G	N1-C6-O6	8.99	125.30	119.90
3	0	385	G	C5-C6-O6	-8.98	123.21	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	132	G	C5-C6-O6	-8.98	123.21	128.60
3	0	208	G	N1-C6-O6	8.98	125.29	119.90
3	0	1363	G	N1-C6-O6	8.98	125.29	119.90
3	0	946	U	C2-N1-C1'	8.97	128.47	117.70
3	0	1293	G	N1-C6-O6	8.97	125.28	119.90
3	0	1695	G	N1-C6-O6	8.97	125.28	119.90
3	0	1741	G	N1-C6-O6	8.97	125.28	119.90
3	0	943	G	N1-C6-O6	8.96	125.28	119.90
3	0	1438	G	N1-C6-O6	8.96	125.28	119.90
3	0	2058	G	N1-C6-O6	8.96	125.28	119.90
3	0	603	G	N1-C6-O6	8.96	125.28	119.90
3	0	2000	G	N1-C6-O6	8.96	125.28	119.90
3	0	1619	G	N1-C6-O6	8.96	125.28	119.90
3	0	220	G	N1-C6-O6	8.96	125.28	119.90
3	0	985	G	N1-C6-O6	8.96	125.28	119.90
3	0	1568	G	N1-C6-O6	8.96	125.28	119.90
3	0	2225	G	N1-C6-O6	8.95	125.27	119.90
3	0	400	G	N1-C6-O6	8.94	125.27	119.90
3	0	1642	G	N1-C6-O6	8.94	125.27	119.90
3	0	1643	G	N1-C6-O6	8.94	125.27	119.90
3	0	1971	C	P-O3'-C3'	8.94	130.43	119.70
3	0	1998	G	N1-C6-O6	8.94	125.26	119.90
3	0	1813	G	C5-C6-O6	-8.94	123.24	128.60
3	0	953	G	C5-C6-O6	-8.94	123.24	128.60
3	0	1870	A	C5-C6-N6	-8.94	116.55	123.70
1	f	1039	ARG	CA-C-N	8.93	134.07	116.20
3	0	1699	G	N1-C6-O6	8.93	125.26	119.90
3	0	2290	G	N1-C6-O6	8.93	125.26	119.90
3	0	591	G	N1-C6-O6	8.92	125.25	119.90
3	0	776	G	N1-C6-O6	8.92	125.25	119.90
3	0	109	G	N1-C6-O6	8.92	125.25	119.90
3	0	628	G	N1-C6-O6	8.91	125.25	119.90
3	0	541	G	C5-C6-O6	-8.90	123.26	128.60
3	0	2066	G	N1-C6-O6	8.90	125.24	119.90
3	0	273	G	C5-C6-O6	-8.90	123.26	128.60
3	0	618	G	N1-C6-O6	8.90	125.24	119.90
3	0	1386	G	N1-C6-O6	8.90	125.24	119.90
3	0	994	G	C5-C6-O6	-8.89	123.26	128.60
3	0	819	G	N1-C6-O6	8.89	125.23	119.90
3	0	1728	G	N1-C6-O6	8.89	125.23	119.90
3	0	2035	G	N1-C6-O6	8.89	125.23	119.90
2	1	9	G	N1-C6-O6	8.88	125.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1803	G	N1-C6-O6	8.88	125.23	119.90
3	0	511	G	N1-C6-O6	8.88	125.23	119.90
3	0	1267	C	O4'-C1'-N1	8.88	115.30	108.20
3	0	664	G	N1-C6-O6	8.87	125.22	119.90
3	0	1268	G	N1-C6-O6	8.87	125.22	119.90
3	0	20	G	N1-C6-O6	8.87	125.22	119.90
2	1	10	G	N1-C6-O6	8.87	125.22	119.90
3	0	1948	G	N1-C6-O6	8.87	125.22	119.90
3	0	1977	G	C5-C6-O6	-8.86	123.28	128.60
3	0	1254	G	N1-C6-O6	8.86	125.22	119.90
3	0	199	G	N1-C6-O6	8.86	125.22	119.90
3	0	1975	G	O4'-C1'-N9	8.86	115.29	108.20
3	0	1586	A	N1-C6-N6	8.86	123.91	118.60
3	0	1926	G	N1-C6-O6	8.85	125.21	119.90
3	0	419	G	N1-C6-O6	8.85	125.21	119.90
3	0	1875	G	N1-C6-O6	8.85	125.21	119.90
3	0	615	G	N1-C6-O6	8.85	125.21	119.90
3	0	909	G	N1-C6-O6	8.85	125.21	119.90
3	0	1690	G	N1-C6-O6	8.85	125.21	119.90
3	0	2184	G	N1-C6-O6	8.85	125.21	119.90
3	0	407	G	N1-C6-O6	8.84	125.21	119.90
3	0	1833	G	N1-C6-O6	8.84	125.21	119.90
3	0	1241	G	N1-C6-O6	8.84	125.20	119.90
3	0	2291	G	N1-C6-O6	8.83	125.20	119.90
3	0	1327	G	N1-C6-O6	8.83	125.20	119.90
3	0	1389	G	N1-C6-O6	8.82	125.19	119.90
3	0	379	G	N1-C6-O6	8.82	125.19	119.90
3	0	1873	G	C5-C6-O6	-8.82	123.31	128.60
3	0	1801	G	N1-C6-O6	8.82	125.19	119.90
3	0	2309	G	C5-C6-O6	-8.82	123.31	128.60
2	1	25	G	C5-C6-O6	-8.81	123.31	128.60
3	0	188	G	N1-C6-O6	8.81	125.19	119.90
3	0	2253	G	N1-C6-O6	8.81	125.19	119.90
3	0	1685	G	N1-C6-O6	8.80	125.18	119.90
3	0	899	G	N1-C6-O6	8.80	125.18	119.90
3	0	1627	G	N1-C6-O6	8.80	125.18	119.90
3	0	2091	G	N1-C6-O6	8.80	125.18	119.90
3	0	1585	G	N1-C6-O6	8.80	125.18	119.90
3	0	924	G	N1-C6-O6	8.80	125.18	119.90
3	0	918	G	N1-C6-O6	8.79	125.18	119.90
3	0	1622	G	C5-C6-O6	-8.79	123.32	128.60
3	0	189	G	C5-C6-O6	-8.79	123.33	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	397	G	N1-C6-O6	8.79	125.17	119.90
3	0	1601	G	N1-C6-O6	8.79	125.17	119.90
3	0	1990	C	O4'-C1'-N1	8.78	115.23	108.20
2	1	22	C	O4'-C1'-N1	8.78	115.23	108.20
3	0	750	C	O4'-C1'-N1	8.78	115.22	108.20
3	0	2022	G	N1-C6-O6	8.78	125.17	119.90
1	f	1175	PRO	C-N-CA	-8.78	99.76	121.70
3	0	1860	G	C5-C6-O6	-8.77	123.34	128.60
3	0	1907	G	N1-C6-O6	8.77	125.16	119.90
2	1	15	G	N1-C6-O6	8.77	125.16	119.90
3	0	1322	G	N1-C6-O6	8.77	125.16	119.90
3	0	1381	G	N1-C6-O6	8.77	125.16	119.90
3	0	867	G	N1-C6-O6	8.77	125.16	119.90
3	0	1524	U	P-O3'-C3'	8.76	130.21	119.70
1	f	1627	ARG	O-C-N	-8.76	108.31	123.20
3	0	272	G	C5-C6-O6	-8.76	123.35	128.60
3	0	989	G	C5-C6-O6	-8.76	123.35	128.60
3	0	1231	G	N1-C6-O6	8.76	125.15	119.90
3	0	1673	G	C5-C6-O6	-8.76	123.35	128.60
3	0	794	G	N1-C6-O6	8.75	125.15	119.90
3	0	1207	G	N1-C6-O6	8.75	125.15	119.90
3	0	1415	G	N1-C6-O6	8.75	125.15	119.90
3	0	205	G	N1-C6-O6	8.75	125.15	119.90
3	0	1697	G	N1-C6-O6	8.74	125.15	119.90
1	f	193	ARG	C-N-CA	8.74	143.54	121.70
3	0	106	G	C5-C6-O6	-8.74	123.36	128.60
3	0	159	G	N1-C6-O6	8.73	125.14	119.90
3	0	1369	G	N1-C6-O6	8.73	125.14	119.90
3	0	1647	G	N1-C6-O6	8.73	125.14	119.90
3	0	120	C	O4'-C1'-N1	8.73	115.18	108.20
3	0	1797	G	N1-C6-O6	8.73	125.14	119.90
3	0	130	G	N1-C6-O6	8.72	125.13	119.90
3	0	1671	G	N1-C6-O6	8.72	125.13	119.90
3	0	1929	G	N1-C6-O6	8.72	125.13	119.90
3	0	1326	G	N1-C6-O6	8.72	125.13	119.90
1	f	1127	VAL	C-N-CD	-8.72	101.42	120.60
3	0	1785	G	N1-C6-O6	8.71	125.13	119.90
3	0	2123	G	N1-C6-O6	8.71	125.13	119.90
3	0	1	G	N1-C6-O6	8.71	125.13	119.90
3	0	1331	G	N1-C6-O6	8.71	125.13	119.90
3	0	1344	G	N1-C6-O6	8.71	125.13	119.90
3	0	1613	G	N1-C6-O6	8.71	125.13	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2129	G	N1-C6-O6	8.71	125.13	119.90
3	0	2217	G	N1-C6-O6	8.71	125.13	119.90
3	0	337	G	N1-C6-O6	8.71	125.12	119.90
3	0	2080	G	N1-C6-O6	8.71	125.12	119.90
3	0	10	G	N1-C6-O6	8.70	125.12	119.90
3	0	878	G	N1-C6-O6	8.70	125.12	119.90
3	0	2101	G	N1-C6-O6	8.70	125.12	119.90
3	0	1880	G	N1-C6-O6	8.70	125.12	119.90
3	0	768	G	N1-C6-O6	8.70	125.12	119.90
3	0	1278	G	N1-C6-O6	8.69	125.12	119.90
2	1	17	G	N1-C6-O6	8.69	125.11	119.90
3	0	179	G	N1-C6-O6	8.69	125.12	119.90
3	0	661	G	N1-C6-O6	8.69	125.11	119.90
3	0	1508	G	N1-C6-O6	8.69	125.11	119.90
3	0	2104	G	N1-C6-O6	8.69	125.11	119.90
3	0	1503	G	N1-C6-O6	8.69	125.11	119.90
3	0	630	G	N1-C6-O6	8.68	125.11	119.90
3	0	1770	G	N1-C6-O6	8.68	125.11	119.90
3	0	2113	G	C5-C6-O6	-8.68	123.39	128.60
2	1	71	U	O4'-C1'-N1	8.68	115.14	108.20
3	0	2111	G	N1-C6-O6	8.68	125.11	119.90
3	0	1294	G	C5-C6-O6	-8.67	123.40	128.60
3	0	682	G	N1-C6-O6	8.67	125.10	119.90
3	0	693	G	N1-C6-O6	8.67	125.10	119.90
3	0	1949	G	N1-C6-O6	8.67	125.10	119.90
3	0	418	G	N1-C6-O6	8.66	125.10	119.90
3	0	1939	G	N1-C6-O6	8.66	125.10	119.90
3	0	289	G	N1-C6-O6	8.66	125.10	119.90
3	0	1068	C	O4'-C1'-N1	8.66	115.13	108.20
3	0	1200	G	N1-C6-O6	8.66	125.09	119.90
3	0	1754	G	C5-C6-O6	-8.65	123.41	128.60
3	0	1351	G	N1-C6-O6	8.65	125.09	119.90
2	1	44	G	N1-C6-O6	8.65	125.09	119.90
3	0	1760	G	N1-C6-O6	8.64	125.09	119.90
2	1	56	G	N1-C6-O6	8.64	125.08	119.90
3	0	424	G	N1-C6-O6	8.64	125.08	119.90
3	0	2218	G	N1-C6-O6	8.64	125.08	119.90
1	f	1220	LEU	CA-C-N	-8.64	98.19	117.20
3	0	744	C	O4'-C1'-N1	8.64	115.11	108.20
3	0	749	C	O4'-C1'-N1	8.63	115.11	108.20
3	0	1195	G	N1-C6-O6	8.63	125.08	119.90
3	0	1456	G	N1-C6-O6	8.63	125.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	871	G	N1-C6-O6	8.63	125.08	119.90
3	0	1001	G	N1-C6-O6	8.63	125.08	119.90
3	0	1187	G	N1-C6-O6	8.63	125.08	119.90
3	0	67	C	O4'-C1'-N1	8.62	115.10	108.20
3	0	92	G	N1-C6-O6	8.63	125.08	119.90
3	0	2268	G	N1-C6-O6	8.62	125.07	119.90
3	0	211	G	C5-C6-O6	-8.62	123.43	128.60
3	0	1714	G	N1-C6-O6	8.62	125.07	119.90
3	0	382	G	N1-C6-O6	8.62	125.07	119.90
3	0	1203	G	N1-C6-O6	8.62	125.07	119.90
3	0	479	G	N1-C6-O6	8.62	125.07	119.90
3	0	519	G	N1-C6-O6	8.62	125.07	119.90
3	0	30	G	C5-C6-O6	-8.62	123.43	128.60
3	0	217	C	O4'-C1'-N1	8.62	115.09	108.20
3	0	1556	G	N1-C6-O6	8.61	125.07	119.90
3	0	1931	G	N1-C6-O6	8.61	125.07	119.90
3	0	539	G	N1-C6-O6	8.61	125.06	119.90
3	0	808	G	N1-C6-O6	8.61	125.07	119.90
3	0	1701	G	N1-C6-O6	8.61	125.06	119.90
3	0	1780	U	O4'-C1'-N1	8.61	115.09	108.20
3	0	1645	G	N1-C6-O6	8.61	125.06	119.90
3	0	1777	G	N1-C6-O6	8.61	125.06	119.90
3	0	1982	G	N1-C6-O6	8.61	125.06	119.90
3	0	2193	G	N1-C6-O6	8.61	125.06	119.90
3	0	2196	G	N1-C6-O6	8.61	125.06	119.90
3	0	1447	C	O4'-C1'-N1	8.60	115.08	108.20
3	0	1071	G	C5-C6-O6	-8.60	123.44	128.60
3	0	1216	G	N1-C6-O6	8.60	125.06	119.90
3	0	1718	G	N1-C6-O6	8.59	125.06	119.90
3	0	200	U	C2-N1-C1'	8.59	128.01	117.70
3	0	2202	G	C5-C6-O6	-8.59	123.45	128.60
3	0	857	G	N1-C6-O6	8.59	125.05	119.90
3	0	116	G	N1-C6-O6	8.58	125.05	119.90
3	0	1196	G	N1-C6-O6	8.58	125.05	119.90
3	0	1818	G	N1-C6-O6	8.58	125.05	119.90
3	0	2102	U	O4'-C1'-N1	8.58	115.06	108.20
3	0	688	G	N1-C6-O6	8.57	125.05	119.90
3	0	2238	G	C5-C6-O6	-8.57	123.46	128.60
3	0	792	G	C5-C6-O6	-8.57	123.46	128.60
3	0	368	G	N1-C6-O6	8.56	125.04	119.90
3	0	445	G	N1-C6-O6	8.56	125.04	119.90
3	0	812	A	P-O3'-C3'	8.56	129.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1591	G	N1-C6-O6	8.56	125.04	119.90
3	0	1772	G	N1-C6-O6	8.55	125.03	119.90
1	f	239	ASN	CB-CA-C	8.55	127.50	110.40
3	0	411	G	N1-C6-O6	8.55	125.03	119.90
3	0	838	G	N1-C6-O6	8.55	125.03	119.90
3	0	1971	C	C2-N1-C1'	8.54	128.20	118.80
3	0	2114	G	N1-C6-O6	8.54	125.03	119.90
3	0	2127	G	C5-C6-O6	-8.54	123.47	128.60
3	0	80	G	N1-C6-O6	8.54	125.03	119.90
3	0	86	G	C5-C6-O6	-8.54	123.48	128.60
3	0	1987	C	O4'-C1'-N1	8.54	115.03	108.20
3	0	919	G	N1-C6-O6	8.54	125.02	119.90
3	0	1520	G	N1-C6-O6	8.54	125.02	119.90
1	f	238	SER	C-N-CA	8.53	143.02	121.70
3	0	88	G	N1-C6-O6	8.53	125.02	119.90
3	0	1409	G	C5-C6-O6	-8.53	123.48	128.60
3	0	1696	G	N1-C6-O6	8.52	125.01	119.90
3	0	150	U	P-O3'-C3'	8.52	129.92	119.70
3	0	840	C	O4'-C1'-N1	8.52	115.01	108.20
3	0	2136	A	O4'-C1'-N9	8.51	115.00	108.20
3	0	1855	C	O4'-C1'-N1	8.50	115.00	108.20
1	f	131	THR	C-N-CA	8.50	142.94	121.70
3	0	741	G	N1-C6-O6	8.50	125.00	119.90
3	0	248	G	N1-C6-O6	8.49	125.00	119.90
3	0	309	G	N1-C6-O6	8.49	124.99	119.90
3	0	1851	C	O4'-C1'-N1	8.49	114.99	108.20
3	0	308	C	C2-N1-C1'	8.48	128.13	118.80
3	0	57	G	C5-C6-O6	-8.48	123.51	128.60
3	0	286	G	N1-C6-O6	8.48	124.99	119.90
3	0	1372	G	C5-C6-O6	-8.48	123.51	128.60
3	0	1189	C	O4'-C1'-N1	8.47	114.98	108.20
3	0	405	G	C5-C6-O6	-8.46	123.52	128.60
3	0	373	G	N1-C6-O6	8.46	124.98	119.90
3	0	1904	C	O4'-C1'-N1	8.46	114.97	108.20
2	1	45	G	N1-C6-O6	8.45	124.97	119.90
3	0	1405	G	N1-C6-O6	8.45	124.97	119.90
43	G	164	ALA	N-CA-CB	8.45	121.93	110.10
3	0	294	G	N1-C6-O6	8.45	124.97	119.90
3	0	2048	G	C5-C6-O6	-8.45	123.53	128.60
3	0	1451	C	O4'-C1'-N1	8.45	114.96	108.20
3	0	1595	G	N1-C6-O6	8.45	124.97	119.90
3	0	221	C	O4'-C1'-N1	8.45	114.96	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1282	G	C5-C6-O6	-8.45	123.53	128.60
3	0	1755	C	O4'-C1'-N1	8.45	114.96	108.20
3	0	1895	C	O4'-C1'-N1	8.44	114.95	108.20
3	0	1740	G	N1-C6-O6	8.43	124.96	119.90
3	0	835	G	C5-C6-O6	-8.43	123.54	128.60
3	0	977	A	O4'-C1'-N9	8.43	114.94	108.20
3	0	1413	G	C5-C6-O6	-8.43	123.54	128.60
2	1	5	C	O4'-C1'-N1	8.42	114.94	108.20
3	0	16	G	N1-C6-O6	8.42	124.95	119.90
3	0	1736	G	C5-C6-O6	-8.42	123.55	128.60
1	f	256	GLU	N-CA-C	8.42	133.72	111.00
3	0	1532	G	N1-C6-O6	8.42	124.95	119.90
3	0	1543	G	N1-C6-O6	8.42	124.95	119.90
3	0	2015	G	N1-C6-O6	8.42	124.95	119.90
3	0	1983	C	O4'-C1'-N1	8.41	114.93	108.20
3	0	2098	U	O4'-C1'-N1	8.41	114.93	108.20
3	0	651	G	C5-C6-O6	-8.41	123.55	128.60
3	0	481	G	N1-C6-O6	8.40	124.94	119.90
3	0	677	G	N1-C6-O6	8.40	124.94	119.90
3	0	204	G	C5-C6-O6	-8.39	123.57	128.60
3	0	754	G	N1-C6-O6	8.39	124.93	119.90
3	0	1445	G	C5-C6-O6	-8.39	123.57	128.60
3	0	921	G	N1-C6-O6	8.38	124.93	119.90
3	0	1486	G	N1-C6-O6	8.38	124.93	119.90
3	0	1623	G	N1-C6-O6	8.38	124.93	119.90
3	0	995	C	O4'-C1'-N1	8.38	114.91	108.20
3	0	2295	C	O4'-C1'-N1	8.38	114.91	108.20
3	0	1596	C	O4'-C1'-N1	8.38	114.90	108.20
3	0	395	G	C5-C6-O6	-8.38	123.58	128.60
3	0	1545	C	O4'-C1'-N1	8.37	114.90	108.20
3	0	2282	C	O4'-C1'-N1	8.37	114.90	108.20
3	0	966	C	O4'-C1'-N1	8.37	114.89	108.20
3	0	1752	C	O4'-C1'-N1	8.37	114.89	108.20
3	0	801	C	O4'-C1'-N1	8.37	114.89	108.20
3	0	167	A	O4'-C1'-N9	8.36	114.89	108.20
3	0	797	G	N1-C6-O6	8.36	124.92	119.90
3	0	2026	G	N1-C6-O6	8.35	124.91	119.90
3	0	2084	G	C5-C6-O6	-8.35	123.59	128.60
3	0	2227	G	C5-C6-O6	-8.35	123.59	128.60
3	0	1869	C	O4'-C1'-N1	8.34	114.88	108.20
3	0	2047	G	N1-C6-O6	8.34	124.90	119.90
3	0	2240	C	O4'-C1'-N1	8.34	114.87	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1626	U	O4'-C1'-N1	8.33	114.87	108.20
3	0	1751	G	C5-C6-O6	-8.33	123.60	128.60
3	0	965	C	O4'-C1'-N1	8.33	114.86	108.20
3	0	1244	G	N1-C6-O6	8.33	124.90	119.90
3	0	553	U	O4'-C1'-N1	8.32	114.86	108.20
1	f	236	SER	O-C-N	-8.32	109.39	122.70
3	0	2316	G	N1-C6-O6	8.32	124.89	119.90
3	0	1716	G	N1-C6-O6	8.32	124.89	119.90
3	0	706	G	C5-C6-O6	-8.31	123.61	128.60
3	0	1398	G	C5-C6-O6	-8.31	123.61	128.60
3	0	136	U	O4'-C1'-N1	8.31	114.85	108.20
3	0	158	C	O4'-C1'-N1	8.31	114.85	108.20
3	0	2241	C	O4'-C1'-N1	8.31	114.84	108.20
3	0	69	C	O4'-C1'-N1	8.30	114.84	108.20
3	0	933	C	O4'-C1'-N1	8.30	114.84	108.20
3	0	547	G	C5-C6-O6	-8.29	123.63	128.60
3	0	1074	G	C5-C6-O6	-8.29	123.63	128.60
3	0	1224	C	O4'-C1'-N1	8.28	114.83	108.20
1	f	1121	CYS	CA-C-N	-8.28	98.99	117.20
3	0	394	G	C5-C6-O6	-8.28	123.63	128.60
3	0	318	C	O4'-C1'-N1	8.28	114.82	108.20
3	0	696	G	C5-C6-O6	-8.28	123.63	128.60
3	0	1192	C	O4'-C1'-N1	8.28	114.82	108.20
3	0	2045	G	C5-C6-O6	-8.28	123.63	128.60
3	0	2199	G	C5-C6-O6	-8.28	123.64	128.60
3	0	834	G	C5-C6-O6	-8.27	123.64	128.60
3	0	1452	C	O4'-C1'-N1	8.27	114.81	108.20
3	0	1927	G	N1-C6-O6	8.27	124.86	119.90
3	0	2028	C	O4'-C1'-N1	8.26	114.81	108.20
3	0	389	G	C5-C6-O6	-8.26	123.64	128.60
3	0	987	G	C5-C6-O6	-8.26	123.65	128.60
3	0	212	G	N1-C6-O6	8.26	124.85	119.90
3	0	1852	C	O4'-C1'-N1	8.25	114.80	108.20
2	1	6	C	O4'-C1'-N1	8.25	114.80	108.20
2	1	64	C	O4'-C1'-N1	8.25	114.80	108.20
3	0	440	C	O4'-C1'-N1	8.25	114.80	108.20
3	0	1587	G	N1-C6-O6	8.25	124.85	119.90
3	0	7	G	C5-C6-O6	-8.25	123.65	128.60
3	0	53	G	C5-C6-O6	-8.24	123.65	128.60
2	1	36	A	O4'-C1'-N9	8.24	114.79	108.20
2	1	40	C	O4'-C1'-N1	8.24	114.79	108.20
3	0	1312	G	C5-C6-O6	-8.24	123.65	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1388	G	N1-C6-O6	8.24	124.84	119.90
3	0	1193	C	O4'-C1'-N1	8.24	114.79	108.20
3	0	1450	G	N1-C6-O6	8.24	124.84	119.90
3	0	1979	C	P-O3'-C3'	8.24	129.58	119.70
3	0	1724	U	O4'-C1'-N1	8.23	114.79	108.20
2	1	52	G	C5-C6-O6	-8.23	123.66	128.60
3	0	725	U	O4'-C1'-N1	8.23	114.78	108.20
3	0	384	G	N1-C6-O6	8.23	124.84	119.90
3	0	466	G	C5-C6-O6	-8.23	123.67	128.60
3	0	1261	C	O4'-C1'-N1	8.23	114.78	108.20
3	0	1387	G	C5-C6-O6	-8.23	123.67	128.60
3	0	1968	G	C5-C6-O6	-8.22	123.67	128.60
3	0	291	G	C5-C6-O6	-8.22	123.67	128.60
3	0	390	C	O4'-C1'-N1	8.21	114.77	108.20
3	0	1874	G	C5-C6-O6	-8.22	123.67	128.60
3	0	980	G	C5-C6-O6	-8.21	123.67	128.60
3	0	971	G	C5-C6-O6	-8.21	123.68	128.60
3	0	1391	G	N1-C6-O6	8.21	124.82	119.90
3	0	719	G	N1-C6-O6	8.20	124.82	119.90
3	0	71	G	C5-C6-O6	-8.20	123.68	128.60
3	0	928	C	O4'-C1'-N1	8.20	114.76	108.20
3	0	1330	C	O4'-C1'-N1	8.19	114.75	108.20
3	0	2163	C	O4'-C1'-N1	8.19	114.75	108.20
3	0	996	G	C5-C6-O6	-8.19	123.69	128.60
3	0	1988	U	O4'-C1'-N1	8.19	114.75	108.20
3	0	837	C	O4'-C1'-N1	8.18	114.75	108.20
3	0	1404	G	C5-C6-O6	-8.18	123.69	128.60
3	0	2005	C	O4'-C1'-N1	8.18	114.74	108.20
3	0	34	G	N1-C6-O6	8.18	124.81	119.90
3	0	828	G	C5-C6-O6	-8.18	123.69	128.60
3	0	2118	G	C5-C6-O6	-8.17	123.70	128.60
3	0	157	G	C5-C6-O6	-8.17	123.70	128.60
3	0	649	G	C5-C6-O6	-8.17	123.70	128.60
3	0	1672	G	N1-C6-O6	8.16	124.80	119.90
3	0	2154	C	O4'-C1'-N1	8.16	114.73	108.20
3	0	1521	G	C5-C6-O6	-8.16	123.71	128.60
3	0	2106	G	C5-C6-O6	-8.16	123.71	128.60
3	0	836	G	C5-C6-O6	-8.15	123.71	128.60
3	0	344	G	C5-C6-O6	-8.15	123.71	128.60
3	0	2032	C	O4'-C1'-N1	8.15	114.72	108.20
3	0	514	G	C5-C6-O6	-8.14	123.71	128.60
3	0	2090	U	O4'-C1'-N1	8.14	114.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	69	G	C5-C6-O6	-8.14	123.72	128.60
3	0	72	C	O4'-C1'-N1	8.14	114.71	108.20
3	0	303	C	O4'-C1'-N1	8.14	114.71	108.20
3	0	1958	G	C5-C6-O6	-8.13	123.72	128.60
1	f	255	TRP	O-C-N	8.13	135.71	122.70
3	0	2128	C	O4'-C1'-N1	8.13	114.71	108.20
3	0	554	C	O4'-C1'-N1	8.13	114.70	108.20
3	0	714	G	N1-C6-O6	8.13	124.78	119.90
3	0	1915	G	C5-C6-O6	-8.12	123.73	128.60
3	0	2119	U	O4'-C1'-N1	8.12	114.70	108.20
3	0	1868	C	O4'-C1'-N1	8.12	114.69	108.20
3	0	134	U	O4'-C1'-N1	8.12	114.69	108.20
3	0	412	G	C5-C6-O6	-8.11	123.73	128.60
3	0	650	C	O4'-C1'-N1	8.11	114.69	108.20
3	0	1186	C	O4'-C1'-N1	8.11	114.69	108.20
3	0	2280	G	C5-C6-O6	-8.11	123.73	128.60
3	0	333	C	O4'-C1'-N1	8.11	114.69	108.20
3	0	148	G	C5-C6-O6	-8.11	123.74	128.60
3	0	1858	C	O4'-C1'-N1	8.11	114.69	108.20
3	0	904	C	O4'-C1'-N1	8.10	114.68	108.20
3	0	238	G	C5-C6-O6	-8.10	123.74	128.60
3	0	1850	C	O4'-C1'-N1	8.10	114.68	108.20
1	f	304	PRO	O-C-N	8.09	135.65	122.70
3	0	926	C	O4'-C1'-N1	8.09	114.67	108.20
3	0	1961	C	O4'-C1'-N1	8.09	114.67	108.20
3	0	218	C	O4'-C1'-N1	8.09	114.67	108.20
2	1	2	G	C5-C6-O6	-8.08	123.75	128.60
3	0	117	C	O4'-C1'-N1	8.08	114.67	108.20
3	0	206	C	O4'-C1'-N1	8.08	114.67	108.20
3	0	488	G	C5-C6-O6	-8.08	123.75	128.60
3	0	668	C	O4'-C1'-N1	8.08	114.67	108.20
3	0	1798	G	C5-C6-O6	-8.08	123.75	128.60
3	0	2213	G	C5-C6-O6	-8.08	123.75	128.60
3	0	1881	G	N1-C6-O6	8.08	124.75	119.90
3	0	2251	C	O4'-C1'-N1	8.08	114.66	108.20
2	1	51	G	C5-C6-O6	-8.08	123.75	128.60
3	0	579	C	O4'-C1'-N1	8.08	114.66	108.20
3	0	708	G	C5-C6-O6	-8.08	123.75	128.60
3	0	1554	G	C5-C6-O6	-8.07	123.75	128.60
3	0	1976	C	O4'-C1'-N1	8.07	114.66	108.20
3	0	751	C	O4'-C1'-N1	8.07	114.65	108.20
3	0	756	G	C5-C6-O6	-8.07	123.76	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	262	U	O4'-C1'-N1	8.06	114.65	108.20
3	0	230	G	C5-C6-O6	-8.06	123.76	128.60
3	0	907	G	C5-C6-O6	-8.06	123.77	128.60
3	0	955	U	O4'-C1'-N1	8.06	114.64	108.20
3	0	435	G	C5-C6-O6	-8.05	123.77	128.60
3	0	1814	C	O4'-C1'-N1	8.05	114.64	108.20
3	0	1262	C	O4'-C1'-N1	8.05	114.64	108.20
3	0	1856	C	O4'-C1'-N1	8.05	114.64	108.20
3	0	1943	C	O4'-C1'-N1	8.05	114.64	108.20
3	0	139	G	C5-C6-O6	-8.05	123.77	128.60
3	0	1066	C	O4'-C1'-N1	8.05	114.64	108.20
3	0	229	G	C5-C6-O6	-8.04	123.78	128.60
3	0	1590	C	O4'-C1'-N1	8.04	114.63	108.20
3	0	1984	G	C5-C6-O6	-8.04	123.78	128.60
3	0	1565	G	N1-C6-O6	8.04	124.72	119.90
3	0	2181	G	C5-C6-O6	-8.04	123.78	128.60
3	0	1276	G	N1-C6-O6	8.04	124.72	119.90
3	0	593	G	N1-C6-O6	8.03	124.72	119.90
3	0	759	C	O4'-C1'-N1	8.03	114.62	108.20
3	0	1702	G	N1-C6-O6	8.03	124.72	119.90
3	0	320	G	C5-C6-O6	-8.03	123.78	128.60
2	1	21	G	C5-C6-O6	-8.02	123.79	128.60
3	0	532	G	C5-C6-O6	-8.02	123.79	128.60
3	0	731	U	O4'-C1'-N1	8.02	114.62	108.20
3	0	580	C	O4'-C1'-N1	8.02	114.62	108.20
3	0	1480	C	O4'-C1'-N1	8.02	114.61	108.20
3	0	1634	C	O4'-C1'-N1	8.02	114.61	108.20
3	0	2028	C	C2-N1-C1'	8.02	127.62	118.80
3	0	2263	C	O4'-C1'-N1	8.02	114.61	108.20
3	0	104	C	O4'-C1'-N1	8.02	114.61	108.20
3	0	264	C	O4'-C1'-N1	8.02	114.61	108.20
3	0	1728	G	P-O3'-C3'	8.02	129.32	119.70
3	0	1906	G	C5-C6-O6	-8.02	123.79	128.60
3	0	108	C	O4'-C1'-N1	8.01	114.61	108.20
3	0	319	C	O4'-C1'-N1	8.01	114.61	108.20
3	0	2210	G	C5-C6-O6	-8.01	123.79	128.60
46	C	411	ARG	NE-CZ-NH1	-8.01	116.30	120.30
3	0	1763	C	O4'-C1'-N1	8.01	114.61	108.20
46	C	411	ARG	CG-CD-NE	8.01	128.62	111.80
3	0	1822	G	C5-C6-O6	-8.00	123.80	128.60
2	1	3	C	O4'-C1'-N1	7.99	114.59	108.20
3	0	1533	C	O4'-C1'-N1	7.99	114.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1753	C	O4'-C1'-N1	7.99	114.59	108.20
3	0	2230	C	O4'-C1'-N1	7.99	114.59	108.20
3	0	2235	C	O4'-C1'-N1	7.99	114.59	108.20
3	0	458	C	O4'-C1'-N1	7.99	114.59	108.20
3	0	1414	G	C5-C6-O6	-7.99	123.81	128.60
3	0	1639	C	O4'-C1'-N1	7.99	114.59	108.20
3	0	869	G	C5-C6-O6	-7.98	123.81	128.60
3	0	812	A	O4'-C1'-N9	7.98	114.59	108.20
3	0	2144	G	C5-C6-O6	-7.98	123.81	128.60
3	0	54	C	O4'-C1'-N1	7.98	114.58	108.20
3	0	437	G	N1-C6-O6	7.98	124.69	119.90
1	f	234	GLY	C-N-CA	-7.98	101.76	121.70
3	0	1683	C	O4'-C1'-N1	7.98	114.58	108.20
3	0	1974	G	O4'-C1'-N9	7.98	114.58	108.20
3	0	2303	G	N1-C6-O6	7.98	124.69	119.90
3	0	156	G	C5-C6-O6	-7.97	123.81	128.60
3	0	542	C	O4'-C1'-N1	7.97	114.58	108.20
3	0	2242	G	C5-C6-O6	-7.97	123.81	128.60
3	0	695	G	C5-C6-O6	-7.97	123.82	128.60
3	0	2216	C	O4'-C1'-N1	7.97	114.58	108.20
2	1	67	G	C5-C6-O6	-7.96	123.82	128.60
3	0	387	C	O4'-C1'-N1	7.96	114.57	108.20
3	0	430	G	C5-C6-O6	-7.96	123.82	128.60
3	0	925	C	O4'-C1'-N1	7.96	114.57	108.20
3	0	182	C	O4'-C1'-N1	7.96	114.57	108.20
3	0	370	G	C5-C6-O6	-7.96	123.83	128.60
3	0	746	A	C5-C6-N6	-7.96	117.33	123.70
3	0	1603	G	C5-C6-O6	-7.96	123.83	128.60
3	0	1878	G	C5-C6-O6	-7.96	123.83	128.60
3	0	2203	C	O4'-C1'-N1	7.96	114.56	108.20
3	0	76	G	C5-C6-O6	-7.95	123.83	128.60
3	0	1442	C	O4'-C1'-N1	7.95	114.56	108.20
3	0	726	C	O4'-C1'-N1	7.95	114.56	108.20
3	0	1412	C	O4'-C1'-N1	7.95	114.56	108.20
3	0	537	C	O4'-C1'-N1	7.95	114.56	108.20
3	0	1179	C	O4'-C1'-N1	7.95	114.56	108.20
3	0	1649	G	C5-C6-O6	-7.95	123.83	128.60
3	0	1896	C	O4'-C1'-N1	7.95	114.56	108.20
3	0	1750	G	N1-C6-O6	7.94	124.67	119.90
3	0	1912	C	O4'-C1'-N1	7.94	114.55	108.20
3	0	251	A	P-O3'-C3'	7.94	129.23	119.70
3	0	1287	C	O4'-C1'-N1	7.94	114.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1578	C	O4'-C1'-N1	7.94	114.55	108.20
3	0	1397	G	C5-C6-O6	-7.94	123.84	128.60
3	0	2301	G	C5-C6-O6	-7.94	123.84	128.60
3	0	763	G	C5-C6-O6	-7.94	123.84	128.60
3	0	1553	C	C2-N1-C1'	7.94	127.53	118.80
3	0	1073	C	O4'-C1'-N1	7.93	114.55	108.20
3	0	1607	C	O4'-C1'-N1	7.93	114.55	108.20
3	0	1621	C	O4'-C1'-N1	7.93	114.54	108.20
3	0	1746	G	N1-C6-O6	7.93	124.66	119.90
3	0	1854	U	O4'-C1'-N1	7.93	114.54	108.20
1	f	1148	ASP	CA-C-N	-7.93	99.76	117.20
3	0	1725	C	O4'-C1'-N1	7.93	114.54	108.20
2	1	57	A	N1-C6-N6	7.93	123.36	118.60
2	1	70	C	O4'-C1'-N1	7.92	114.54	108.20
3	0	347	G	C5-C6-O6	-7.92	123.85	128.60
3	0	1228	C	O4'-C1'-N1	7.92	114.54	108.20
3	0	1687	U	O4'-C1'-N1	7.92	114.54	108.20
2	1	55	C	O4'-C1'-N1	7.92	114.54	108.20
3	0	678	G	C5-C6-O6	-7.92	123.85	128.60
3	0	2149	G	C5-C6-O6	-7.92	123.85	128.60
3	0	1876	G	C5-C6-O6	-7.91	123.85	128.60
3	0	2025	G	C5-C6-O6	-7.91	123.85	128.60
3	0	1905	G	C5-C6-O6	-7.91	123.85	128.60
3	0	147	G	N1-C6-O6	7.91	124.64	119.90
3	0	1225	G	C5-C6-O6	-7.91	123.86	128.60
3	0	2260	C	O4'-C1'-N1	7.91	114.53	108.20
3	0	548	C	O4'-C1'-N1	7.91	114.52	108.20
3	0	1891	G	C5-C6-O6	-7.91	123.86	128.60
3	0	2162	C	O4'-C1'-N1	7.91	114.53	108.20
3	0	1256	C	O4'-C1'-N1	7.90	114.52	108.20
3	0	1505	C	O4'-C1'-N1	7.90	114.52	108.20
3	0	2270	G	C5-C6-O6	-7.90	123.86	128.60
3	0	31	C	O4'-C1'-N1	7.90	114.52	108.20
3	0	853	C	O4'-C1'-N1	7.90	114.52	108.20
2	1	11	C	O4'-C1'-N1	7.90	114.52	108.20
3	0	109	G	O4'-C1'-N9	7.90	114.52	108.20
3	0	1511	C	O4'-C1'-N1	7.90	114.52	108.20
1	f	193	ARG	O-C-N	-7.89	110.07	122.70
3	0	1853	U	O4'-C1'-N1	7.89	114.52	108.20
3	0	1239	G	C5-C6-O6	-7.89	123.86	128.60
1	f	240	PHE	CA-C-N	-7.89	99.84	117.20
3	0	409	G	C5-C6-O6	-7.89	123.87	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2303	G	O4'-C1'-N9	7.89	114.51	108.20
3	0	2271	G	C5-C6-O6	-7.89	123.87	128.60
3	0	402	C	O4'-C1'-N1	7.89	114.51	108.20
3	0	508	G	C5-C6-O6	-7.88	123.87	128.60
3	0	950	G	C5-C6-O6	-7.88	123.87	128.60
3	0	2283	G	C5-C6-O6	-7.88	123.87	128.60
3	0	2300	G	C5-C6-O6	-7.88	123.87	128.60
3	0	224	C	O4'-C1'-N1	7.88	114.50	108.20
3	0	964	U	O4'-C1'-N1	7.88	114.50	108.20
3	0	1076	C	O4'-C1'-N1	7.88	114.50	108.20
3	0	240	G	C5-C6-O6	-7.87	123.88	128.60
3	0	2142	C	O4'-C1'-N1	7.87	114.50	108.20
3	0	1359	C	O4'-C1'-N1	7.87	114.50	108.20
3	0	1761	G	C5-C6-O6	-7.87	123.88	128.60
3	0	2138	C	O4'-C1'-N1	7.87	114.50	108.20
3	0	410	G	C5-C6-O6	-7.87	123.88	128.60
3	0	789	C	O4'-C1'-N1	7.87	114.49	108.20
3	0	1406	C	O4'-C1'-N1	7.86	114.49	108.20
3	0	1940	C	O4'-C1'-N1	7.86	114.49	108.20
3	0	404	G	C5-C6-O6	-7.86	123.88	128.60
3	0	1397	G	O4'-C1'-N9	7.86	114.49	108.20
3	0	698	C	O4'-C1'-N1	7.86	114.49	108.20
1	f	1654	GLY	N-CA-C	7.86	132.74	113.10
2	1	23	G	C5-C6-O6	-7.85	123.89	128.60
3	0	1315	C	O4'-C1'-N1	7.85	114.48	108.20
3	0	2211	G	C5-C6-O6	-7.85	123.89	128.60
3	0	578	C	O4'-C1'-N1	7.85	114.48	108.20
3	0	1555	C	O4'-C1'-N1	7.85	114.48	108.20
3	0	263	G	C5-C6-O6	-7.85	123.89	128.60
3	0	550	U	O4'-C1'-N1	7.85	114.48	108.20
3	0	1401	G	C5-C6-O6	-7.85	123.89	128.60
2	1	38	C	O4'-C1'-N1	7.84	114.47	108.20
3	0	1688	C	O4'-C1'-N1	7.84	114.47	108.20
3	0	1877	G	C5-C6-O6	-7.84	123.89	128.60
3	0	1937	G	C5-C6-O6	-7.84	123.89	128.60
3	0	332	C	O4'-C1'-N1	7.84	114.47	108.20
3	0	1551	C	O4'-C1'-N1	7.84	114.47	108.20
3	0	830	C	O4'-C1'-N1	7.84	114.47	108.20
3	0	1560	G	C5-C6-O6	-7.84	123.90	128.60
3	0	641	C	O4'-C1'-N1	7.84	114.47	108.20
3	0	713	G	N1-C6-O6	7.84	124.60	119.90
3	0	1768	G	C5-C6-O6	-7.84	123.90	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	297	THR	C-N-CA	7.83	141.29	121.70
3	0	311	G	C5-C6-O6	-7.83	123.90	128.60
3	0	1548	C	O4'-C1'-N1	7.83	114.47	108.20
3	0	1790	C	O4'-C1'-N1	7.83	114.47	108.20
3	0	914	C	O4'-C1'-N1	7.83	114.47	108.20
3	0	2246	G	C5-C6-O6	-7.83	123.90	128.60
3	0	1959	C	O4'-C1'-N1	7.83	114.46	108.20
1	f	1254	ALA	O-C-N	7.83	135.22	122.70
3	0	6	G	C5-C6-O6	-7.83	123.90	128.60
3	0	192	G	C5-C6-O6	-7.83	123.90	128.60
3	0	1235	G	C5-C6-O6	-7.83	123.90	128.60
1	f	293	LYS	O-C-N	-7.83	110.18	122.70
3	0	1781	G	C5-C6-O6	-7.83	123.91	128.60
3	0	228	G	C5-C6-O6	-7.82	123.91	128.60
3	0	815	G	C5-C6-O6	-7.82	123.91	128.60
3	0	1540	U	O4'-C1'-N1	7.82	114.46	108.20
3	0	1774	U	O4'-C1'-N1	7.82	114.46	108.20
3	0	2275	C	O4'-C1'-N1	7.82	114.46	108.20
3	0	1721	C	O4'-C1'-N1	7.82	114.46	108.20
3	0	2059	G	N1-C6-O6	7.82	124.59	119.90
3	0	186	C	O4'-C1'-N1	7.82	114.45	108.20
3	0	1826	C	O4'-C1'-N1	7.82	114.45	108.20
3	0	2229	G	C5-C6-O6	-7.82	123.91	128.60
3	0	133	G	C5-C6-O6	-7.81	123.91	128.60
3	0	165	C	O4'-C1'-N1	7.81	114.45	108.20
3	0	423	C	O4'-C1'-N1	7.81	114.45	108.20
3	0	1732	C	O4'-C1'-N1	7.81	114.45	108.20
3	0	1885	U	O4'-C1'-N1	7.81	114.45	108.20
3	0	2018	U	P-O3'-C3'	7.81	129.07	119.70
3	0	2192	C	O4'-C1'-N1	7.81	114.45	108.20
3	0	268	C	O4'-C1'-N1	7.81	114.45	108.20
3	0	89	C	O4'-C1'-N1	7.81	114.45	108.20
3	0	470	G	C5-C6-O6	-7.81	123.92	128.60
3	0	1241	G	O4'-C1'-N9	7.81	114.45	108.20
3	0	1782	G	C5-C6-O6	-7.81	123.92	128.60
1	f	303	ASN	CB-CA-C	7.80	126.01	110.40
3	0	1502	C	O4'-C1'-N1	7.80	114.44	108.20
3	0	214	C	O4'-C1'-N1	7.80	114.44	108.20
3	0	629	C	O4'-C1'-N1	7.80	114.44	108.20
3	0	859	C	O4'-C1'-N1	7.80	114.44	108.20
3	0	2148	C	O4'-C1'-N1	7.80	114.44	108.20
3	0	623	C	O4'-C1'-N1	7.80	114.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	780	C	O4'-C1'-N1	7.80	114.44	108.20
3	0	1691	G	C5-C6-O6	-7.80	123.92	128.60
3	0	480	C	O4'-C1'-N1	7.79	114.43	108.20
3	0	376	C	O4'-C1'-N1	7.79	114.43	108.20
3	0	744	C	C2-N1-C1'	7.79	127.37	118.80
3	0	1574	G	C5-C6-O6	-7.78	123.93	128.60
3	0	1650	C	O4'-C1'-N1	7.78	114.42	108.20
3	0	1640	G	C5-C6-O6	-7.78	123.93	128.60
3	0	2252	C	O4'-C1'-N1	7.78	114.42	108.20
3	0	2156	U	O4'-C1'-N1	7.77	114.42	108.20
3	0	2224	C	O4'-C1'-N1	7.77	114.42	108.20
3	0	461	C	O4'-C1'-N1	7.77	114.42	108.20
3	0	1478	U	O4'-C1'-N1	7.77	114.42	108.20
3	0	2030	U	O4'-C1'-N1	7.77	114.42	108.20
3	0	1661	G	C5-C6-O6	-7.77	123.94	128.60
3	0	2220	C	O4'-C1'-N1	7.77	114.41	108.20
3	0	176	C	O4'-C1'-N1	7.76	114.41	108.20
3	0	2161	G	C5-C6-O6	-7.76	123.94	128.60
3	0	2249	C	O4'-C1'-N1	7.76	114.41	108.20
3	0	232	C	O4'-C1'-N1	7.76	114.41	108.20
3	0	455	C	O4'-C1'-N1	7.76	114.41	108.20
3	0	2063	C	O4'-C1'-N1	7.76	114.41	108.20
3	0	2089	U	O4'-C1'-N1	7.76	114.41	108.20
3	0	1277	C	O4'-C1'-N1	7.76	114.41	108.20
3	0	1985	C	O4'-C1'-N1	7.76	114.41	108.20
28	5	267	SER	CA-C-N	7.76	134.27	117.20
3	0	79	G	C5-C6-O6	-7.76	123.95	128.60
3	0	391	C	O4'-C1'-N1	7.76	114.41	108.20
3	0	1354	G	C5-C6-O6	-7.75	123.95	128.60
3	0	1744	G	C5-C6-O6	-7.75	123.95	128.60
3	0	1969	U	O4'-C1'-N1	7.75	114.40	108.20
3	0	155	U	O4'-C1'-N1	7.75	114.40	108.20
3	0	164	G	C5-C6-O6	-7.75	123.95	128.60
3	0	1337	G	C5-C6-O6	-7.75	123.95	128.60
3	0	2198	U	O4'-C1'-N1	7.75	114.40	108.20
3	0	1821	G	C5-C6-O6	-7.75	123.95	128.60
3	0	1796	C	O4'-C1'-N1	7.74	114.39	108.20
1	f	1218	VAL	O-C-N	-7.74	110.31	122.70
3	0	1069	U	O4'-C1'-N1	7.74	114.39	108.20
3	0	931	G	C5-C6-O6	-7.74	123.96	128.60
3	0	2220	C	P-O3'-C3'	7.74	128.99	119.70
3	0	2222	G	C5-C6-O6	-7.74	123.96	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2110	C	O4'-C1'-N1	7.73	114.39	108.20
3	0	365	C	O4'-C1'-N1	7.73	114.38	108.20
3	0	478	C	O4'-C1'-N1	7.73	114.39	108.20
3	0	1376	C	O4'-C1'-N1	7.73	114.38	108.20
3	0	2297	G	C5-C6-O6	-7.73	123.96	128.60
3	0	441	C	O4'-C1'-N1	7.72	114.38	108.20
3	0	566	G	C5-C6-O6	-7.72	123.97	128.60
3	0	1215	G	C5-C6-O6	-7.72	123.97	128.60
3	0	321	G	C5-C6-O6	-7.72	123.97	128.60
2	1	68	U	O4'-C1'-N1	7.72	114.37	108.20
3	0	897	U	O4'-C1'-N1	7.71	114.37	108.20
3	0	1506	G	C5-C6-O6	-7.71	123.97	128.60
3	0	517	G	C5-C6-O6	-7.71	123.97	128.60
3	0	1668	C	O4'-C1'-N1	7.71	114.37	108.20
3	0	901	A	O4'-C1'-N9	7.71	114.37	108.20
3	0	235	C	O4'-C1'-N1	7.71	114.37	108.20
3	0	686	U	O4'-C1'-N1	7.71	114.37	108.20
3	0	1218	G	C5-C6-O6	-7.71	123.98	128.60
3	0	2168	G	C5-C6-O6	-7.71	123.98	128.60
3	0	565	G	N1-C6-O6	7.71	124.52	119.90
3	0	1599	G	C5-C6-O6	-7.71	123.98	128.60
3	0	715	U	O4'-C1'-N1	7.70	114.36	108.20
3	0	2191	C	O4'-C1'-N1	7.70	114.36	108.20
3	0	225	C	O4'-C1'-N1	7.70	114.36	108.20
3	0	606	G	C5-C6-O6	-7.70	123.98	128.60
3	0	640	G	C5-C6-O6	-7.70	123.98	128.60
3	0	1867	C	O4'-C1'-N1	7.70	114.36	108.20
3	0	84	C	O4'-C1'-N1	7.70	114.36	108.20
3	0	1474	C	O4'-C1'-N1	7.70	114.36	108.20
3	0	796	G	C5-C6-O6	-7.69	123.98	128.60
3	0	431	G	C5-C6-O6	-7.69	123.98	128.60
3	0	1894	U	O4'-C1'-N1	7.69	114.35	108.20
2	1	7	G	C5-C6-O6	-7.69	123.99	128.60
3	0	1962	C	O4'-C1'-N1	7.69	114.35	108.20
3	0	568	G	C5-C6-O6	-7.69	123.99	128.60
3	0	2032	C	C2-N1-C1'	7.69	127.26	118.80
3	0	2233	C	O4'-C1'-N1	7.69	114.35	108.20
3	0	251	A	O4'-C1'-N9	7.68	114.35	108.20
3	0	760	C	O4'-C1'-N1	7.68	114.35	108.20
3	0	1002	G	C5-C6-O6	-7.68	123.99	128.60
3	0	2014	C	O4'-C1'-N1	7.68	114.35	108.20
3	0	236	C	O4'-C1'-N1	7.68	114.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	77	C	O4'-C1'-N1	7.68	114.34	108.20
3	0	705	G	C5-C6-O6	-7.68	123.99	128.60
3	0	244	G	C5-C6-O6	-7.68	123.99	128.60
3	0	563	U	O4'-C1'-N1	7.67	114.34	108.20
3	0	1628	G	C5-C6-O6	-7.67	124.00	128.60
3	0	983	C	O4'-C1'-N1	7.67	114.34	108.20
3	0	787	C	O4'-C1'-N1	7.67	114.33	108.20
3	0	1553	C	O4'-C1'-N1	7.67	114.33	108.20
3	0	1576	C	O4'-C1'-N1	7.67	114.33	108.20
3	0	605	G	C5-C6-O6	-7.67	124.00	128.60
3	0	1233	G	C5-C6-O6	-7.67	124.00	128.60
3	0	1515	U	O4'-C1'-N1	7.67	114.33	108.20
3	0	1749	U	O4'-C1'-N1	7.67	114.33	108.20
3	0	681	C	O4'-C1'-N1	7.67	114.33	108.20
3	0	1000	G	C5-C6-O6	-7.66	124.00	128.60
3	0	1259	C	O4'-C1'-N1	7.66	114.33	108.20
3	0	490	C	O4'-C1'-N1	7.66	114.33	108.20
3	0	1708	C	O4'-C1'-N1	7.66	114.33	108.20
3	0	2126	G	C5-C6-O6	-7.66	124.00	128.60
3	0	1377	C	O4'-C1'-N1	7.66	114.33	108.20
3	0	1416	C	O4'-C1'-N1	7.66	114.33	108.20
3	0	1449	C	O4'-C1'-N1	7.66	114.33	108.20
3	0	2274	G	C5-C6-O6	-7.66	124.00	128.60
3	0	213	G	N1-C6-O6	7.66	124.49	119.90
2	1	13	C	O4'-C1'-N1	7.66	114.33	108.20
3	0	774	C	O4'-C1'-N1	7.66	114.32	108.20
3	0	939	U	O4'-C1'-N1	7.66	114.32	108.20
3	0	374	G	N1-C6-O6	7.65	124.49	119.90
2	1	61	C	O4'-C1'-N1	7.65	114.32	108.20
3	0	1693	C	O4'-C1'-N1	7.65	114.32	108.20
3	0	477	G	C5-C6-O6	-7.65	124.01	128.60
3	0	530	G	C5-C6-O6	-7.65	124.01	128.60
3	0	757	G	C5-C6-O6	-7.64	124.01	128.60
3	0	896	U	O4'-C1'-N1	7.64	114.32	108.20
3	0	934	C	O4'-C1'-N1	7.64	114.32	108.20
3	0	968	U	O4'-C1'-N1	7.64	114.31	108.20
3	0	489	C	O4'-C1'-N1	7.64	114.31	108.20
3	0	1374	C	O4'-C1'-N1	7.64	114.31	108.20
3	0	1945	G	C5-C6-O6	-7.64	124.01	128.60
1	f	1267	LEU	N-CA-C	-7.64	90.37	111.00
1	f	304	PRO	CA-C-O	-7.64	101.87	120.20
3	0	2130	C	O4'-C1'-N1	7.64	114.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1419	G	C5-C6-O6	-7.64	124.02	128.60
1	f	1670	CYS	C-N-CA	7.63	140.78	121.70
3	0	377	G	C5-C6-O6	-7.63	124.02	128.60
3	0	2147	C	O4'-C1'-N1	7.63	114.31	108.20
3	0	1324	G	C5-C6-O6	-7.63	124.02	128.60
3	0	888	G	C5-C6-O6	-7.63	124.02	128.60
3	0	1221	G	C5-C6-O6	-7.63	124.02	128.60
3	0	2100	G	C5-C6-O6	-7.63	124.02	128.60
3	0	1436	C	O4'-C1'-N1	7.62	114.30	108.20
3	0	1598	A	C4-C5-C6	7.62	120.81	117.00
3	0	1654	U	O4'-C1'-N1	7.62	114.30	108.20
3	0	1722	U	O4'-C1'-N1	7.62	114.30	108.20
3	0	2034	U	O4'-C1'-N1	7.62	114.30	108.20
3	0	334	G	C5-C6-O6	-7.62	124.03	128.60
3	0	882	U	O4'-C1'-N1	7.62	114.29	108.20
3	0	259	C	O4'-C1'-N1	7.62	114.29	108.20
3	0	842	G	C5-C6-O6	-7.62	124.03	128.60
2	1	65	C	O4'-C1'-N1	7.61	114.29	108.20
3	0	317	G	C5-C6-O6	-7.61	124.03	128.60
3	0	709	C	O4'-C1'-N1	7.61	114.29	108.20
3	0	1816	C	O4'-C1'-N1	7.61	114.29	108.20
3	0	1309	C	O4'-C1'-N1	7.61	114.29	108.20
2	1	48	G	C5-C6-O6	-7.61	124.04	128.60
3	0	23	G	C5-C6-O6	-7.61	124.04	128.60
3	0	1004	G	C5-C6-O6	-7.61	124.04	128.60
3	0	1257	C	O4'-C1'-N1	7.60	114.28	108.20
3	0	2062	U	O4'-C1'-N1	7.60	114.28	108.20
3	0	572	U	O4'-C1'-N1	7.60	114.28	108.20
3	0	1579	A	O4'-C1'-N9	7.60	114.28	108.20
3	0	1911	C	O4'-C1'-N1	7.60	114.28	108.20
3	0	2080	G	O4'-C1'-N9	7.60	114.28	108.20
3	0	560	C	O4'-C1'-N1	7.59	114.28	108.20
3	0	1664	U	O4'-C1'-N1	7.59	114.28	108.20
3	0	732	C	O4'-C1'-N1	7.59	114.27	108.20
3	0	1706	G	C5-C6-O6	-7.59	124.05	128.60
3	0	1765	G	N1-C6-O6	7.59	124.45	119.90
2	1	12	G	C5-C6-O6	-7.59	124.05	128.60
3	0	1468	U	P-O5'-C5'	7.59	133.04	120.90
3	0	2189	U	O4'-C1'-N1	7.58	114.27	108.20
3	0	727	C	O4'-C1'-N1	7.58	114.27	108.20
3	0	223	G	C5-C6-O6	-7.58	124.05	128.60
3	0	1182	C	O4'-C1'-N1	7.58	114.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	807	U	O4'-C1'-N1	7.58	114.26	108.20
3	0	1938	G	C5-C6-O6	-7.58	124.05	128.60
3	0	1834	C	O4'-C1'-N1	7.58	114.26	108.20
3	0	2180	C	O4'-C1'-N1	7.57	114.26	108.20
1	f	1264	LEU	CA-C-N	7.57	133.84	117.20
3	0	364	G	C5-C6-O6	-7.57	124.06	128.60
3	0	197	C	O4'-C1'-N1	7.56	114.25	108.20
3	0	1923	C	O4'-C1'-N1	7.56	114.25	108.20
3	0	2178	C	O4'-C1'-N1	7.56	114.25	108.20
3	0	2266	U	O4'-C1'-N1	7.56	114.25	108.20
3	0	464	C	O4'-C1'-N1	7.56	114.25	108.20
3	0	620	C	O4'-C1'-N1	7.56	114.25	108.20
3	0	734	G	C5-C6-O6	-7.56	124.06	128.60
2	1	29	G	C5-C6-O6	-7.56	124.07	128.60
3	0	42	G	C5-C6-O6	-7.55	124.07	128.60
3	0	495	G	C5-C6-O6	-7.55	124.07	128.60
3	0	94	C	O4'-C1'-N1	7.55	114.24	108.20
3	0	849	U	O4'-C1'-N1	7.55	114.24	108.20
3	0	403	G	C5-C6-O6	-7.55	124.07	128.60
3	0	2183	C	O4'-C1'-N1	7.54	114.24	108.20
3	0	355	G	C5-C6-O6	-7.54	124.07	128.60
3	0	2298	U	O4'-C1'-N1	7.54	114.23	108.20
3	0	153	C	O4'-C1'-N1	7.54	114.23	108.20
3	0	944	G	C5-C6-O6	-7.54	124.08	128.60
3	0	1080	G	C5-C6-O6	-7.54	124.08	128.60
3	0	421	U	O4'-C1'-N1	7.54	114.23	108.20
3	0	1509	G	C5-C6-O6	-7.54	124.08	128.60
3	0	298	C	O4'-C1'-N1	7.53	114.23	108.20
3	0	1584	G	C5-C6-O6	-7.53	124.08	128.60
3	0	328	U	O4'-C1'-N1	7.53	114.22	108.20
3	0	2294	G	C5-C6-O6	-7.53	124.08	128.60
3	0	2307	C	O4'-C1'-N1	7.53	114.22	108.20
3	0	551	U	O4'-C1'-N1	7.53	114.22	108.20
3	0	1293	G	C5-C6-O6	-7.53	124.08	128.60
3	0	2215	U	O4'-C1'-N1	7.52	114.22	108.20
3	0	1648	U	O4'-C1'-N1	7.52	114.22	108.20
3	0	1955	G	C5-C6-O6	-7.52	124.09	128.60
3	0	1310	A	C4-C5-C6	7.52	120.76	117.00
3	0	927	U	O4'-C1'-N1	7.52	114.22	108.20
3	0	2137	U	O4'-C1'-N1	7.52	114.22	108.20
3	0	2159	C	O4'-C1'-N1	7.52	114.21	108.20
3	0	824	G	C5-C6-O6	-7.51	124.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	997	G	C5-C6-O6	-7.51	124.09	128.60
3	0	375	C	O4'-C1'-N1	7.51	114.21	108.20
3	0	1332	A	C4-C5-C6	7.51	120.75	117.00
3	0	1408	U	O4'-C1'-N1	7.51	114.21	108.20
3	0	2046	U	O4'-C1'-N1	7.51	114.21	108.20
3	0	742	A	C5-C6-N6	-7.51	117.69	123.70
3	0	513	G	C5-C6-O6	-7.51	124.09	128.60
3	0	590	C	O4'-C1'-N1	7.51	114.21	108.20
3	0	166	C	O4'-C1'-N1	7.51	114.20	108.20
3	0	515	C	O4'-C1'-N1	7.50	114.20	108.20
3	0	758	U	O4'-C1'-N1	7.50	114.20	108.20
3	0	1561	C	O4'-C1'-N1	7.50	114.20	108.20
3	0	25	C	O4'-C1'-N1	7.50	114.20	108.20
3	0	963	G	C5-C6-O6	-7.50	124.10	128.60
3	0	2033	U	O4'-C1'-N1	7.50	114.20	108.20
3	0	2087	U	O4'-C1'-N1	7.50	114.20	108.20
3	0	1234	C	O4'-C1'-N1	7.50	114.20	108.20
3	0	2157	C	O4'-C1'-N1	7.50	114.20	108.20
3	0	791	G	C5-C6-O6	-7.50	124.10	128.60
3	0	1608	U	O4'-C1'-N1	7.50	114.20	108.20
1	f	194	PHE	CA-C-N	-7.50	100.71	117.20
3	0	2315	G	C5-C6-O6	-7.49	124.11	128.60
2	1	28	G	C5-C6-O6	-7.49	124.11	128.60
3	0	170	C	O4'-C1'-N1	7.49	114.19	108.20
3	0	1193	C	N3-C4-N4	7.49	123.24	118.00
3	0	1953	G	N1-C6-O6	7.49	124.39	119.90
3	0	452	C	O4'-C1'-N1	7.48	114.19	108.20
3	0	903	G	C5-C6-O6	-7.48	124.11	128.60
3	0	2146	G	C5-C6-O6	-7.48	124.11	128.60
3	0	844	G	C5-C6-O6	-7.48	124.11	128.60
3	0	982	G	C5-C6-O6	-7.48	124.11	128.60
3	0	998	C	O4'-C1'-N1	7.48	114.19	108.20
3	0	1807	C	O4'-C1'-N1	7.48	114.18	108.20
3	0	1195	G	O4'-C1'-N9	7.48	114.18	108.20
3	0	353	C	O4'-C1'-N1	7.48	114.18	108.20
3	0	1204	G	C5-C6-O6	-7.48	124.11	128.60
3	0	1531	A	OP2-P-O3'	-7.48	88.75	105.20
3	0	436	G	C5-C6-O6	-7.47	124.12	128.60
3	0	699	C	O4'-C1'-N1	7.47	114.17	108.20
3	0	802	U	O4'-C1'-N1	7.47	114.17	108.20
3	0	2085	A	C5-C6-N6	-7.46	117.73	123.70
10	u	35	LYS	N-CA-C	7.46	131.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	335	G	C5-C6-O6	-7.46	124.12	128.60
3	0	617	U	O4'-C1'-N1	7.46	114.17	108.20
3	0	2079	G	C5-C6-O6	-7.46	124.12	128.60
3	0	469	G	C5-C6-O6	-7.46	124.12	128.60
3	0	1460	A	O4'-C1'-N9	7.46	114.17	108.20
3	0	18	C	O4'-C1'-N1	7.46	114.17	108.20
3	0	1290	C	O4'-C1'-N1	7.46	114.17	108.20
3	0	2179	C	O4'-C1'-N1	7.46	114.17	108.20
3	0	1336	U	O4'-C1'-N1	7.46	114.16	108.20
3	0	1674	G	N1-C6-O6	7.45	124.37	119.90
3	0	48	G	C5-C6-O6	-7.45	124.13	128.60
3	0	1342	G	C5-C6-O6	-7.45	124.13	128.60
3	0	1075	C	O4'-C1'-N1	7.45	114.16	108.20
3	0	1861	G	C5-C6-O6	-7.45	124.13	128.60
3	0	2132	G	C5-C6-O6	-7.44	124.13	128.60
3	0	2200	G	C5-C6-O6	-7.44	124.14	128.60
3	0	350	C	O4'-C1'-N1	7.44	114.15	108.20
3	0	413	G	C5-C6-O6	-7.44	124.14	128.60
3	0	1659	U	O4'-C1'-N1	7.44	114.15	108.20
3	0	1994	G	N1-C6-O6	7.44	124.36	119.90
3	0	2029	C	O4'-C1'-N1	7.44	114.15	108.20
3	0	1773	A	C4-C5-C6	7.43	120.72	117.00
3	0	2078	G	C5-C6-O6	-7.43	124.14	128.60
3	0	1325	G	C5-C6-O6	-7.43	124.14	128.60
3	0	1541	C	O4'-C1'-N1	7.43	114.14	108.20
3	0	87	C	O4'-C1'-N1	7.43	114.14	108.20
3	0	140	C	O4'-C1'-N1	7.43	114.14	108.20
3	0	1208	G	C5-C6-O6	-7.43	124.14	128.60
3	0	2187	G	C5-C6-O6	-7.43	124.14	128.60
3	0	2290	G	C5-C6-O6	-7.43	124.14	128.60
3	0	1898	U	O4'-C1'-N1	7.43	114.14	108.20
3	0	15	U	O4'-C1'-N1	7.43	114.14	108.20
3	0	208	G	C5-C6-O6	-7.43	124.14	128.60
3	0	1494	U	O4'-C1'-N1	7.43	114.14	108.20
3	0	2261	U	O4'-C1'-N1	7.43	114.14	108.20
3	0	1288	U	O4'-C1'-N1	7.42	114.14	108.20
3	0	2080	G	C5-C6-O6	-7.42	124.15	128.60
3	0	947	U	O4'-C1'-N1	7.42	114.14	108.20
3	0	1211	G	C5-C6-O6	-7.42	124.15	128.60
3	0	1950	U	O4'-C1'-N1	7.42	114.14	108.20
3	0	220	G	C5-C6-O6	-7.42	124.15	128.60
3	0	1879	C	O4'-C1'-N1	7.42	114.14	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1974	G	C5-C6-O6	-7.42	124.15	128.60
3	0	1329	U	O4'-C1'-N1	7.42	114.13	108.20
3	0	358	C	O4'-C1'-N1	7.41	114.13	108.20
3	0	643	C	O4'-C1'-N1	7.41	114.13	108.20
3	0	1302	C	O4'-C1'-N1	7.41	114.13	108.20
3	0	1357	C	O4'-C1'-N1	7.41	114.13	108.20
3	0	742	A	C4-C5-C6	7.41	120.71	117.00
49	I	211	TYR	CB-CG-CD1	-7.41	116.55	121.00
3	0	1710	G	C5-C6-O6	-7.41	124.15	128.60
3	0	738	G	C5-C6-O6	-7.41	124.16	128.60
3	0	1072	U	O4'-C1'-N1	7.41	114.13	108.20
3	0	63	G	C5-C6-O6	-7.40	124.16	128.60
3	0	1948	G	C5-C6-O6	-7.40	124.16	128.60
3	0	2107	C	O4'-C1'-N1	7.40	114.12	108.20
10	u	35	LYS	CB-CA-C	-7.39	95.61	110.40
3	0	518	C	O4'-C1'-N1	7.39	114.11	108.20
3	0	207	G	C5-C6-O6	-7.39	124.17	128.60
3	0	1723	U	O4'-C1'-N1	7.39	114.11	108.20
1	f	1148	ASP	O-C-N	7.39	134.52	122.70
3	0	205	G	C5-C6-O6	-7.39	124.17	128.60
1	f	240	PHE	O-C-N	7.38	134.51	122.70
3	0	1410	G	C5-C6-O6	-7.38	124.17	128.60
3	0	428	C	O4'-C1'-N1	7.38	114.11	108.20
3	0	1594	C	O4'-C1'-N1	7.38	114.11	108.20
3	0	41	G	C5-C6-O6	-7.38	124.17	128.60
3	0	911	U	O4'-C1'-N1	7.38	114.10	108.20
3	0	930	G	C5-C6-O6	-7.38	124.17	128.60
3	0	2155	G	C5-C6-O6	-7.37	124.18	128.60
3	0	755	U	O4'-C1'-N1	7.37	114.10	108.20
3	0	2195	U	O4'-C1'-N1	7.37	114.10	108.20
3	0	818	U	O4'-C1'-N1	7.37	114.09	108.20
3	0	935	A	O4'-C1'-N9	7.37	114.09	108.20
3	0	222	U	O4'-C1'-N1	7.37	114.09	108.20
3	0	465	G	C5-C6-O6	-7.37	124.18	128.60
3	0	1308	U	O4'-C1'-N1	7.37	114.09	108.20
3	0	378	U	O4'-C1'-N1	7.36	114.09	108.20
2	1	30	G	C5-C6-O6	-7.36	124.18	128.60
3	0	2076	U	O4'-C1'-N1	7.36	114.09	108.20
3	0	2086	G	C5-C6-O6	-7.36	124.18	128.60
3	0	2206	U	O4'-C1'-N1	7.36	114.09	108.20
3	0	456	C	O4'-C1'-N1	7.36	114.09	108.20
3	0	540	U	O4'-C1'-N1	7.36	114.09	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	804	U	O4'-C1'-N1	7.36	114.09	108.20
3	0	1766	U	O4'-C1'-N1	7.36	114.09	108.20
3	0	1446	U	O4'-C1'-N1	7.36	114.08	108.20
3	0	1581	G	N1-C6-O6	7.36	124.31	119.90
3	0	1435	C	O4'-C1'-N1	7.35	114.08	108.20
3	0	1396	U	O4'-C1'-N1	7.35	114.08	108.20
3	0	473	G	C5-C6-O6	-7.35	124.19	128.60
3	0	1230	G	C5-C6-O6	-7.35	124.19	128.60
3	0	2105	C	O4'-C1'-N1	7.35	114.08	108.20
3	0	188	G	C5-C6-O6	-7.35	124.19	128.60
3	0	2002	G	C5-C6-O6	-7.35	124.19	128.60
3	0	1712	U	O4'-C1'-N1	7.35	114.08	108.20
3	0	344	G	O4'-C1'-N9	7.34	114.08	108.20
3	0	1444	C	O4'-C1'-N1	7.34	114.08	108.20
3	0	1519	G	N1-C6-O6	7.34	124.31	119.90
3	0	1188	G	C5-C6-O6	-7.34	124.19	128.60
1	f	1633	HIS	N-CA-CB	-7.34	97.39	110.60
3	0	644	C	O4'-C1'-N1	7.34	114.07	108.20
3	0	1296	U	O4'-C1'-N1	7.34	114.07	108.20
3	0	1316	C	O4'-C1'-N1	7.34	114.07	108.20
3	0	1493	G	C5-C6-O6	-7.34	124.20	128.60
3	0	1699	G	C5-C6-O6	-7.34	124.20	128.60
3	0	1779	U	O4'-C1'-N1	7.34	114.07	108.20
3	0	114	C	O4'-C1'-N1	7.33	114.07	108.20
3	0	135	C	O4'-C1'-N1	7.33	114.07	108.20
1	f	289	ASP	C-N-CA	7.33	140.03	121.70
3	0	239	C	O4'-C1'-N1	7.33	114.07	108.20
3	0	534	C	O4'-C1'-N1	7.33	114.06	108.20
3	0	2306	C	O4'-C1'-N1	7.33	114.06	108.20
3	0	429	C	O4'-C1'-N1	7.33	114.06	108.20
3	0	697	G	C5-C6-O6	-7.33	124.20	128.60
3	0	1320	G	C5-C6-O6	-7.33	124.20	128.60
3	0	131	C	O4'-C1'-N1	7.33	114.06	108.20
3	0	670	G	C5-C6-O6	-7.32	124.21	128.60
3	0	1229	U	O4'-C1'-N1	7.32	114.06	108.20
3	0	2120	C	N3-C4-N4	7.32	123.12	118.00
3	0	276	G	C5-C6-O6	-7.31	124.21	128.60
3	0	1485	U	O4'-C1'-N1	7.31	114.05	108.20
3	0	49	C	O4'-C1'-N1	7.31	114.05	108.20
3	0	2247	U	O4'-C1'-N1	7.31	114.05	108.20
3	0	2257	U	O4'-C1'-N1	7.31	114.05	108.20
1	f	258	GLU	C-N-CA	-7.31	103.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	303	ASN	CA-C-O	7.31	135.45	120.10
3	0	408	C	O4'-C1'-N1	7.31	114.05	108.20
3	0	622	G	C5-C6-O6	-7.31	124.22	128.60
3	0	1479	U	O4'-C1'-N1	7.31	114.05	108.20
3	0	956	U	O4'-C1'-N1	7.30	114.04	108.20
3	0	2310	C	O4'-C1'-N1	7.30	114.04	108.20
3	0	119	G	C5-C6-O6	-7.30	124.22	128.60
3	0	524	G	C5-C6-O6	-7.30	124.22	128.60
3	0	1502	C	C2-N1-C1'	7.30	126.83	118.80
3	0	2208	C	O4'-C1'-N1	7.30	114.04	108.20
39	E	279	TYR	CB-CG-CD1	7.30	125.38	121.00
3	0	776	G	C5-C6-O6	-7.30	124.22	128.60
3	0	874	C	O4'-C1'-N1	7.30	114.04	108.20
3	0	1352	U	O4'-C1'-N1	7.30	114.04	108.20
3	0	2049	G	C5-C6-O6	-7.29	124.22	128.60
3	0	45	U	O4'-C1'-N1	7.29	114.03	108.20
3	0	50	C	O4'-C1'-N1	7.29	114.03	108.20
3	0	2143	U	O4'-C1'-N1	7.29	114.03	108.20
3	0	881	G	C5-C6-O6	-7.29	124.23	128.60
3	0	1470	C	O4'-C1'-N1	7.29	114.03	108.20
3	0	1518	C	O4'-C1'-N1	7.29	114.03	108.20
1	f	1670	CYS	CA-C-N	7.28	133.22	117.20
3	0	603	G	C5-C6-O6	-7.28	124.23	128.60
3	0	482	C	O4'-C1'-N1	7.28	114.02	108.20
3	0	2188	U	O4'-C1'-N1	7.28	114.03	108.20
1	f	301	GLU	O-C-N	7.28	134.35	122.70
3	0	1651	G	C5-C6-O6	-7.28	124.23	128.60
1	f	236	SER	C-N-CA	7.27	139.88	121.70
3	0	169	G	C5-C6-O6	-7.27	124.24	128.60
3	0	546	U	O4'-C1'-N1	7.27	114.02	108.20
3	0	2066	G	O4'-C1'-N9	7.27	114.02	108.20
3	0	833	A	C5-C6-N6	-7.27	117.88	123.70
3	0	1349	U	O4'-C1'-N1	7.27	114.02	108.20
3	0	1407	G	C5-C6-O6	-7.27	124.24	128.60
3	0	954	G	C5-C6-O6	-7.27	124.24	128.60
3	0	856	U	O4'-C1'-N1	7.26	114.01	108.20
3	0	1767	G	C5-C6-O6	-7.26	124.24	128.60
3	0	2065	C	O4'-C1'-N1	7.26	114.01	108.20
3	0	841	C	O4'-C1'-N1	7.26	114.01	108.20
3	0	1448	U	O4'-C1'-N1	7.26	114.01	108.20
3	0	2287	C	O4'-C1'-N1	7.26	114.01	108.20
3	0	1437	C	O4'-C1'-N1	7.26	114.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	527	A	O4'-C1'-N9	7.26	114.01	108.20
1	f	1038	GLY	C-N-CA	7.25	139.83	121.70
3	0	1833	G	O4'-C1'-N9	7.25	114.00	108.20
3	0	970	G	C5-C6-O6	-7.25	124.25	128.60
3	0	1627	G	C5-C6-O6	-7.25	124.25	128.60
3	0	1792	U	O4'-C1'-N1	7.25	114.00	108.20
3	0	266	U	O4'-C1'-N1	7.25	114.00	108.20
2	1	8	U	O4'-C1'-N1	7.25	114.00	108.20
3	0	2071	C	O4'-C1'-N1	7.25	114.00	108.20
3	0	2133	C	O4'-C1'-N1	7.25	114.00	108.20
3	0	2151	U	O4'-C1'-N1	7.25	114.00	108.20
3	0	171	U	O4'-C1'-N1	7.24	114.00	108.20
3	0	313	G	C5-C6-O6	-7.24	124.25	128.60
3	0	338	U	O4'-C1'-N1	7.24	113.99	108.20
3	0	1422	U	O4'-C1'-N1	7.24	113.99	108.20
3	0	1537	U	O4'-C1'-N1	7.24	113.99	108.20
3	0	91	U	O4'-C1'-N1	7.23	113.99	108.20
2	1	49	U	O4'-C1'-N1	7.23	113.98	108.20
3	0	1886	C	O4'-C1'-N1	7.23	113.98	108.20
3	0	1526	U	O4'-C1'-N1	7.23	113.98	108.20
2	1	35	U	O4'-C1'-N1	7.23	113.98	108.20
3	0	101	C	O4'-C1'-N1	7.23	113.98	108.20
3	0	468	G	C5-C6-O6	-7.23	124.26	128.60
3	0	282	C	O4'-C1'-N1	7.22	113.98	108.20
3	0	978	U	C2-N1-C1'	7.22	126.37	117.70
3	0	583	C	O4'-C1'-N1	7.22	113.98	108.20
3	0	615	G	C5-C6-O6	-7.22	124.27	128.60
3	0	58	C	O4'-C1'-N1	7.22	113.97	108.20
3	0	929	U	O4'-C1'-N1	7.22	113.97	108.20
3	0	2024	C	O4'-C1'-N1	7.21	113.97	108.20
3	0	183	C	O4'-C1'-N1	7.21	113.97	108.20
3	0	1982	G	C5-C6-O6	-7.21	124.27	128.60
3	0	1322	G	C5-C6-O6	-7.21	124.27	128.60
3	0	1568	G	C5-C6-O6	-7.21	124.27	128.60
3	0	1644	A	C5-C6-N6	-7.21	117.94	123.70
3	0	1705	U	O4'-C1'-N1	7.21	113.96	108.20
3	0	459	U	O4'-C1'-N1	7.20	113.96	108.20
3	0	1418	U	O4'-C1'-N1	7.20	113.96	108.20
3	0	415	U	O4'-C1'-N1	7.20	113.96	108.20
3	0	1546	U	O4'-C1'-N1	7.20	113.96	108.20
2	1	10	G	C5-C6-O6	-7.20	124.28	128.60
3	0	212	G	C5-C6-O6	-7.20	124.28	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	265	C	O4'-C1'-N1	7.20	113.96	108.20
3	0	611	G	C5-C6-O6	-7.20	124.28	128.60
3	0	2313	C	O4'-C1'-N1	7.20	113.96	108.20
3	0	829	C	O4'-C1'-N1	7.20	113.96	108.20
3	0	331	U	O4'-C1'-N1	7.19	113.95	108.20
3	0	543	U	O4'-C1'-N1	7.19	113.95	108.20
3	0	1334	G	C5-C6-O6	-7.19	124.29	128.60
3	0	93	G	C5-C6-O6	-7.19	124.29	128.60
3	0	1911	C	C2-N1-C1'	7.19	126.70	118.80
3	0	2255	U	O4'-C1'-N1	7.18	113.95	108.20
3	0	707	C	C2-N1-C1'	7.18	126.70	118.80
3	0	1734	C	O4'-C1'-N1	7.18	113.94	108.20
3	0	2000	G	C5-C6-O6	-7.18	124.29	128.60
3	0	2092	C	O4'-C1'-N1	7.18	113.94	108.20
3	0	1928	U	O4'-C1'-N1	7.18	113.94	108.20
3	0	1356	C	O4'-C1'-N1	7.17	113.94	108.20
3	0	1629	C	O4'-C1'-N1	7.17	113.94	108.20
3	0	1762	U	O4'-C1'-N1	7.17	113.94	108.20
3	0	800	C	O4'-C1'-N1	7.17	113.94	108.20
3	0	832	G	C5-C6-O6	-7.17	124.30	128.60
3	0	1775	U	O4'-C1'-N1	7.17	113.94	108.20
3	0	2175	C	O4'-C1'-N1	7.17	113.94	108.20
3	0	642	U	O4'-C1'-N1	7.17	113.94	108.20
3	0	1582	G	C5-C6-O6	-7.17	124.30	128.60
3	0	753	U	O4'-C1'-N1	7.16	113.93	108.20
3	0	1619	G	C5-C6-O6	-7.16	124.31	128.60
3	0	790	G	C5-C6-O6	-7.15	124.31	128.60
3	0	1567	G	C5-C6-O6	-7.15	124.31	128.60
1	f	1149	TYR	N-CA-C	-7.15	91.69	111.00
3	0	981	G	C5-C6-O6	-7.15	124.31	128.60
3	0	1432	C	O4'-C1'-N1	7.15	113.92	108.20
3	0	908	G	C5-C6-O6	-7.15	124.31	128.60
3	0	407	G	C5-C6-O6	-7.14	124.31	128.60
3	0	733	G	C5-C6-O6	-7.14	124.31	128.60
3	0	1248	U	O4'-C1'-N1	7.14	113.92	108.20
3	0	346	C	N3-C4-N4	7.14	123.00	118.00
3	0	162	A	C4-C5-C6	7.14	120.57	117.00
3	0	552	G	C5-C6-O6	-7.14	124.32	128.60
3	0	1206	G	C5-C6-O6	-7.14	124.32	128.60
3	0	1857	G	C5-C6-O6	-7.14	124.32	128.60
3	0	396	C	O4'-C1'-N1	7.13	113.91	108.20
3	0	1824	U	O4'-C1'-N1	7.13	113.91	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	301	GLU	CA-C-O	-7.13	105.12	120.10
3	0	1653	U	O4'-C1'-N1	7.13	113.91	108.20
3	0	962	A	C5-C6-N6	-7.13	118.00	123.70
3	0	27	U	O4'-C1'-N1	7.13	113.90	108.20
3	0	2082	C	O4'-C1'-N1	7.13	113.90	108.20
3	0	368	G	O4'-C1'-N9	7.13	113.90	108.20
3	0	144	A	C5-C6-N6	-7.12	118.00	123.70
3	0	1242	G	C5-C6-O6	-7.12	124.33	128.60
3	0	714	G	P-O5'-C5'	7.12	132.29	120.90
3	0	1219	G	C5-C6-O6	-7.12	124.33	128.60
3	0	1652	G	C5-C6-O6	-7.12	124.33	128.60
3	0	451	G	C5-C6-O6	-7.12	124.33	128.60
3	0	1386	G	C5-C6-O6	-7.12	124.33	128.60
3	0	1490	U	O4'-C1'-N1	7.12	113.89	108.20
3	0	1993	U	O4'-C1'-N1	7.12	113.89	108.20
3	0	2117	U	O4'-C1'-N1	7.12	113.89	108.20
3	0	943	G	C5-C6-O6	-7.12	124.33	128.60
3	0	1899	C	O4'-C1'-N1	7.11	113.89	108.20
1	f	304	PRO	N-CA-C	7.11	130.59	112.10
3	0	1003	U	O4'-C1'-N1	7.11	113.89	108.20
3	0	693	G	P-O3'-C3'	7.11	128.23	119.70
2	1	18	G	C5-C6-O6	-7.11	124.34	128.60
3	0	1232	U	O4'-C1'-N1	7.11	113.89	108.20
3	0	2201	U	O4'-C1'-N1	7.11	113.89	108.20
3	0	616	G	C5-C6-O6	-7.10	124.34	128.60
3	0	652	U	O4'-C1'-N1	7.10	113.88	108.20
3	0	2237	U	O4'-C1'-N1	7.10	113.88	108.20
3	0	1434	U	O4'-C1'-N1	7.10	113.88	108.20
3	0	1492	C	O4'-C1'-N1	7.10	113.88	108.20
3	0	1831	U	O4'-C1'-N1	7.10	113.88	108.20
39	E	83	TYR	CB-CG-CD2	-7.10	116.74	121.00
2	1	50	U	O4'-C1'-N1	7.10	113.88	108.20
3	0	873	C	O4'-C1'-N1	7.10	113.88	108.20
3	0	2069	G	C5-C6-O6	-7.10	124.34	128.60
3	0	150	U	O4'-C1'-N1	7.10	113.88	108.20
3	0	857	G	C5-C6-O6	-7.10	124.34	128.60
3	0	2318	U	O4'-C1'-N1	7.10	113.88	108.20
3	0	252	G	C5-C6-O6	-7.10	124.34	128.60
3	0	175	A	C5-C6-N6	-7.09	118.03	123.70
3	0	109	G	C5-C6-O6	-7.09	124.35	128.60
3	0	433	G	C5-C6-O6	-7.09	124.35	128.60
3	0	626	C	O4'-C1'-N1	7.09	113.87	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1489	C	O4'-C1'-N1	7.09	113.87	108.20
3	0	2083	C	O4'-C1'-N1	7.09	113.87	108.20
3	0	1361	C	O4'-C1'-N1	7.08	113.87	108.20
3	0	312	C	O4'-C1'-N1	7.08	113.87	108.20
3	0	81	A	O4'-C1'-N9	7.08	113.86	108.20
3	0	138	C	O4'-C1'-N1	7.08	113.87	108.20
3	0	323	U	O4'-C1'-N1	7.08	113.87	108.20
3	0	345	A	O4'-C1'-N9	7.08	113.86	108.20
3	0	1217	G	C5-C6-O6	-7.08	124.35	128.60
3	0	1231	G	C5-C6-O6	-7.08	124.35	128.60
3	0	113	U	O4'-C1'-N1	7.08	113.86	108.20
3	0	1872	G	C5-C6-O6	-7.08	124.35	128.60
3	0	683	U	O4'-C1'-N1	7.08	113.86	108.20
3	0	2269	A	C4-C5-C6	7.07	120.53	117.00
3	0	243	U	O4'-C1'-N1	7.07	113.85	108.20
3	0	1973	G	C5-C6-O6	-7.07	124.36	128.60
3	0	2259	U	O4'-C1'-N1	7.07	113.85	108.20
1	f	199	PHE	N-CA-CB	-7.06	97.89	110.60
2	1	66	G	C5-C6-O6	-7.06	124.36	128.60
3	0	1810	G	C5-C6-O6	-7.06	124.36	128.60
3	0	2055	C	O4'-C1'-N1	7.06	113.85	108.20
3	0	476	G	C5-C6-O6	-7.06	124.36	128.60
3	0	591	G	C5-C6-O6	-7.06	124.36	128.60
3	0	310	U	O4'-C1'-N1	7.06	113.85	108.20
3	0	2158	C	O4'-C1'-N1	7.06	113.85	108.20
3	0	1411	U	O4'-C1'-N1	7.06	113.84	108.20
3	0	1363	G	C5-C6-O6	-7.05	124.37	128.60
3	0	2312	G	C5-C6-O6	-7.05	124.37	128.60
3	0	264	C	N3-C4-N4	7.05	122.94	118.00
3	0	322	G	C5-C6-O6	-7.05	124.37	128.60
3	0	1672	G	C5-C6-O6	-7.05	124.37	128.60
3	0	710	A	C4-C5-C6	7.05	120.52	117.00
3	0	739	G	N1-C6-O6	7.05	124.13	119.90
3	0	1078	U	O4'-C1'-N1	7.05	113.84	108.20
3	0	1300	U	O4'-C1'-N1	7.05	113.84	108.20
3	0	1530	C	O4'-C1'-N1	7.05	113.84	108.20
3	0	574	U	O4'-C1'-N1	7.05	113.84	108.20
3	0	2081	A	P-O3'-C3'	7.05	128.16	119.70
3	0	1963	U	O4'-C1'-N1	7.04	113.84	108.20
1	f	1106	TYR	CB-CG-CD2	-7.04	116.77	121.00
3	0	1884	U	O4'-C1'-N1	7.04	113.83	108.20
3	0	548	C	N3-C4-N4	7.04	122.93	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1815	C	O4'-C1'-N1	7.04	113.83	108.20
3	0	2258	U	O4'-C1'-N1	7.04	113.83	108.20
3	0	20	G	C5-C6-O6	-7.04	124.38	128.60
3	0	83	U	O4'-C1'-N1	7.04	113.83	108.20
3	0	816	C	O4'-C1'-N1	7.04	113.83	108.20
3	0	1980	A	C4-C5-C6	7.04	120.52	117.00
3	0	2186	U	O4'-C1'-N1	7.04	113.83	108.20
3	0	353	C	N3-C4-N4	7.04	122.92	118.00
3	0	2190	U	O4'-C1'-N1	7.04	113.83	108.20
3	0	564	G	C5-C6-O6	-7.03	124.38	128.60
3	0	850	U	O4'-C1'-N1	7.03	113.83	108.20
3	0	938	G	N1-C6-O6	7.03	124.12	119.90
3	0	324	U	O4'-C1'-N1	7.03	113.83	108.20
3	0	511	G	C5-C6-O6	-7.03	124.38	128.60
3	0	627	C	O4'-C1'-N1	7.03	113.83	108.20
3	0	821	C	O4'-C1'-N1	7.03	113.82	108.20
3	0	1384	U	O4'-C1'-N1	7.03	113.82	108.20
3	0	1914	U	O4'-C1'-N1	7.03	113.82	108.20
3	0	1920	G	N1-C6-O6	7.03	124.12	119.90
3	0	923	A	C4-C5-C6	7.03	120.51	117.00
3	0	1421	U	O4'-C1'-N1	7.03	113.82	108.20
3	0	2020	U	O4'-C1'-N1	7.03	113.82	108.20
3	0	1741	G	C5-C6-O6	-7.02	124.39	128.60
3	0	2066	G	C5-C6-O6	-7.02	124.39	128.60
5	s	250	TYR	CB-CG-CD2	-7.02	116.79	121.00
3	0	656	U	O4'-C1'-N1	7.02	113.82	108.20
3	0	906	U	O4'-C1'-N1	7.02	113.82	108.20
2	1	39	C	O4'-C1'-N1	7.02	113.81	108.20
3	0	422	U	O4'-C1'-N1	7.02	113.81	108.20
3	0	827	U	O4'-C1'-N1	7.01	113.81	108.20
3	0	900	A	O4'-C1'-N9	7.01	113.81	108.20
3	0	1184	C	O4'-C1'-N1	7.01	113.81	108.20
3	0	5	U	O4'-C1'-N1	7.01	113.81	108.20
3	0	973	G	C5-C6-O6	-7.01	124.39	128.60
3	0	1670	C	O4'-C1'-N1	7.01	113.81	108.20
3	0	420	G	C5-C6-O6	-7.01	124.39	128.60
3	0	1789	C	O4'-C1'-N1	7.01	113.81	108.20
3	0	2248	U	O4'-C1'-N1	7.01	113.81	108.20
3	0	187	C	O4'-C1'-N1	7.01	113.81	108.20
3	0	1268	G	C5-C6-O6	-7.01	124.40	128.60
3	0	1530	C	OP1-P-O3'	7.01	120.61	105.20
49	I	211	TYR	CB-CG-CD2	7.00	125.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	118	C	O4'-C1'-N1	7.00	113.80	108.20
3	0	439	G	C5-C6-O6	-7.00	124.40	128.60
3	0	741	G	C5-C6-O6	-7.00	124.40	128.60
3	0	1588	U	O4'-C1'-N1	7.00	113.80	108.20
3	0	557	U	O4'-C1'-N1	7.00	113.80	108.20
3	0	1241	G	C5-C6-O6	-7.00	124.40	128.60
2	1	60	C	O4'-C1'-N1	7.00	113.80	108.20
3	0	1327	G	C5-C6-O6	-7.00	124.40	128.60
3	0	1764	G	C5-C6-O6	-7.00	124.40	128.60
3	0	1913	U	O4'-C1'-N1	7.00	113.80	108.20
3	0	1250	C	O4'-C1'-N1	7.00	113.80	108.20
2	1	14	A	C4-C5-C6	6.99	120.50	117.00
3	0	1592	U	O4'-C1'-N1	6.99	113.80	108.20
3	0	1289	U	O4'-C1'-N1	6.99	113.79	108.20
3	0	382	G	C5-C6-O6	-6.99	124.41	128.60
3	0	723	C	N3-C4-N4	6.99	122.89	118.00
3	0	1283	C	O4'-C1'-N1	6.99	113.79	108.20
3	0	855	G	C5-C6-O6	-6.99	124.41	128.60
3	0	1917	U	O4'-C1'-N1	6.99	113.79	108.20
3	0	384	G	C5-C6-O6	-6.99	124.41	128.60
3	0	559	U	O4'-C1'-N1	6.99	113.79	108.20
3	0	2184	G	C5-C6-O6	-6.98	124.41	128.60
3	0	1512	C	O4'-C1'-N1	6.98	113.79	108.20
3	0	270	C	O4'-C1'-N1	6.98	113.78	108.20
3	0	1801	G	C5-C6-O6	-6.98	124.41	128.60
3	0	1825	U	O4'-C1'-N1	6.98	113.78	108.20
3	0	339	C	O4'-C1'-N1	6.98	113.78	108.20
3	0	1605	A	C4-C5-C6	6.98	120.49	117.00
3	0	2232	U	O4'-C1'-N1	6.98	113.78	108.20
3	0	1530	C	O3'-P-O5'	6.97	117.25	104.00
3	0	474	C	O4'-C1'-N1	6.97	113.78	108.20
3	0	1258	G	C5-C6-O6	-6.97	124.42	128.60
1	f	1265	HIS	O-C-N	-6.97	107.86	121.10
1	f	1702	LEU	C-N-CA	-6.97	107.67	122.30
3	0	97	A	C4-C5-C6	6.97	120.48	117.00
3	0	1459	U	O4'-C1'-N1	6.97	113.78	108.20
3	0	748	G	C5-C6-O6	-6.97	124.42	128.60
3	0	937	C	O4'-C1'-N1	6.97	113.77	108.20
3	0	1442	C	N3-C4-N4	6.97	122.88	118.00
3	0	397	G	C5-C6-O6	-6.96	124.42	128.60
2	1	44	G	C5-C6-O6	-6.96	124.42	128.60
3	0	631	G	C5-C6-O6	-6.96	124.42	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2057	C	O4'-C1'-N1	6.96	113.77	108.20
2	1	33	C	O4'-C1'-N1	6.96	113.77	108.20
3	0	1438	G	C5-C6-O6	-6.96	124.42	128.60
3	0	803	U	O4'-C1'-N1	6.96	113.77	108.20
3	0	868	U	O4'-C1'-N1	6.96	113.77	108.20
3	0	1900	U	O4'-C1'-N1	6.96	113.77	108.20
3	0	613	C	O4'-C1'-N1	6.96	113.76	108.20
3	0	2225	G	C5-C6-O6	-6.96	124.43	128.60
3	0	1369	G	C5-C6-O6	-6.95	124.43	128.60
3	0	302	U	O4'-C1'-N1	6.95	113.76	108.20
3	0	986	U	O4'-C1'-N1	6.95	113.76	108.20
3	0	1347	C	O4'-C1'-N1	6.95	113.76	108.20
3	0	1583	G	C5-C6-O6	-6.95	124.43	128.60
3	0	292	U	O4'-C1'-N1	6.95	113.76	108.20
3	0	1487	G	C5-C6-O6	-6.95	124.43	128.60
3	0	1777	G	C5-C6-O6	-6.95	124.43	128.60
3	0	1793	C	O4'-C1'-N1	6.95	113.76	108.20
3	0	1931	G	C5-C6-O6	-6.95	124.43	128.60
3	0	2212	U	O4'-C1'-N1	6.95	113.76	108.20
1	f	198	PHE	CA-C-N	6.95	132.48	117.20
3	0	1660	U	O4'-C1'-N1	6.95	113.76	108.20
3	0	1882	U	O4'-C1'-N1	6.95	113.76	108.20
3	0	362	C	O4'-C1'-N1	6.94	113.75	108.20
3	0	1213	U	O4'-C1'-N1	6.94	113.75	108.20
3	0	628	G	C5-C6-O6	-6.94	124.44	128.60
3	0	766	C	O4'-C1'-N1	6.94	113.75	108.20
3	0	1690	G	C5-C6-O6	-6.94	124.44	128.60
3	0	1869	C	N3-C4-N4	6.94	122.86	118.00
3	0	234	U	O4'-C1'-N1	6.94	113.75	108.20
3	0	1803	G	C5-C6-O6	-6.94	124.44	128.60
3	0	1617	U	O4'-C1'-N1	6.93	113.75	108.20
3	0	1495	U	O4'-C1'-N1	6.93	113.75	108.20
3	0	1833	G	C5-C6-O6	-6.93	124.44	128.60
3	0	2022	G	C5-C6-O6	-6.93	124.44	128.60
3	0	2262	U	O4'-C1'-N1	6.93	113.75	108.20
3	0	819	G	C5-C6-O6	-6.93	124.44	128.60
3	0	1471	G	C5-C6-O6	-6.93	124.44	128.60
3	0	957	U	O4'-C1'-N1	6.93	113.74	108.20
3	0	1286	U	O4'-C1'-N1	6.93	113.74	108.20
3	0	510	U	O4'-C1'-N1	6.92	113.74	108.20
3	0	1971	C	C6-N1-C1'	-6.92	112.49	120.80
3	0	969	U	O4'-C1'-N1	6.92	113.74	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	295	ASN	N-CA-C	6.92	129.69	111.00
3	0	14	C	O4'-C1'-N1	6.92	113.74	108.20
3	0	2043	G	C5-C6-O6	-6.92	124.45	128.60
3	0	1247	A	C4-C5-C6	6.92	120.46	117.00
3	0	985	G	C5-C6-O6	-6.91	124.45	128.60
3	0	1577	U	O4'-C1'-N1	6.91	113.73	108.20
3	0	1811	C	O4'-C1'-N1	6.91	113.73	108.20
3	0	664	G	C5-C6-O6	-6.91	124.45	128.60
3	0	1226	U	O4'-C1'-N1	6.91	113.73	108.20
3	0	2124	U	O4'-C1'-N1	6.91	113.73	108.20
3	0	691	U	O4'-C1'-N1	6.91	113.73	108.20
3	0	2061	A	C5-C6-N6	-6.91	118.17	123.70
3	0	460	U	O4'-C1'-N1	6.91	113.72	108.20
3	0	1079	U	O4'-C1'-N1	6.91	113.72	108.20
3	0	1518	C	N3-C4-N4	6.91	122.83	118.00
3	0	2302	U	O4'-C1'-N1	6.91	113.72	108.20
3	0	1677	C	O4'-C1'-N1	6.90	113.72	108.20
1	f	1110	GLY	C-N-CA	6.90	136.79	122.30
3	0	1580	G	C5-C6-O6	-6.90	124.46	128.60
3	0	1936	U	O4'-C1'-N1	6.90	113.72	108.20
3	0	1631	C	O4'-C1'-N1	6.90	113.72	108.20
3	0	1771	U	O4'-C1'-N1	6.90	113.72	108.20
3	0	33	U	O4'-C1'-N1	6.90	113.72	108.20
3	0	1380	U	O4'-C1'-N1	6.89	113.72	108.20
3	0	2165	U	O4'-C1'-N1	6.89	113.71	108.20
3	0	505	A	O4'-C1'-N9	6.89	113.71	108.20
3	0	661	G	C5-C6-O6	-6.89	124.47	128.60
3	0	1406	C	N3-C4-N4	6.89	122.82	118.00
3	0	437	G	O4'-C1'-N9	6.89	113.71	108.20
3	0	669	U	O4'-C1'-N1	6.89	113.71	108.20
3	0	1616	A	C4-C5-C6	6.88	120.44	117.00
3	0	1618	U	O4'-C1'-N1	6.88	113.71	108.20
3	0	1743	G	C5-C6-O6	-6.88	124.47	128.60
3	0	418	G	C5-C6-O6	-6.88	124.47	128.60
3	0	497	C	O4'-C1'-N1	6.88	113.70	108.20
3	0	584	C	N3-C4-N4	6.88	122.81	118.00
3	0	2123	G	C5-C6-O6	-6.88	124.47	128.60
3	0	337	G	C5-C6-O6	-6.88	124.47	128.60
3	0	379	G	C5-C6-O6	-6.88	124.47	128.60
3	0	1216	G	C5-C6-O6	-6.88	124.47	128.60
3	0	2285	A	C5-C6-N6	-6.88	118.20	123.70
3	0	479	G	C5-C6-O6	-6.87	124.48	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2236	U	O4'-C1'-N1	6.87	113.69	108.20
3	0	37	U	O4'-C1'-N1	6.87	113.69	108.20
3	0	1207	G	O4'-C1'-N9	6.87	113.69	108.20
3	0	2152	U	C2-N1-C1'	6.87	125.94	117.70
3	0	685	G	C5-C6-O6	-6.86	124.48	128.60
3	0	1298	C	O4'-C1'-N1	6.86	113.69	108.20
3	0	1378	C	O4'-C1'-N1	6.86	113.69	108.20
3	0	839	C	O4'-C1'-N1	6.86	113.69	108.20
3	0	419	G	C5-C6-O6	-6.86	124.48	128.60
3	0	794	G	C5-C6-O6	-6.86	124.48	128.60
3	0	154	U	O4'-C1'-N1	6.86	113.69	108.20
3	0	286	G	C5-C6-O6	-6.86	124.48	128.60
3	0	199	G	C5-C6-O6	-6.86	124.48	128.60
3	0	657	U	O4'-C1'-N1	6.86	113.69	108.20
3	0	1665	C	O4'-C1'-N1	6.86	113.69	108.20
3	0	1772	G	C5-C6-O6	-6.86	124.48	128.60
3	0	247	U	O4'-C1'-N1	6.86	113.68	108.20
3	0	443	G	C5-C6-O6	-6.86	124.49	128.60
3	0	772	U	O4'-C1'-N1	6.86	113.68	108.20
3	0	1391	G	C5-C6-O6	-6.86	124.49	128.60
3	0	1504	G	C5-C6-O6	-6.85	124.49	128.60
3	0	216	A	O4'-C1'-N9	6.85	113.68	108.20
3	0	441	C	N3-C4-N4	6.85	122.80	118.00
1	f	303	ASN	CA-C-N	-6.85	97.93	117.10
3	0	500	A	C4-C5-C6	6.85	120.42	117.00
3	0	233	G	C5-C6-O6	-6.84	124.49	128.60
3	0	1187	G	O4'-C1'-N9	6.84	113.67	108.20
3	0	1456	G	C5-C6-O6	-6.84	124.49	128.60
3	0	2058	G	C5-C6-O6	-6.84	124.49	128.60
3	0	52	U	O4'-C1'-N1	6.84	113.67	108.20
3	0	92	G	C5-C6-O6	-6.84	124.50	128.60
3	0	630	G	C5-C6-O6	-6.84	124.50	128.60
3	0	2035	G	C5-C6-O6	-6.84	124.50	128.60
3	0	2134	U	O4'-C1'-N1	6.84	113.67	108.20
3	0	1484	U	O4'-C1'-N1	6.84	113.67	108.20
3	0	637	C	O4'-C1'-N1	6.83	113.67	108.20
3	0	1693	C	N3-C4-N4	6.83	122.78	118.00
3	0	1513	U	O4'-C1'-N1	6.83	113.67	108.20
3	0	1598	A	C5-C6-N1	-6.83	114.28	117.70
3	0	1773	A	C5-C6-N1	-6.83	114.28	117.70
3	0	508	G	O4'-C1'-N9	6.83	113.67	108.20
3	0	932	G	O4'-C1'-N9	6.83	113.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	1177	PRO	CB-CA-C	6.83	129.07	112.00
3	0	301	U	O4'-C1'-N1	6.83	113.66	108.20
3	0	662	C	O4'-C1'-N1	6.83	113.66	108.20
3	0	1488	U	O4'-C1'-N1	6.83	113.66	108.20
3	0	1695	G	C5-C6-O6	-6.83	124.50	128.60
3	0	1922	G	C5-C6-O6	-6.83	124.50	128.60
3	0	2194	A	C4-C5-C6	6.82	120.41	117.00
3	0	1620	A	C5-C6-N6	-6.82	118.24	123.70
3	0	40	A	C4-C5-C6	6.82	120.41	117.00
3	0	230	G	O4'-C1'-N9	6.82	113.66	108.20
3	0	277	U	O4'-C1'-N1	6.82	113.66	108.20
3	0	1977	G	O4'-C1'-N9	6.82	113.65	108.20
3	0	364	G	O4'-C1'-N9	6.82	113.65	108.20
3	0	1326	G	C5-C6-O6	-6.82	124.51	128.60
3	0	1916	U	O4'-C1'-N1	6.82	113.65	108.20
3	0	2019	C	O4'-C1'-N1	6.82	113.65	108.20
3	0	918	G	C5-C6-O6	-6.81	124.51	128.60
3	0	1776	U	O4'-C1'-N1	6.81	113.65	108.20
3	0	1949	G	C5-C6-O6	-6.81	124.51	128.60
3	0	949	U	O4'-C1'-N1	6.81	113.65	108.20
3	0	1702	G	O4'-C1'-N9	6.81	113.65	108.20
3	0	1339	U	O4'-C1'-N1	6.81	113.65	108.20
3	0	38	C	O4'-C1'-N1	6.81	113.65	108.20
3	0	327	U	O4'-C1'-N1	6.81	113.65	108.20
3	0	336	C	O4'-C1'-N1	6.81	113.65	108.20
3	0	1647	G	C5-C6-O6	-6.81	124.51	128.60
3	0	1720	U	O4'-C1'-N1	6.81	113.65	108.20
3	0	375	C	N3-C4-N4	6.81	122.77	118.00
3	0	909	G	C5-C6-O6	-6.81	124.52	128.60
3	0	1981	C	P-O3'-C3'	6.81	127.87	119.70
3	0	400	G	C5-C6-O6	-6.81	124.52	128.60
3	0	1697	G	C5-C6-O6	-6.81	124.52	128.60
5	s	250	TYR	CB-CG-CD1	6.81	125.08	121.00
3	0	116	G	C5-C6-O6	-6.80	124.52	128.60
3	0	1381	G	C5-C6-O6	-6.80	124.52	128.60
3	0	1682	C	O4'-C1'-N1	6.80	113.64	108.20
3	0	1	G	C5-C6-O6	-6.80	124.52	128.60
3	0	1439	U	O4'-C1'-N1	6.80	113.64	108.20
3	0	1462	U	O4'-C1'-N1	6.79	113.64	108.20
3	0	619	C	O4'-C1'-N1	6.79	113.64	108.20
3	0	808	G	C5-C6-O6	-6.79	124.52	128.60
3	0	1473	G	C5-C6-O6	-6.79	124.52	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2166	U	O4'-C1'-N1	6.79	113.64	108.20
3	0	2228	U	O4'-C1'-N1	6.79	113.63	108.20
3	0	899	G	C5-C6-O6	-6.79	124.53	128.60
3	0	2007	A	O4'-C1'-N9	6.79	113.63	108.20
3	0	722	C	N3-C4-N4	6.78	122.75	118.00
3	0	1575	U	O4'-C1'-N1	6.78	113.63	108.20
3	0	1636	A	C5-C6-N6	-6.78	118.27	123.70
3	0	2139	A	C4-C5-C6	6.78	120.39	117.00
3	0	2145	U	O4'-C1'-N1	6.78	113.63	108.20
3	0	2141	A	C5-C6-N6	-6.78	118.27	123.70
2	1	24	C	O4'-C1'-N1	6.78	113.62	108.20
3	0	1559	A	C4-C5-C6	6.78	120.39	117.00
3	0	439	G	O4'-C1'-N9	6.78	113.62	108.20
3	0	1585	G	C5-C6-O6	-6.78	124.53	128.60
3	0	1855	C	N3-C4-N4	6.78	122.74	118.00
3	0	130	G	C5-C6-O6	-6.78	124.53	128.60
3	0	274	C	N3-C4-N4	6.78	122.74	118.00
3	0	815	G	O4'-C1'-N9	6.78	113.62	108.20
3	0	1265	G	C5-C6-O6	-6.78	124.53	128.60
3	0	1468	U	O4'-C1'-N1	6.78	113.62	108.20
3	0	948	U	O4'-C1'-N1	6.77	113.62	108.20
3	0	893	G	C5-C6-O6	-6.77	124.54	128.60
3	0	1187	G	C5-C6-O6	-6.77	124.54	128.60
3	0	1593	U	O4'-C1'-N1	6.77	113.62	108.20
3	0	805	C	N3-C4-N4	6.77	122.74	118.00
3	0	930	G	O4'-C1'-N9	6.77	113.61	108.20
3	0	638	C	O4'-C1'-N1	6.76	113.61	108.20
3	0	780	C	N3-C4-N4	6.76	122.73	118.00
3	0	1549	U	O4'-C1'-N1	6.76	113.61	108.20
3	0	1641	U	O4'-C1'-N1	6.76	113.61	108.20
3	0	1883	A	C4-C5-C6	6.76	120.38	117.00
3	0	671	U	O4'-C1'-N1	6.76	113.61	108.20
43	G	164	ALA	CB-CA-C	6.76	120.24	110.10
2	1	9	G	C5-C6-O6	-6.76	124.54	128.60
3	0	341	U	O4'-C1'-N1	6.76	113.61	108.20
3	0	1483	U	O4'-C1'-N1	6.76	113.61	108.20
3	0	1760	G	C5-C6-O6	-6.76	124.54	128.60
3	0	1770	G	C5-C6-O6	-6.76	124.54	128.60
3	0	1806	C	O4'-C1'-N1	6.76	113.61	108.20
3	0	1929	G	C5-C6-O6	-6.75	124.55	128.60
3	0	2167	U	O4'-C1'-N1	6.75	113.60	108.20
3	0	2244	A	C4-C5-C6	6.75	120.38	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1524	U	O4'-C1'-N1	6.75	113.60	108.20
3	0	1880	G	C5-C6-O6	-6.75	124.55	128.60
3	0	1281	G	C5-C6-O6	-6.75	124.55	128.60
3	0	2273	A	C5-C6-N6	-6.75	118.30	123.70
3	0	711	A	C5-C6-N1	-6.74	114.33	117.70
3	0	1559	A	C5-C6-N6	-6.74	118.31	123.70
3	0	688	G	C5-C6-O6	-6.74	124.56	128.60
3	0	2054	C	O4'-C1'-N1	6.74	113.59	108.20
3	0	2086	G	O4'-C1'-N9	6.74	113.59	108.20
3	0	542	C	N3-C4-N4	6.74	122.72	118.00
3	0	890	C	O4'-C1'-N1	6.74	113.59	108.20
3	0	946	U	C6-N1-C1'	-6.74	111.77	121.20
3	0	1482	U	O4'-C1'-N1	6.74	113.59	108.20
3	0	2150	A	C4-C5-C6	6.74	120.37	117.00
3	0	826	A	C4-C5-C6	6.73	120.37	117.00
3	0	2253	G	C5-C6-O6	-6.73	124.56	128.60
3	0	1001	G	C5-C6-O6	-6.73	124.56	128.60
3	0	32	U	O4'-C1'-N1	6.73	113.58	108.20
3	0	596	A	O4'-C1'-N9	6.73	113.58	108.20
3	0	1998	G	C5-C6-O6	-6.73	124.56	128.60
3	0	1353	A	C4-C5-C6	6.73	120.36	117.00
3	0	85	U	O4'-C1'-N1	6.73	113.58	108.20
3	0	843	U	O4'-C1'-N1	6.73	113.58	108.20
3	0	1075	C	N3-C4-N4	6.73	122.71	118.00
3	0	750	C	N3-C4-N4	6.72	122.71	118.00
3	0	2131	A	C4-C5-C6	6.72	120.36	117.00
3	0	1477	A	P-O3'-C3'	6.72	127.77	119.70
3	0	1429	U	O4'-C1'-N1	6.72	113.58	108.20
3	0	1671	G	C5-C6-O6	-6.72	124.57	128.60
3	0	2281	U	O4'-C1'-N1	6.72	113.58	108.20
1	f	259	PHE	CA-C-O	-6.72	106.00	120.10
3	0	558	U	O4'-C1'-N1	6.72	113.57	108.20
3	0	582	U	O4'-C1'-N1	6.72	113.57	108.20
3	0	1486	G	C5-C6-O6	-6.72	124.57	128.60
3	0	602	G	C5-C6-O6	-6.71	124.57	128.60
3	0	692	U	O4'-C1'-N1	6.71	113.57	108.20
3	0	931	G	O4'-C1'-N9	6.71	113.57	108.20
3	0	2217	G	C5-C6-O6	-6.71	124.57	128.60
3	0	938	G	O4'-C1'-N9	6.71	113.57	108.20
3	0	1443	U	O4'-C1'-N1	6.71	113.57	108.20
3	0	2114	G	C5-C6-O6	-6.71	124.57	128.60
2	1	1	A	C5-C6-N1	-6.71	114.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	411	G	C5-C6-O6	-6.71	124.58	128.60
3	0	442	U	O4'-C1'-N1	6.71	113.57	108.20
2	1	31	C	O4'-C1'-N1	6.71	113.56	108.20
3	0	126	U	O4'-C1'-N1	6.71	113.56	108.20
3	0	424	G	C5-C6-O6	-6.71	124.58	128.60
3	0	519	G	C5-C6-O6	-6.71	124.58	128.60
3	0	924	G	C5-C6-O6	-6.71	124.58	128.60
3	0	2171	C	O4'-C1'-N1	6.71	113.56	108.20
3	0	1832	U	P-O3'-C3'	6.70	127.75	119.70
3	0	4	C	O4'-C1'-N1	6.70	113.56	108.20
3	0	1630	A	C4-C5-C6	6.70	120.35	117.00
3	0	1991	A	C5-C6-N6	-6.70	118.34	123.70
3	0	1385	U	O4'-C1'-N1	6.70	113.56	108.20
3	0	2308	U	O4'-C1'-N1	6.70	113.56	108.20
39	E	83	TYR	CB-CG-CD1	6.70	125.02	121.00
3	0	2147	C	N3-C4-N4	6.69	122.69	118.00
3	0	878	G	C5-C6-O6	-6.69	124.58	128.60
3	0	1181	A	C5-C6-N6	-6.69	118.35	123.70
3	0	2104	G	C5-C6-O6	-6.69	124.58	128.60
3	0	255	A	C4-C5-C6	6.69	120.34	117.00
3	0	1783	U	O4'-C1'-N1	6.69	113.55	108.20
10	u	35	LYS	N-CA-CB	-6.69	98.56	110.60
3	0	1609	U	O4'-C1'-N1	6.69	113.55	108.20
3	0	368	G	C5-C6-O6	-6.68	124.59	128.60
3	0	354	U	O4'-C1'-N1	6.68	113.55	108.20
3	0	1702	G	C5-C6-O6	-6.68	124.59	128.60
3	0	1612	A	C4-C5-C6	6.68	120.34	117.00
3	0	388	U	O4'-C1'-N1	6.68	113.54	108.20
3	0	209	C	O4'-C1'-N1	6.68	113.54	108.20
3	0	998	C	N3-C4-N4	6.68	122.67	118.00
3	0	1203	G	C5-C6-O6	-6.68	124.59	128.60
3	0	1645	G	C5-C6-O6	-6.68	124.59	128.60
3	0	1553	C	C6-N1-C1'	-6.67	112.79	120.80
3	0	2042	A	O4'-C1'-N9	6.67	113.54	108.20
3	0	2254	A	C4-C5-C6	6.67	120.34	117.00
3	0	2091	G	C5-C6-O6	-6.67	124.60	128.60
3	0	225	C	N3-C4-N4	6.67	122.67	118.00
3	0	1729	A	C4-C5-C6	6.67	120.33	117.00
3	0	1881	G	O4'-C1'-N9	6.67	113.54	108.20
1	f	1214	ARG	CA-C-N	-6.67	102.53	117.20
3	0	492	A	C5-C6-N6	-6.67	118.37	123.70
3	0	768	G	C5-C6-O6	-6.67	124.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2101	G	C5-C6-O6	-6.67	124.60	128.60
3	0	24	U	O4'-C1'-N1	6.67	113.53	108.20
3	0	1314	A	C5-C6-N6	-6.67	118.37	123.70
3	0	1714	G	C5-C6-O6	-6.67	124.60	128.60
3	0	127	C	O4'-C1'-N1	6.67	113.53	108.20
3	0	1441	C	O4'-C1'-N1	6.67	113.53	108.20
3	0	871	G	C5-C6-O6	-6.66	124.60	128.60
3	0	275	A	C4-C5-C6	6.66	120.33	117.00
3	0	445	G	C5-C6-O6	-6.66	124.60	128.60
3	0	2130	C	N3-C4-N4	6.66	122.66	118.00
3	0	2220	C	N3-C4-N4	6.66	122.66	118.00
3	0	1379	A	C4-C5-C6	6.66	120.33	117.00
3	0	1249	U	O4'-C1'-N1	6.66	113.53	108.20
3	0	1907	G	C5-C6-O6	-6.66	124.60	128.60
3	0	2047	G	C5-C6-O6	-6.66	124.61	128.60
3	0	446	A	C4-C5-C6	6.66	120.33	117.00
3	0	1556	G	C5-C6-O6	-6.66	124.61	128.60
3	0	1715	A	C5-C6-N6	-6.66	118.38	123.70
3	0	1946	C	N3-C4-N4	6.66	122.66	118.00
3	0	265	C	N3-C4-N4	6.65	122.66	118.00
3	0	667	G	N1-C6-O6	6.65	123.89	119.90
3	0	340	U	O4'-C1'-N1	6.65	113.52	108.20
3	0	654	U	O4'-C1'-N1	6.65	113.52	108.20
3	0	680	U	O4'-C1'-N1	6.65	113.52	108.20
3	0	1460	A	C5-C6-N6	-6.65	118.38	123.70
3	0	84	C	N3-C4-N4	6.65	122.65	118.00
3	0	1643	G	C5-C6-O6	-6.65	124.61	128.60
3	0	88	G	C5-C6-O6	-6.65	124.61	128.60
3	0	1520	G	O4'-C1'-N9	6.65	113.52	108.20
2	1	27	U	O4'-C1'-N1	6.65	113.52	108.20
3	0	298	C	N3-C4-N4	6.65	122.65	118.00
3	0	1301	U	O4'-C1'-N1	6.65	113.52	108.20
3	0	2291	G	C5-C6-O6	-6.65	124.61	128.60
3	0	687	U	O4'-C1'-N1	6.64	113.52	108.20
3	0	1739	U	O4'-C1'-N1	6.64	113.52	108.20
3	0	259	C	N3-C4-N4	6.64	122.65	118.00
3	0	309	G	C5-C6-O6	-6.64	124.61	128.60
3	0	533	C	O4'-C1'-N1	6.64	113.51	108.20
3	0	1184	C	N3-C4-N4	6.64	122.65	118.00
3	0	1428	U	O4'-C1'-N1	6.64	113.51	108.20
3	0	2017	C	N3-C4-N4	6.64	122.65	118.00
3	0	2111	G	C5-C6-O6	-6.64	124.61	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	K	141	TYR	CB-CG-CD1	-6.64	117.01	121.00
2	1	37	A	C5-C6-N6	-6.64	118.39	123.70
3	0	372	U	O4'-C1'-N1	6.64	113.51	108.20
3	0	2296	U	O4'-C1'-N1	6.64	113.51	108.20
3	0	838	G	C5-C6-O6	-6.64	124.62	128.60
3	0	867	G	C5-C6-O6	-6.64	124.62	128.60
3	0	679	U	O4'-C1'-N1	6.63	113.51	108.20
3	0	1818	G	C5-C6-O6	-6.63	124.62	128.60
3	0	1875	G	C5-C6-O6	-6.63	124.62	128.60
2	1	72	A	P-O3'-C3'	6.63	127.66	119.70
3	0	203	C	O4'-C1'-N1	6.63	113.50	108.20
3	0	2182	U	O4'-C1'-N1	6.63	113.50	108.20
3	0	1785	G	C5-C6-O6	-6.63	124.62	128.60
3	0	58	C	N3-C4-N4	6.63	122.64	118.00
3	0	820	U	O4'-C1'-N1	6.63	113.50	108.20
3	0	1344	G	C5-C6-O6	-6.63	124.62	128.60
3	0	1971	C	O4'-C1'-N1	6.63	113.50	108.20
3	0	172	A	C4-C5-C6	6.62	120.31	117.00
3	0	235	C	N3-C4-N4	6.62	122.64	118.00
3	0	1602	U	O4'-C1'-N1	6.62	113.50	108.20
3	0	366	C	O4'-C1'-N1	6.62	113.50	108.20
3	0	484	A	C4-C5-C6	6.62	120.31	117.00
3	0	1214	C	O4'-C1'-N1	6.62	113.50	108.20
3	0	2038	C	O4'-C1'-N1	6.62	113.50	108.20
3	0	321	G	O4'-C1'-N9	6.62	113.50	108.20
3	0	1901	C	O4'-C1'-N1	6.62	113.49	108.20
3	0	218	C	N3-C4-N4	6.62	122.63	118.00
3	0	2017	C	O4'-C1'-N1	6.62	113.49	108.20
3	0	592	A	C4-C5-C6	6.62	120.31	117.00
3	0	618	G	C5-C6-O6	-6.62	124.63	128.60
3	0	1688	C	N3-C4-N4	6.62	122.63	118.00
3	0	10	G	C5-C6-O6	-6.61	124.63	128.60
3	0	146	U	O4'-C1'-N1	6.61	113.49	108.20
3	0	494	U	O4'-C1'-N1	6.61	113.49	108.20
3	0	289	G	C5-C6-O6	-6.61	124.63	128.60
3	0	1532	G	C5-C6-O6	-6.61	124.63	128.60
3	0	1745	U	O4'-C1'-N1	6.61	113.49	108.20
3	0	1191	U	O4'-C1'-N1	6.61	113.49	108.20
3	0	1791	G	C5-C6-O6	-6.61	124.63	128.60
3	0	1975	G	C5-C6-O6	-6.61	124.63	128.60
3	0	1278	G	C5-C6-O6	-6.61	124.63	128.60
3	0	1245	A	C4-C5-C6	6.61	120.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1498	U	O4'-C1'-N1	6.61	113.49	108.20
3	0	1402	U	O4'-C1'-N1	6.60	113.48	108.20
3	0	535	G	C5-C6-O6	-6.60	124.64	128.60
3	0	1678	U	O4'-C1'-N1	6.60	113.48	108.20
3	0	1604	A	C4-C5-C6	6.60	120.30	117.00
3	0	1536	G	C5-C6-O6	-6.60	124.64	128.60
3	0	17	C	N3-C4-N4	6.60	122.62	118.00
3	0	1420	A	C4-C5-C6	6.60	120.30	117.00
3	0	1701	G	C5-C6-O6	-6.60	124.64	128.60
3	0	1992	A	C4-C5-C6	6.60	120.30	117.00
3	0	2029	C	N3-C4-N4	6.59	122.62	118.00
3	0	2268	G	C5-C6-O6	-6.59	124.64	128.60
3	0	82	A	P-O3'-C3'	6.59	127.61	119.70
3	0	634	A	C4-C5-C6	6.59	120.30	117.00
3	0	1536	G	O4'-C1'-N9	6.59	113.47	108.20
3	0	1646	C	O4'-C1'-N1	6.59	113.47	108.20
3	0	2094	A	C4-C5-C6	6.59	120.30	117.00
3	0	453	U	O4'-C1'-N1	6.59	113.47	108.20
3	0	1921	C	O4'-C1'-N1	6.59	113.47	108.20
3	0	159	G	C5-C6-O6	-6.59	124.65	128.60
3	0	219	U	O4'-C1'-N1	6.59	113.47	108.20
3	0	1196	G	C5-C6-O6	-6.59	124.65	128.60
3	0	1926	G	C5-C6-O6	-6.59	124.65	128.60
20	X	32	ASN	C-N-CA	6.59	138.16	121.70
3	0	872	A	C4-C5-C6	6.58	120.29	117.00
3	0	2026	G	C5-C6-O6	-6.58	124.65	128.60
3	0	1728	G	C5-C6-O6	-6.58	124.65	128.60
3	0	1696	G	C5-C6-O6	-6.58	124.65	128.60
3	0	2136	A	C4-C5-C6	6.58	120.29	117.00
3	0	357	C	O4'-C1'-N1	6.58	113.46	108.20
3	0	1323	U	O4'-C1'-N1	6.58	113.46	108.20
2	1	15	G	C5-C6-O6	-6.58	124.66	128.60
3	0	1718	G	C5-C6-O6	-6.58	124.66	128.60
3	0	1726	U	O4'-C1'-N1	6.58	113.46	108.20
1	f	297	THR	O-C-N	6.57	133.22	122.70
3	0	294	G	C5-C6-O6	-6.57	124.66	128.60
3	0	316	A	C4-C5-C6	6.57	120.28	117.00
3	0	846	U	O4'-C1'-N1	6.57	113.46	108.20
3	0	1960	U	O4'-C1'-N1	6.57	113.46	108.20
3	0	95	U	O4'-C1'-N1	6.57	113.45	108.20
3	0	1450	G	C5-C6-O6	-6.57	124.66	128.60
3	0	2185	U	O4'-C1'-N1	6.57	113.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	82	A	O4'-C1'-N9	6.56	113.45	108.20
3	0	1508	G	C5-C6-O6	-6.56	124.66	128.60
3	0	2009	A	O4'-C1'-N9	6.56	113.45	108.20
2	1	56	G	C5-C6-O6	-6.56	124.67	128.60
46	C	53	ARG	O-C-N	-6.56	112.20	122.70
3	0	489	C	N3-C4-N4	6.56	122.59	118.00
3	0	2316	G	C5-C6-O6	-6.56	124.67	128.60
2	1	42	U	O4'-C1'-N1	6.55	113.44	108.20
3	0	16	G	C5-C6-O6	-6.55	124.67	128.60
3	0	1805	U	O4'-C1'-N1	6.55	113.44	108.20
2	1	43	A	C5-C6-N6	-6.55	118.46	123.70
3	0	614	U	O4'-C1'-N1	6.55	113.44	108.20
3	0	1503	G	C5-C6-O6	-6.55	124.67	128.60
2	1	36	A	C4-C5-C6	6.55	120.27	117.00
3	0	577	A	C4-C5-C6	6.55	120.27	117.00
3	0	665	U	O4'-C1'-N1	6.55	113.44	108.20
3	0	1389	G	C5-C6-O6	-6.55	124.67	128.60
3	0	1800	C	O4'-C1'-N1	6.55	113.44	108.20
3	0	299	A	C4-C5-C6	6.55	120.27	117.00
3	0	1200	G	C5-C6-O6	-6.55	124.67	128.60
3	0	1451	C	N3-C4-N4	6.55	122.58	118.00
3	0	2223	U	O4'-C1'-N1	6.55	113.44	108.20
3	0	1454	A	C4-C5-C6	6.54	120.27	117.00
3	0	2008	G	C5-C6-O6	-6.54	124.67	128.60
3	0	80	G	C5-C6-O6	-6.54	124.67	128.60
3	0	115	U	O4'-C1'-N1	6.54	113.43	108.20
3	0	919	G	C5-C6-O6	-6.54	124.67	128.60
3	0	254	A	C4-C5-C6	6.54	120.27	117.00
3	0	1195	G	C5-C6-O6	-6.54	124.67	128.60
3	0	1464	A	C4-C5-C6	6.54	120.27	117.00
3	0	1538	U	O4'-C1'-N1	6.54	113.43	108.20
3	0	194	U	O4'-C1'-N1	6.54	113.43	108.20
3	0	496	U	O4'-C1'-N1	6.54	113.43	108.20
3	0	797	G	C5-C6-O6	-6.54	124.68	128.60
3	0	1501	A	O4'-C1'-N9	6.54	113.43	108.20
3	0	1709	A	C4-C5-C6	6.54	120.27	117.00
3	0	1199	U	O4'-C1'-N1	6.54	113.43	108.20
3	0	2041	A	C4-C5-C6	6.54	120.27	117.00
3	0	1436	C	N3-C4-N4	6.53	122.57	118.00
3	0	1531	A	C4-C5-C6	6.53	120.27	117.00
3	0	831	A	C5-C6-N6	-6.53	118.47	123.70
3	0	676	G	C5-C6-O6	-6.53	124.68	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	759	C	N3-C4-N4	6.53	122.57	118.00
3	0	1601	G	C5-C6-O6	-6.53	124.68	128.60
3	0	1814	C	N3-C4-N4	6.53	122.57	118.00
3	0	2209	A	C4-C5-C6	6.53	120.27	117.00
47	8	453	ARG	C-N-CA	6.53	138.03	121.70
3	0	383	U	O4'-C1'-N1	6.53	113.42	108.20
3	0	1197	A	P-O3'-C3'	6.53	127.53	119.70
3	0	2064	A	C4-C5-C6	6.53	120.26	117.00
3	0	51	A	C5-C6-N6	-6.52	118.48	123.70
3	0	951	U	O4'-C1'-N1	6.52	113.42	108.20
3	0	1266	A	O4'-C1'-N9	6.52	113.42	108.20
3	0	952	U	O4'-C1'-N1	6.52	113.42	108.20
3	0	1637	G	O4'-C1'-N9	6.52	113.42	108.20
3	0	471	C	O4'-C1'-N1	6.52	113.42	108.20
3	0	599	A	C4-C5-C6	6.52	120.26	117.00
3	0	2031	A	C5-C6-N6	-6.52	118.48	123.70
3	0	2081	A	O3'-P-O5'	6.52	116.39	104.00
2	1	30	G	O4'-C1'-N9	6.52	113.41	108.20
3	0	740	U	O4'-C1'-N1	6.52	113.41	108.20
3	0	1587	G	C5-C6-O6	-6.52	124.69	128.60
3	0	1623	G	C5-C6-O6	-6.52	124.69	128.60
3	0	1737	A	C5-C6-N6	-6.52	118.49	123.70
3	0	1477	A	O4'-C1'-N9	6.52	113.41	108.20
3	0	2115	A	C4-C5-C6	6.52	120.26	117.00
3	0	373	G	C5-C6-O6	-6.51	124.69	128.60
3	0	1727	C	O4'-C1'-N1	6.51	113.41	108.20
3	0	2081	A	O4'-C1'-N9	6.51	113.41	108.20
3	0	179	G	C5-C6-O6	-6.51	124.69	128.60
3	0	693	G	C5-C6-O6	-6.51	124.69	128.60
3	0	1606	A	C4-C5-C6	6.51	120.25	117.00
3	0	2176	C	O4'-C1'-N1	6.51	113.41	108.20
3	0	371	A	C4-C5-C6	6.51	120.25	117.00
3	0	720	U	O4'-C1'-N1	6.51	113.41	108.20
3	0	1684	A	C5-C6-N1	-6.51	114.45	117.70
3	0	77	C	N3-C4-N4	6.50	122.55	118.00
3	0	256	A	C5-C6-N6	-6.50	118.50	123.70
3	0	839	C	N3-C4-N4	6.50	122.55	118.00
3	0	138	C	N3-C4-N4	6.50	122.55	118.00
3	0	2218	G	C5-C6-O6	-6.50	124.70	128.60
3	0	346	C	O4'-C1'-N1	6.50	113.40	108.20
3	0	900	A	C4-C5-C6	6.50	120.25	117.00
3	0	1274	C	O4'-C1'-N1	6.50	113.40	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2109	A	C4-C5-C6	6.50	120.25	117.00
3	0	573	U	O4'-C1'-N1	6.50	113.40	108.20
3	0	754	G	C5-C6-O6	-6.50	124.70	128.60
3	0	886	U	O4'-C1'-N1	6.50	113.40	108.20
3	0	1642	G	C5-C6-O6	-6.50	124.70	128.60
3	0	1904	C	N3-C4-N4	6.50	122.55	118.00
3	0	2040	A	C4-C5-C6	6.50	120.25	117.00
3	0	191	U	O4'-C1'-N1	6.50	113.40	108.20
3	0	1360	A	C5-C6-N6	-6.50	118.50	123.70
3	0	1435	C	N3-C4-N4	6.50	122.55	118.00
1	f	136	LEU	CA-C-O	-6.49	106.47	120.10
3	0	481	G	C5-C6-O6	-6.49	124.70	128.60
3	0	1355	U	O4'-C1'-N1	6.49	113.39	108.20
2	1	45	G	C5-C6-O6	-6.49	124.71	128.60
3	0	1812	U	O4'-C1'-N1	6.49	113.39	108.20
3	0	2183	C	N3-C4-N4	6.49	122.54	118.00
3	0	18	C	N3-C4-N4	6.49	122.54	118.00
3	0	1663	C	O4'-C1'-N1	6.49	113.39	108.20
3	0	2169	U	O4'-C1'-N1	6.49	113.39	108.20
3	0	136	U	C2-N1-C1'	6.49	125.48	117.70
3	0	1472	U	O4'-C1'-N1	6.49	113.39	108.20
2	1	17	G	C5-C6-O6	-6.48	124.71	128.60
3	0	677	G	C5-C6-O6	-6.48	124.71	128.60
3	0	831	A	C4-C5-C6	6.48	120.24	117.00
3	0	864	A	C5-C6-N6	-6.48	118.51	123.70
3	0	1222	A	O4'-C1'-N9	6.48	113.39	108.20
3	0	1496	U	O4'-C1'-N1	6.48	113.39	108.20
3	0	2274	G	O4'-C1'-N9	6.48	113.39	108.20
3	0	70	U	O4'-C1'-N1	6.48	113.38	108.20
3	0	111	A	C5-C6-N6	-6.48	118.52	123.70
3	0	456	C	N3-C4-N4	6.48	122.54	118.00
3	0	1797	G	C5-C6-O6	-6.48	124.71	128.60
3	0	220	G	O4'-C1'-N9	6.48	113.38	108.20
3	0	1561	C	N3-C4-N4	6.48	122.53	118.00
3	0	357	C	N3-C4-N4	6.48	122.53	118.00
3	0	200	U	C6-N1-C1'	-6.47	112.14	121.20
3	0	745	C	O4'-C1'-N1	6.47	113.38	108.20
3	0	1923	C	N3-C4-N4	6.47	122.53	118.00
3	0	879	C	O4'-C1'-N1	6.47	113.38	108.20
3	0	1202	A	O4'-C1'-N9	6.47	113.38	108.20
3	0	1242	G	N3-C2-N2	6.47	124.43	119.90
3	0	21	U	O4'-C1'-N1	6.47	113.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	544	U	O4'-C1'-N1	6.47	113.38	108.20
3	0	895	A	C4-C5-C6	6.47	120.23	117.00
3	0	992	A	C4-C5-C6	6.47	120.23	117.00
3	0	1202	A	C4-C5-C6	6.47	120.23	117.00
3	0	1254	G	C5-C6-O6	-6.47	124.72	128.60
3	0	144	A	C4-C5-C6	6.46	120.23	117.00
3	0	1348	A	C4-C5-C6	6.46	120.23	117.00
3	0	2097	A	O4'-C1'-N9	6.46	113.37	108.20
3	0	2243	A	C4-C5-C6	6.46	120.23	117.00
3	0	710	A	C5-C6-N6	-6.46	118.53	123.70
3	0	1595	G	C5-C6-O6	-6.46	124.72	128.60
3	0	1804	A	C4-C5-C6	6.46	120.23	117.00
3	0	2196	G	C5-C6-O6	-6.46	124.72	128.60
3	0	2277	A	C4-C5-C6	6.46	120.23	117.00
3	0	3	U	O4'-C1'-N1	6.46	113.36	108.20
3	0	462	U	O4'-C1'-N1	6.46	113.36	108.20
3	0	479	G	O4'-C1'-N9	6.46	113.36	108.20
3	0	1700	A	C5-C6-N6	-6.46	118.53	123.70
1	f	1127	VAL	C-N-CA	6.45	149.11	122.00
2	1	26	A	C5-C6-N6	-6.45	118.54	123.70
3	0	31	C	N3-C4-N4	6.45	122.52	118.00
3	0	261	A	C5-C6-N6	-6.45	118.54	123.70
3	0	609	A	C4-C5-C6	6.45	120.23	117.00
3	0	1333	A	C4-C5-C6	6.45	120.23	117.00
3	0	2293	A	C5-C6-N6	-6.45	118.54	123.70
2	1	64	C	N3-C4-N4	6.45	122.52	118.00
3	0	556	U	O4'-C1'-N1	6.45	113.36	108.20
3	0	1388	G	C5-C6-O6	-6.45	124.73	128.60
3	0	1939	G	C5-C6-O6	-6.45	124.73	128.60
3	0	359	U	O4'-C1'-N1	6.45	113.36	108.20
3	0	1264	A	C4-C5-C6	6.45	120.22	117.00
3	0	2028	C	C6-N1-C1'	-6.45	113.06	120.80
3	0	2085	A	C4-C5-C6	6.45	120.22	117.00
5	s	126	PHE	CB-CG-CD1	6.45	125.31	120.80
3	0	147	G	C5-C6-O6	-6.45	124.73	128.60
3	0	1510	G	C5-C6-O6	-6.45	124.73	128.60
3	0	1573	A	C4-C5-C6	6.45	120.22	117.00
3	0	1669	A	C4-C5-C6	6.45	120.22	117.00
3	0	308	C	C6-N1-C1'	-6.44	113.07	120.80
3	0	1244	G	C5-C6-O6	-6.44	124.73	128.60
3	0	752	U	O4'-C1'-N1	6.44	113.35	108.20
3	0	778	A	C4-C5-C6	6.44	120.22	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1525	A	C4-C5-C6	6.44	120.22	117.00
3	0	2003	A	C5-C6-N6	-6.44	118.55	123.70
5	s	126	PHE	CB-CG-CD2	-6.44	116.29	120.80
3	0	876	A	N1-C6-N6	6.44	122.46	118.60
3	0	1756	U	O4'-C1'-N1	6.44	113.35	108.20
3	0	1620	A	C4-C5-C6	6.44	120.22	117.00
3	0	1954	U	O4'-C1'-N1	6.44	113.35	108.20
3	0	1529	U	O4'-C1'-N1	6.44	113.35	108.20
3	0	1666	A	C4-C5-C6	6.44	120.22	117.00
3	0	1862	U	O4'-C1'-N1	6.44	113.35	108.20
3	0	254	A	C5-C6-N1	-6.44	114.48	117.70
3	0	485	A	C4-C5-C6	6.44	120.22	117.00
3	0	854	U	O4'-C1'-N1	6.44	113.35	108.20
3	0	2224	C	N3-C4-N4	6.44	122.50	118.00
2	1	26	A	C4-C5-C6	6.43	120.22	117.00
3	0	744	C	C6-N1-C1'	-6.43	113.08	120.80
3	0	1902	U	O4'-C1'-N1	6.43	113.35	108.20
3	0	2263	C	N3-C4-N4	6.43	122.50	118.00
3	0	597	C	O4'-C1'-N1	6.43	113.35	108.20
3	0	2160	U	O4'-C1'-N1	6.43	113.35	108.20
3	0	151	A	C4-C5-C6	6.43	120.22	117.00
3	0	892	U	O4'-C1'-N1	6.43	113.34	108.20
3	0	1346	C	O4'-C1'-N1	6.43	113.34	108.20
3	0	35	U	O4'-C1'-N1	6.43	113.34	108.20
3	0	1228	C	N3-C4-N4	6.43	122.50	118.00
3	0	34	G	C5-C6-O6	-6.43	124.74	128.60
3	0	883	C	O4'-C1'-N1	6.43	113.34	108.20
3	0	326	U	O4'-C1'-N1	6.43	113.34	108.20
3	0	1591	G	C5-C6-O6	-6.43	124.74	128.60
3	0	1634	C	N3-C4-N4	6.42	122.50	118.00
3	0	1691	G	C4-N9-C1'	6.42	134.85	126.50
1	f	292	ARG	C-N-CA	6.42	137.76	121.70
3	0	217	C	N3-C4-N4	6.42	122.50	118.00
3	0	1450	G	O4'-C1'-N9	6.42	113.34	108.20
3	0	1627	G	O4'-C1'-N9	6.42	113.34	108.20
3	0	2015	G	C5-C6-O6	-6.42	124.75	128.60
3	0	118	C	N3-C4-N4	6.42	122.49	118.00
3	0	1547	U	O4'-C1'-N1	6.42	113.34	108.20
3	0	901	A	C4-C5-C6	6.42	120.21	117.00
3	0	2024	C	N3-C4-N4	6.42	122.49	118.00
3	0	209	C	N3-C4-N4	6.42	122.49	118.00
3	0	509	A	C5-C6-N6	-6.42	118.57	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2101	G	O4'-C1'-N9	6.42	113.33	108.20
1	f	137	CYS	N-CA-C	-6.42	93.68	111.00
1	f	1128	PRO	CA-C-N	6.41	131.31	117.20
3	0	932	G	C5-C6-O6	-6.41	124.75	128.60
3	0	1985	C	N3-C4-N4	6.41	122.49	118.00
3	0	2303	G	C5-C6-O6	-6.41	124.75	128.60
3	0	437	G	C5-C6-O6	-6.41	124.75	128.60
3	0	2193	G	C5-C6-O6	-6.41	124.75	128.60
3	0	2260	C	N3-C4-N4	6.41	122.49	118.00
3	0	1717	U	O4'-C1'-N1	6.41	113.33	108.20
3	0	1865	U	O4'-C1'-N1	6.41	113.32	108.20
3	0	2104	G	O4'-C1'-N9	6.41	113.33	108.20
3	0	1207	G	C5-C6-O6	-6.40	124.76	128.60
3	0	570	U	P-O3'-C3'	6.40	127.38	119.70
3	0	698	C	N3-C4-N4	6.40	122.48	118.00
3	0	1073	C	N3-C4-N4	6.40	122.48	118.00
3	0	1935	U	O4'-C1'-N1	6.40	113.32	108.20
2	1	3	C	N3-C4-N4	6.40	122.48	118.00
3	0	505	A	C4-C5-C6	6.40	120.20	117.00
3	0	588	A	C4-C5-C6	6.40	120.20	117.00
3	0	1415	G	C5-C6-O6	-6.40	124.76	128.60
3	0	1447	C	N3-C4-N4	6.40	122.48	118.00
3	0	2039	A	O4'-C1'-N9	6.40	113.32	108.20
3	0	260	A	C4-C5-C6	6.39	120.20	117.00
2	1	37	A	C4-C5-C6	6.39	120.20	117.00
3	0	1399	U	O4'-C1'-N1	6.39	113.31	108.20
3	0	1636	A	C4-C5-C6	6.39	120.20	117.00
3	0	2311	A	C5-C6-N6	-6.39	118.59	123.70
1	f	1106	TYR	CB-CG-CD1	6.39	124.83	121.00
3	0	61	C	O4'-C1'-N1	6.39	113.31	108.20
3	0	1686	A	C4-C5-C6	6.39	120.19	117.00
3	0	1795	A	C4-C5-C6	6.39	120.19	117.00
2	1	21	G	O4'-C1'-N9	6.39	113.31	108.20
3	0	178	U	O4'-C1'-N1	6.39	113.31	108.20
3	0	509	A	C4-C5-C6	6.39	120.19	117.00
3	0	719	G	C5-C6-O6	-6.39	124.77	128.60
3	0	650	C	N3-C4-N4	6.38	122.47	118.00
3	0	1657	A	C4-C5-C6	6.38	120.19	117.00
3	0	1780	U	C2-N1-C1'	6.38	125.36	117.70
3	0	1932	A	C4-C5-C6	6.38	120.19	117.00
3	0	103	U	O4'-C1'-N1	6.38	113.31	108.20
3	0	402	C	N3-C4-N4	6.38	122.47	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	862	A	C5-C6-N6	-6.38	118.60	123.70
3	0	2004	A	O4'-C1'-N9	6.38	113.30	108.20
1	f	775	GLY	C-N-CA	6.38	135.69	122.30
3	0	87	C	N3-C4-N4	6.38	122.47	118.00
3	0	812	A	C4-C5-C6	6.38	120.19	117.00
2	1	39	C	N3-C4-N4	6.38	122.46	118.00
3	0	774	C	P-O3'-C3'	6.38	127.35	119.70
3	0	2313	C	N3-C4-N4	6.38	122.46	118.00
3	0	68	A	C4-C5-C6	6.38	120.19	117.00
3	0	260	A	C5-C6-N6	-6.38	118.60	123.70
3	0	1716	G	C5-C6-O6	-6.38	124.78	128.60
3	0	1331	G	C5-C6-O6	-6.37	124.78	128.60
44	K	30	TYR	CB-CG-CD2	-6.37	117.18	121.00
3	0	1284	A	C5-C6-N6	-6.37	118.60	123.70
3	0	1522	A	C4-C5-C6	6.37	120.19	117.00
3	0	1632	C	O4'-C1'-N1	6.37	113.30	108.20
3	0	1788	U	O4'-C1'-N1	6.37	113.30	108.20
3	0	2027	A	O4'-C1'-N9	6.37	113.29	108.20
1	f	239	ASN	C-N-CA	6.37	137.61	121.70
3	0	410	G	O4'-C1'-N9	6.37	113.29	108.20
3	0	801	C	N3-C4-N4	6.37	122.46	118.00
3	0	2306	C	N3-C4-N4	6.36	122.45	118.00
3	0	2252	C	N3-C4-N4	6.36	122.45	118.00
3	0	105	A	C4-C5-C6	6.36	120.18	117.00
3	0	245	A	C5-C6-N6	-6.36	118.61	123.70
3	0	2013	A	C4-C5-C6	6.36	120.18	117.00
3	0	170	C	N3-C4-N4	6.36	122.45	118.00
3	0	1930	A	C5-C6-N6	-6.36	118.61	123.70
3	0	593	G	C5-C6-O6	-6.36	124.78	128.60
3	0	1292	A	C5-C6-N6	-6.36	118.61	123.70
3	0	1504	G	O4'-C1'-N9	6.36	113.28	108.20
3	0	1345	A	C4-C5-C6	6.36	120.18	117.00
3	0	2013	A	C5-C6-N6	-6.36	118.62	123.70
3	0	2036	A	O4'-C1'-N9	6.35	113.28	108.20
3	0	114	C	N3-C4-N4	6.35	122.45	118.00
3	0	940	U	O4'-C1'-N1	6.35	113.28	108.20
3	0	1715	A	C4-C5-C6	6.35	120.17	117.00
3	0	702	U	O4'-C1'-N1	6.35	113.28	108.20
3	0	596	A	C4-C5-C6	6.35	120.17	117.00
3	0	777	A	C4-C5-C6	6.35	120.17	117.00
3	0	1784	U	O4'-C1'-N1	6.35	113.28	108.20
3	0	1431	U	O4'-C1'-N1	6.34	113.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1566	A	C4-C5-C6	6.34	120.17	117.00
3	0	2279	A	C5-C6-N6	-6.34	118.62	123.70
3	0	861	A	O4'-C1'-N9	6.34	113.27	108.20
3	0	1802	A	C4-C5-C6	6.34	120.17	117.00
3	0	2180	C	N3-C4-N4	6.34	122.44	118.00
3	0	2265	A	C4-C5-C6	6.34	120.17	117.00
3	0	941	U	O4'-C1'-N1	6.34	113.27	108.20
3	0	1506	G	O4'-C1'-N9	6.34	113.27	108.20
3	0	745	C	N3-C4-C5	-6.34	119.36	121.90
3	0	2320	A	C4-C5-C6	6.34	120.17	117.00
3	0	864	A	C4-C5-C6	6.33	120.17	117.00
3	0	984	A	C5-C6-N6	-6.33	118.63	123.70
3	0	1942	A	C4-C5-C6	6.33	120.17	117.00
3	0	1257	C	N3-C4-N4	6.33	122.43	118.00
3	0	1944	A	C4-C5-C6	6.33	120.17	117.00
26	J	103	TYR	CB-CG-CD2	-6.33	117.20	121.00
3	0	14	C	N3-C4-C5	-6.33	119.37	121.90
3	0	167	A	C4-C5-C6	6.33	120.17	117.00
3	0	770	C	O4'-C1'-N1	6.33	113.27	108.20
3	0	883	C	N3-C4-N4	6.33	122.43	118.00
3	0	475	A	C4-C5-C6	6.33	120.17	117.00
3	0	1070	C	N3-C4-N4	6.33	122.43	118.00
3	0	1600	A	C4-C5-C6	6.33	120.17	117.00
3	0	1871	A	C4-C5-C6	6.33	120.17	117.00
3	0	936	C	N3-C4-N4	6.33	122.43	118.00
3	0	1318	A	O4'-C1'-N9	6.33	113.26	108.20
3	0	1633	A	C4-C5-C6	6.33	120.16	117.00
3	0	2250	A	C5-C6-N6	-6.33	118.64	123.70
3	0	365	C	N3-C4-N4	6.33	122.43	118.00
3	0	1454	A	C5-C6-N1	-6.33	114.54	117.70
3	0	2273	A	C4-C5-C6	6.33	120.16	117.00
2	1	47	C	O4'-C1'-N1	6.32	113.26	108.20
3	0	880	A	O4'-C1'-N9	6.32	113.26	108.20
3	0	1405	G	C5-C6-O6	-6.32	124.81	128.60
3	0	1951	C	N3-C4-N4	6.32	122.43	118.00
3	0	2249	C	N3-C4-N4	6.32	122.43	118.00
3	0	516	A	C4-C5-C6	6.32	120.16	117.00
3	0	131	C	N3-C4-N4	6.32	122.42	118.00
3	0	198	U	O4'-C1'-N1	6.32	113.26	108.20
3	0	345	A	C4-C5-C6	6.32	120.16	117.00
3	0	465	G	O4'-C1'-N9	6.32	113.26	108.20
3	0	880	A	C4-C5-C6	6.32	120.16	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2088	A	C5-C6-N6	-6.32	118.64	123.70
2	1	61	C	N3-C4-N4	6.32	122.42	118.00
3	0	703	A	O4'-C1'-N9	6.32	113.25	108.20
3	0	1307	A	C4-C5-C6	6.32	120.16	117.00
3	0	2311	A	C4-C5-C6	6.32	120.16	117.00
2	1	67	G	O4'-C1'-N9	6.32	113.25	108.20
3	0	223	G	O4'-C1'-N9	6.32	113.25	108.20
3	0	342	U	O4'-C1'-N1	6.32	113.25	108.20
3	0	697	G	O4'-C1'-N9	6.32	113.25	108.20
3	0	1863	U	O4'-C1'-N1	6.32	113.25	108.20
3	0	1947	A	O4'-C1'-N9	6.32	113.25	108.20
3	0	2007	A	C5-C6-N6	-6.31	118.65	123.70
3	0	1700	A	O4'-C1'-N9	6.31	113.25	108.20
3	0	2157	C	N3-C4-N4	6.31	122.42	118.00
3	0	2251	C	N3-C4-N4	6.31	122.42	118.00
3	0	842	G	O4'-C1'-N9	6.31	113.25	108.20
3	0	1315	C	N3-C4-N4	6.31	122.41	118.00
2	1	19	A	C5-C6-N6	-6.30	118.66	123.70
3	0	210	A	C5-C6-N6	-6.30	118.66	123.70
3	0	1181	A	C4-C5-C6	6.30	120.15	117.00
3	0	1370	A	C4-C5-C6	6.30	120.15	117.00
3	0	1558	A	C4-C5-C6	6.30	120.15	117.00
3	0	1655	U	O4'-C1'-N1	6.30	113.24	108.20
1	f	1703	GLY	C-N-CA	-6.30	105.94	121.70
3	0	538	A	C5-C6-N1	-6.30	114.55	117.70
3	0	645	A	C4-C5-C6	6.30	120.15	117.00
48	W	165	TRP	N-CA-C	6.30	128.02	111.00
3	0	860	U	O4'-C1'-N1	6.30	113.24	108.20
3	0	877	A	C4-C5-C6	6.30	120.15	117.00
3	0	1405	G	O4'-C1'-N9	6.30	113.24	108.20
3	0	1710	G	O4'-C1'-N9	6.30	113.24	108.20
3	0	2064	A	C5-C6-N1	-6.30	114.55	117.70
1	f	194	PHE	O-C-N	6.30	132.78	122.70
3	0	852	A	C5-C6-N6	-6.30	118.66	123.70
3	0	1520	G	C5-C6-O6	-6.30	124.82	128.60
3	0	1574	G	O4'-C1'-N9	6.30	113.24	108.20
3	0	149	A	C4-C5-C6	6.30	120.15	117.00
3	0	1270	A	C4-C5-C6	6.30	120.15	117.00
3	0	1307	A	C5-C6-N6	-6.30	118.66	123.70
39	E	316	TYR	CB-CG-CD1	6.30	124.78	121.00
3	0	788	A	O4'-C1'-N9	6.29	113.24	108.20
3	0	992	A	O4'-C1'-N9	6.29	113.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1852	C	N3-C4-N4	6.29	122.41	118.00
3	0	1243	U	O4'-C1'-N1	6.29	113.23	108.20
3	0	2036	A	C4-C5-C6	6.29	120.15	117.00
6	j	80	PHE	CB-CG-CD1	6.29	125.20	120.80
3	0	206	C	N3-C4-N4	6.29	122.40	118.00
3	0	305	U	O4'-C1'-N1	6.29	113.23	108.20
3	0	1713	U	O4'-C1'-N1	6.29	113.23	108.20
3	0	1746	G	C5-C6-O6	-6.29	124.83	128.60
3	0	51	A	C4-C5-C6	6.28	120.14	117.00
3	0	483	A	C4-C5-C6	6.28	120.14	117.00
3	0	647	A	O4'-C1'-N9	6.28	113.23	108.20
3	0	961	A	C4-C5-C6	6.28	120.14	117.00
3	0	2031	A	C4-C5-C6	6.28	120.14	117.00
2	1	75	A	O4'-C1'-N9	6.28	113.22	108.20
3	0	1820	A	C4-C5-C6	6.28	120.14	117.00
3	0	73	A	C5-C6-N6	-6.28	118.68	123.70
3	0	90	A	C4-C5-C6	6.28	120.14	117.00
3	0	199	G	O4'-C1'-N9	6.28	113.22	108.20
3	0	1502	C	C6-N1-C1'	-6.28	113.27	120.80
3	0	1910	U	O4'-C1'-N1	6.28	113.22	108.20
3	0	524	G	O4'-C1'-N9	6.28	113.22	108.20
3	0	718	A	C4-C5-C6	6.28	120.14	117.00
3	0	816	C	N3-C4-N4	6.28	122.39	118.00
3	0	1271	C	O4'-C1'-N1	6.28	113.22	108.20
3	0	2006	A	O4'-C1'-N9	6.28	113.22	108.20
3	0	2035	G	O4'-C1'-N9	6.28	113.22	108.20
3	0	47	A	C4-C5-C6	6.27	120.14	117.00
3	0	1685	G	C5-C6-O6	-6.27	124.84	128.60
3	0	1881	G	C5-C6-O6	-6.27	124.84	128.60
3	0	1927	G	C5-C6-O6	-6.27	124.84	128.60
3	0	800	C	N3-C4-N4	6.27	122.39	118.00
3	0	988	U	O4'-C1'-N1	6.27	113.22	108.20
3	0	36	U	O4'-C1'-N1	6.27	113.22	108.20
3	0	249	A	C5-C6-N6	-6.27	118.69	123.70
3	0	269	A	O4'-C1'-N9	6.27	113.22	108.20
3	0	921	G	C5-C6-O6	-6.27	124.84	128.60
3	0	1365	A	C5-C6-N6	-6.27	118.68	123.70
3	0	1967	U	O4'-C1'-N1	6.27	113.22	108.20
3	0	2103	C	N3-C4-N4	6.27	122.39	118.00
3	0	19	A	O4'-C1'-N9	6.27	113.22	108.20
3	0	255	A	C5-C6-N1	-6.27	114.57	117.70
3	0	1340	U	O4'-C1'-N1	6.27	113.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1850	C	N3-C4-N4	6.27	122.39	118.00
3	0	2211	G	O4'-C1'-N9	6.27	113.22	108.20
3	0	1557	A	C4-C5-C6	6.27	120.13	117.00
3	0	129	U	O4'-C1'-N1	6.26	113.21	108.20
3	0	713	G	O4'-C1'-N9	6.26	113.21	108.20
3	0	576	A	C5-C6-N6	-6.26	118.69	123.70
3	0	1895	C	N3-C4-N4	6.26	122.38	118.00
3	0	251	A	C4-C5-C6	6.26	120.13	117.00
3	0	499	A	C4-C5-C6	6.26	120.13	117.00
3	0	501	A	C4-C5-C6	6.26	120.13	117.00
3	0	2239	A	C4-C5-C6	6.26	120.13	117.00
3	0	455	C	N3-C4-N4	6.26	122.38	118.00
3	0	723	C	O4'-C1'-N1	6.26	113.20	108.20
3	0	1180	A	C4-C5-C6	6.26	120.13	117.00
3	0	1517	A	C4-C5-C6	6.26	120.13	117.00
3	0	2072	C	O4'-C1'-N1	6.26	113.20	108.20
3	0	2315	G	O4'-C1'-N9	6.26	113.21	108.20
3	0	851	U	O4'-C1'-N1	6.25	113.20	108.20
3	0	1212	U	O4'-C1'-N1	6.25	113.20	108.20
3	0	1452	C	N3-C4-N4	6.25	122.38	118.00
3	0	119	G	O4'-C1'-N9	6.25	113.20	108.20
3	0	498	A	C4-C5-C6	6.25	120.12	117.00
3	0	549	A	C5-C6-N1	-6.25	114.58	117.70
3	0	1328	A	C4-C5-C6	6.25	120.12	117.00
3	0	1978	A	C5-C6-N6	-6.25	118.70	123.70
3	0	2097	A	C4-C5-C6	6.25	120.12	117.00
3	0	2282	C	N3-C4-N4	6.25	122.37	118.00
3	0	785	A	C4-C5-C6	6.25	120.12	117.00
3	0	1786	A	C4-C5-C6	6.25	120.12	117.00
2	1	53	A	C4-C5-C6	6.25	120.12	117.00
3	0	386	A	C4-C5-C6	6.24	120.12	117.00
3	0	392	A	C4-C5-C6	6.24	120.12	117.00
3	0	414	A	C4-C5-C6	6.24	120.12	117.00
3	0	875	A	C4-C5-C6	6.24	120.12	117.00
3	0	1507	A	C4-C5-C6	6.24	120.12	117.00
3	0	2158	C	N3-C4-N4	6.24	122.37	118.00
2	1	46	A	C4-C5-C6	6.24	120.12	117.00
48	W	166	VAL	N-CA-C	-6.24	94.14	111.00
2	1	54	U	O4'-C1'-N1	6.24	113.19	108.20
3	0	181	A	C4-C5-C6	6.24	120.12	117.00
3	0	858	A	C4-C5-C6	6.24	120.12	117.00
3	0	1430	U	O4'-C1'-N1	6.24	113.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1986	A	C5-C6-N6	-6.24	118.71	123.70
28	5	283	GLY	N-CA-C	6.24	128.70	113.10
1	f	266	GLU	C-N-CA	6.24	137.29	121.70
1	f	1152	LEU	C-N-CA	-6.24	106.10	121.70
3	0	130	G	O4'-C1'-N9	6.24	113.19	108.20
3	0	863	A	C4-C5-C6	6.24	120.12	117.00
3	0	141	A	C5-C6-N6	-6.24	118.71	123.70
3	0	204	G	O4'-C1'-N9	6.24	113.19	108.20
3	0	448	A	C4-C5-C6	6.24	120.12	117.00
3	0	515	C	N3-C4-N4	6.24	122.36	118.00
3	0	526	A	C4-C5-C6	6.24	120.12	117.00
3	0	829	C	N3-C4-N4	6.24	122.36	118.00
3	0	1501	A	C4-C5-C6	6.24	120.12	117.00
14	q	127	PHE	CB-CG-CD1	6.24	125.17	120.80
3	0	430	G	O4'-C1'-N9	6.23	113.19	108.20
3	0	560	C	N3-C4-N4	6.23	122.36	118.00
3	0	610	A	C4-C5-C6	6.23	120.12	117.00
3	0	2294	G	O4'-C1'-N9	6.23	113.19	108.20
3	0	252	G	O4'-C1'-N9	6.23	113.19	108.20
3	0	1255	A	C4-C5-C6	6.23	120.12	117.00
3	0	1594	C	N3-C4-N4	6.23	122.36	118.00
3	0	1873	G	O4'-C1'-N9	6.23	113.19	108.20
46	C	690	TYR	CB-CG-CD2	-6.23	117.26	121.00
3	0	713	G	P-O3'-C3'	-6.23	112.22	119.70
3	0	937	C	N3-C4-N4	6.23	122.36	118.00
3	0	22	A	C4-C5-C6	6.23	120.11	117.00
3	0	2172	A	C4-C5-C6	6.23	120.11	117.00
3	0	682	G	C5-C6-O6	-6.23	124.86	128.60
3	0	1737	A	C4-C5-C6	6.22	120.11	117.00
3	0	1943	C	N3-C4-N4	6.22	122.36	118.00
3	0	72	C	N3-C4-N4	6.22	122.36	118.00
3	0	598	A	C4-C5-C6	6.22	120.11	117.00
3	0	730	U	O4'-C1'-N1	6.22	113.18	108.20
3	0	2235	C	N3-C4-N4	6.22	122.36	118.00
3	0	523	A	C5-C6-N1	-6.22	114.59	117.70
3	0	2108	A	C5-C6-N6	-6.22	118.72	123.70
3	0	2285	A	C4-C5-C6	6.22	120.11	117.00
3	0	529	A	C4-C5-C6	6.22	120.11	117.00
3	0	1685	G	O4'-C1'-N9	6.22	113.18	108.20
3	0	1964	C	O4'-C1'-N1	6.22	113.17	108.20
3	0	884	A	C5-C6-N6	-6.22	118.73	123.70
2	1	32	U	O4'-C1'-N1	6.22	113.17	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	250	A	O4'-C1'-N9	6.22	113.17	108.20
3	0	789	C	N3-C4-N4	6.22	122.35	118.00
3	0	2050	A	C4-C5-C6	6.22	120.11	117.00
3	0	190	A	C5-C6-N1	-6.21	114.59	117.70
3	0	1700	A	C4-C5-C6	6.21	120.11	117.00
3	0	978	U	C6-N1-C1'	-6.21	112.50	121.20
3	0	1639	C	N3-C4-N4	6.21	122.35	118.00
3	0	1686	A	C5-C6-N6	-6.21	118.73	123.70
3	0	1981	C	N3-C4-N4	6.21	122.35	118.00
3	0	2088	A	C4-C5-C6	6.21	120.11	117.00
3	0	1679	U	O4'-C1'-N1	6.21	113.17	108.20
2	1	5	C	N3-C4-N4	6.21	122.35	118.00
3	0	423	C	N3-C4-N4	6.21	122.35	118.00
3	0	996	G	O4'-C1'-N9	6.21	113.17	108.20
3	0	2026	G	O4'-C1'-N9	6.21	113.17	108.20
3	0	695	G	O4'-C1'-N9	6.21	113.17	108.20
3	0	735	A	C5-C6-N1	-6.21	114.60	117.70
3	0	913	A	C4-C5-C6	6.21	120.10	117.00
3	0	2059	G	C5-C6-O6	-6.21	124.88	128.60
3	0	587	A	C4-C5-C6	6.21	120.10	117.00
3	0	248	G	C5-C6-O6	-6.20	124.88	128.60
3	0	1382	A	C4-C5-C6	6.20	120.10	117.00
3	0	1896	C	N3-C4-N4	6.20	122.34	118.00
3	0	1600	A	C5-C6-N6	-6.20	118.74	123.70
3	0	161	A	C4-C5-C6	6.20	120.10	117.00
3	0	1311	A	C4-C5-C6	6.20	120.10	117.00
3	0	1532	G	O3'-P-O5'	-6.20	92.22	104.00
3	0	1576	C	N3-C4-N4	6.20	122.34	118.00
3	0	1867	C	N3-C4-N4	6.20	122.34	118.00
3	0	180	A	C4-C5-C6	6.20	120.10	117.00
3	0	245	A	C4-C5-C6	6.20	120.10	117.00
3	0	674	A	C4-C5-C6	6.20	120.10	117.00
3	0	1192	C	N3-C4-N4	6.20	122.34	118.00
3	0	1250	C	N3-C4-N4	6.20	122.34	118.00
3	0	261	A	C4-C5-C6	6.20	120.10	117.00
3	0	539	G	C5-C6-O6	-6.20	124.88	128.60
1	f	1219	HIS	O-C-N	-6.20	112.79	122.70
3	0	613	C	N3-C4-N4	6.20	122.34	118.00
3	0	2129	G	C5-C6-O6	-6.20	124.88	128.60
3	0	2279	A	O4'-C1'-N9	6.20	113.16	108.20
3	0	741	G	O4'-C1'-N9	6.19	113.16	108.20
3	0	2	A	C4-C5-C6	6.19	120.10	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	216	A	C4-C5-C6	6.19	120.10	117.00
3	0	2310	C	N3-C4-N4	6.19	122.33	118.00
3	0	506	A	C4-C5-C6	6.19	120.09	117.00
3	0	704	A	C4-C5-C6	6.19	120.10	117.00
3	0	1269	A	C4-C5-C6	6.19	120.09	117.00
3	0	1707	A	C4-C5-C6	6.19	120.09	117.00
3	0	1709	A	C5-C6-N1	-6.19	114.61	117.70
3	0	2193	G	N3-C2-N2	6.19	124.23	119.90
3	0	977	A	C4-C5-C6	6.19	120.09	117.00
3	0	1190	A	C4-C5-C6	6.19	120.09	117.00
3	0	1295	A	C5-C6-N6	-6.19	118.75	123.70
3	0	1539	A	O4'-C1'-N9	6.19	113.15	108.20
3	0	2155	G	O4'-C1'-N9	6.19	113.15	108.20
3	0	166	C	N3-C4-N4	6.19	122.33	118.00
3	0	425	A	C4-C5-C6	6.19	120.09	117.00
3	0	431	G	O4'-C1'-N9	6.19	113.15	108.20
49	I	216	SER	N-CA-CB	6.19	119.78	110.50
3	0	744	C	N3-C4-N4	6.19	122.33	118.00
3	0	2052	A	C5-C6-N6	-6.19	118.75	123.70
3	0	722	C	N3-C4-C5	-6.18	119.43	121.90
3	0	806	C	N3-C4-N4	6.18	122.33	118.00
3	0	1887	G	N1-C6-O6	6.18	123.61	119.90
3	0	1996	C	O4'-C1'-N1	6.18	113.15	108.20
28	5	267	SER	C-N-CA	6.18	137.16	121.70
3	0	125	A	C4-C5-C6	6.18	120.09	117.00
3	0	300	A	C4-C5-C6	6.18	120.09	117.00
3	0	746	A	C5-C6-N1	-6.18	114.61	117.70
3	0	1331	G	N3-C2-N2	6.18	124.23	119.90
3	0	1667	A	C4-C5-C6	6.18	120.09	117.00
44	K	176	PHE	CB-CG-CD1	6.18	125.13	120.80
3	0	278	A	C4-C5-C6	6.18	120.09	117.00
3	0	1965	A	C4-C5-C6	6.18	120.09	117.00
3	0	1276	G	C5-C6-O6	-6.18	124.89	128.60
3	0	2196	G	O4'-C1'-N9	6.18	113.14	108.20
3	0	681	C	N3-C4-N4	6.18	122.33	118.00
3	0	826	A	C5-C6-N6	-6.18	118.76	123.70
3	0	993	A	C4-C5-C6	6.18	120.09	117.00
3	0	1205	A	C5-C6-N6	-6.18	118.76	123.70
3	0	1651	G	O4'-C1'-N9	6.18	113.14	108.20
3	0	1830	A	C4-C5-C6	6.17	120.09	117.00
3	0	2264	A	C4-C5-C6	6.17	120.09	117.00
3	0	590	C	N3-C4-N4	6.17	122.32	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	242	A	C4-C5-C6	6.17	120.08	117.00
3	0	604	A	C5-C6-N6	-6.17	118.76	123.70
3	0	1800	C	N3-C4-N4	6.17	122.32	118.00
3	0	2037	U	O4'-C1'-N1	6.17	113.14	108.20
3	0	2221	A	C4-C5-C6	6.17	120.09	117.00
3	0	2173	C	O4'-C1'-N1	6.17	113.13	108.20
3	0	1290	C	N3-C4-N4	6.17	122.32	118.00
3	0	1650	C	N3-C4-N4	6.17	122.32	118.00
3	0	267	U	O4'-C1'-N1	6.17	113.13	108.20
1	f	139	MET	N-CA-CB	-6.16	99.51	110.60
3	0	78	A	C4-C5-C6	6.16	120.08	117.00
3	0	539	G	O4'-C1'-N9	6.16	113.13	108.20
3	0	1403	A	C4-C5-C6	6.16	120.08	117.00
3	0	1426	A	C4-C5-C6	6.16	120.08	117.00
3	0	2275	C	N3-C4-N4	6.16	122.31	118.00
3	0	1285	U	O4'-C1'-N1	6.16	113.13	108.20
3	0	2299	A	C4-C5-C6	6.16	120.08	117.00
3	0	224	C	N3-C4-N4	6.16	122.31	118.00
3	0	713	G	C5-C6-O6	-6.16	124.90	128.60
2	1	55	C	N3-C4-N4	6.16	122.31	118.00
3	0	467	A	O4'-C1'-N9	6.16	113.13	108.20
3	0	554	C	N3-C4-C5	-6.16	119.44	121.90
3	0	699	C	N3-C4-N4	6.16	122.31	118.00
3	0	1351	G	C5-C6-O6	-6.16	124.91	128.60
3	0	2093	A	C4-C5-C6	6.16	120.08	117.00
3	0	73	A	C4-C5-C6	6.16	120.08	117.00
3	0	646	A	C5-C6-N6	-6.16	118.78	123.70
3	0	1531	A	O5'-C5'-C4'	6.16	123.39	111.70
3	0	2060	A	C4-C5-C6	6.16	120.08	117.00
3	0	226	A	C4-C5-C6	6.15	120.08	117.00
3	0	764	A	C4-C5-C6	6.15	120.08	117.00
3	0	1358	A	C4-C5-C6	6.15	120.08	117.00
3	0	1624	A	C5-C6-N1	-6.15	114.62	117.70
3	0	1711	A	O4'-C1'-N9	6.15	113.12	108.20
3	0	295	A	C4-C5-C6	6.15	120.08	117.00
3	0	2239	A	C5-C6-N6	-6.15	118.78	123.70
3	0	1694	A	O4'-C1'-N9	6.15	113.12	108.20
3	0	2027	A	C4-C5-C6	6.15	120.08	117.00
3	0	1275	A	C4-C5-C6	6.15	120.07	117.00
3	0	1554	G	O4'-C1'-N9	6.15	113.12	108.20
3	0	1799	A	C4-C5-C6	6.15	120.07	117.00
3	0	141	A	C4-C5-C6	6.15	120.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1911	C	C6-N1-C1'	-6.15	113.42	120.80
3	0	61	C	C2-N1-C1'	6.14	125.56	118.80
3	0	314	A	C4-C5-C6	6.14	120.07	117.00
3	0	562	A	O4'-C1'-N9	6.14	113.12	108.20
3	0	1347	C	N3-C4-N4	6.14	122.30	118.00
3	0	1764	G	O4'-C1'-N9	6.14	113.11	108.20
3	0	1828	G	O4'-C1'-N9	6.14	113.11	108.20
3	0	2191	C	N3-C4-N4	6.14	122.30	118.00
3	0	637	C	N3-C4-N4	6.14	122.30	118.00
3	0	832	G	O4'-C1'-N9	6.14	113.11	108.20
3	0	1325	G	O4'-C1'-N9	6.14	113.11	108.20
3	0	1941	A	C4-C5-C6	6.14	120.07	117.00
3	0	1197	A	C4-C5-C6	6.14	120.07	117.00
3	0	1460	A	C4-C5-C6	6.14	120.07	117.00
3	0	2256	A	C4-C5-C6	6.14	120.07	117.00
2	1	70	C	N3-C4-N4	6.14	122.30	118.00
3	0	159	G	N3-C2-N2	6.14	124.20	119.90
3	0	190	A	C4-C5-C6	6.14	120.07	117.00
3	0	870	U	O4'-C1'-N1	6.14	113.11	108.20
3	0	1694	A	C5-C6-N6	-6.14	118.79	123.70
3	0	1738	A	C4-C5-C6	6.14	120.07	117.00
3	0	1966	A	C4-C5-C6	6.14	120.07	117.00
3	0	1589	A	C4-C5-C6	6.14	120.07	117.00
1	f	1259	CYS	C-N-CA	-6.14	106.36	121.70
3	0	55	A	C4-C5-C6	6.14	120.07	117.00
3	0	184	A	C4-C5-C6	6.14	120.07	117.00
3	0	406	A	C4-C5-C6	6.14	120.07	117.00
3	0	1311	A	O4'-C1'-N9	6.14	113.11	108.20
3	0	1829	A	O4'-C1'-N9	6.14	113.11	108.20
3	0	2061	A	C4-C5-C6	6.14	120.07	117.00
3	0	2170	A	C4-C5-C6	6.14	120.07	117.00
3	0	810	U	O4'-C1'-N1	6.13	113.11	108.20
3	0	1806	C	N3-C4-N4	6.13	122.29	118.00
3	0	1892	U	O4'-C1'-N1	6.13	113.11	108.20
3	0	502	A	C4-C5-C6	6.13	120.07	117.00
3	0	552	G	O4'-C1'-N9	6.13	113.11	108.20
3	0	1179	C	N3-C4-N4	6.13	122.29	118.00
3	0	1492	C	N3-C4-N4	6.13	122.29	118.00
3	0	1613	G	C5-C6-O6	-6.13	124.92	128.60
3	0	504	A	C4-C5-C6	6.13	120.06	117.00
3	0	1621	C	N3-C4-N4	6.13	122.29	118.00
3	0	1956	A	C4-C5-C6	6.13	120.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1324	G	O4'-C1'-N9	6.13	113.10	108.20
3	0	1373	A	C4-C5-C6	6.13	120.06	117.00
3	0	124	A	C4-C5-C6	6.13	120.06	117.00
3	0	399	U	O4'-C1'-N1	6.13	113.10	108.20
3	0	658	A	C4-C5-C6	6.13	120.06	117.00
3	0	1420	A	C5-C6-N6	-6.13	118.80	123.70
3	0	1449	C	N3-C4-N4	6.13	122.29	118.00
3	0	1989	A	C5-C6-N1	-6.13	114.64	117.70
3	0	2003	A	O4'-C1'-N9	6.13	113.10	108.20
39	E	316	TYR	CB-CG-CD2	-6.13	117.32	121.00
3	0	168	A	C5-C6-N6	-6.13	118.80	123.70
3	0	1820	A	C5-C6-N6	-6.13	118.80	123.70
2	1	62	A	C5-C6-N6	-6.12	118.80	123.70
3	0	257	A	C4-C5-C6	6.12	120.06	117.00
3	0	1317	A	C4-C5-C6	6.12	120.06	117.00
3	0	1367	A	C4-C5-C6	6.12	120.06	117.00
3	0	1872	G	O4'-C1'-N9	6.12	113.10	108.20
3	0	2200	G	O4'-C1'-N9	6.12	113.10	108.20
1	f	1153	ASP	C-N-CA	6.12	137.00	121.70
3	0	137	C	N3-C4-N4	6.12	122.28	118.00
3	0	783	A	C4-C5-C6	6.12	120.06	117.00
3	0	1264	A	C5-C6-N6	-6.12	118.80	123.70
3	0	1662	A	C4-C5-C6	6.12	120.06	117.00
3	0	1982	G	C5'-C4'-C3'	-6.12	106.21	116.00
3	0	472	A	C4-C5-C6	6.12	120.06	117.00
3	0	719	G	O4'-C1'-N9	6.12	113.09	108.20
3	0	2187	G	O4'-C1'-N9	6.12	113.09	108.20
3	0	392	A	C5-C6-N1	-6.12	114.64	117.70
3	0	39	A	O4'-C1'-N9	6.11	113.09	108.20
3	0	889	A	C4-C5-C6	6.11	120.06	117.00
3	0	1294	G	O4'-C1'-N9	6.11	113.09	108.20
3	0	1458	A	C4-C5-C6	6.11	120.06	117.00
3	0	1522	A	C5-C6-N6	-6.11	118.81	123.70
3	0	1601	G	O4'-C1'-N9	6.11	113.09	108.20
3	0	1944	A	O4'-C1'-N9	6.11	113.09	108.20
3	0	1378	C	N3-C4-N4	6.11	122.28	118.00
3	0	312	C	N3-C4-N4	6.11	122.28	118.00
3	0	585	A	C4-C5-C6	6.11	120.06	117.00
3	0	920	A	C4-C5-C6	6.11	120.06	117.00
3	0	1001	G	O4'-C1'-N9	6.11	113.09	108.20
3	0	1263	A	C4-C5-C6	6.11	120.06	117.00
3	0	1309	C	N3-C4-N4	6.11	122.28	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1689	C	O4'-C1'-N1	6.11	113.09	108.20
3	0	817	A	C4-C5-C6	6.11	120.06	117.00
3	0	583	C	N3-C4-N4	6.11	122.28	118.00
3	0	2125	A	C4-C5-C6	6.11	120.05	117.00
3	0	1542	U	O4'-C1'-N1	6.10	113.08	108.20
3	0	212	G	O4'-C1'-N9	6.10	113.08	108.20
3	0	1581	G	C5-C6-O6	-6.10	124.94	128.60
3	0	1763	C	N3-C4-N4	6.10	122.27	118.00
30	i	121	ALA	N-CA-CB	6.10	118.64	110.10
3	0	208	G	O4'-C1'-N9	6.10	113.08	108.20
3	0	2051	A	C5-C6-N6	-6.10	118.82	123.70
3	0	2319	C	O4'-C1'-N1	6.10	113.08	108.20
1	f	1039	ARG	CB-CA-C	6.10	122.60	110.40
2	1	24	C	N3-C4-N4	6.10	122.27	118.00
3	0	22	A	C5-C6-N6	-6.10	118.82	123.70
3	0	865	A	C4-C5-C6	6.10	120.05	117.00
3	0	1489	C	N3-C4-N4	6.10	122.27	118.00
3	0	2032	C	C6-N1-C1'	-6.10	113.48	120.80
3	0	2153	A	O4'-C1'-N9	6.10	113.08	108.20
3	0	569	A	C4-C5-C6	6.10	120.05	117.00
3	0	1185	A	C5-C6-N6	-6.10	118.82	123.70
3	0	1505	C	N3-C4-N4	6.10	122.27	118.00
3	0	349	A	C4-C5-C6	6.10	120.05	117.00
3	0	718	A	C5-C6-N6	-6.10	118.82	123.70
3	0	417	A	C4-C5-C6	6.09	120.05	117.00
3	0	1201	A	C4-C5-C6	6.09	120.05	117.00
3	0	1319	A	C5-C6-N6	-6.09	118.83	123.70
33	N	19	THR	N-CA-CB	6.09	121.88	110.30
3	0	1469	A	O4'-C1'-N9	6.09	113.07	108.20
3	0	2074	A	C4-C5-C6	6.09	120.05	117.00
46	C	331	ARG	C-N-CA	6.09	136.93	121.70
3	0	54	C	N3-C4-N4	6.09	122.27	118.00
3	0	334	G	O4'-C1'-N9	6.09	113.07	108.20
3	0	520	A	C4-C5-C6	6.09	120.05	117.00
3	0	879	C	N3-C4-N4	6.09	122.27	118.00
3	0	916	A	C4-C5-C6	6.09	120.05	117.00
3	0	1332	A	C5-C6-N1	-6.09	114.65	117.70
3	0	1444	C	N3-C4-N4	6.09	122.26	118.00
3	0	536	A	O4'-C1'-N9	6.09	113.07	108.20
3	0	2010	A	C4-C5-C6	6.09	120.04	117.00
3	0	2172	A	C5-C6-N6	-6.09	118.83	123.70
3	0	1740	G	C5-C6-O6	-6.09	124.95	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	K	23	PHE	CB-CG-CD2	6.09	125.06	120.80
3	0	905	A	C4-C5-C6	6.09	120.04	117.00
3	0	1223	A	C5-C6-N6	-6.09	118.83	123.70
2	1	58	A	C4-C5-C6	6.08	120.04	117.00
3	0	1518	C	N3-C4-C5	-6.08	119.47	121.90
3	0	1635	A	C4-C5-C6	6.08	120.04	117.00
3	0	1787	U	O4'-C1'-N1	6.08	113.07	108.20
22	F	85	PHE	CB-CG-CD1	6.08	125.06	120.80
2	1	34	A	C4-C5-C6	6.08	120.04	117.00
3	0	653	A	C4-C5-C6	6.08	120.04	117.00
3	0	701	C	O4'-C1'-N1	6.08	113.07	108.20
3	0	737	U	O4'-C1'-N1	6.08	113.07	108.20
3	0	1646	C	N3-C4-N4	6.08	122.26	118.00
3	0	2110	C	N3-C4-N4	6.08	122.26	118.00
3	0	694	A	C4-C5-C6	6.08	120.04	117.00
3	0	1186	C	N3-C4-N4	6.08	122.26	118.00
3	0	1395	U	O4'-C1'-N1	6.08	113.07	108.20
3	0	607	A	C4-C5-C6	6.08	120.04	117.00
3	0	1354	G	O4'-C1'-N9	6.08	113.06	108.20
3	0	160	A	O4'-C1'-N9	6.08	113.06	108.20
3	0	461	C	N3-C4-N4	6.08	122.25	118.00
3	0	586	A	C4-C5-C6	6.08	120.04	117.00
3	0	1314	A	C4-C5-C6	6.08	120.04	117.00
3	0	1597	A	C4-C5-C6	6.08	120.04	117.00
3	0	287	A	C4-C5-C6	6.08	120.04	117.00
1	f	772	TYR	C-N-CA	6.08	136.89	121.70
3	0	434	A	C5-C6-N1	-6.08	114.66	117.70
3	0	450	A	C5-C6-N6	-6.08	118.84	123.70
3	0	769	A	C4-C5-C6	6.08	120.04	117.00
3	0	1333	A	O4'-C1'-N9	6.08	113.06	108.20
3	0	2081	A	C5-C6-N6	-6.08	118.84	123.70
3	0	1373	A	C5-C6-N6	-6.07	118.84	123.70
3	0	975	U	O4'-C1'-N1	6.07	113.06	108.20
3	0	1403	A	C5-C6-N1	-6.07	114.66	117.70
3	0	2317	A	C4-C5-C6	6.07	120.04	117.00
2	1	59	A	C4-C5-C6	6.07	120.03	117.00
3	0	99	U	O4'-C1'-N1	6.07	113.06	108.20
3	0	185	A	C4-C5-C6	6.07	120.03	117.00
3	0	272	G	P-O3'-C3'	6.07	126.98	119.70
3	0	1374	C	N3-C4-N4	6.07	122.25	118.00
3	0	1795	A	C5-C6-N6	-6.07	118.84	123.70
33	N	93	ALA	N-CA-CB	6.07	118.60	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	293	LYS	C-N-CA	6.07	136.87	121.70
3	0	863	A	C5-C6-N6	-6.07	118.84	123.70
3	0	1932	A	C5-C6-N6	-6.07	118.84	123.70
3	0	2226	A	C4-C5-C6	6.07	120.03	117.00
3	0	2286	A	C5-C6-N1	-6.07	114.67	117.70
46	C	262	ALA	N-CA-CB	6.07	118.60	110.10
3	0	833	A	O4'-C1'-N9	6.07	113.06	108.20
3	0	995	C	N3-C4-N4	6.07	122.25	118.00
3	0	1670	C	N3-C4-N4	6.07	122.25	118.00
3	0	107	A	C4-C5-C6	6.07	120.03	117.00
3	0	111	A	C4-C5-C6	6.07	120.03	117.00
3	0	330	A	C4-C5-C6	6.07	120.03	117.00
3	0	684	A	C4-C5-C6	6.07	120.03	117.00
3	0	2023	U	O4'-C1'-N1	6.07	113.05	108.20
3	0	66	U	O4'-C1'-N1	6.06	113.05	108.20
3	0	285	A	O4'-C1'-N9	6.06	113.05	108.20
3	0	972	A	C4-C5-C6	6.06	120.03	117.00
3	0	1989	A	O4'-C1'-N9	6.06	113.05	108.20
3	0	503	A	C4-C5-C6	6.06	120.03	117.00
3	0	570	U	O4'-C1'-N1	6.06	113.05	108.20
3	0	923	A	C5-C6-N6	-6.06	118.85	123.70
3	0	1674	G	O4'-C1'-N9	6.06	113.05	108.20
3	0	11	A	C4-C5-C6	6.06	120.03	117.00
3	0	429	C	N3-C4-N4	6.06	122.24	118.00
3	0	862	A	C4-C5-C6	6.06	120.03	117.00
3	0	49	C	N3-C4-N4	6.06	122.24	118.00
3	0	132	G	O4'-C1'-N9	6.06	113.05	108.20
3	0	531	A	C4-C5-C6	6.06	120.03	117.00
3	0	833	A	C4-C5-C6	6.06	120.03	117.00
3	0	869	G	O4'-C1'-N9	6.06	113.05	108.20
3	0	48	G	O4'-C1'-N9	6.06	113.05	108.20
3	0	760	C	N3-C4-N4	6.06	122.24	118.00
3	0	910	A	C4-C5-C6	6.06	120.03	117.00
3	0	1330	C	N3-C4-N4	6.06	122.24	118.00
3	0	2068	A	C5-C6-N6	-6.06	118.85	123.70
3	0	2081	A	C4-C5-C6	6.06	120.03	117.00
3	0	153	C	N3-C4-N4	6.06	122.24	118.00
3	0	1341	A	C4-C5-C6	6.06	120.03	117.00
3	0	1427	U	O4'-C1'-N1	6.06	113.05	108.20
3	0	1956	A	O4'-C1'-N9	6.06	113.05	108.20
3	0	1979	C	O4'-C1'-N1	6.06	113.04	108.20
3	0	454	A	C4-C5-C6	6.05	120.03	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	621	A	C4-C5-C6	6.05	120.03	117.00
3	0	866	A	C4-C5-C6	6.05	120.03	117.00
3	0	2164	A	C4-C5-C6	6.05	120.03	117.00
3	0	2240	C	N3-C4-N4	6.05	122.24	118.00
1	f	1333	ALA	N-CA-CB	6.05	118.57	110.10
3	0	64	A	C4-C5-C6	6.05	120.03	117.00
3	0	168	A	C4-C5-C6	6.05	120.03	117.00
3	0	450	A	C4-C5-C6	6.05	120.03	117.00
3	0	581	A	C4-C5-C6	6.05	120.03	117.00
3	0	747	U	O4'-C1'-N1	6.05	113.04	108.20
3	0	749	C	N3-C4-N4	6.05	122.24	118.00
3	0	917	A	C4-C5-C6	6.05	120.03	117.00
3	0	1541	C	N3-C4-N4	6.05	122.24	118.00
46	C	630	TYR	CA-C-N	6.05	128.30	116.20
3	0	110	U	O4'-C1'-N1	6.05	113.04	108.20
3	0	202	C	N3-C4-N4	6.05	122.23	118.00
3	0	333	C	N3-C4-N4	6.05	122.23	118.00
3	0	715	U	C2-N1-C1'	6.05	124.96	117.70
3	0	773	U	O4'-C1'-N1	6.05	113.04	108.20
3	0	1453	A	C4-C5-C6	6.05	120.02	117.00
3	0	1552	A	O4'-C1'-N9	6.05	113.04	108.20
3	0	2219	A	O4'-C1'-N9	6.05	113.04	108.20
3	0	279	A	C5-C6-N6	-6.05	118.86	123.70
3	0	659	A	C4-C5-C6	6.05	120.02	117.00
2	1	74	C	O4'-C1'-N1	6.05	113.04	108.20
3	0	258	C	N3-C4-C5	-6.05	119.48	121.90
3	0	1415	G	O4'-C1'-N9	6.05	113.04	108.20
3	0	1959	C	N3-C4-N4	6.05	122.23	118.00
39	E	313	LEU	C-N-CA	6.05	135.00	122.30
3	0	1796	C	N3-C4-N4	6.04	122.23	118.00
3	0	2221	A	C5-C6-N6	-6.04	118.86	123.70
2	1	4	A	O4'-C1'-N9	6.04	113.03	108.20
3	0	65	A	C4-C5-C6	6.04	120.02	117.00
3	0	173	A	C4-C5-C6	6.04	120.02	117.00
3	0	965	C	N3-C4-N4	6.04	122.23	118.00
3	0	1360	A	C4-C5-C6	6.04	120.02	117.00
3	0	1465	A	C4-C5-C6	6.04	120.02	117.00
3	0	1544	A	C4-C5-C6	6.04	120.02	117.00
3	0	576	A	C4-C5-C6	6.04	120.02	117.00
3	0	721	C	O4'-C1'-N1	6.04	113.03	108.20
3	0	959	A	O4'-C1'-N9	6.04	113.03	108.20
3	0	1287	C	N3-C4-N4	6.04	122.23	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	293	U	O4'-C1'-N1	6.04	113.03	108.20
3	0	808	G	O4'-C1'-N9	6.04	113.03	108.20
3	0	232	C	N3-C4-N4	6.04	122.23	118.00
3	0	249	A	C4-C5-C6	6.04	120.02	117.00
3	0	581	A	C5-C6-N6	-6.04	118.87	123.70
3	0	786	A	C4-C5-C6	6.04	120.02	117.00
3	0	1681	A	C5-C6-N6	-6.04	118.87	123.70
3	0	374	G	C5-C6-O6	-6.04	124.98	128.60
3	0	528	U	O4'-C1'-N1	6.04	113.03	108.20
3	0	1227	A	C5-C6-N1	-6.04	114.68	117.70
3	0	160	A	C4-C5-C6	6.04	120.02	117.00
3	0	1246	A	C4-C5-C6	6.04	120.02	117.00
3	0	1457	A	C4-C5-C6	6.04	120.02	117.00
2	1	20	A	C4-C5-C6	6.03	120.02	117.00
3	0	177	A	C4-C5-C6	6.03	120.02	117.00
3	0	742	A	O4'-C1'-N9	6.03	113.03	108.20
3	0	928	C	N3-C4-N4	6.03	122.22	118.00
3	0	1761	G	O4'-C1'-N9	6.03	113.03	108.20
3	0	575	A	C4-C5-C6	6.03	120.02	117.00
3	0	1614	A	C4-C5-C6	6.03	120.02	117.00
3	0	1893	A	C4-C5-C6	6.03	120.02	117.00
3	0	2276	A	C4-C5-C6	6.03	120.02	117.00
3	0	2288	A	C4-C5-C6	6.03	120.02	117.00
2	1	1	A	C4-C5-C6	6.03	120.02	117.00
3	0	889	A	C5-C6-N1	-6.03	114.68	117.70
3	0	1794	A	C4-C5-C6	6.03	120.02	117.00
3	0	2012	A	C5-C6-N6	-6.03	118.88	123.70
3	0	2120	C	O4'-C1'-N1	6.03	113.03	108.20
3	0	447	A	C4-C5-C6	6.03	120.01	117.00
3	0	658	A	C5-C6-N6	-6.03	118.88	123.70
3	0	688	G	O4'-C1'-N9	6.03	113.02	108.20
3	0	728	A	C4-C5-C6	6.03	120.01	117.00
3	0	981	G	O4'-C1'-N9	6.03	113.02	108.20
3	0	710	A	C5-C6-N1	-6.03	114.69	117.70
3	0	1231	G	O4'-C1'-N9	6.03	113.02	108.20
3	0	2009	A	C4-C5-C6	6.03	120.01	117.00
3	0	518	C	N3-C4-N4	6.03	122.22	118.00
3	0	855	G	O4'-C1'-N9	6.03	113.02	108.20
3	0	1322	G	O4'-C1'-N9	6.03	113.02	108.20
3	0	1957	U	O4'-C1'-N1	6.03	113.02	108.20
3	0	2243	A	C5-C6-N1	-6.03	114.69	117.70
3	0	128	U	O4'-C1'-N1	6.02	113.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	771	A	C4-C5-C6	6.02	120.01	117.00
3	0	2207	A	C4-C5-C6	6.02	120.01	117.00
3	0	102	A	C4-C5-C6	6.02	120.01	117.00
3	0	595	A	C4-C5-C6	6.02	120.01	117.00
3	0	703	A	C4-C5-C6	6.02	120.01	117.00
3	0	724	A	O4'-C1'-N9	6.02	113.02	108.20
3	0	1222	A	C4-C5-C6	6.02	120.01	117.00
3	0	2079	G	N3-C2-N2	6.02	124.11	119.90
3	0	122	A	C4-C5-C6	6.02	120.01	117.00
3	0	175	A	C4-C5-C6	6.02	120.01	117.00
3	0	467	A	C4-C5-C6	6.02	120.01	117.00
3	0	568	G	O4'-C1'-N9	6.02	113.01	108.20
3	0	898	A	C4-C5-C6	6.02	120.01	117.00
3	0	1297	A	C4-C5-C6	6.02	120.01	117.00
3	0	1657	A	C5-C6-N1	-6.02	114.69	117.70
3	0	1983	C	P-O5'-C5'	6.02	130.53	120.90
3	0	1989	A	C4-C5-C6	6.02	120.01	117.00
3	0	525	A	C4-C5-C6	6.02	120.01	117.00
3	0	933	C	N3-C4-N4	6.02	122.21	118.00
3	0	1924	A	C4-C5-C6	6.02	120.01	117.00
3	0	2304	A	C4-C5-C6	6.01	120.01	117.00
2	1	43	A	C4-C5-C6	6.01	120.01	117.00
3	0	358	C	N3-C4-N4	6.01	122.21	118.00
3	0	414	A	C5-C6-N6	-6.01	118.89	123.70
3	0	925	C	N3-C4-N4	6.01	122.21	118.00
3	0	2270	G	O4'-C1'-N9	6.01	113.01	108.20
3	0	526	A	C5-C6-N6	-6.01	118.89	123.70
3	0	1615	A	C4-C5-C6	6.01	120.00	117.00
3	0	1925	A	O4'-C1'-N9	6.01	113.01	108.20
3	0	2133	C	N3-C4-N4	6.01	122.21	118.00
3	0	845	A	C4-C5-C6	6.01	120.00	117.00
3	0	356	C	N3-C4-N4	6.01	122.20	118.00
3	0	960	A	C4-C5-C6	6.01	120.00	117.00
3	0	1807	C	N3-C4-N4	6.01	122.20	118.00
3	0	123	A	C4-C5-C6	6.01	120.00	117.00
3	0	915	A	C4-C5-C6	6.01	120.00	117.00
3	0	1337	G	O4'-C1'-N9	6.01	113.00	108.20
3	0	1458	A	O4'-C1'-N9	6.01	113.00	108.20
3	0	1669	A	O4'-C1'-N9	6.01	113.00	108.20
2	1	28	G	O4'-C1'-N9	6.00	113.00	108.20
3	0	257	A	C5-C6-N1	-6.00	114.70	117.70
3	0	997	G	O4'-C1'-N9	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1318	A	C4-C5-C6	6.00	120.00	117.00
3	0	1359	C	N3-C4-N4	6.00	122.20	118.00
3	0	1614	A	C5-C6-N1	-6.00	114.70	117.70
3	0	1681	A	C4-C5-C6	6.00	120.00	117.00
3	0	2040	A	O4'-C1'-N9	6.00	113.00	108.20
3	0	1516	A	O4'-C1'-N9	6.00	113.00	108.20
3	0	1539	A	C4-C5-C6	6.00	120.00	117.00
3	0	970	G	O4'-C1'-N9	6.00	113.00	108.20
3	0	2131	A	O4'-C1'-N9	6.00	113.00	108.20
3	0	2299	A	C5-C6-N6	-6.00	118.90	123.70
3	0	215	A	C4-C5-C6	6.00	120.00	117.00
3	0	638	C	N3-C4-N4	6.00	122.20	118.00
3	0	690	A	C4-C5-C6	6.00	120.00	117.00
3	0	775	A	C4-C5-C6	6.00	120.00	117.00
3	0	1205	A	O4'-C1'-N9	6.00	113.00	108.20
3	0	1247	A	O4'-C1'-N9	6.00	113.00	108.20
3	0	2242	G	O4'-C1'-N9	6.00	113.00	108.20
3	0	76	G	O4'-C1'-N9	6.00	113.00	108.20
3	0	797	G	O4'-C1'-N9	6.00	113.00	108.20
3	0	984	A	C4-C5-C6	5.99	120.00	117.00
3	0	1388	G	O4'-C1'-N9	5.99	112.99	108.20
3	0	1642	G	N3-C2-N2	5.99	124.09	119.90
3	0	1735	U	O4'-C1'-N1	5.99	112.99	108.20
3	0	304	A	C4-C5-C6	5.99	120.00	117.00
3	0	1638	A	C5-C6-N6	-5.99	118.91	123.70
3	0	2001	A	C4-C5-C6	5.99	120.00	117.00
3	0	428	C	N3-C4-N4	5.99	122.19	118.00
3	0	643	C	N3-C4-N4	5.99	122.19	118.00
3	0	959	A	C4-C5-C6	5.99	119.99	117.00
3	0	1220	A	C4-C5-C6	5.99	119.99	117.00
3	0	1811	C	N3-C4-C5	-5.99	119.50	121.90
3	0	1875	G	O4'-C1'-N9	5.99	112.99	108.20
3	0	2267	A	C4-C5-C6	5.99	120.00	117.00
3	0	1066	C	N3-C4-N4	5.99	122.19	118.00
3	0	1605	A	C5-C6-N1	-5.99	114.71	117.70
3	0	2039	A	C4-C5-C6	5.99	119.99	117.00
3	0	380	U	O4'-C1'-N1	5.99	112.99	108.20
3	0	1785	G	O4'-C1'-N9	5.99	112.99	108.20
3	0	2239	A	O4'-C1'-N9	5.99	112.99	108.20
3	0	1383	A	O4'-C1'-N9	5.98	112.99	108.20
3	0	536	A	C5-C6-N1	-5.98	114.71	117.70
3	0	910	A	C5-C6-N6	-5.98	118.91	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	912	A	C4-C5-C6	5.98	119.99	117.00
3	0	2293	A	C4-C5-C6	5.98	119.99	117.00
3	0	174	U	O4'-C1'-N1	5.98	112.98	108.20
3	0	522	A	C5-C6-N1	-5.98	114.71	117.70
3	0	554	C	N3-C4-N4	5.98	122.19	118.00
3	0	562	A	C4-C5-C6	5.98	119.99	117.00
3	0	782	A	C4-C5-C6	5.98	119.99	117.00
3	0	795	U	O4'-C1'-N1	5.98	112.98	108.20
3	0	1539	A	C5-C6-N1	-5.98	114.71	117.70
3	0	1946	C	O4'-C1'-N1	5.98	112.98	108.20
2	1	11	C	N3-C4-N4	5.98	122.19	118.00
3	0	360	A	C4-C5-C6	5.98	119.99	117.00
3	0	902	A	C4-C5-C6	5.98	119.99	117.00
3	0	1555	C	N3-C4-N4	5.98	122.19	118.00
3	0	1815	C	N3-C4-N4	5.98	122.19	118.00
2	1	62	A	C4-C5-C6	5.98	119.99	117.00
3	0	463	A	C4-C5-C6	5.98	119.99	117.00
3	0	1361	C	N3-C4-N4	5.98	122.18	118.00
3	0	1365	A	C4-C5-C6	5.98	119.99	117.00
3	0	1523	A	C4-C5-C6	5.98	119.99	117.00
3	0	1578	C	N3-C4-N4	5.98	122.18	118.00
3	0	348	A	C4-C5-C6	5.98	119.99	117.00
3	0	2142	C	N3-C4-N4	5.98	122.18	118.00
3	0	125	A	C5-C6-N1	-5.97	114.71	117.70
3	0	1266	A	C5-C6-N6	-5.97	118.92	123.70
3	0	381	A	C4-C5-C6	5.97	119.99	117.00
3	0	626	C	N3-C4-N4	5.97	122.18	118.00
3	0	711	A	C4-C5-C6	5.97	119.99	117.00
3	0	1357	C	N3-C4-N4	5.97	122.18	118.00
3	0	1711	A	C4-C5-C6	5.97	119.99	117.00
3	0	2063	C	N3-C4-C5	-5.97	119.51	121.90
3	0	2205	A	C4-C5-C6	5.97	119.99	117.00
3	0	2226	A	C5-C6-N6	-5.97	118.92	123.70
3	0	2320	A	C5-C6-N6	-5.97	118.92	123.70
3	0	149	A	C5-C6-N6	-5.97	118.92	123.70
3	0	1570	U	O4'-C1'-N1	5.97	112.98	108.20
3	0	2021	U	O4'-C1'-N1	5.97	112.98	108.20
2	1	63	A	O4'-C1'-N9	5.97	112.98	108.20
3	0	434	A	C4-C5-C6	5.97	119.98	117.00
3	0	467	A	C5-C6-N6	-5.97	118.92	123.70
3	0	608	C	O4'-C1'-N1	5.97	112.97	108.20
3	0	668	C	N3-C4-N4	5.97	122.18	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	852	A	C4-C5-C6	5.97	119.98	117.00
3	0	1982	G	C3'-C2'-C1'	5.97	106.27	101.50
1	f	192	ALA	O-C-N	5.97	132.25	122.70
1	f	294	ALA	O-C-N	5.97	132.25	122.70
3	0	69	C	N3-C4-N4	5.97	122.18	118.00
3	0	303	C	N3-C4-N4	5.97	122.18	118.00
3	0	444	A	C4-C5-C6	5.97	119.98	117.00
3	0	571	A	C4-C5-C6	5.97	119.98	117.00
3	0	784	A	C4-C5-C6	5.97	119.98	117.00
3	0	1827	A	C4-C5-C6	5.97	119.98	117.00
3	0	26	A	O4'-C1'-N9	5.96	112.97	108.20
3	0	44	C	O4'-C1'-N1	5.96	112.97	108.20
3	0	639	A	C4-C5-C6	5.96	119.98	117.00
3	0	689	A	C4-C5-C6	5.96	119.98	117.00
3	0	974	A	C5-C6-N6	-5.96	118.93	123.70
3	0	1437	C	N3-C4-N4	5.96	122.17	118.00
3	0	1675	A	C4-C5-C6	5.96	119.98	117.00
43	G	136	TRP	CA-CB-CG	5.96	125.03	113.70
3	0	2141	A	C4-C5-C6	5.96	119.98	117.00
3	0	2153	A	C4-C5-C6	5.96	119.98	117.00
3	0	306	U	O4'-C1'-N1	5.96	112.97	108.20
3	0	716	U	O4'-C1'-N1	5.96	112.97	108.20
3	0	1832	U	O4'-C1'-N1	5.96	112.97	108.20
3	0	2234	A	C5-C6-N6	-5.96	118.93	123.70
3	0	700	U	O4'-C1'-N1	5.96	112.97	108.20
3	0	884	A	C4-C5-C6	5.96	119.98	117.00
3	0	1477	A	C4-C5-C6	5.96	119.98	117.00
46	C	690	TYR	CB-CG-CD1	5.96	124.58	121.00
3	0	474	C	N3-C4-N4	5.96	122.17	118.00
3	0	497	C	N3-C4-N4	5.96	122.17	118.00
3	0	861	A	C4-C5-C6	5.96	119.98	117.00
26	J	189	TYR	CB-CG-CD2	-5.96	117.43	121.00
3	0	250	A	C4-C5-C6	5.96	119.98	117.00
3	0	480	C	N3-C4-N4	5.96	122.17	118.00
3	0	2006	A	C4-C5-C6	5.96	119.98	117.00
3	0	164	G	O4'-C1'-N9	5.95	112.96	108.20
3	0	512	A	C4-C5-C6	5.95	119.98	117.00
3	0	754	G	O4'-C1'-N9	5.95	112.96	108.20
3	0	934	C	N3-C4-C5	-5.95	119.52	121.90
3	0	1209	U	O4'-C1'-N1	5.95	112.96	108.20
3	0	1298	C	N3-C4-N4	5.95	122.17	118.00
3	0	1534	A	C5-C6-N6	-5.95	118.94	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2054	C	N3-C4-N4	5.95	122.17	118.00
3	0	2287	C	N3-C4-N4	5.95	122.17	118.00
2	1	41	A	C5-C6-N6	-5.95	118.94	123.70
3	0	352	A	C4-C5-C6	5.95	119.98	117.00
3	0	278	A	O4'-C1'-N9	5.95	112.96	108.20
3	0	894	A	C4-C5-C6	5.95	119.97	117.00
3	0	1188	G	O4'-C1'-N9	5.95	112.96	108.20
3	0	1615	A	O4'-C1'-N9	5.95	112.96	108.20
3	0	1629	C	N3-C4-N4	5.95	122.17	118.00
3	0	1769	A	C4-C5-C6	5.95	119.97	117.00
3	0	701	C	N3-C4-N4	5.95	122.16	118.00
3	0	1475	A	C4-C5-C6	5.95	119.97	117.00
3	0	1750	G	C5-C6-O6	-5.95	125.03	128.60
3	0	2044	A	C4-C5-C6	5.95	119.97	117.00
3	0	2205	A	C5-C6-N6	-5.95	118.94	123.70
3	0	2234	A	C4-C5-C6	5.95	119.97	117.00
3	0	396	C	N3-C4-N4	5.95	122.16	118.00
3	0	1986	A	C4-C5-C6	5.95	119.97	117.00
3	0	2272	A	O4'-C1'-N9	5.95	112.96	108.20
2	1	4	A	C5-C6-N6	-5.95	118.94	123.70
3	0	788	A	C4-C5-C6	5.95	119.97	117.00
3	0	1240	A	C5-C6-N6	-5.95	118.94	123.70
3	0	1356	C	N3-C4-N4	5.95	122.16	118.00
3	0	6	G	O4'-C1'-N9	5.94	112.95	108.20
3	0	401	A	C4-C5-C6	5.94	119.97	117.00
3	0	527	A	C4-C5-C6	5.94	119.97	117.00
3	0	1926	G	O4'-C1'-N9	5.94	112.95	108.20
3	0	387	C	N3-C4-N4	5.94	122.16	118.00
3	0	561	A	C5-C6-N6	-5.94	118.95	123.70
3	0	604	A	C4-C5-C6	5.94	119.97	117.00
3	0	645	A	C5-C6-N6	-5.94	118.94	123.70
3	0	798	U	O4'-C1'-N1	5.94	112.95	108.20
3	0	1223	A	C4-C5-C6	5.94	119.97	117.00
3	0	2011	A	C4-C5-C6	5.94	119.97	117.00
2	1	60	C	N3-C4-N4	5.94	122.16	118.00
3	0	121	A	C4-C5-C6	5.94	119.97	117.00
3	0	646	A	C4-C5-C6	5.94	119.97	117.00
3	0	872	A	C5-C6-N6	-5.94	118.95	123.70
3	0	1313	A	C4-C5-C6	5.94	119.97	117.00
3	0	1733	C	O4'-C1'-N1	5.94	112.95	108.20
3	0	1789	C	N3-C4-N4	5.94	122.16	118.00
3	0	98	U	O4'-C1'-N1	5.94	112.95	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1236	U	O4'-C1'-N1	5.94	112.95	108.20
3	0	197	C	N3-C4-N4	5.94	122.16	118.00
3	0	793	A	C4-C5-C6	5.94	119.97	117.00
3	0	1398	G	O4'-C1'-N9	5.94	112.95	108.20
3	0	1921	C	N3-C4-N4	5.94	122.16	118.00
3	0	236	C	N3-C4-N4	5.94	122.16	118.00
3	0	1665	C	N3-C4-N4	5.94	122.16	118.00
3	0	307	C	O4'-C1'-N1	5.93	112.95	108.20
3	0	967	A	C4-C5-C6	5.93	119.97	117.00
3	0	1230	G	O4'-C1'-N9	5.93	112.95	108.20
3	0	1262	C	N3-C4-N4	5.93	122.15	118.00
3	0	1292	A	C4-C5-C6	5.93	119.97	117.00
3	0	1851	C	N3-C4-N4	5.93	122.15	118.00
3	0	549	A	C4-C5-C6	5.93	119.97	117.00
3	0	735	A	C5-C6-N6	-5.93	118.95	123.70
3	0	1234	C	N3-C4-N4	5.93	122.15	118.00
3	0	1253	A	C4-C5-C6	5.93	119.97	117.00
3	0	2099	U	O4'-C1'-N1	5.93	112.95	108.20
3	0	1674	G	C5-C6-O6	-5.93	125.04	128.60
3	0	43	A	C4-C5-C6	5.93	119.97	117.00
3	0	62	A	C4-C5-C6	5.93	119.96	117.00
3	0	256	A	C4-C5-C6	5.93	119.97	117.00
3	0	269	A	C4-C5-C6	5.93	119.97	117.00
3	0	806	C	N3-C4-C5	-5.93	119.53	121.90
3	0	841	C	N3-C4-N4	5.93	122.15	118.00
3	0	1607	C	N3-C4-N4	5.93	122.15	118.00
3	0	1656	A	C4-C5-C6	5.93	119.97	117.00
3	0	1725	C	N3-C4-N4	5.93	122.15	118.00
3	0	239	C	N3-C4-N4	5.93	122.15	118.00
3	0	363	A	C4-C5-C6	5.93	119.96	117.00
3	0	707	C	C6-N1-C1'	-5.93	113.69	120.80
3	0	1765	G	C5-C6-O6	-5.93	125.04	128.60
3	0	319	C	N3-C4-N4	5.93	122.15	118.00
3	0	633	A	C4-C5-C6	5.93	119.96	117.00
3	0	858	A	C5-C6-N6	-5.93	118.96	123.70
3	0	2271	G	O4'-C1'-N9	5.93	112.94	108.20
1	f	1653	CYS	CA-C-N	-5.92	104.35	116.20
3	0	905	A	O4'-C1'-N9	5.92	112.94	108.20
3	0	1240	A	C4-C5-C6	5.92	119.96	117.00
3	0	1276	G	O4'-C1'-N9	5.92	112.94	108.20
3	0	1310	A	C5-C6-N1	-5.92	114.74	117.70
3	0	1683	C	N3-C4-N4	5.92	122.15	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1826	C	N3-C4-N4	5.92	122.15	118.00
3	0	1997	A	C5-C6-N1	-5.92	114.74	117.70
3	0	1068	C	N3-C4-N4	5.92	122.15	118.00
3	0	1265	G	O4'-C1'-N9	5.92	112.94	108.20
1	f	1694	ALA	N-CA-CB	5.92	118.39	110.10
3	0	28	A	C4-C5-C6	5.92	119.96	117.00
3	0	1344	G	O4'-C1'-N9	5.92	112.94	108.20
3	0	2238	G	O4'-C1'-N9	5.92	112.94	108.20
3	0	655	A	C4-C5-C6	5.92	119.96	117.00
3	0	2146	G	O4'-C1'-N9	5.92	112.93	108.20
3	0	1433	A	C4-C5-C6	5.91	119.96	117.00
3	0	133	G	O4'-C1'-N9	5.91	112.93	108.20
3	0	493	A	C4-C5-C6	5.91	119.96	117.00
3	0	1438	G	O4'-C1'-N9	5.91	112.93	108.20
3	0	1908	A	C5-C6-N6	-5.91	118.97	123.70
3	0	2174	A	C4-C5-C6	5.91	119.96	117.00
2	1	65	C	N3-C4-N4	5.91	122.14	118.00
3	0	64	A	C5-C6-N1	-5.91	114.74	117.70
3	0	81	A	C4-C5-C6	5.91	119.96	117.00
3	0	351	A	C4-C5-C6	5.91	119.95	117.00
3	0	523	A	C4-C5-C6	5.91	119.96	117.00
3	0	962	A	C4-C5-C6	5.91	119.95	117.00
3	0	1291	A	C5-C6-N1	-5.91	114.75	117.70
3	0	1306	A	C5-C6-N6	-5.91	118.97	123.70
3	0	2278	A	C4-C5-C6	5.91	119.96	117.00
3	0	1591	G	O4'-C1'-N9	5.91	112.93	108.20
3	0	1682	C	N3-C4-C5	-5.91	119.54	121.90
3	0	1748	A	O4'-C1'-N9	5.91	112.93	108.20
3	0	2052	A	C5-C6-N1	-5.91	114.75	117.70
3	0	2140	A	C4-C5-C6	5.91	119.95	117.00
3	0	281	A	C4-C5-C6	5.91	119.95	117.00
3	0	787	C	N3-C4-N4	5.91	122.13	118.00
3	0	1461	U	O4'-C1'-N1	5.91	112.92	108.20
3	0	1581	G	O4'-C1'-N9	5.91	112.92	108.20
3	0	1740	G	O4'-C1'-N9	5.91	112.92	108.20
2	1	13	C	N3-C4-N4	5.90	122.13	118.00
3	0	537	C	N3-C4-N4	5.90	122.13	118.00
3	0	922	C	O4'-C1'-N1	5.90	112.92	108.20
3	0	1375	A	C4-C5-C6	5.90	119.95	117.00
3	0	1423	A	C4-C5-C6	5.90	119.95	117.00
3	0	195	C	O4'-C1'-N1	5.90	112.92	108.20
3	0	332	C	N3-C4-N4	5.90	122.13	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	530	G	O4'-C1'-N9	5.90	112.92	108.20
3	0	1366	A	C4-C5-C6	5.90	119.95	117.00
3	0	1952	U	O4'-C1'-N1	5.90	112.92	108.20
3	0	2197	A	C4-C5-C6	5.90	119.95	117.00
3	0	160	A	C5-C6-N6	-5.90	118.98	123.70
3	0	263	G	O4'-C1'-N9	5.90	112.92	108.20
3	0	311	G	O4'-C1'-N9	5.90	112.92	108.20
3	0	432	A	O4'-C1'-N9	5.90	112.92	108.20
3	0	853	C	N3-C4-N4	5.90	122.13	118.00
3	0	1453	A	C5-C6-N6	-5.90	118.98	123.70
3	0	1686	A	O4'-C1'-N9	5.90	112.92	108.20
3	0	231	A	O4'-C1'-N9	5.90	112.92	108.20
3	0	1689	C	N3-C4-N4	5.90	122.13	118.00
3	0	1908	A	C4-C5-C6	5.90	119.95	117.00
3	0	12	U	O4'-C1'-N1	5.90	112.92	108.20
3	0	958	U	O4'-C1'-N1	5.90	112.92	108.20
3	0	1991	A	C4-C5-C6	5.90	119.95	117.00
3	0	2184	G	O4'-C1'-N9	5.90	112.92	108.20
3	0	458	C	N3-C4-N4	5.90	122.13	118.00
3	0	1377	C	N3-C4-N4	5.90	122.13	118.00
3	0	158	C	N3-C4-N4	5.89	122.13	118.00
3	0	533	C	N3-C4-N4	5.89	122.13	118.00
3	0	1937	G	O4'-C1'-N9	5.89	112.92	108.20
3	0	104	C	N3-C4-N4	5.89	122.12	118.00
3	0	1616	A	C5-C6-N1	-5.89	114.75	117.70
3	0	1809	A	C4-C5-C6	5.89	119.95	117.00
3	0	2070	A	C4-C5-C6	5.89	119.95	117.00
3	0	2192	C	N3-C4-N4	5.89	122.12	118.00
3	0	1522	A	C5-C6-N1	-5.89	114.75	117.70
3	0	2053	A	C4-C5-C6	5.89	119.95	117.00
3	0	214	C	N3-C4-N4	5.89	122.12	118.00
3	0	1403	A	C5-C6-N6	-5.89	118.99	123.70
3	0	2108	A	C4-C5-C6	5.89	119.94	117.00
3	0	2133	C	N3-C4-C5	-5.89	119.54	121.90
3	0	2265	A	C5-C6-N1	-5.89	114.75	117.70
3	0	1947	A	C4-C5-C6	5.89	119.94	117.00
3	0	123	A	C5-C6-N6	-5.89	118.99	123.70
3	0	177	A	C5-C6-N1	-5.89	114.76	117.70
3	0	390	C	N3-C4-N4	5.89	122.12	118.00
3	0	967	A	O4'-C1'-N9	5.89	112.91	108.20
3	0	1543	G	C5-C6-O6	-5.89	125.07	128.60
3	0	1992	A	C5-C6-N1	-5.89	114.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	241	A	C4-C5-C6	5.88	119.94	117.00
3	0	371	A	C5-C6-N6	-5.88	118.99	123.70
3	0	1216	G	O4'-C1'-N9	5.88	112.91	108.20
3	0	1319	A	C4-C5-C6	5.88	119.94	117.00
3	0	1738	A	O4'-C1'-N9	5.88	112.91	108.20
3	0	2116	A	C5-C6-N6	-5.88	118.99	123.70
3	0	2135	C	N3-C4-N4	5.88	122.12	118.00
3	0	1754	G	O4'-C1'-N9	5.88	112.91	108.20
3	0	1939	G	O4'-C1'-N9	5.88	112.91	108.20
3	0	1183	U	O4'-C1'-N1	5.88	112.91	108.20
3	0	1220	A	C5-C6-N6	-5.88	119.00	123.70
3	0	1233	G	O4'-C1'-N9	5.88	112.91	108.20
3	0	1291	A	C4-C5-C6	5.88	119.94	117.00
3	0	1644	A	C4-C5-C6	5.88	119.94	117.00
3	0	1883	A	C5-C6-N6	-5.88	119.00	123.70
3	0	1927	G	O4'-C1'-N9	5.88	112.90	108.20
3	0	2075	C	N3-C4-N4	5.88	122.12	118.00
3	0	2116	A	C4-C5-C6	5.88	119.94	117.00
39	E	276	LEU	C-N-CA	5.88	136.41	121.70
3	0	96	C	N3-C4-N4	5.88	122.12	118.00
3	0	1306	A	C4-C5-C6	5.88	119.94	117.00
3	0	112	A	C4-C5-C6	5.88	119.94	117.00
3	0	735	A	C4-C5-C6	5.88	119.94	117.00
3	0	142	A	C4-C5-C6	5.88	119.94	117.00
3	0	281	A	C5-C6-N1	-5.88	114.76	117.70
3	0	317	G	O4'-C1'-N9	5.88	112.90	108.20
3	0	1480	C	N3-C4-N4	5.88	122.11	118.00
3	0	2095	U	O4'-C1'-N1	5.88	112.90	108.20
3	0	26	A	C4-C5-C6	5.88	119.94	117.00
3	0	78	A	C5-C6-N6	-5.88	119.00	123.70
3	0	775	A	C5-C6-N6	-5.88	119.00	123.70
3	0	1981	C	N3-C4-C5	-5.88	119.55	121.90
3	0	2082	C	N3-C4-N4	5.88	122.11	118.00
3	0	890	C	N3-C4-N4	5.87	122.11	118.00
3	0	1205	A	C4-C5-C6	5.87	119.94	117.00
3	0	1321	U	O4'-C1'-N1	5.87	112.90	108.20
3	0	2063	C	N3-C4-N4	5.87	122.11	118.00
3	0	2256	A	C5-C6-N6	-5.87	119.00	123.70
3	0	183	C	N3-C4-N4	5.87	122.11	118.00
3	0	521	A	C4-C5-C6	5.87	119.94	117.00
3	0	1295	A	O4'-C1'-N9	5.87	112.90	108.20
3	0	2286	A	C4-C5-C6	5.87	119.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	43	A	C5-C6-N6	-5.87	119.00	123.70
3	0	1571	A	C4-C5-C6	5.87	119.94	117.00
3	0	2074	A	C5-C6-N6	-5.87	119.00	123.70
1	f	306	ARG	C-N-CA	5.87	136.37	121.70
3	0	2	A	O4'-C1'-N9	5.87	112.89	108.20
3	0	1874	G	O4'-C1'-N9	5.87	112.89	108.20
3	0	2103	C	O4'-C1'-N1	5.87	112.89	108.20
3	0	165	C	N3-C4-N4	5.87	122.11	118.00
3	0	465	G	P-O3'-C3'	5.87	126.74	119.70
3	0	767	A	C4-C5-C6	5.87	119.93	117.00
3	0	1214	C	N3-C4-N4	5.87	122.11	118.00
3	0	1610	A	C5-C6-N1	-5.87	114.77	117.70
3	0	1827	A	C5-C6-N1	-5.87	114.77	117.70
3	0	2014	C	N3-C4-N4	5.87	122.11	118.00
3	0	648	A	C4-C5-C6	5.86	119.93	117.00
3	0	1273	A	C5-C6-N6	-5.86	119.01	123.70
3	0	1997	A	C5-C6-N6	-5.86	119.01	123.70
3	0	2051	A	C4-C5-C6	5.86	119.93	117.00
3	0	2162	C	N3-C4-N4	5.86	122.11	118.00
3	0	2289	A	C4-C5-C6	5.86	119.93	117.00
3	0	2305	A	C4-C5-C6	5.86	119.93	117.00
3	0	283	U	O4'-C1'-N1	5.86	112.89	108.20
3	0	527	A	C5-C6-N6	-5.86	119.01	123.70
3	0	1982	G	O4'-C1'-N9	5.86	112.89	108.20
3	0	161	A	C5-C6-N1	-5.86	114.77	117.70
3	0	210	A	C4-C5-C6	5.86	119.93	117.00
3	0	308	C	C6-N1-C2	-5.86	117.96	120.30
3	0	531	A	C5-C6-N6	-5.86	119.01	123.70
3	0	569	A	C5-C6-N6	-5.86	119.02	123.70
3	0	974	A	C4-C5-C6	5.86	119.93	117.00
3	0	1198	A	C4-C5-C6	5.86	119.93	117.00
3	0	1565	G	C5-C6-O6	-5.86	125.09	128.60
3	0	1721	C	N3-C4-N4	5.86	122.10	118.00
3	0	2004	A	C4-C5-C6	5.86	119.93	117.00
3	0	13	U	O4'-C1'-N1	5.86	112.88	108.20
3	0	17	C	O4'-C1'-N1	5.86	112.88	108.20
3	0	522	A	C4-C5-C6	5.86	119.93	117.00
3	0	1259	C	N3-C4-N4	5.86	122.10	118.00
3	0	1343	A	C4-C5-C6	5.86	119.93	117.00
49	I	262	PHE	CB-CG-CD1	5.86	124.90	120.80
3	0	578	C	N3-C4-N4	5.85	122.10	118.00
3	0	1765	G	O4'-C1'-N9	5.85	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2197	A	O4'-C1'-N9	5.85	112.88	108.20
22	F	85	PHE	CB-CG-CD2	-5.85	116.70	120.80
1	f	256	GLU	N-CA-CB	-5.85	100.07	110.60
3	0	187	C	N3-C4-N4	5.85	122.10	118.00
3	0	1521	G	O4'-C1'-N9	5.85	112.88	108.20
3	0	2204	A	C4-C5-C6	5.85	119.93	117.00
3	0	392	A	C5-C6-N6	-5.85	119.02	123.70
3	0	612	U	O4'-C1'-N1	5.85	112.88	108.20
3	0	1264	A	C5-C6-N1	-5.85	114.78	117.70
3	0	1972	U	O4'-C1'-N1	5.85	112.88	108.20
1	f	143	LEU	C-N-CA	5.85	136.32	121.70
3	0	788	A	C5-C6-N6	-5.85	119.02	123.70
3	0	990	A	C5-C6-N6	-5.85	119.02	123.70
3	0	1930	A	O4'-C1'-N9	5.85	112.88	108.20
1	f	150	PHE	CB-CG-CD1	5.85	124.89	120.80
2	1	14	A	O4'-C1'-N9	5.85	112.88	108.20
3	0	117	C	N3-C4-N4	5.85	122.09	118.00
3	0	280	C	O4'-C1'-N1	5.85	112.88	108.20
3	0	1534	A	C5-C6-N1	-5.85	114.78	117.70
3	0	1856	C	N3-C4-N4	5.85	122.09	118.00
3	0	169	G	O4'-C1'-N9	5.85	112.88	108.20
3	0	1445	G	O4'-C1'-N9	5.85	112.88	108.20
3	0	1516	A	C4-C5-C6	5.85	119.92	117.00
3	0	1558	A	C5-C6-N1	-5.85	114.78	117.70
3	0	1823	A	C4-C5-C6	5.85	119.92	117.00
3	0	82	A	C4-C5-C6	5.84	119.92	117.00
3	0	627	C	N3-C4-N4	5.84	122.09	118.00
3	0	920	A	C5-C6-N1	-5.84	114.78	117.70
3	0	1335	A	C4-C5-C6	5.84	119.92	117.00
3	0	1580	G	O4'-C1'-N9	5.84	112.88	108.20
3	0	1625	A	C4-C5-C6	5.84	119.92	117.00
3	0	1829	A	C4-C5-C6	5.84	119.92	117.00
1	f	1044	VAL	CA-C-N	-5.84	104.35	117.20
3	0	19	A	C4-C5-C6	5.84	119.92	117.00
3	0	861	A	C5-C6-N1	-5.84	114.78	117.70
3	0	28	A	C5-C6-N6	-5.84	119.03	123.70
3	0	246	A	O4'-C1'-N9	5.84	112.87	108.20
3	0	1313	A	C5-C6-N6	-5.84	119.03	123.70
3	0	1596	C	N3-C4-N4	5.84	122.09	118.00
3	0	1676	A	C4-C5-C6	5.84	119.92	117.00
3	0	1817	A	C4-C5-C6	5.84	119.92	117.00
3	0	2171	C	N3-C4-N4	5.84	122.09	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	457	A	C4-C5-C6	5.84	119.92	117.00
3	0	668	C	N3-C4-C5	-5.84	119.56	121.90
3	0	1425	U	O4'-C1'-N1	5.84	112.87	108.20
3	0	1551	C	N3-C4-N4	5.84	122.09	118.00
3	0	1987	C	N3-C4-N4	5.84	122.09	118.00
3	0	2214	A	C5-C6-N1	-5.84	114.78	117.70
50	H	212	ARG	N-CA-CB	5.84	121.11	110.60
3	0	491	C	O4'-C1'-N1	5.84	112.87	108.20
3	0	1662	A	C5-C6-N6	-5.84	119.03	123.70
3	0	983	C	N3-C4-N4	5.84	122.08	118.00
3	0	1878	G	P-O3'-C3'	5.84	126.70	119.70
3	0	1974	G	C4'-C3'-C2'	-5.84	96.76	102.60
3	0	2071	C	N3-C4-C5	-5.84	119.56	121.90
3	0	2272	A	C4-C5-C6	5.84	119.92	117.00
2	1	63	A	C4-C5-C6	5.83	119.92	117.00
3	0	330	A	C5-C6-N6	-5.83	119.03	123.70
3	0	1790	C	N3-C4-N4	5.83	122.08	118.00
3	0	2279	A	C4-C5-C6	5.83	119.92	117.00
3	0	438	A	C4-C5-C6	5.83	119.92	117.00
3	0	538	A	C4-C5-C6	5.83	119.92	117.00
3	0	813	U	O4'-C1'-N1	5.83	112.87	108.20
3	0	1512	C	N3-C4-N4	5.83	122.08	118.00
3	0	2061	A	O4'-C1'-N9	5.83	112.87	108.20
3	0	2164	A	O4'-C1'-N9	5.83	112.87	108.20
3	0	641	C	N3-C4-N4	5.83	122.08	118.00
3	0	2016	A	C5-C6-N6	-5.83	119.03	123.70
3	0	231	A	C4-C5-C6	5.83	119.92	117.00
3	0	406	A	C5-C6-N6	-5.83	119.04	123.70
3	0	1381	G	O4'-C1'-N9	5.83	112.86	108.20
3	0	336	C	N3-C4-N4	5.83	122.08	118.00
3	0	901	A	C5-C6-N6	-5.83	119.04	123.70
3	0	571	A	C5-C6-N1	-5.83	114.79	117.70
2	1	41	A	C4-C5-C6	5.83	119.91	117.00
3	0	386	A	C5-C6-N1	-5.83	114.79	117.70
3	0	885	U	O4'-C1'-N1	5.83	112.86	108.20
3	0	1283	C	N3-C4-N4	5.83	122.08	118.00
3	0	1823	A	C5-C6-N6	-5.83	119.04	123.70
3	0	1925	A	C5-C6-N6	-5.83	119.04	123.70
3	0	2199	G	O4'-C1'-N9	5.83	112.86	108.20
26	J	103	TYR	CB-CG-CD1	5.83	124.50	121.00
1	f	257	PRO	O-C-N	-5.82	113.38	122.70
3	0	790	G	O4'-C1'-N9	5.82	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1067	A	C4-C5-C6	5.82	119.91	117.00
3	0	1273	A	C4-C5-C6	5.82	119.91	117.00
3	0	1829	A	C5-C6-N6	-5.82	119.04	123.70
3	0	2214	A	C4-C5-C6	5.82	119.91	117.00
3	0	1210	A	C5-C6-N6	-5.82	119.04	123.70
3	0	1507	A	C5-C6-N6	-5.82	119.04	123.70
3	0	1704	U	O4'-C1'-N1	5.82	112.86	108.20
3	0	2144	G	O4'-C1'-N9	5.82	112.86	108.20
3	0	646	A	C5-C6-N1	-5.82	114.79	117.70
3	0	1868	C	N3-C4-C5	-5.82	119.57	121.90
3	0	2210	G	O4'-C1'-N9	5.82	112.86	108.20
3	0	2253	G	N3-C2-N2	5.82	123.97	119.90
3	0	135	C	N3-C4-N4	5.82	122.07	118.00
3	0	781	A	C4-C5-C6	5.82	119.91	117.00
3	0	1682	C	N3-C4-N4	5.82	122.07	118.00
3	0	2203	C	N3-C4-N4	5.82	122.07	118.00
3	0	221	C	N3-C4-N4	5.82	122.07	118.00
3	0	304	A	C5-C6-N6	-5.82	119.05	123.70
3	0	704	A	C5-C6-N6	-5.82	119.05	123.70
3	0	724	A	C5-C6-N1	-5.82	114.79	117.70
3	0	745	C	N3-C4-N4	5.82	122.07	118.00
3	0	784	A	C5-C6-N6	-5.82	119.05	123.70
3	0	1383	A	C4-C5-C6	5.82	119.91	117.00
3	0	468	G	O4'-C1'-N9	5.81	112.85	108.20
3	0	967	A	C5-C6-N1	-5.81	114.79	117.70
3	0	1266	A	C4-C5-C6	5.81	119.91	117.00
3	0	1350	U	O4'-C1'-N1	5.81	112.85	108.20
3	0	1986	A	C5-C6-N1	-5.81	114.79	117.70
3	0	1227	A	C4-C5-C6	5.81	119.91	117.00
3	0	2008	G	O4'-C1'-N9	5.81	112.85	108.20
3	0	1500	U	O4'-C1'-N1	5.81	112.85	108.20
3	0	1661	G	O4'-C1'-N9	5.81	112.85	108.20
3	0	2178	C	N3-C4-N4	5.81	122.07	118.00
3	0	1210	A	C4-C5-C6	5.81	119.90	117.00
3	0	156	G	O4'-C1'-N9	5.81	112.85	108.20
3	0	451	G	O4'-C1'-N9	5.81	112.85	108.20
3	0	1519	G	O4'-C1'-N9	5.81	112.85	108.20
3	0	2297	G	O4'-C1'-N9	5.81	112.85	108.20
3	0	2300	G	O4'-C1'-N9	5.81	112.85	108.20
23	d	197	PHE	CB-CG-CD1	5.81	124.86	120.80
3	0	416	U	O4'-C1'-N1	5.81	112.84	108.20
3	0	1755	C	N3-C4-N4	5.81	122.06	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2016	A	C4-C5-C6	5.81	119.90	117.00
3	0	44	C	N3-C4-N4	5.80	122.06	118.00
3	0	499	A	O4'-C1'-N9	5.80	112.84	108.20
3	0	673	A	C4-C5-C6	5.80	119.90	117.00
3	0	894	A	C5-C6-N6	-5.80	119.06	123.70
3	0	1246	A	C5-C6-N6	-5.80	119.06	123.70
3	0	1620	A	O4'-C1'-N9	5.80	112.84	108.20
3	0	1830	A	O4'-C1'-N9	5.80	112.84	108.20
3	0	1624	A	C4-C5-C6	5.80	119.90	117.00
3	0	2132	G	O4'-C1'-N9	5.80	112.84	108.20
3	0	148	G	O4'-C1'-N9	5.80	112.84	108.20
3	0	746	A	C4-C5-C6	5.80	119.90	117.00
1	f	1022	ALA	N-CA-CB	5.80	118.22	110.10
3	0	94	C	N3-C4-N4	5.80	122.06	118.00
3	0	836	G	O4'-C1'-N9	5.80	112.84	108.20
3	0	2244	A	C5-C6-N6	-5.80	119.06	123.70
3	0	783	A	C5-C6-N6	-5.80	119.06	123.70
3	0	1252	U	O4'-C1'-N1	5.80	112.84	108.20
3	0	1326	G	O4'-C1'-N9	5.80	112.84	108.20
3	0	1221	G	O4'-C1'-N9	5.80	112.84	108.20
3	0	1238	A	C4-C5-C6	5.80	119.90	117.00
3	0	1769	A	C5-C6-N6	-5.79	119.06	123.70
3	0	1925	A	C4-C5-C6	5.79	119.90	117.00
3	0	1932	A	O4'-C1'-N9	5.79	112.84	108.20
28	5	114	PHE	CB-CG-CD1	5.79	124.86	120.80
3	0	142	A	C5-C6-N6	-5.79	119.06	123.70
3	0	318	C	N3-C4-N4	5.79	122.06	118.00
3	0	1463	A	C4-C5-C6	5.79	119.89	117.00
3	0	1786	A	C5-C6-N6	-5.79	119.07	123.70
6	j	80	PHE	CB-CG-CD2	-5.79	116.75	120.80
30	i	86	PRO	C-N-CA	5.79	136.18	121.70
39	E	318	LEU	C-N-CA	5.79	136.18	121.70
3	0	366	C	N3-C4-C5	-5.79	119.58	121.90
3	0	1194	A	C5-C6-N1	-5.79	114.81	117.70
3	0	1523	A	C5-C6-N1	-5.79	114.81	117.70
3	0	1535	C	N3-C4-N4	5.79	122.05	118.00
3	0	1870	A	C4-C5-C6	5.79	119.89	117.00
3	0	1955	G	C4-N9-C1'	5.79	134.03	126.50
3	0	2299	A	O4'-C1'-N9	5.79	112.83	108.20
3	0	2307	C	N3-C4-N4	5.79	122.05	118.00
3	0	624	A	C4-C5-C6	5.79	119.89	117.00
3	0	1299	C	N3-C4-N4	5.79	122.05	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	765	A	C4-C5-C6	5.79	119.89	117.00
3	0	1263	A	C5-C6-N6	-5.79	119.07	123.70
3	0	107	A	C5-C6-N6	-5.78	119.07	123.70
3	0	961	A	O4'-C1'-N9	5.78	112.83	108.20
3	0	561	A	O4'-C1'-N9	5.78	112.83	108.20
3	0	619	C	N3-C4-N4	5.78	122.05	118.00
3	0	1275	A	C5-C6-N6	-5.78	119.07	123.70
3	0	1335	A	C5-C6-N6	-5.78	119.08	123.70
3	0	1866	A	C4-C5-C6	5.78	119.89	117.00
3	0	2148	C	N3-C4-N4	5.78	122.05	118.00
1	f	264	ASP	C-N-CA	5.78	134.44	122.30
3	0	143	C	O4'-C1'-N1	5.78	112.83	108.20
3	0	963	G	O4'-C1'-N9	5.78	112.82	108.20
3	0	2197	A	C5-C6-N1	-5.78	114.81	117.70
3	0	1733	C	N3-C4-N4	5.78	122.05	118.00
1	f	1653	CYS	O-C-N	5.78	133.02	123.20
3	0	434	A	C5-C6-N6	-5.78	119.08	123.70
3	0	520	A	C5-C6-N6	-5.78	119.08	123.70
3	0	1877	G	O4'-C1'-N9	5.78	112.82	108.20
2	1	72	A	C5-C6-N6	-5.78	119.08	123.70
3	0	349	A	C5-C6-N6	-5.78	119.08	123.70
3	0	1180	A	C5-C6-N1	-5.78	114.81	117.70
3	0	1201	A	C5-C6-N1	-5.78	114.81	117.70
3	0	1220	A	O4'-C1'-N9	5.78	112.82	108.20
3	0	1753	C	N3-C4-N4	5.78	122.04	118.00
3	0	1961	C	N3-C4-N4	5.78	122.04	118.00
3	0	2088	A	C5-C6-N1	-5.78	114.81	117.70
3	0	2092	C	N3-C4-N4	5.78	122.04	118.00
2	1	63	A	C5-C6-N6	-5.77	119.08	123.70
3	0	352	A	C5-C6-N6	-5.77	119.08	123.70
3	0	659	A	C5-C6-N6	-5.77	119.08	123.70
3	0	779	A	C5-C6-N6	-5.77	119.08	123.70
3	0	246	A	C4-C5-C6	5.77	119.89	117.00
3	0	279	A	C4-C5-C6	5.77	119.89	117.00
3	0	314	A	C5-C6-N6	-5.77	119.08	123.70
3	0	315	A	C5-C6-N6	-5.77	119.08	123.70
3	0	1206	G	O4'-C1'-N9	5.77	112.82	108.20
3	0	1600	A	C5-C6-N1	-5.77	114.81	117.70
3	0	291	G	O4'-C1'-N9	5.77	112.82	108.20
3	0	483	A	C5-C6-N6	-5.77	119.08	123.70
3	0	916	A	C5-C6-N6	-5.77	119.08	123.70
3	0	1365	A	O4'-C1'-N9	5.77	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	384	G	O4'-C1'-N9	5.77	112.82	108.20
3	0	881	G	O4'-C1'-N9	5.77	112.82	108.20
3	0	971	G	O4'-C1'-N9	5.77	112.82	108.20
3	0	1579	A	C4-C5-C6	5.77	119.88	117.00
3	0	2068	A	C4-C5-C6	5.77	119.89	117.00
3	0	308	C	N3-C4-C5	-5.77	119.59	121.90
3	0	936	C	O4'-C1'-N1	5.77	112.81	108.20
3	0	1605	A	O4'-C1'-N9	5.77	112.81	108.20
3	0	1638	A	C4-C5-C6	5.77	119.88	117.00
3	0	1707	A	C5-C6-N1	-5.77	114.82	117.70
3	0	610	A	C5-C6-N1	-5.77	114.82	117.70
3	0	1194	A	C4-C5-C6	5.77	119.88	117.00
2	1	19	A	C4-C5-C6	5.76	119.88	117.00
2	1	34	A	C5-C6-N6	-5.76	119.09	123.70
3	0	350	C	N3-C4-N4	5.76	122.03	118.00
3	0	1571	A	C5-C6-N6	-5.76	119.09	123.70
3	0	1677	C	N3-C4-N4	5.76	122.03	118.00
3	0	2112	A	C4-C5-C6	5.76	119.88	117.00
3	0	288	A	C4-C5-C6	5.76	119.88	117.00
3	0	1297	A	C5-C6-N6	-5.76	119.09	123.70
3	0	1924	A	C5-C6-N6	-5.76	119.09	123.70
2	1	62	A	C5-C6-N1	-5.76	114.82	117.70
3	0	639	A	C5-C6-N6	-5.76	119.09	123.70
3	0	935	A	C4-C5-C6	5.76	119.88	117.00
3	0	1893	A	C5-C6-N6	-5.76	119.09	123.70
3	0	2011	A	C5-C6-N6	-5.76	119.09	123.70
3	0	522	A	C5-C6-N6	-5.76	119.09	123.70
3	0	972	A	O4'-C1'-N9	5.76	112.81	108.20
3	0	1002	G	O4'-C1'-N9	5.76	112.81	108.20
2	1	52	G	O4'-C1'-N9	5.76	112.81	108.20
3	0	11	A	C5-C6-N1	-5.76	114.82	117.70
3	0	315	A	P-O3'-C3'	5.76	126.61	119.70
3	0	433	G	O4'-C1'-N9	5.76	112.81	108.20
3	0	438	A	C5-C6-N1	-5.76	114.82	117.70
3	0	2094	A	C5-C6-N1	-5.76	114.82	117.70
3	0	2225	G	O4'-C1'-N9	5.76	112.81	108.20
3	0	2264	A	O4'-C1'-N9	5.76	112.81	108.20
3	0	2269	A	C5-C6-N6	-5.76	119.09	123.70
5	s	394	TYR	C-N-CA	5.76	136.09	121.70
3	0	577	A	C5-C6-N1	-5.75	114.82	117.70
47	8	434	TYR	CB-CG-CD2	-5.75	117.55	121.00
3	0	1180	A	O4'-C1'-N9	5.75	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1469	A	C4-C5-C6	5.75	119.88	117.00
1	f	1279	PHE	CB-CG-CD2	-5.75	116.77	120.80
3	0	20	G	O4'-C1'-N9	5.75	112.80	108.20
3	0	1579	A	C5-C6-N6	-5.75	119.10	123.70
3	0	2178	C	N3-C4-C5	-5.75	119.60	121.90
3	0	2250	A	C4-C5-C6	5.75	119.88	117.00
44	K	176	PHE	CB-CG-CD2	-5.75	116.77	120.80
3	0	432	A	C4-C5-C6	5.75	119.88	117.00
2	1	16	U	O4'-C1'-N1	5.75	112.80	108.20
3	0	256	A	O4'-C1'-N9	5.75	112.80	108.20
3	0	38	C	N3-C4-C5	-5.75	119.60	121.90
3	0	100	A	C4-C5-C6	5.75	119.87	117.00
3	0	258	C	N3-C4-N4	5.75	122.02	118.00
3	0	1770	G	O4'-C1'-N9	5.75	112.80	108.20
3	0	1804	A	C5-C6-N6	-5.75	119.10	123.70
3	0	2163	C	N3-C4-N4	5.75	122.02	118.00
3	0	2272	A	C5-C6-N6	-5.75	119.10	123.70
1	f	197	VAL	N-CA-CB	-5.75	98.86	111.50
3	0	2056	C	C2-N1-C1'	5.75	125.12	118.80
3	0	308	C	N3-C4-N4	5.74	122.02	118.00
3	0	492	A	C4-C5-C6	5.74	119.87	117.00
3	0	724	A	C4-C5-C6	5.74	119.87	117.00
3	0	778	A	C5-C6-N1	-5.74	114.83	117.70
3	0	809	A	C4-C5-C6	5.74	119.87	117.00
3	0	1925	A	C5-C6-N1	-5.74	114.83	117.70
3	0	241	A	C5-C6-N6	-5.74	119.11	123.70
3	0	586	A	C5-C6-N6	-5.74	119.11	123.70
3	0	990	A	C4-C5-C6	5.74	119.87	117.00
3	0	1305	C	N3-C4-N4	5.74	122.02	118.00
3	0	161	A	O4'-C1'-N9	5.74	112.79	108.20
3	0	242	A	C5-C6-N6	-5.74	119.11	123.70
3	0	653	A	C5-C6-N6	-5.74	119.11	123.70
3	0	837	C	N3-C4-N4	5.74	122.02	118.00
3	0	1808	A	C4-C5-C6	5.74	119.87	117.00
3	0	1966	A	C5-C6-N1	-5.74	114.83	117.70
3	0	2128	C	N3-C4-N4	5.74	122.02	118.00
3	0	2139	A	C5-C6-N1	-5.74	114.83	117.70
3	0	565	G	O4'-C1'-N9	5.74	112.79	108.20
3	0	840	C	N3-C4-N4	5.74	122.02	118.00
3	0	1435	C	N3-C4-C5	-5.74	119.61	121.90
3	0	1559	A	C5-C6-N1	-5.74	114.83	117.70
3	0	1835	C	N3-C4-N4	5.74	122.02	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2105	C	N3-C4-N4	5.74	122.02	118.00
3	0	2135	C	O4'-C1'-N1	5.74	112.79	108.20
3	0	2179	C	N3-C4-N4	5.74	122.02	118.00
3	0	498	A	C5-C6-N6	-5.74	119.11	123.70
51	A	3	PHE	C-N-CA	5.74	136.04	121.70
3	0	39	A	C5-C6-N6	-5.74	119.11	123.70
3	0	213	G	C5-C6-O6	-5.74	125.16	128.60
3	0	447	A	C5-C6-N6	-5.74	119.11	123.70
3	0	960	A	O4'-C1'-N9	5.74	112.79	108.20
3	0	1185	A	C4-C5-C6	5.74	119.87	117.00
3	0	1390	A	C4-C5-C6	5.74	119.87	117.00
3	0	1866	A	C5-C6-N6	-5.74	119.11	123.70
3	0	2267	A	C5-C6-N6	-5.74	119.11	123.70
3	0	2295	C	N3-C4-N4	5.74	122.02	118.00
22	F	206	PHE	CB-CG-CD1	5.74	124.81	120.80
23	d	217	PHE	CB-CG-CD1	5.74	124.81	120.80
3	0	1886	C	N3-C4-N4	5.73	122.01	118.00
3	0	565	G	C5-C6-O6	-5.73	125.16	128.60
3	0	645	A	C5-C6-N1	-5.73	114.83	117.70
3	0	1256	C	N3-C4-N4	5.73	122.01	118.00
3	0	1375	A	O4'-C1'-N9	5.73	112.79	108.20
3	0	1532	G	O4'-C1'-N9	5.73	112.79	108.20
3	0	2205	A	O4'-C1'-N9	5.73	112.79	108.20
3	0	391	C	N3-C4-N4	5.73	122.01	118.00
3	0	943	G	O4'-C1'-N9	5.73	112.78	108.20
3	0	1516	A	C5-C6-N6	-5.73	119.12	123.70
3	0	1727	C	N3-C4-N4	5.73	122.01	118.00
3	0	1886	C	N3-C4-C5	-5.73	119.61	121.90
3	0	393	U	O4'-C1'-N1	5.73	112.78	108.20
3	0	205	G	O4'-C1'-N9	5.73	112.78	108.20
3	0	432	A	C5-C6-N6	-5.73	119.12	123.70
3	0	452	C	N3-C4-N4	5.73	122.01	118.00
3	0	1597	A	O4'-C1'-N9	5.73	112.78	108.20
3	0	1997	A	O4'-C1'-N9	5.73	112.78	108.20
3	0	821	C	N3-C4-C5	-5.73	119.61	121.90
3	0	1649	G	O4'-C1'-N9	5.73	112.78	108.20
3	0	2083	C	N3-C4-N4	5.73	122.01	118.00
3	0	255	A	O4'-C1'-N9	5.72	112.78	108.20
3	0	330	A	O4'-C1'-N9	5.72	112.78	108.20
3	0	536	A	C4-C5-C6	5.72	119.86	117.00
3	0	1295	A	C5-C6-N1	-5.72	114.84	117.70
3	0	1481	U	O4'-C1'-N1	5.72	112.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1621	C	N3-C4-C5	-5.72	119.61	121.90
3	0	1944	A	C5-C6-N1	-5.72	114.84	117.70
3	0	2019	C	N3-C4-C5	-5.72	119.61	121.90
3	0	38	C	N3-C4-N4	5.72	122.01	118.00
3	0	525	A	C5-C6-N6	-5.72	119.12	123.70
3	0	729	C	N3-C4-N4	5.72	122.00	118.00
3	0	1767	G	O4'-C1'-N9	5.72	112.78	108.20
3	0	1920	G	O4'-C1'-N9	5.72	112.78	108.20
3	0	472	A	C5-C6-N6	-5.72	119.12	123.70
3	0	215	A	O4'-C1'-N9	5.72	112.78	108.20
3	0	561	A	C4-C5-C6	5.72	119.86	117.00
3	0	765	A	C5-C6-N1	-5.72	114.84	117.70
3	0	1692	A	C4-C5-C6	5.72	119.86	117.00
2	1	46	A	O4'-C1'-N9	5.72	112.77	108.20
3	0	934	C	N3-C4-N4	5.72	122.00	118.00
2	1	69	G	O4'-C1'-N9	5.72	112.77	108.20
3	0	799	A	C4-C5-C6	5.72	119.86	117.00
3	0	828	G	O4'-C1'-N9	5.72	112.77	108.20
26	J	189	TYR	CB-CG-CD1	5.72	124.43	121.00
3	0	63	G	O4'-C1'-N9	5.71	112.77	108.20
3	0	503	A	O4'-C1'-N9	5.71	112.77	108.20
3	0	1376	C	N3-C4-N4	5.71	122.00	118.00
3	0	1597	A	C5-C6-N1	-5.71	114.84	117.70
3	0	1738	A	C5-C6-N6	-5.71	119.13	123.70
3	0	88	G	O4'-C1'-N9	5.71	112.77	108.20
3	0	367	A	C4-C5-C6	5.71	119.86	117.00
3	0	751	C	N3-C4-N4	5.71	122.00	118.00
3	0	1375	A	C5-C6-N6	-5.71	119.13	123.70
3	0	1912	C	N3-C4-C5	-5.71	119.62	121.90
3	0	2112	A	O4'-C1'-N9	5.71	112.77	108.20
3	0	2264	A	C5-C6-N6	-5.71	119.13	123.70
3	0	56	U	O4'-C1'-N1	5.71	112.77	108.20
3	0	1684	A	C4-C5-C6	5.71	119.86	117.00
3	0	2241	C	N3-C4-N4	5.71	122.00	118.00
1	f	307	LEU	CB-CA-C	-5.71	99.35	110.20
2	1	46	A	C5-C6-N6	-5.71	119.13	123.70
3	0	600	U	O4'-C1'-N1	5.71	112.77	108.20
3	0	1586	A	C4-C5-C6	5.71	119.86	117.00
3	0	1625	A	C5-C6-N1	-5.71	114.85	117.70
3	0	255	A	C5-C6-N6	-5.71	119.14	123.70
3	0	593	G	O4'-C1'-N9	5.71	112.77	108.20
3	0	295	A	C5-C6-N6	-5.71	119.14	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	f	241	SER	CA-C-N	-5.70	104.65	117.20
3	0	60	U	O4'-C1'-N1	5.70	112.76	108.20
3	0	585	A	C5-C6-N6	-5.70	119.14	123.70
3	0	707	C	N3-C4-C5	-5.70	119.62	121.90
3	0	1303	C	N3-C4-N4	5.70	121.99	118.00
3	0	1348	A	C5-C6-N6	-5.70	119.14	123.70
3	0	362	C	N3-C4-C5	-5.70	119.62	121.90
3	0	913	A	C5-C6-N6	-5.70	119.14	123.70
3	0	966	C	N3-C4-N4	5.70	121.99	118.00
3	0	2031	A	O4'-C1'-N9	5.70	112.76	108.20
2	1	47	C	N3-C4-C5	-5.70	119.62	121.90
3	0	186	C	N3-C4-N4	5.70	121.99	118.00
3	0	1858	C	N3-C4-N4	5.70	121.99	118.00
3	0	2070	A	O4'-C1'-N9	5.70	112.76	108.20
1	f	774	LEU	O-C-N	-5.70	113.52	123.20
3	0	733	G	O4'-C1'-N9	5.70	112.76	108.20
3	0	2164	A	C5-C6-N6	-5.70	119.14	123.70
3	0	499	A	C5-C6-N6	-5.70	119.14	123.70
3	0	712	U	O4'-C1'-N1	5.70	112.76	108.20
3	0	821	C	N3-C4-N4	5.70	121.99	118.00
3	0	822	A	C4-C5-C6	5.70	119.85	117.00
3	0	1343	A	O4'-C1'-N9	5.70	112.76	108.20
3	0	2042	A	C4-C5-C6	5.70	119.85	117.00
3	0	278	A	C5-C6-N6	-5.69	119.14	123.70
3	0	534	C	N3-C4-N4	5.69	121.99	118.00
3	0	1222	A	C5-C6-N6	-5.69	119.14	123.70
3	0	1423	A	C5-C6-N6	-5.69	119.15	123.70
3	0	1737	A	O4'-C1'-N9	5.69	112.75	108.20
3	0	761	G	N1-C6-O6	5.69	123.31	119.90
3	0	1338	A	C4-C5-C6	5.69	119.84	117.00
3	0	1379	A	C5-C6-N6	-5.69	119.15	123.70
3	0	2231	U	O4'-C1'-N1	5.69	112.75	108.20
3	0	1341	A	C5-C6-N6	-5.69	119.15	123.70
3	0	1819	U	O4'-C1'-N1	5.69	112.75	108.20
3	0	250	A	C5-C6-N6	-5.69	119.15	123.70
3	0	592	A	C5-C6-N6	-5.69	119.15	123.70
3	0	905	A	C5-C6-N6	-5.69	119.15	123.70
3	0	1808	A	C5-C6-N1	-5.69	114.86	117.70
3	0	2068	A	O4'-C1'-N9	5.69	112.75	108.20
3	0	269	A	C5-C6-N6	-5.69	119.15	123.70
3	0	599	A	C5-C6-N1	-5.69	114.86	117.70
3	0	935	A	C5-C6-N6	-5.69	119.15	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1246	A	C5-C6-N1	-5.69	114.86	117.70
3	0	1400	C	N3-C4-N4	5.69	121.98	118.00
3	0	1752	C	N3-C4-N4	5.69	121.98	118.00
49	I	379	PHE	CB-CG-CD1	-5.69	116.82	120.80
3	0	781	A	O4'-C1'-N9	5.68	112.75	108.20
3	0	1632	C	N3-C4-N4	5.68	121.98	118.00
3	0	2022	G	O4'-C1'-N9	5.68	112.75	108.20
3	0	105	A	C5-C6-N6	-5.68	119.15	123.70
3	0	647	A	C5-C6-N6	-5.68	119.15	123.70
3	0	1663	C	N3-C4-N4	5.68	121.98	118.00
3	0	1706	G	O4'-C1'-N9	5.68	112.75	108.20
3	0	2245	A	C4-C5-C6	5.68	119.84	117.00
3	0	362	C	N3-C4-N4	5.68	121.98	118.00
3	0	708	G	O4'-C1'-N9	5.68	112.75	108.20
1	f	1306	TRP	CA-CB-CG	5.68	124.49	113.70
1	f	240	PHE	CB-CG-CD1	5.68	124.77	120.80
3	0	122	A	C5-C6-N6	-5.68	119.16	123.70
3	0	633	A	C5-C6-N6	-5.68	119.16	123.70
3	0	1222	A	C5-C6-N1	-5.68	114.86	117.70
3	0	1306	A	O4'-C1'-N9	5.68	112.74	108.20
3	0	1579	A	C5-C6-N1	-5.68	114.86	117.70
3	0	2014	C	N3-C4-C5	-5.68	119.63	121.90
3	0	2016	A	C5-C6-N1	-5.68	114.86	117.70
3	0	2127	G	O4'-C1'-N9	5.68	112.74	108.20
2	1	14	A	C5-C6-N1	-5.67	114.86	117.70
3	0	587	A	C5-C6-N6	-5.67	119.16	123.70
3	0	1284	A	C4-C5-C6	5.67	119.84	117.00
3	0	1313	A	C5-C6-N1	-5.67	114.86	117.70
3	0	1992	A	C5-C6-N6	-5.67	119.16	123.70
3	0	2233	C	N3-C4-N4	5.67	121.97	118.00
3	0	347	G	O4'-C1'-N9	5.67	112.74	108.20
3	0	569	A	C5-C6-N1	-5.67	114.86	117.70
3	0	777	A	C5-C6-N1	-5.67	114.86	117.70
3	0	920	A	C5-C6-N6	-5.67	119.16	123.70
3	0	2045	G	O4'-C1'-N9	5.67	112.74	108.20
3	0	2213	G	O4'-C1'-N9	5.67	112.74	108.20
11	m	105	PHE	CB-CG-CD1	5.67	124.77	120.80
3	0	1328	A	O4'-C1'-N9	5.67	112.74	108.20
3	0	2018	U	O4'-C1'-N1	5.67	112.74	108.20
3	0	62	A	C5-C6-N6	-5.67	119.16	123.70
3	0	599	A	O4'-C1'-N9	5.67	112.74	108.20
3	0	1748	A	C4-C5-C6	5.67	119.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2041	A	C5-C6-N1	-5.67	114.86	117.70
3	0	1709	A	C5-C6-N6	-5.67	119.17	123.70
3	0	2007	A	C4-C5-C6	5.67	119.83	117.00
40	Y	366	ALA	N-CA-CB	5.67	118.03	110.10
3	0	9	U	O4'-C1'-N1	5.67	112.73	108.20
3	0	82	A	C5-C6-N6	-5.67	119.17	123.70
3	0	181	A	C5-C6-N6	-5.67	119.17	123.70
3	0	580	C	N3-C4-N4	5.67	121.97	118.00
3	0	624	A	C5-C6-N1	-5.67	114.87	117.70
3	0	880	A	C5-C6-N1	-5.67	114.87	117.70
3	0	1611	A	C4-C5-C6	5.67	119.83	117.00
3	0	457	A	C5-C6-N6	-5.67	119.17	123.70
3	0	1194	A	O4'-C1'-N9	5.67	112.73	108.20
3	0	29	U	O4'-C1'-N1	5.66	112.73	108.20
3	0	369	C	O4'-C1'-N1	5.66	112.73	108.20
3	0	478	C	N3-C4-N4	5.66	121.97	118.00
3	0	1267	C	N3-C4-N4	5.66	121.96	118.00
3	0	709	C	N3-C4-C5	-5.66	119.64	121.90
3	0	1544	A	O4'-C1'-N9	5.66	112.73	108.20
3	0	2131	A	C5-C6-N1	-5.66	114.87	117.70
1	f	255	TRP	CA-C-N	-5.66	104.75	117.20
3	0	65	A	C5-C6-N6	-5.66	119.17	123.70
3	0	226	A	C5-C6-N6	-5.66	119.17	123.70
3	0	504	A	C5-C6-N6	-5.66	119.17	123.70
3	0	525	A	C5-C6-N1	-5.66	114.87	117.70
3	0	913	A	O4'-C1'-N9	5.66	112.73	108.20
3	0	61	C	N3-C4-C5	-5.66	119.64	121.90
3	0	258	C	O4'-C1'-N1	5.66	112.73	108.20
3	0	348	A	O4'-C1'-N9	5.66	112.73	108.20
3	0	507	A	C4-C5-C6	5.66	119.83	117.00
3	0	588	A	C5-C6-N6	-5.66	119.17	123.70
3	0	1530	C	N3-C4-N4	5.66	121.96	118.00
3	0	1552	A	C4-C5-C6	5.66	119.83	117.00
3	0	203	C	N3-C4-N4	5.66	121.96	118.00
3	0	769	A	C5-C6-N6	-5.66	119.17	123.70
3	0	1390	A	C5-C6-N6	-5.66	119.18	123.70
3	0	1426	A	O4'-C1'-N9	5.66	112.72	108.20
3	0	2234	A	C5-C6-N1	-5.66	114.87	117.70
3	0	140	C	N3-C4-N4	5.65	121.96	118.00
3	0	592	A	C5-C6-N1	-5.65	114.87	117.70
3	0	764	A	C5-C6-N6	-5.65	119.18	123.70
3	0	2027	A	C5-C6-N6	-5.65	119.18	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2219	A	C4-C5-C6	5.65	119.83	117.00
3	0	105	A	C5-C6-N1	-5.65	114.87	117.70
3	0	257	A	C5-C6-N6	-5.65	119.18	123.70
3	0	1260	A	C5-C6-N6	-5.65	119.18	123.70
3	0	1280	A	C5-C6-N6	-5.65	119.18	123.70
3	0	1305	C	C2-N1-C1'	5.65	125.02	118.80
3	0	2207	A	C5-C6-N6	-5.65	119.18	123.70
3	0	59	C	N3-C4-N4	5.65	121.96	118.00
3	0	502	A	O4'-C1'-N9	5.65	112.72	108.20
3	0	743	C	N3-C4-C5	-5.65	119.64	121.90
3	0	1280	A	C4-C5-C6	5.65	119.83	117.00
3	0	1597	A	C5-C6-N6	-5.65	119.18	123.70
3	0	1809	A	C5-C6-N1	-5.65	114.88	117.70
3	0	2305	A	O4'-C1'-N9	5.65	112.72	108.20
1	f	1440	GLU	N-CA-CB	5.65	120.77	110.60
3	0	237	A	O4'-C1'-N9	5.65	112.72	108.20
3	0	490	C	N3-C4-N4	5.65	121.95	118.00
3	0	581	A	C5-C6-N1	-5.65	114.88	117.70
3	0	1255	A	C5-C6-N1	-5.65	114.88	117.70
3	0	2284	U	O4'-C1'-N1	5.65	112.72	108.20
3	0	484	A	C5-C6-N6	-5.65	119.18	123.70
3	0	1260	A	C4-C5-C6	5.65	119.82	117.00
3	0	1270	A	C5-C6-N6	-5.65	119.18	123.70
3	0	1751	G	O4'-C1'-N9	5.65	112.72	108.20
3	0	1931	G	O4'-C1'-N9	5.65	112.72	108.20
3	0	2204	A	O4'-C1'-N9	5.65	112.72	108.20
1	f	237	ILE	C-N-CA	5.65	135.81	121.70
3	0	506	A	C5-C6-N6	-5.65	119.18	123.70
3	0	1519	G	C5-C6-O6	-5.65	125.21	128.60
3	0	417	A	O4'-C1'-N9	5.64	112.72	108.20
3	0	689	A	C5-C6-N1	-5.64	114.88	117.70
3	0	1821	G	O4'-C1'-N9	5.64	112.72	108.20
3	0	2204	A	C5-C6-N6	-5.64	119.18	123.70
3	0	714	G	C5-C6-O6	-5.64	125.21	128.60
3	0	1251	U	O4'-C1'-N1	5.64	112.71	108.20
3	0	1979	C	N3-C4-C5	-5.64	119.64	121.90
3	0	2040	A	C5-C6-N6	-5.64	119.19	123.70
3	0	2229	G	O4'-C1'-N9	5.64	112.71	108.20
3	0	153	C	N3-C4-C5	-5.64	119.64	121.90
3	0	675	A	C5-C6-N1	-5.64	114.88	117.70
3	0	1423	A	O4'-C1'-N9	5.64	112.71	108.20
2	1	53	A	C5-C6-N6	-5.64	119.19	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	284	C	O4'-C1'-N1	5.64	112.71	108.20
3	0	666	U	O4'-C1'-N1	5.64	112.71	108.20
3	0	825	C	N3-C4-C5	-5.64	119.64	121.90
3	0	1711	A	C5-C6-N1	-5.64	114.88	117.70
3	0	1794	A	C5-C6-N6	-5.64	119.19	123.70
3	0	1809	A	C5-C6-N6	-5.64	119.19	123.70
3	0	1953	G	C5-C6-O6	-5.64	125.22	128.60
3	0	595	A	C5-C6-N6	-5.64	119.19	123.70
3	0	771	A	C5-C6-N6	-5.64	119.19	123.70
3	0	2301	G	O4'-C1'-N9	5.64	112.71	108.20
3	0	172	A	C5-C6-N1	-5.64	114.88	117.70
3	0	1527	C	N3-C4-N4	5.64	121.94	118.00
3	0	1544	A	C5-C6-N6	-5.64	119.19	123.70
3	0	73	A	O4'-C1'-N9	5.63	112.71	108.20
3	0	233	G	O4'-C1'-N9	5.63	112.71	108.20
3	0	858	A	C5-C6-N1	-5.63	114.88	117.70
3	0	926	C	N3-C4-C5	-5.63	119.65	121.90
3	0	875	A	C5-C6-N6	-5.63	119.19	123.70
3	0	1180	A	C5-C6-N6	-5.63	119.19	123.70
3	0	2047	G	O4'-C1'-N9	5.63	112.71	108.20
3	0	173	A	C5-C6-N1	-5.63	114.89	117.70
3	0	313	G	C4-N9-C1'	5.63	133.82	126.50
3	0	500	A	C5-C6-N6	-5.63	119.19	123.70
3	0	779	A	C4-C5-C6	5.63	119.82	117.00
3	0	1871	A	C5-C6-N6	-5.63	119.19	123.70
3	0	413	G	O4'-C1'-N9	5.63	112.70	108.20
46	C	215	ARG	N-CA-C	5.63	126.20	111.00
3	0	381	A	C5-C6-N6	-5.63	119.20	123.70
3	0	426	U	O4'-C1'-N1	5.63	112.70	108.20
3	0	767	A	C5-C6-N1	-5.63	114.89	117.70
3	0	1196	G	O4'-C1'-N9	5.63	112.70	108.20
3	0	1634	C	N3-C4-C5	-5.63	119.65	121.90
3	0	2039	A	C5-C6-N6	-5.63	119.20	123.70
3	0	2091	G	O4'-C1'-N9	5.63	112.70	108.20
3	0	2216	C	N3-C4-N4	5.63	121.94	118.00
3	0	538	A	O4'-C1'-N9	5.63	112.70	108.20
3	0	623	C	N3-C4-N4	5.63	121.94	118.00
3	0	774	C	N3-C4-N4	5.63	121.94	118.00
3	0	811	U	O4'-C1'-N1	5.63	112.70	108.20
3	0	898	A	C5-C6-N1	-5.63	114.89	117.70
3	0	1335	A	O4'-C1'-N9	5.63	112.70	108.20
3	0	2044	A	C5-C6-N6	-5.63	119.20	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2246	G	O4'-C1'-N9	5.63	112.70	108.20
1	f	264	ASP	N-CA-CB	5.62	120.72	110.60
3	0	101	C	N3-C4-C5	-5.62	119.65	121.90
3	0	591	G	O4'-C1'-N9	5.62	112.70	108.20
3	0	718	A	P-O5'-C5'	5.62	129.90	120.90
3	0	501	A	C5-C6-N6	-5.62	119.20	123.70
3	0	785	A	O4'-C1'-N9	5.62	112.70	108.20
3	0	1487	G	O4'-C1'-N9	5.62	112.70	108.20
3	0	1782	G	O4'-C1'-N9	5.62	112.70	108.20
3	0	280	C	N3-C4-N4	5.62	121.94	118.00
3	0	647	A	C4-C5-C6	5.62	119.81	117.00
3	0	675	A	C4-C5-C6	5.62	119.81	117.00
3	0	817	A	C5-C6-N6	-5.62	119.20	123.70
3	0	1370	A	C5-C6-N6	-5.62	119.20	123.70
3	0	1530	C	N3-C4-C5	-5.62	119.65	121.90
1	f	296	TYR	O-C-N	-5.62	113.71	122.70
3	0	449	U	O4'-C1'-N1	5.62	112.70	108.20
3	0	2043	G	O4'-C1'-N9	5.62	112.70	108.20
3	0	2268	G	N3-C2-N2	5.62	123.83	119.90
3	0	596	A	C5-C6-N6	-5.62	119.20	123.70
3	0	1525	A	O4'-C1'-N9	5.62	112.69	108.20
3	0	1666	A	C5-C6-N1	-5.62	114.89	117.70
3	0	2055	C	N3-C4-N4	5.62	121.93	118.00
3	0	2277	A	C5-C6-N1	-5.62	114.89	117.70
3	0	1253	A	C5-C6-N6	-5.62	119.21	123.70
3	0	1362	U	O4'-C1'-N1	5.62	112.69	108.20
3	0	1457	A	C5-C6-N6	-5.62	119.21	123.70
44	K	30	TYR	CB-CG-CD1	5.62	124.37	121.00
3	0	2	A	C5-C6-N6	-5.62	119.21	123.70
3	0	122	A	C5-C6-N1	-5.62	114.89	117.70
3	0	469	G	O4'-C1'-N9	5.62	112.69	108.20
3	0	1949	G	O4'-C1'-N9	5.62	112.69	108.20
3	0	2052	A	C4-C5-C6	5.62	119.81	117.00
3	0	809	A	C5-C6-N6	-5.61	119.21	123.70
3	0	1545	C	N3-C4-N4	5.61	121.93	118.00
3	0	1956	A	C5-C6-N1	-5.61	114.89	117.70
41	Q	33	ARG	N-CA-CB	5.61	120.70	110.60
3	0	112	A	C5-C6-N6	-5.61	119.21	123.70
3	0	202	C	N3-C4-C5	-5.61	119.66	121.90
3	0	248	G	N3-C2-N2	5.61	123.83	119.90
3	0	339	C	N3-C4-C5	-5.61	119.66	121.90
3	0	367	A	C5-C6-N6	-5.61	119.21	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	917	A	C5-C6-N6	-5.61	119.21	123.70
3	0	1562	U	O4'-C1'-N1	5.61	112.69	108.20
3	0	1903	G	O4'-C1'-N9	5.61	112.69	108.20
3	0	2150	A	C5-C6-N1	-5.61	114.89	117.70
3	0	2154	C	N3-C4-N4	5.61	121.93	118.00
3	0	1345	A	C5-C6-N1	-5.61	114.89	117.70
3	0	1501	A	C5-C6-N6	-5.61	119.21	123.70
3	0	912	A	C5-C6-N6	-5.61	119.21	123.70
3	0	1291	A	C5-C6-N6	-5.61	119.21	123.70
3	0	1335	A	C5-C6-N1	-5.61	114.90	117.70
3	0	1511	C	N3-C4-C5	-5.61	119.66	121.90
3	0	1566	A	C5-C6-N1	-5.61	114.90	117.70
3	0	2319	C	N3-C4-N4	5.61	121.92	118.00
44	K	175	THR	C-N-CA	5.61	135.72	121.70
2	1	51	G	O4'-C1'-N9	5.61	112.68	108.20
3	0	180	A	C5-C6-N6	-5.61	119.22	123.70
3	0	529	A	C5-C6-N1	-5.61	114.90	117.70
3	0	782	A	C5-C6-N6	-5.61	119.22	123.70
3	0	866	A	C5-C6-N1	-5.61	114.90	117.70
3	0	1067	A	O4'-C1'-N9	5.61	112.68	108.20
3	0	1182	C	N3-C4-C5	-5.61	119.66	121.90
3	0	1507	A	C5-C6-N1	-5.61	114.90	117.70
3	0	1834	C	N3-C4-C5	-5.61	119.66	121.90
3	0	1964	C	C2-N1-C1'	5.61	124.97	118.80
3	0	2207	A	C5-C6-N1	-5.61	114.90	117.70
3	0	2221	A	O4'-C1'-N9	5.61	112.68	108.20
3	0	348	A	C5-C6-N6	-5.60	119.22	123.70
3	0	953	G	O4'-C1'-N9	5.60	112.68	108.20
2	1	40	C	N3-C4-N4	5.60	121.92	118.00
2	1	58	A	C5-C6-N1	-5.60	114.90	117.70
3	0	910	A	O4'-C1'-N9	5.60	112.68	108.20
3	0	1269	A	C5-C6-N6	-5.60	119.22	123.70
3	0	1345	A	O4'-C1'-N9	5.60	112.68	108.20
3	0	2067	U	O4'-C1'-N1	5.60	112.68	108.20
1	f	1214	ARG	O-C-N	-5.60	113.74	122.70
3	0	1887	G	O4'-C1'-N9	5.60	112.68	108.20
3	0	2069	G	O4'-C1'-N9	5.60	112.68	108.20
3	0	502	A	C5-C6-N6	-5.60	119.22	123.70
3	0	1691	G	C8-N9-C1'	-5.60	119.72	127.00
3	0	1888	C	N3-C4-N4	5.60	121.92	118.00
1	f	308	ARG	O-C-N	-5.60	113.74	122.70
2	1	66	G	O4'-C1'-N9	5.60	112.68	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	147	G	O4'-C1'-N9	5.60	112.68	108.20
3	0	1389	G	O4'-C1'-N9	5.60	112.68	108.20
3	0	1748	A	C5-C6-N6	-5.60	119.22	123.70
3	0	476	G	O4'-C1'-N9	5.60	112.68	108.20
3	0	1930	A	C4-C5-C6	5.60	119.80	117.00
3	0	2041	A	C5-C6-N6	-5.60	119.22	123.70
3	0	452	C	N3-C4-C5	-5.59	119.66	121.90
3	0	902	A	C5-C6-N6	-5.59	119.22	123.70
3	0	954	G	O4'-C1'-N9	5.59	112.68	108.20
3	0	1441	C	N3-C4-N4	5.59	121.92	118.00
3	0	1667	A	C5-C6-N6	-5.59	119.22	123.70
3	0	1829	A	C5-C6-N1	-5.59	114.90	117.70
3	0	152	A	C4-C5-C6	5.59	119.80	117.00
3	0	781	A	C5-C6-N6	-5.59	119.22	123.70
3	0	1227	A	C5-C6-N6	-5.59	119.23	123.70
3	0	1822	G	O4'-C1'-N9	5.59	112.67	108.20
3	0	84	C	N3-C4-C5	-5.59	119.66	121.90
3	0	307	C	N3-C4-N4	5.59	121.91	118.00
3	0	923	A	C5-C6-N1	-5.59	114.91	117.70
3	0	2267	A	C5-C6-N1	-5.59	114.91	117.70
3	0	300	A	C5-C6-N6	-5.59	119.23	123.70
3	0	505	A	C5-C6-N1	-5.59	114.91	117.70
3	0	1271	C	N3-C4-N4	5.59	121.91	118.00
3	0	1856	C	N3-C4-C5	-5.59	119.66	121.90
49	I	379	PHE	CB-CG-CD2	5.59	124.71	120.80
3	0	499	A	C5-C6-N1	-5.59	114.91	117.70
3	0	526	A	O4'-C1'-N9	5.59	112.67	108.20
3	0	718	A	C5-C6-N1	-5.59	114.91	117.70
3	0	972	A	C5-C6-N1	-5.59	114.91	117.70
3	0	1067	A	C5-C6-N6	-5.59	119.23	123.70
3	0	1318	A	C5-C6-N6	-5.59	119.23	123.70
3	0	1604	A	C5-C6-N1	-5.59	114.91	117.70
3	0	1990	C	N3-C4-N4	5.59	121.91	118.00
3	0	285	A	C4-C5-C6	5.59	119.79	117.00
3	0	454	A	C5-C6-N6	-5.59	119.23	123.70
3	0	566	G	O4'-C1'-N9	5.59	112.67	108.20
3	0	945	C	O4'-C1'-N1	5.59	112.67	108.20
3	0	993	A	C5-C6-N6	-5.59	119.23	123.70
3	0	1590	C	N3-C4-N4	5.59	121.91	118.00
3	0	1768	G	O4'-C1'-N9	5.59	112.67	108.20
3	0	1876	G	O4'-C1'-N9	5.59	112.67	108.20
3	0	2230	C	N3-C4-N4	5.59	121.91	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	E	42	THR	N-CA-CB	5.59	120.92	110.30
50	H	115	TYR	CB-CG-CD2	-5.59	117.65	121.00
3	0	503	A	C5-C6-N1	-5.58	114.91	117.70
3	0	575	A	C5-C6-N1	-5.58	114.91	117.70
3	0	898	A	C5-C6-N6	-5.58	119.23	123.70
3	0	1198	A	C5-C6-N6	-5.58	119.23	123.70
3	0	1281	G	O4'-C1'-N9	5.58	112.67	108.20
3	0	1464	A	C5-C6-N1	-5.58	114.91	117.70
3	0	1984	G	O4'-C1'-N9	5.58	112.67	108.20
3	0	2276	A	C5-C6-N6	-5.58	119.23	123.70
39	E	313	LEU	CA-C-N	5.58	127.37	116.20
2	1	20	A	C5-C6-N1	-5.58	114.91	117.70
3	0	674	A	C5-C6-N6	-5.58	119.23	123.70
3	0	726	C	N3-C4-N4	5.58	121.91	118.00
3	0	761	G	N3-C2-N2	5.58	123.81	119.90
3	0	2060	A	C5-C6-N6	-5.58	119.23	123.70
3	0	214	C	N3-C4-C5	-5.58	119.67	121.90
3	0	805	C	O4'-C1'-N1	5.58	112.66	108.20
3	0	865	A	C5-C6-N6	-5.58	119.24	123.70
3	0	1351	G	N3-C2-N2	5.58	123.81	119.90
14	q	127	PHE	CB-CG-CD2	-5.58	116.89	120.80
3	0	585	A	O4'-C1'-N9	5.58	112.66	108.20
3	0	639	A	C5-C6-N1	-5.58	114.91	117.70
3	0	1223	A	C5-C6-N1	-5.58	114.91	117.70
3	0	1511	C	N3-C4-N4	5.58	121.91	118.00
3	0	1799	A	C5-C6-N6	-5.58	119.24	123.70
3	0	1994	G	C5-C6-O6	-5.58	125.25	128.60
3	0	1798	G	O4'-C1'-N9	5.58	112.66	108.20
3	0	1866	A	O4'-C1'-N9	5.58	112.66	108.20
3	0	2304	A	C5-C6-N6	-5.58	119.24	123.70
3	0	287	A	C5-C6-N6	-5.58	119.24	123.70
3	0	1316	C	N3-C4-N4	5.58	121.90	118.00
3	0	2136	A	C5-C6-N6	-5.58	119.24	123.70
1	f	233	VAL	CA-C-N	5.57	127.35	116.20
3	0	183	C	N3-C4-C5	-5.57	119.67	121.90
3	0	904	C	N3-C4-N4	5.57	121.90	118.00
3	0	1261	C	N3-C4-N4	5.57	121.90	118.00
3	0	1404	G	O4'-C1'-N9	5.57	112.66	108.20
3	0	1966	A	O4'-C1'-N9	5.57	112.66	108.20
3	0	1992	A	O4'-C1'-N9	5.57	112.66	108.20
3	0	2154	C	N3-C4-C5	-5.57	119.67	121.90
3	0	2304	A	C5-C6-N1	-5.57	114.91	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	E	77	GLU	C-N-CA	5.57	135.63	121.70
39	E	215	PHE	C-N-CA	5.57	135.64	121.70
3	0	50	C	N3-C4-C5	-5.57	119.67	121.90
3	0	231	A	C5-C6-N1	-5.57	114.91	117.70
3	0	237	A	C4-C5-C6	5.57	119.79	117.00
3	0	690	A	O4'-C1'-N9	5.57	112.66	108.20
3	0	1696	G	O4'-C1'-N9	5.57	112.66	108.20
3	0	1947	A	C5-C6-N6	-5.57	119.24	123.70
3	0	51	A	O4'-C1'-N9	5.57	112.66	108.20
3	0	124	A	C5-C6-N6	-5.57	119.24	123.70
3	0	215	A	C5-C6-N6	-5.57	119.24	123.70
3	0	812	A	C5-C6-N1	-5.57	114.92	117.70
3	0	822	A	C5-C6-N6	-5.57	119.24	123.70
3	0	1312	G	O4'-C1'-N9	5.57	112.66	108.20
3	0	1475	A	C5-C6-N6	-5.57	119.24	123.70
3	0	1491	U	O4'-C1'-N1	5.57	112.66	108.20
3	0	1610	A	C5-C6-N6	-5.57	119.24	123.70
3	0	1732	C	N3-C4-N4	5.57	121.90	118.00
3	0	2075	C	N3-C4-C5	-5.57	119.67	121.90
3	0	2085	A	O4'-C1'-N9	5.57	112.66	108.20
3	0	481	G	O4'-C1'-N9	5.57	112.65	108.20
3	0	703	A	C5-C6-N6	-5.57	119.25	123.70
3	0	748	G	O4'-C1'-N9	5.57	112.65	108.20
3	0	962	A	O4'-C1'-N9	5.57	112.66	108.20
2	1	36	A	C5-C6-N6	-5.57	119.25	123.70
3	0	8	U	O4'-C1'-N1	5.57	112.65	108.20
3	0	142	A	C5-C6-N1	-5.57	114.92	117.70
3	0	405	G	O4'-C1'-N9	5.57	112.65	108.20
3	0	845	A	C5-C6-N6	-5.57	119.25	123.70
3	0	1676	A	C5-C6-N1	-5.57	114.92	117.70
3	0	316	A	C5-C6-N1	-5.56	114.92	117.70
3	0	339	C	N3-C4-N4	5.56	121.89	118.00
3	0	424	G	O4'-C1'-N9	5.56	112.65	108.20
3	0	607	A	C5-C6-N1	-5.56	114.92	117.70
3	0	961	A	C5-C6-N6	-5.56	119.25	123.70
3	0	1638	A	C5-C6-N1	-5.56	114.92	117.70
3	0	2112	A	C5-C6-N6	-5.56	119.25	123.70
3	0	2214	A	C5-C6-N6	-5.56	119.25	123.70
3	0	1245	A	C5-C6-N6	-5.56	119.25	123.70
3	0	1557	A	C5-C6-N1	-5.56	114.92	117.70
1	f	1279	PHE	CB-CG-CD1	5.56	124.69	120.80
2	1	4	A	C4-C5-C6	5.56	119.78	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	167	A	C5-C6-N6	-5.56	119.25	123.70
3	0	184	A	C5-C6-N1	-5.56	114.92	117.70
3	0	1364	C	O4'-C1'-N1	5.56	112.65	108.20
3	0	1465	A	C5-C6-N6	-5.56	119.25	123.70
3	0	1759	U	O4'-C1'-N1	5.56	112.65	108.20
3	0	1793	C	N3-C4-N4	5.56	121.89	118.00
3	0	1940	C	N3-C4-N4	5.56	121.89	118.00
3	0	1983	C	N3-C4-N4	5.56	121.89	118.00
3	0	2053	A	C5-C6-N6	-5.56	119.25	123.70
3	0	2071	C	N3-C4-N4	5.56	121.89	118.00
3	0	2208	C	N3-C4-N4	5.56	121.89	118.00
49	I	262	PHE	CB-CG-CD2	-5.56	116.91	120.80
2	1	53	A	O4'-C1'-N9	5.56	112.65	108.20
3	0	97	A	C5-C6-N6	-5.56	119.25	123.70
3	0	97	A	O4'-C1'-N9	5.56	112.65	108.20
3	0	315	A	C4-C5-C6	5.56	119.78	117.00
3	0	608	C	N3-C4-N4	5.56	121.89	118.00
3	0	1493	G	O4'-C1'-N9	5.56	112.65	108.20
3	0	1734	C	N3-C4-N4	5.56	121.89	118.00
3	0	1835	C	N3-C4-C5	-5.56	119.68	121.90
3	0	1858	C	N3-C4-C5	-5.56	119.68	121.90
3	0	728	A	C5-C6-N6	-5.56	119.26	123.70
3	0	1367	A	C5-C6-N6	-5.56	119.25	123.70
3	0	162	A	C5-C6-N1	-5.55	114.92	117.70
3	0	709	C	N3-C4-N4	5.55	121.89	118.00
3	0	777	A	C5-C6-N6	-5.55	119.26	123.70
3	0	786	A	C5-C6-N6	-5.55	119.26	123.70
3	0	1980	A	C5-C6-N6	-5.55	119.26	123.70
2	1	6	C	N3-C4-N4	5.55	121.89	118.00
3	0	2041	A	O4'-C1'-N9	5.55	112.64	108.20
3	0	92	G	O4'-C1'-N9	5.55	112.64	108.20
3	0	514	G	O4'-C1'-N9	5.55	112.64	108.20
3	0	1548	C	N3-C4-N4	5.55	121.89	118.00
3	0	1781	G	O4'-C1'-N9	5.55	112.64	108.20
3	0	1803	G	O4'-C1'-N9	5.55	112.64	108.20
3	0	2009	A	C5-C6-N6	-5.55	119.26	123.70
3	0	2245	A	C5-C6-N6	-5.55	119.26	123.70
26	J	149	SER	C-N-CA	5.55	135.58	121.70
2	1	38	C	N3-C4-N4	5.55	121.88	118.00
2	1	59	A	C5-C6-N6	-5.55	119.26	123.70
3	0	1189	C	N3-C4-N4	5.55	121.89	118.00
3	0	1247	A	C5-C6-N1	-5.55	114.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1358	A	C5-C6-N6	-5.55	119.26	123.70
3	0	1871	A	C5-C6-N1	-5.55	114.92	117.70
3	0	2003	A	C4-C5-C6	5.55	119.77	117.00
3	0	2065	C	N3-C4-N4	5.55	121.88	118.00
3	0	1358	A	C5-C6-N1	-5.55	114.93	117.70
3	0	1368	C	N3-C4-N4	5.55	121.88	118.00
3	0	1439	U	C2-N1-C1'	5.55	124.36	117.70
3	0	900	A	C5-C6-N6	-5.55	119.26	123.70
3	0	1386	G	O4'-C1'-N9	5.55	112.64	108.20
3	0	1392	U	O4'-C1'-N1	5.55	112.64	108.20
3	0	1695	G	O4'-C1'-N9	5.55	112.64	108.20
3	0	2286	A	C5-C6-N6	-5.55	119.26	123.70
3	0	143	C	N3-C4-N4	5.54	121.88	118.00
3	0	154	U	P-O3'-C3'	5.54	126.35	119.70
3	0	646	A	O4'-C1'-N9	5.54	112.64	108.20
3	0	1811	C	N3-C4-N4	5.54	121.88	118.00
3	0	2019	C	N3-C4-N4	5.54	121.88	118.00
3	0	195	C	N3-C4-N4	5.54	121.88	118.00
3	0	588	A	C5-C6-N1	-5.54	114.93	117.70
3	0	689	A	C5-C6-N6	-5.54	119.27	123.70
3	0	767	A	C5-C6-N6	-5.54	119.27	123.70
3	0	819	G	O4'-C1'-N9	5.54	112.63	108.20
3	0	915	A	C5-C6-N6	-5.54	119.27	123.70
3	0	2105	C	N3-C4-C5	-5.54	119.68	121.90
3	0	2140	A	C5-C6-N1	-5.54	114.93	117.70
3	0	2278	A	C5-C6-N6	-5.54	119.27	123.70
3	0	106	G	O4'-C1'-N9	5.54	112.63	108.20
3	0	774	C	N3-C4-C5	-5.54	119.68	121.90
3	0	848	U	O4'-C1'-N1	5.54	112.63	108.20
3	0	994	G	O4'-C1'-N9	5.54	112.63	108.20
3	0	1564	U	O4'-C1'-N1	5.54	112.63	108.20
46	C	330	GLN	O-C-N	5.54	131.57	122.70
3	0	246	A	C5-C6-N1	-5.54	114.93	117.70
3	0	1684	A	C5-C6-N6	-5.54	119.27	123.70
3	0	1890	U	O4'-C1'-N1	5.54	112.63	108.20
3	0	80	G	O4'-C1'-N9	5.54	112.63	108.20
3	0	112	A	C5-C6-N1	-5.54	114.93	117.70
3	0	1656	A	C5-C6-N6	-5.54	119.27	123.70
3	0	1990	C	N3-C4-C5	-5.54	119.68	121.90
3	0	2226	A	O4'-C1'-N9	5.54	112.63	108.20
3	0	2288	A	C5-C6-N6	-5.54	119.27	123.70
3	0	945	C	N3-C4-N4	5.54	121.88	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1407	G	O4'-C1'-N9	5.54	112.63	108.20
3	0	1995	U	O4'-C1'-N1	5.54	112.63	108.20
3	0	450	A	O4'-C1'-N9	5.54	112.63	108.20
3	0	454	A	C5-C6-N1	-5.54	114.93	117.70
3	0	529	A	C5-C6-N6	-5.54	119.27	123.70
3	0	644	C	N3-C4-C5	-5.54	119.69	121.90
3	0	667	G	C5-C6-O6	-5.54	125.28	128.60
3	0	1534	A	C4-C5-C6	5.54	119.77	117.00
3	0	1689	C	N3-C4-C5	-5.54	119.69	121.90
3	0	2061	A	C5-C6-N1	-5.54	114.93	117.70
3	0	2256	A	O4'-C1'-N9	5.54	112.63	108.20
3	0	11	A	C5-C6-N6	-5.53	119.27	123.70
3	0	139	G	O4'-C1'-N9	5.53	112.63	108.20
3	0	231	A	C5-C6-N6	-5.53	119.27	123.70
3	0	280	C	N3-C4-C5	-5.53	119.69	121.90
3	0	637	C	N3-C4-C5	-5.53	119.69	121.90
3	0	738	G	O4'-C1'-N9	5.53	112.63	108.20
3	0	793	A	C5-C6-N6	-5.53	119.27	123.70
3	0	1273	A	C5-C6-N1	-5.53	114.93	117.70
3	0	1470	C	N3-C4-N4	5.53	121.87	118.00
3	0	2100	G	O4'-C1'-N9	5.53	112.63	108.20
3	0	2254	A	C5-C6-N6	-5.53	119.27	123.70
3	0	505	A	C5-C6-N6	-5.53	119.28	123.70
3	0	674	A	C5-C6-N1	-5.53	114.94	117.70
3	0	694	A	C5-C6-N6	-5.53	119.28	123.70
3	0	962	A	C5-C6-N1	-5.53	114.94	117.70
3	0	1302	C	N3-C4-N4	5.53	121.87	118.00
3	0	1502	C	N3-C4-N4	5.53	121.87	118.00
3	0	1517	A	C5-C6-N6	-5.53	119.28	123.70
3	0	2093	A	C5-C6-N1	-5.53	114.94	117.70
7	n	279	TYR	CB-CG-CD2	-5.53	117.68	121.00
3	0	1182	C	N3-C4-N4	5.53	121.87	118.00
3	0	2241	C	N3-C4-C5	-5.53	119.69	121.90
3	0	121	A	C5-C6-N6	-5.53	119.28	123.70
3	0	182	C	N3-C4-N4	5.53	121.87	118.00
3	0	765	A	C5-C6-N6	-5.53	119.28	123.70
3	0	959	A	C5-C6-N6	-5.53	119.28	123.70
3	0	1578	C	N3-C4-C5	-5.53	119.69	121.90
3	0	1716	G	O4'-C1'-N9	5.53	112.62	108.20
3	0	1912	C	N3-C4-N4	5.53	121.87	118.00
3	0	2227	G	O4'-C1'-N9	5.53	112.62	108.20
1	f	302	ALA	CA-C-O	-5.53	108.50	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	152	A	C5-C6-N6	-5.53	119.28	123.70
3	0	386	A	C5-C6-N6	-5.53	119.28	123.70
3	0	560	C	N3-C4-C5	-5.53	119.69	121.90
3	0	607	A	C5-C6-N6	-5.53	119.28	123.70
3	0	1295	A	C4-C5-C6	5.53	119.76	117.00
3	0	1387	G	O4'-C1'-N9	5.52	112.62	108.20
3	0	1802	A	C5-C6-N6	-5.52	119.28	123.70
3	0	2244	A	C5-C6-N1	-5.52	114.94	117.70
3	0	68	A	C5-C6-N6	-5.52	119.28	123.70
3	0	440	C	N3-C4-N4	5.52	121.86	118.00
3	0	547	G	O4'-C1'-N9	5.52	112.62	108.20
3	0	564	G	O4'-C1'-N9	5.52	112.62	108.20
3	0	1076	C	N3-C4-N4	5.52	121.86	118.00
3	0	1624	A	C5-C6-N6	-5.52	119.28	123.70
47	8	366	ALA	N-CA-CB	5.52	117.83	110.10
3	0	407	G	O4'-C1'-N9	5.52	112.61	108.20
3	0	729	C	N3-C4-C5	-5.52	119.69	121.90
3	0	1277	C	N3-C4-N4	5.52	121.86	118.00
3	0	1864	U	O4'-C1'-N1	5.52	112.62	108.20
3	0	2082	C	N3-C4-C5	-5.52	119.69	121.90
3	0	55	A	C5-C6-N6	-5.52	119.29	123.70
3	0	369	C	N3-C4-N4	5.52	121.86	118.00
3	0	619	C	N3-C4-C5	-5.52	119.69	121.90
3	0	1237	C	N3-C4-N4	5.52	121.86	118.00
3	0	1284	A	C5-C6-N1	-5.52	114.94	117.70
3	0	1369	G	O4'-C1'-N9	5.52	112.61	108.20
3	0	1451	C	N3-C4-C5	-5.52	119.69	121.90
3	0	1610	A	C4-C5-C6	5.52	119.76	117.00
3	0	2050	A	C5-C6-N1	-5.52	114.94	117.70
3	0	2138	C	N3-C4-N4	5.52	121.86	118.00
49	I	383	TYR	CB-CG-CD2	-5.52	117.69	121.00
3	0	403	G	O4'-C1'-N9	5.52	112.61	108.20
3	0	1589	A	O4'-C1'-N9	5.52	112.61	108.20
1	f	1267	LEU	N-CA-CB	5.51	121.43	110.40
3	0	597	C	N3-C4-N4	5.51	121.86	118.00
3	0	1353	A	O4'-C1'-N9	5.51	112.61	108.20
3	0	348	A	C5-C6-N1	-5.51	114.94	117.70
3	0	1922	G	O4'-C1'-N9	5.51	112.61	108.20
3	0	282	C	N3-C4-N4	5.51	121.86	118.00
3	0	799	A	O4'-C1'-N9	5.51	112.61	108.20
3	0	926	C	N3-C4-N4	5.51	121.86	118.00
3	0	1458	A	C5-C6-N1	-5.51	114.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1808	A	O4'-C1'-N9	5.51	112.61	108.20
2	1	58	A	C5-C6-N6	-5.51	119.29	123.70
3	0	7	G	O4'-C1'-N9	5.51	112.61	108.20
3	0	516	A	C5-C6-N6	-5.51	119.29	123.70
3	0	1201	A	C5-C6-N6	-5.51	119.29	123.70
3	0	1224	C	N3-C4-N4	5.51	121.86	118.00
3	0	1234	C	N3-C4-C5	-5.51	119.70	121.90
3	0	1345	A	C5-C6-N6	-5.51	119.29	123.70
3	0	493	A	C5-C6-N6	-5.51	119.29	123.70
3	0	1794	A	C5-C6-N1	-5.51	114.95	117.70
3	0	2001	A	C5-C6-N1	-5.51	114.95	117.70
3	0	329	U	O4'-C1'-N1	5.51	112.61	108.20
3	0	736	U	O4'-C1'-N1	5.51	112.61	108.20
3	0	743	C	O4'-C1'-N1	5.51	112.61	108.20
3	0	1293	G	O4'-C1'-N9	5.51	112.61	108.20
3	0	1416	C	N3-C4-N4	5.51	121.85	118.00
3	0	1732	C	N3-C4-C5	-5.51	119.70	121.90
3	0	78	A	C5-C6-N1	-5.50	114.95	117.70
3	0	1528	C	N3-C4-N4	5.50	121.85	118.00
3	0	2142	C	N3-C4-C5	-5.50	119.70	121.90
3	0	457	A	C5-C6-N1	-5.50	114.95	117.70
3	0	1533	C	N3-C4-N4	5.50	121.85	118.00
3	0	1615	A	C5-C6-N1	-5.50	114.95	117.70
3	0	1633	A	C5-C6-N6	-5.50	119.30	123.70
23	d	197	PHE	CB-CG-CD2	-5.50	116.95	120.80
23	d	217	PHE	CB-CG-CD2	-5.50	116.95	120.80
3	0	1795	A	C5-C6-N1	-5.50	114.95	117.70
3	0	438	A	C5-C6-N6	-5.50	119.30	123.70
3	0	771	A	O4'-C1'-N9	5.50	112.60	108.20
1	f	296	TYR	N-CA-CB	-5.50	100.70	110.60
2	1	75	A	C4-C5-C6	5.50	119.75	117.00
3	0	4	C	N3-C4-C5	-5.50	119.70	121.90
3	0	463	A	C5-C6-N6	-5.50	119.30	123.70
3	0	817	A	C5-C6-N1	-5.50	114.95	117.70
3	0	1663	C	N3-C4-C5	-5.50	119.70	121.90
3	0	1669	A	C5-C6-N1	-5.50	114.95	117.70
3	0	1933	U	O4'-C1'-N1	5.50	112.60	108.20
28	5	172	PHE	C-N-CD	5.50	139.95	128.40
3	0	176	C	N3-C4-N4	5.50	121.85	118.00
3	0	373	G	O4'-C1'-N9	5.50	112.60	108.20
3	0	672	U	O4'-C1'-N1	5.50	112.60	108.20
3	0	721	C	N3-C4-N4	5.50	121.85	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1379	A	C5-C6-N1	-5.50	114.95	117.70
3	0	1414	G	O4'-C1'-N9	5.50	112.60	108.20
3	0	1426	A	C5-C6-N6	-5.50	119.30	123.70
3	0	1942	A	C5-C6-N6	-5.50	119.30	123.70
3	0	2006	A	C5-C6-N6	-5.50	119.30	123.70
1	f	1153	ASP	O-C-N	-5.49	113.91	122.70
3	0	298	C	N3-C4-C5	-5.49	119.70	121.90
3	0	562	A	C5-C6-N1	-5.49	114.95	117.70
3	0	1383	A	C5-C6-N6	-5.49	119.30	123.70
3	0	1631	C	N3-C4-N4	5.49	121.84	118.00
3	0	1714	G	O4'-C1'-N9	5.49	112.59	108.20
3	0	1793	C	N3-C4-C5	-5.49	119.70	121.90
3	0	2070	A	C5-C6-N6	-5.49	119.31	123.70
3	0	387	C	N3-C4-C5	-5.49	119.70	121.90
3	0	936	C	N3-C4-C5	-5.49	119.70	121.90
3	0	1736	G	O4'-C1'-N9	5.49	112.59	108.20
2	1	47	C	N3-C4-N4	5.49	121.84	118.00
3	0	355	G	O4'-C1'-N9	5.49	112.59	108.20
3	0	789	C	N3-C4-C5	-5.49	119.70	121.90
3	0	1393	U	O4'-C1'-N1	5.49	112.59	108.20
3	0	2150	A	C5-C6-N6	-5.49	119.31	123.70
3	0	172	A	C5-C6-N6	-5.49	119.31	123.70
3	0	509	A	O4'-C1'-N9	5.49	112.59	108.20
3	0	673	A	C5-C6-N6	-5.49	119.31	123.70
3	0	1604	A	C5-C6-N6	-5.49	119.31	123.70
3	0	1606	A	C5-C6-N6	-5.49	119.31	123.70
3	0	2152	U	C6-N1-C1'	-5.49	113.52	121.20
3	0	2276	A	C5-C6-N1	-5.49	114.96	117.70
47	8	453	ARG	CA-C-N	5.49	129.27	117.20
3	0	175	A	C5-C6-N1	-5.49	114.96	117.70
3	0	629	C	N3-C4-C5	-5.49	119.70	121.90
3	0	960	A	C5-C6-N6	-5.49	119.31	123.70
3	0	1403	A	O4'-C1'-N9	5.49	112.59	108.20
3	0	121	A	O4'-C1'-N9	5.49	112.59	108.20
3	0	487	U	O4'-C1'-N1	5.49	112.59	108.20
3	0	549	A	O4'-C1'-N9	5.49	112.59	108.20
3	0	766	C	N3-C4-N4	5.49	121.84	118.00
3	0	984	A	C5-C6-N1	-5.49	114.96	117.70
3	0	1197	A	C5-C6-N6	-5.49	119.31	123.70
3	0	1202	A	C5-C6-N1	-5.49	114.96	117.70
3	0	1274	C	N3-C4-N4	5.49	121.84	118.00
3	0	1275	A	C5-C6-N1	-5.49	114.96	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1477	A	C5-C6-N6	-5.49	119.31	123.70
3	0	1733	C	N3-C4-C5	-5.49	119.71	121.90
3	0	1808	A	C5-C6-N6	-5.49	119.31	123.70
1	f	1158	MET	CG-SD-CE	-5.48	91.42	100.20
3	0	254	A	C5-C6-N6	-5.48	119.31	123.70
3	0	1424	U	O4'-C1'-N1	5.48	112.59	108.20
3	0	2088	A	O4'-C1'-N9	5.48	112.59	108.20
2	1	57	A	C4-C5-C6	5.48	119.74	117.00
3	0	314	A	C5-C6-N1	-5.48	114.96	117.70
3	0	498	A	C5-C6-N1	-5.48	114.96	117.70
3	0	675	A	C5-C6-N6	-5.48	119.31	123.70
3	0	1887	G	C5-C6-O6	-5.48	125.31	128.60
3	0	1971	C	N3-C4-C5	-5.48	119.71	121.90
3	0	14	C	N3-C4-N4	5.48	121.84	118.00
3	0	143	C	N3-C4-C5	-5.48	119.71	121.90
3	0	887	C	N3-C4-N4	5.48	121.84	118.00
3	0	2044	A	O4'-C1'-N9	5.48	112.58	108.20
3	0	444	A	C5-C6-N6	-5.48	119.32	123.70
3	0	44	C	N3-C4-C5	-5.48	119.71	121.90
3	0	690	A	C5-C6-N1	-5.48	114.96	117.70
3	0	1258	G	O4'-C1'-N9	5.48	112.58	108.20
3	0	1272	U	O4'-C1'-N1	5.48	112.58	108.20
3	0	1669	A	C5-C6-N6	-5.48	119.32	123.70
2	1	33	C	N3-C4-N4	5.47	121.83	118.00
3	0	26	A	C5-C6-N1	-5.47	114.96	117.70
3	0	1742	U	O4'-C1'-N1	5.47	112.58	108.20
3	0	1830	A	C5-C6-N6	-5.47	119.32	123.70
3	0	2289	A	C5-C6-N6	-5.47	119.32	123.70
44	K	23	PHE	CB-CG-CD1	-5.47	116.97	120.80
2	1	74	C	N3-C4-N4	5.47	121.83	118.00
3	0	102	A	C5-C6-N6	-5.47	119.32	123.70
3	0	125	A	O4'-C1'-N9	5.47	112.58	108.20
3	0	411	G	N3-C2-N2	5.47	123.73	119.90
3	0	585	A	C5-C6-N1	-5.47	114.96	117.70
3	0	809	A	O4'-C1'-N9	5.47	112.58	108.20
3	0	834	G	O4'-C1'-N9	5.47	112.58	108.20
3	0	1368	C	O4'-C1'-N1	5.47	112.58	108.20
3	0	1432	C	N3-C4-C5	-5.47	119.71	121.90
3	0	1962	C	N3-C4-N4	5.47	121.83	118.00
3	0	61	C	N3-C4-N4	5.47	121.83	118.00
3	0	1378	C	N3-C4-C5	-5.47	119.71	121.90
3	0	40	A	C5-C6-N1	-5.47	114.97	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	185	A	C5-C6-N6	-5.47	119.32	123.70
3	0	270	C	N3-C4-C5	-5.47	119.71	121.90
3	0	345	A	C5-C6-N6	-5.47	119.33	123.70
3	0	446	A	C5-C6-N1	-5.47	114.97	117.70
3	0	676	G	O4'-C1'-N9	5.47	112.58	108.20
3	0	750	C	N3-C4-C5	-5.47	119.71	121.90
3	0	1274	C	N3-C4-C5	-5.47	119.71	121.90
3	0	1299	C	N3-C4-C5	-5.47	119.71	121.90
3	0	2001	A	O4'-C1'-N9	5.47	112.57	108.20
3	0	2056	C	O4'-C1'-N1	5.47	112.57	108.20
3	0	2107	C	N3-C4-C5	-5.47	119.71	121.90
3	0	2265	A	O4'-C1'-N9	5.47	112.57	108.20
3	0	124	A	C5-C6-N1	-5.47	114.97	117.70
3	0	187	C	N3-C4-C5	-5.47	119.71	121.90
3	0	270	C	N3-C4-N4	5.47	121.83	118.00
3	0	417	A	C5-C6-N6	-5.47	119.33	123.70
3	0	690	A	C5-C6-N6	-5.47	119.33	123.70
3	0	743	C	N3-C4-N4	5.47	121.83	118.00
3	0	1313	A	O4'-C1'-N9	5.47	112.57	108.20
3	0	1544	A	C5-C6-N1	-5.47	114.97	117.70
3	0	2028	C	N3-C4-C5	-5.47	119.71	121.90
3	0	2131	A	C5-C6-N6	-5.47	119.33	123.70
1	f	199	PHE	N-CA-C	-5.46	96.25	111.00
1	f	214	PHE	CB-CG-CD1	5.46	124.62	120.80
2	1	31	C	N3-C4-C5	-5.46	119.71	121.90
3	0	418	G	O4'-C1'-N9	5.46	112.57	108.20
3	0	598	A	O4'-C1'-N9	5.46	112.57	108.20
3	0	1263	A	C5-C6-N1	-5.46	114.97	117.70
3	0	1317	A	C5-C6-N6	-5.46	119.33	123.70
3	0	1416	C	N3-C4-C5	-5.46	119.71	121.90
3	0	2264	A	C5-C6-N1	-5.46	114.97	117.70
3	0	598	A	C5-C6-N6	-5.46	119.33	123.70
3	0	1283	C	N3-C4-C5	-5.46	119.72	121.90
3	0	1606	A	O4'-C1'-N9	5.46	112.57	108.20
3	0	4	C	N3-C4-N4	5.46	121.82	118.00
3	0	25	C	N3-C4-N4	5.46	121.82	118.00
3	0	75	U	O4'-C1'-N1	5.46	112.57	108.20
3	0	616	G	O4'-C1'-N9	5.46	112.57	108.20
3	0	648	A	C5-C6-N1	-5.46	114.97	117.70
3	0	1573	A	C5-C6-N6	-5.46	119.33	123.70
3	0	2140	A	C5-C6-N6	-5.46	119.33	123.70
3	0	982	G	O4'-C1'-N9	5.46	112.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1901	C	N3-C4-N4	5.46	121.82	118.00
1	f	144	SER	N-CA-CB	5.46	118.69	110.50
3	0	1401	G	O4'-C1'-N9	5.46	112.57	108.20
3	0	1625	A	C5-C6-N6	-5.46	119.33	123.70
3	0	2038	C	N3-C4-N4	5.46	121.82	118.00
3	0	2305	A	C5-C6-N1	-5.46	114.97	117.70
3	0	366	C	N3-C4-N4	5.46	121.82	118.00
3	0	472	A	O4'-C1'-N9	5.46	112.56	108.20
3	0	867	G	N3-C2-N2	5.46	123.72	119.90
3	0	1244	G	O4'-C1'-N9	5.46	112.57	108.20
3	0	1382	A	C5-C6-N1	-5.46	114.97	117.70
3	0	2170	A	C5-C6-N1	-5.46	114.97	117.70
3	0	1260	A	C5-C6-N1	-5.46	114.97	117.70
3	0	28	A	O4'-C1'-N9	5.45	112.56	108.20
3	0	401	A	C5-C6-N1	-5.45	114.97	117.70
3	0	491	C	N3-C4-N4	5.45	121.82	118.00
3	0	717	U	O4'-C1'-N1	5.45	112.56	108.20
3	0	1190	A	C5-C6-N6	-5.45	119.34	123.70
3	0	2250	A	C5-C6-N1	-5.45	114.97	117.70
3	0	2250	A	O4'-C1'-N9	5.45	112.56	108.20
3	0	241	A	O4'-C1'-N9	5.45	112.56	108.20
3	0	1525	A	C5-C6-N1	-5.45	114.97	117.70
3	0	1979	C	N3-C4-N4	5.45	121.81	118.00
2	1	33	C	N3-C4-C5	-5.45	119.72	121.90
3	0	464	C	N3-C4-C5	-5.45	119.72	121.90
3	0	471	C	N3-C4-C5	-5.45	119.72	121.90
3	0	485	A	C5-C6-N1	-5.45	114.98	117.70
3	0	1302	C	N3-C4-C5	-5.45	119.72	121.90
3	0	1328	A	C5-C6-N1	-5.45	114.98	117.70
50	H	96	THR	CA-C-N	5.45	132.36	117.10
3	0	330	A	C5-C6-N1	-5.45	114.98	117.70
3	0	598	A	C5-C6-N1	-5.45	114.98	117.70
3	0	648	A	C5-C6-N6	-5.45	119.34	123.70
3	0	812	A	C5-C6-N6	-5.45	119.34	123.70
3	0	874	C	N3-C4-N4	5.45	121.81	118.00
3	0	1834	C	N3-C4-N4	5.45	121.81	118.00
3	0	2314	U	O4'-C1'-N1	5.44	112.56	108.20
3	0	729	C	O4'-C1'-N1	5.44	112.55	108.20
3	0	817	A	O4'-C1'-N9	5.44	112.55	108.20
3	0	1552	A	C5-C6-N6	-5.44	119.35	123.70
3	0	2317	A	O4'-C1'-N9	5.44	112.55	108.20
3	0	111	A	O4'-C1'-N9	5.44	112.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	210	A	O4'-C1'-N9	5.44	112.55	108.20
3	0	484	A	C5-C6-N1	-5.44	114.98	117.70
3	0	917	A	C5-C6-N1	-5.44	114.98	117.70
3	0	586	A	C5-C6-N1	-5.44	114.98	117.70
3	0	1194	A	C5-C6-N6	-5.44	119.35	123.70
3	0	1260	A	O4'-C1'-N9	5.44	112.55	108.20
3	0	2153	A	C5-C6-N6	-5.44	119.35	123.70
3	0	18	C	N3-C4-C5	-5.44	119.72	121.90
3	0	425	A	C5-C6-N6	-5.44	119.35	123.70
3	0	799	A	C5-C6-N6	-5.44	119.35	123.70
3	0	867	G	O4'-C1'-N9	5.44	112.55	108.20
3	0	1469	A	C5-C6-N6	-5.44	119.35	123.70
3	0	1475	A	O4'-C1'-N9	5.44	112.55	108.20
3	0	1888	C	N3-C4-C5	-5.44	119.72	121.90
3	0	279	A	O4'-C1'-N9	5.44	112.55	108.20
3	0	351	A	C5-C6-N6	-5.44	119.35	123.70
3	0	599	A	C5-C6-N6	-5.44	119.35	123.70
3	0	938	G	C5-C6-O6	-5.44	125.34	128.60
3	0	1245	A	C5-C6-N1	-5.44	114.98	117.70
3	0	1311	A	C5-C6-N6	-5.44	119.35	123.70
3	0	1551	C	N3-C4-C5	-5.44	119.73	121.90
3	0	117	C	N3-C4-C5	-5.43	119.73	121.90
3	0	624	A	C5-C6-N6	-5.43	119.35	123.70
3	0	1729	A	C5-C6-N1	-5.43	114.98	117.70
3	0	1804	A	C5-C6-N1	-5.43	114.98	117.70
3	0	2010	A	O4'-C1'-N9	5.43	112.55	108.20
3	0	2245	A	O4'-C1'-N9	5.43	112.55	108.20
44	K	141	TYR	CB-CG-CD2	5.43	124.26	121.00
3	0	335	G	O4'-C1'-N9	5.43	112.55	108.20
3	0	584	C	O4'-C1'-N1	5.43	112.55	108.20
3	0	1067	A	C5-C6-N1	-5.43	114.98	117.70
3	0	1474	C	N3-C4-C5	-5.43	119.73	121.90
3	0	1566	A	C5-C6-N6	-5.43	119.35	123.70
3	0	1997	A	C4-C5-C6	5.43	119.72	117.00
3	0	215	A	C5-C6-N1	-5.43	114.98	117.70
3	0	526	A	C5-C6-N1	-5.43	114.98	117.70
3	0	1262	C	N3-C4-C5	-5.43	119.73	121.90
3	0	1631	C	N3-C4-C5	-5.43	119.73	121.90
3	0	1953	G	O4'-C1'-N9	5.43	112.55	108.20
2	1	20	A	C5-C6-N6	-5.43	119.36	123.70
3	0	2	A	C5-C6-N1	-5.43	114.98	117.70
3	0	284	C	N3-C4-C5	-5.43	119.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	874	C	N3-C4-C5	-5.43	119.73	121.90
3	0	912	A	C5-C6-N1	-5.43	114.98	117.70
3	0	961	A	C5-C6-N1	-5.43	114.98	117.70
3	0	382	G	O4'-C1'-N9	5.43	112.54	108.20
3	0	1480	C	N3-C4-C5	-5.43	119.73	121.90
3	0	1823	A	O4'-C1'-N9	5.43	112.54	108.20
3	0	2038	C	N3-C4-C5	-5.43	119.73	121.90
3	0	61	C	C6-N1-C1'	-5.43	114.29	120.80
3	0	64	A	C5-C6-N6	-5.43	119.36	123.70
3	0	242	A	O4'-C1'-N9	5.43	112.54	108.20
3	0	316	A	C5-C6-N6	-5.43	119.36	123.70
3	0	595	A	C5-C6-N1	-5.43	114.99	117.70
3	0	1070	C	N3-C4-C5	-5.43	119.73	121.90
3	0	1225	G	O4'-C1'-N9	5.43	112.54	108.20
3	0	1600	A	O4'-C1'-N9	5.43	112.54	108.20
3	0	2319	C	N3-C4-C5	-5.43	119.73	121.90
3	0	732	C	N3-C4-N4	5.42	121.80	118.00
3	0	1240	A	O4'-C1'-N9	5.42	112.54	108.20
3	0	2010	A	C5-C6-N6	-5.42	119.36	123.70
3	0	825	C	N3-C4-N4	5.42	121.80	118.00
3	0	1596	C	N3-C4-C5	-5.42	119.73	121.90
3	0	1941	A	C5-C6-N6	-5.42	119.36	123.70
1	f	292	ARG	O-C-N	-5.42	114.03	122.70
3	0	140	C	N3-C4-C5	-5.42	119.73	121.90
3	0	190	A	C5-C6-N6	-5.42	119.36	123.70
3	0	662	C	N3-C4-N4	5.42	121.80	118.00
3	0	785	A	C5-C6-N6	-5.42	119.36	123.70
3	0	877	A	O4'-C1'-N9	5.42	112.54	108.20
3	0	980	G	O4'-C1'-N9	5.42	112.54	108.20
3	0	1432	C	N3-C4-N4	5.42	121.79	118.00
3	0	1965	A	C5-C6-N1	-5.42	114.99	117.70
3	0	2277	A	C5-C6-N6	-5.42	119.36	123.70
3	0	611	G	O4'-C1'-N9	5.42	112.54	108.20
3	0	1978	A	P-O5'-C5'	5.42	129.57	120.90
3	0	2108	A	O4'-C1'-N9	5.42	112.54	108.20
3	0	28	A	C5-C6-N1	-5.42	114.99	117.70
3	0	727	C	N3-C4-N4	5.42	121.79	118.00
3	0	1267	C	N3-C4-C5	-5.42	119.73	121.90
3	0	1962	C	N3-C4-C5	-5.42	119.73	121.90
3	0	404	G	O4'-C1'-N9	5.42	112.53	108.20
3	0	742	A	C5-C6-N1	-5.42	114.99	117.70
3	0	2036	A	C5-C6-N6	-5.42	119.37	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	914	C	N3-C4-N4	5.42	121.79	118.00
3	0	1458	A	C5-C6-N6	-5.42	119.37	123.70
3	0	2064	A	C5-C6-N6	-5.42	119.37	123.70
3	0	1590	C	N3-C4-C5	-5.41	119.73	121.90
3	0	1797	G	O4'-C1'-N9	5.41	112.53	108.20
3	0	2141	A	C5-C6-N1	-5.41	114.99	117.70
3	0	268	C	N3-C4-N4	5.41	121.79	118.00
3	0	475	A	C5-C6-N6	-5.41	119.37	123.70
3	0	788	A	C5-C6-N1	-5.41	114.99	117.70
3	0	1076	C	N3-C4-C5	-5.41	119.73	121.90
3	0	1729	A	O4'-C1'-N9	5.41	112.53	108.20
3	0	778	A	C5-C6-N6	-5.41	119.37	123.70
3	0	1516	A	C5-C6-N1	-5.41	115.00	117.70
3	0	1747	C	N3-C4-N4	5.41	121.79	118.00
3	0	1942	A	C5-C6-N1	-5.41	114.99	117.70
3	0	2050	A	C5-C6-N6	-5.41	119.37	123.70
2	1	73	C	N3-C4-C5	-5.41	119.74	121.90
3	0	120	C	N3-C4-C5	-5.41	119.74	121.90
3	0	256	A	C5-C6-N1	-5.41	115.00	117.70
3	0	609	A	C5-C6-N1	-5.41	115.00	117.70
3	0	976	U	O4'-C1'-N1	5.41	112.53	108.20
3	0	1420	A	C5-C6-N1	-5.41	115.00	117.70
3	0	1703	A	C4-C5-C6	5.41	119.70	117.00
3	0	503	A	C5-C6-N6	-5.41	119.37	123.70
3	0	1370	A	C5-C6-N1	-5.41	115.00	117.70
3	0	1612	A	C5-C6-N1	-5.41	115.00	117.70
3	0	19	A	C5-C6-N6	-5.41	119.38	123.70
3	0	120	C	N3-C4-N4	5.41	121.78	118.00
3	0	482	C	N3-C4-N4	5.41	121.78	118.00
3	0	876	A	O4'-C1'-N9	5.41	112.52	108.20
3	0	1328	A	C5-C6-N6	-5.41	119.38	123.70
3	0	1666	A	O4'-C1'-N9	5.41	112.53	108.20
3	0	1879	C	N3-C4-N4	5.41	121.78	118.00
2	1	31	C	N3-C4-N4	5.40	121.78	118.00
3	0	638	C	N3-C4-C5	-5.40	119.74	121.90
3	0	770	C	N3-C4-N4	5.40	121.78	118.00
3	0	1338	A	C5-C6-N6	-5.40	119.38	123.70
3	0	1780	U	C6-N1-C1'	-5.40	113.64	121.20
3	0	2110	C	N3-C4-C5	-5.40	119.74	121.90
3	0	322	G	O4'-C1'-N9	5.40	112.52	108.20
3	0	428	C	N3-C4-C5	-5.40	119.74	121.90
3	0	698	C	N3-C4-C5	-5.40	119.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1665	C	N3-C4-C5	-5.40	119.74	121.90
3	0	89	C	N3-C4-N4	5.40	121.78	118.00
3	0	295	A	C5-C6-N1	-5.40	115.00	117.70
3	0	463	A	C5-C6-N1	-5.40	115.00	117.70
3	0	728	A	C5-C6-N1	-5.40	115.00	117.70
3	0	877	A	C5-C6-N6	-5.40	119.38	123.70
3	0	1643	G	O4'-C1'-N9	5.40	112.52	108.20
3	0	1868	C	N3-C4-N4	5.40	121.78	118.00
3	0	2097	A	C5-C6-N1	-5.40	115.00	117.70
3	0	2306	C	N3-C4-C5	-5.40	119.74	121.90
3	0	1879	C	N3-C4-C5	-5.40	119.74	121.90
3	0	389	G	O4'-C1'-N9	5.40	112.52	108.20
3	0	605	G	O4'-C1'-N9	5.40	112.52	108.20
3	0	887	C	O4'-C1'-N1	5.40	112.52	108.20
3	0	1190	A	C5-C6-N1	-5.40	115.00	117.70
3	0	408	C	N3-C4-N4	5.40	121.78	118.00
3	0	1198	A	C5-C6-N1	-5.40	115.00	117.70
3	0	1616	A	O4'-C1'-N9	5.40	112.52	108.20
3	0	107	A	C5-C6-N1	-5.39	115.00	117.70
3	0	351	A	O4'-C1'-N9	5.39	112.52	108.20
3	0	446	A	C5-C6-N6	-5.39	119.38	123.70
3	0	909	G	O4'-C1'-N9	5.39	112.52	108.20
3	0	1796	C	N3-C4-C5	-5.39	119.74	121.90
3	0	2116	A	O4'-C1'-N9	5.39	112.52	108.20
3	0	1463	A	C5-C6-N6	-5.39	119.39	123.70
3	0	2256	A	C5-C6-N1	-5.39	115.00	117.70
2	1	37	A	O4'-C1'-N9	5.39	112.51	108.20
3	0	86	G	O4'-C1'-N9	5.39	112.51	108.20
3	0	1453	A	O4'-C1'-N9	5.39	112.51	108.20
3	0	1528	C	N3-C4-C5	-5.39	119.74	121.90
3	0	1615	A	C5-C6-N6	-5.39	119.39	123.70
3	0	1924	A	C5-C6-N1	-5.39	115.00	117.70
2	1	71	U	O3'-P-O5'	5.39	114.24	104.00
3	0	39	A	C4-C5-C6	5.39	119.69	117.00
3	0	177	A	C5-C6-N6	-5.39	119.39	123.70
3	0	409	G	O4'-C1'-N9	5.39	112.51	108.20
3	0	516	A	C5-C6-N1	-5.39	115.00	117.70
3	0	707	C	N3-C4-N4	5.39	121.77	118.00
3	0	889	A	C5-C6-N6	-5.39	119.39	123.70
3	0	1692	A	O4'-C1'-N9	5.39	112.51	108.20
3	0	1728	G	O4'-C1'-N9	5.39	112.51	108.20
3	0	1731	C	N3-C4-N4	5.39	121.77	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1924	A	O4'-C1'-N9	5.39	112.51	108.20
3	0	2170	A	C5-C6-N6	-5.39	119.39	123.70
3	0	562	A	C5-C6-N6	-5.39	119.39	123.70
3	0	1203	G	O4'-C1'-N9	5.39	112.51	108.20
3	0	1400	C	O4'-C1'-N1	5.39	112.51	108.20
3	0	1476	U	O4'-C1'-N1	5.39	112.51	108.20
3	0	1855	C	N3-C4-C5	-5.39	119.75	121.90
3	0	47	A	C5-C6-N1	-5.39	115.01	117.70
3	0	47	A	C5-C6-N6	-5.39	119.39	123.70
3	0	50	C	N3-C4-N4	5.39	121.77	118.00
3	0	127	C	N3-C4-N4	5.39	121.77	118.00
3	0	244	G	O4'-C1'-N9	5.39	112.51	108.20
3	0	784	A	O4'-C1'-N9	5.39	112.51	108.20
3	0	873	C	N3-C4-C5	-5.39	119.75	121.90
3	0	928	C	N3-C4-C5	-5.39	119.75	121.90
3	0	1711	A	C5-C6-N6	-5.39	119.39	123.70
3	0	1743	G	O4'-C1'-N9	5.39	112.51	108.20
1	f	192	ALA	CA-C-N	-5.38	105.35	117.20
3	0	246	A	C5-C6-N6	-5.38	119.39	123.70
3	0	274	C	N3-C4-C5	-5.38	119.75	121.90
3	0	1553	C	N3-C4-C5	-5.38	119.75	121.90
3	0	2013	A	C5-C6-N1	-5.38	115.01	117.70
3	0	902	A	C5-C6-N1	-5.38	115.01	117.70
3	0	1457	A	C5-C6-N1	-5.38	115.01	117.70
3	0	1871	A	O4'-C1'-N9	5.38	112.51	108.20
3	0	1978	A	C4-C5-C6	5.38	119.69	117.00
3	0	2197	A	C5-C6-N6	-5.38	119.39	123.70
3	0	2292	U	O4'-C1'-N1	5.38	112.51	108.20
3	0	282	C	N3-C4-C5	-5.38	119.75	121.90
3	0	769	A	C5-C6-N1	-5.38	115.01	117.70
3	0	2072	C	N3-C4-C5	-5.38	119.75	121.90
3	0	53	G	O4'-C1'-N9	5.38	112.50	108.20
3	0	471	C	N3-C4-N4	5.38	121.76	118.00
3	0	571	A	C5-C6-N6	-5.38	119.40	123.70
3	0	580	C	N3-C4-C5	-5.38	119.75	121.90
3	0	1966	A	C5-C6-N6	-5.38	119.40	123.70
3	0	2218	G	N3-C2-N2	5.38	123.67	119.90
3	0	504	A	C5-C6-N1	-5.38	115.01	117.70
3	0	673	A	P-O3'-C3'	5.38	126.15	119.70
3	0	1675	A	O4'-C1'-N9	5.38	112.50	108.20
3	0	1827	A	O4'-C1'-N9	5.38	112.50	108.20
3	0	1897	U	O4'-C1'-N1	5.38	112.50	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2254	A	C5-C6-N1	-5.38	115.01	117.70
11	m	105	PHE	CB-CG-CD2	-5.38	117.04	120.80
3	0	866	A	C5-C6-N6	-5.38	119.40	123.70
3	0	1270	A	C5-C6-N1	-5.38	115.01	117.70
3	0	1636	A	O4'-C1'-N9	5.38	112.50	108.20
2	1	72	A	C4-C5-C6	5.37	119.69	117.00
3	0	180	A	C5-C6-N1	-5.37	115.01	117.70
3	0	239	C	N3-C4-C5	-5.37	119.75	121.90
3	0	337	G	O4'-C1'-N9	5.37	112.50	108.20
3	0	841	C	N3-C4-C5	-5.37	119.75	121.90
3	0	1492	C	N3-C4-C5	-5.37	119.75	121.90
3	0	1883	A	C5-C6-N1	-5.37	115.01	117.70
3	0	583	C	N3-C4-C5	-5.37	119.75	121.90
3	0	977	A	C5-C6-N6	-5.37	119.40	123.70
3	0	1817	A	C5-C6-N6	-5.37	119.40	123.70
3	0	213	G	O4'-C1'-N9	5.37	112.50	108.20
3	0	1297	A	C5-C6-N1	-5.37	115.02	117.70
3	0	197	C	N3-C4-C5	-5.37	119.75	121.90
3	0	606	G	O4'-C1'-N9	5.37	112.50	108.20
3	0	1271	C	N3-C4-C5	-5.37	119.75	121.90
3	0	1433	A	C5-C6-N1	-5.37	115.02	117.70
3	0	1501	A	C5-C6-N1	-5.37	115.02	117.70
3	0	1893	A	C5-C6-N1	-5.37	115.02	117.70
3	0	2194	A	O4'-C1'-N9	5.37	112.50	108.20
3	0	2305	A	C5-C6-N6	-5.37	119.41	123.70
3	0	2313	C	N3-C4-C5	-5.37	119.75	121.90
3	0	444	A	O4'-C1'-N9	5.37	112.49	108.20
3	0	783	A	C5-C6-N1	-5.37	115.02	117.70
3	0	786	A	O4'-C1'-N9	5.37	112.49	108.20
1	f	1177	PRO	N-CA-C	-5.37	98.15	112.10
3	0	81	A	C5-C6-N1	-5.37	115.02	117.70
3	0	771	A	C5-C6-N1	-5.37	115.02	117.70
3	0	876	A	C4-C5-C6	5.37	119.68	117.00
3	0	1474	C	N3-C4-N4	5.37	121.76	118.00
3	0	2129	G	O4'-C1'-N9	5.37	112.49	108.20
3	0	2174	A	C5-C6-N6	-5.37	119.41	123.70
3	0	2230	C	N3-C4-C5	-5.37	119.75	121.90
3	0	959	A	C5-C6-N1	-5.36	115.02	117.70
3	0	1256	C	N3-C4-C5	-5.36	119.75	121.90
3	0	1464	A	C5-C6-N6	-5.36	119.41	123.70
3	0	1965	A	C5-C6-N6	-5.36	119.41	123.70
50	H	175	SER	N-CA-CB	5.36	118.55	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2116	A	C5-C6-N1	-5.36	115.02	117.70
3	0	163	C	N3-C4-C5	-5.36	119.76	121.90
3	0	376	C	N3-C4-N4	5.36	121.75	118.00
3	0	483	A	C5-C6-N1	-5.36	115.02	117.70
3	0	523	A	O4'-C1'-N9	5.36	112.49	108.20
3	0	610	A	C5-C6-N6	-5.36	119.41	123.70
3	0	1548	C	N3-C4-C5	-5.36	119.76	121.90
3	0	2115	A	C5-C6-N6	-5.36	119.41	123.70
3	0	2173	C	N3-C4-N4	5.36	121.75	118.00
3	0	2214	A	O4'-C1'-N9	5.36	112.49	108.20
2	1	63	A	C5-C6-N1	-5.36	115.02	117.70
3	0	274	C	O4'-C1'-N1	5.36	112.49	108.20
3	0	1382	A	C5-C6-N6	-5.36	119.41	123.70
3	0	2321	U	O4'-C1'-N1	5.36	112.49	108.20
3	0	116	G	O4'-C1'-N9	5.36	112.49	108.20
3	0	1668	C	N3-C4-N4	5.36	121.75	118.00
3	0	1672	G	O4'-C1'-N9	5.36	112.49	108.20
3	0	54	C	N3-C4-C5	-5.36	119.76	121.90
3	0	188	G	O4'-C1'-N9	5.36	112.48	108.20
3	0	269	A	C5-C6-N1	-5.36	115.02	117.70
3	0	641	C	N3-C4-C5	-5.36	119.76	121.90
3	0	1254	G	N3-C2-N2	5.36	123.65	119.90
3	0	226	A	O4'-C1'-N9	5.35	112.48	108.20
3	0	495	G	O4'-C1'-N9	5.35	112.48	108.20
3	0	1470	C	N3-C4-C5	-5.35	119.76	121.90
3	0	587	A	C5-C6-N1	-5.35	115.02	117.70
3	0	914	C	N3-C4-C5	-5.35	119.76	121.90
3	0	1315	C	N3-C4-C5	-5.35	119.76	121.90
3	0	1859	G	O4'-C1'-N9	5.35	112.48	108.20
3	0	1956	A	C5-C6-N6	-5.35	119.42	123.70
3	0	101	C	N3-C4-N4	5.35	121.74	118.00
3	0	108	C	N3-C4-N4	5.35	121.74	118.00
3	0	185	A	C5-C6-N1	-5.35	115.03	117.70
3	0	655	A	O4'-C1'-N9	5.35	112.48	108.20
3	0	793	A	C5-C6-N1	-5.35	115.03	117.70
3	0	1539	A	C5-C6-N6	-5.35	119.42	123.70
3	0	1558	A	C5-C6-N6	-5.35	119.42	123.70
3	0	2138	C	N3-C4-C5	-5.35	119.76	121.90
3	0	1505	C	N3-C4-C5	-5.35	119.76	121.90
3	0	2097	A	C5-C6-N6	-5.35	119.42	123.70
3	0	2204	A	C5-C6-N1	-5.35	115.03	117.70
3	0	435	G	O4'-C1'-N9	5.35	112.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1919	U	O4'-C1'-N1	5.35	112.48	108.20
3	0	159	G	O4'-C1'-N9	5.34	112.47	108.20
3	0	163	C	N3-C4-N4	5.34	121.74	118.00
3	0	288	A	C5-C6-N6	-5.34	119.42	123.70
3	0	1240	A	C5-C6-N1	-5.34	115.03	117.70
3	0	1830	A	C5-C6-N1	-5.34	115.03	117.70
3	0	1891	G	O4'-C1'-N9	5.34	112.48	108.20
3	0	1911	C	N3-C4-C5	-5.34	119.76	121.90
3	0	2243	A	C5-C6-N6	-5.34	119.42	123.70
3	0	112	A	O4'-C1'-N9	5.34	112.47	108.20
3	0	1264	A	O4'-C1'-N9	5.34	112.47	108.20
3	0	1475	A	C5-C6-N1	-5.34	115.03	117.70
3	0	43	A	C5-C6-N1	-5.34	115.03	117.70
3	0	502	A	C5-C6-N1	-5.34	115.03	117.70
3	0	1334	G	O4'-C1'-N9	5.34	112.47	108.20
3	0	1628	G	O4'-C1'-N9	5.34	112.47	108.20
3	0	1699	G	O4'-C1'-N9	5.34	112.47	108.20
3	0	1799	A	C5-C6-N1	-5.34	115.03	117.70
3	0	1869	C	N3-C4-C5	-5.34	119.76	121.90
3	0	2036	A	C5-C6-N1	-5.34	115.03	117.70
3	0	2278	A	C5-C6-N1	-5.34	115.03	117.70
44	K	26	PHE	CB-CG-CD1	5.34	124.54	120.80
2	1	55	C	N3-C4-C5	-5.34	119.76	121.90
3	0	237	A	C5-C6-N6	-5.34	119.43	123.70
3	0	845	A	C5-C6-N1	-5.34	115.03	117.70
3	0	1377	C	N3-C4-C5	-5.34	119.76	121.90
3	0	1721	C	N3-C4-C5	-5.34	119.76	121.90
3	0	1827	A	C5-C6-N6	-5.34	119.43	123.70
3	0	2012	A	O4'-C1'-N9	5.34	112.47	108.20
3	0	2126	G	O4'-C1'-N9	5.34	112.47	108.20
3	0	2317	A	C5-C6-N1	-5.34	115.03	117.70
3	0	663	U	O4'-C1'-N1	5.34	112.47	108.20
3	0	1632	C	N3-C4-C5	-5.34	119.77	121.90
3	0	65	A	C5-C6-N1	-5.34	115.03	117.70
3	0	114	C	N3-C4-C5	-5.34	119.77	121.90
3	0	506	A	C5-C6-N1	-5.34	115.03	117.70
3	0	707	C	O4'-C1'-N1	5.34	112.47	108.20
3	0	2072	C	N3-C4-N4	5.34	121.73	118.00
22	F	206	PHE	CB-CG-CD2	-5.34	117.06	120.80
3	0	727	C	N3-C4-C5	-5.33	119.77	121.90
3	0	1944	A	C5-C6-N6	-5.33	119.43	123.70
2	1	74	C	N3-C4-C5	-5.33	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	240	G	O4'-C1'-N9	5.33	112.47	108.20
3	0	275	A	C5-C6-N1	-5.33	115.03	117.70
3	0	786	A	C5-C6-N1	-5.33	115.03	117.70
3	0	894	A	C5-C6-N1	-5.33	115.03	117.70
3	0	1224	C	N3-C4-C5	-5.33	119.77	121.90
3	0	300	A	C5-C6-N1	-5.33	115.03	117.70
3	0	414	A	O4'-C1'-N9	5.33	112.47	108.20
3	0	455	C	N3-C4-C5	-5.33	119.77	121.90
3	0	915	A	C5-C6-N1	-5.33	115.03	117.70
3	0	942	C	N3-C4-C5	-5.33	119.77	121.90
3	0	1684	A	O4'-C1'-N9	5.33	112.47	108.20
3	0	1791	G	O4'-C1'-N9	5.33	112.47	108.20
3	0	1920	G	C5-C6-O6	-5.33	125.40	128.60
3	0	2003	A	C5-C6-N1	-5.33	115.03	117.70
3	0	2130	C	N3-C4-C5	-5.33	119.77	121.90
23	d	223	TYR	CB-CG-CD2	-5.33	117.80	121.00
51	A	4	GLU	N-CA-CB	5.33	120.20	110.60
3	0	2226	A	C5-C6-N1	-5.33	115.03	117.70
3	0	603	G	O4'-C1'-N9	5.33	112.46	108.20
3	0	859	C	N3-C4-N4	5.33	121.73	118.00
3	0	900	A	C5-C6-N1	-5.33	115.04	117.70
3	0	992	A	C5-C6-N6	-5.33	119.44	123.70
3	0	1364	C	N3-C4-N4	5.33	121.73	118.00
3	0	1550	U	O4'-C1'-N1	5.33	112.46	108.20
3	0	284	C	N3-C4-N4	5.33	121.73	118.00
3	0	596	A	C5-C6-N1	-5.33	115.04	117.70
3	0	1638	A	O4'-C1'-N9	5.33	112.46	108.20
3	0	1701	G	O4'-C1'-N9	5.33	112.46	108.20
3	0	1719	U	O4'-C1'-N1	5.33	112.46	108.20
3	0	1918	U	O4'-C1'-N1	5.33	112.46	108.20
3	0	2122	C	N3-C4-N4	5.33	121.73	118.00
1	f	236	SER	CA-C-N	5.33	128.92	117.20
3	0	482	C	N3-C4-C5	-5.33	119.77	121.90
3	0	537	C	N3-C4-C5	-5.33	119.77	121.90
3	0	626	C	N3-C4-C5	-5.33	119.77	121.90
3	0	942	C	N3-C4-N4	5.33	121.73	118.00
3	0	1227	A	O4'-C1'-N9	5.33	112.46	108.20
3	0	1523	A	C5-C6-N6	-5.33	119.44	123.70
3	0	1816	C	N3-C4-N4	5.33	121.73	118.00
3	0	1987	C	N3-C4-C5	-5.33	119.77	121.90
3	0	2208	C	N3-C4-C5	-5.33	119.77	121.90
3	0	285	A	C5-C6-N1	-5.32	115.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	993	A	C5-C6-N1	-5.32	115.04	117.70
3	0	1218	G	O4'-C1'-N9	5.32	112.46	108.20
3	0	1305	C	N3-C4-C5	-5.32	119.77	121.90
3	0	1307	A	O4'-C1'-N9	5.32	112.46	108.20
3	0	49	C	N3-C4-C5	-5.32	119.77	121.90
3	0	507	A	C5-C6-N6	-5.32	119.44	123.70
3	0	287	A	C5-C6-N1	-5.32	115.04	117.70
3	0	779	A	C5-C6-N1	-5.32	115.04	117.70
3	0	1465	A	C5-C6-N1	-5.32	115.04	117.70
3	0	1734	C	N3-C4-C5	-5.32	119.77	121.90
3	0	1813	G	O4'-C1'-N9	5.32	112.46	108.20
3	0	2027	A	C5-C6-N1	-5.32	115.04	117.70
3	0	2239	A	C5-C6-N1	-5.32	115.04	117.70
3	0	623	C	N3-C4-C5	-5.32	119.77	121.90
3	0	764	A	C5-C6-N1	-5.32	115.04	117.70
3	0	1703	A	C5-C6-N6	-5.32	119.44	123.70
28	5	114	PHE	CB-CG-CD2	-5.32	117.08	120.80
3	0	406	A	O4'-C1'-N9	5.32	112.45	108.20
3	0	1531	A	OP1-P-O3'	-5.32	93.50	105.20
3	0	1826	C	N3-C4-C5	-5.32	119.77	121.90
3	0	1943	C	N3-C4-C5	-5.32	119.77	121.90
3	0	2107	C	N3-C4-N4	5.32	121.72	118.00
1	f	305	TYR	C-N-CA	5.32	134.99	121.70
1	f	1494	THR	C-N-CA	5.32	134.99	121.70
2	1	6	C	N3-C4-C5	-5.32	119.77	121.90
3	0	1074	G	O4'-C1'-N9	5.32	112.45	108.20
3	0	1583	G	O4'-C1'-N9	5.32	112.45	108.20
3	0	1635	A	C5-C6-N6	-5.32	119.45	123.70
3	0	1680	U	O4'-C1'-N1	5.32	112.45	108.20
3	0	1786	A	C5-C6-N1	-5.32	115.04	117.70
3	0	2322	U	O4'-C1'-N1	5.32	112.45	108.20
3	0	168	A	C5-C6-N1	-5.31	115.04	117.70
3	0	783	A	O4'-C1'-N9	5.31	112.45	108.20
3	0	1584	G	O4'-C1'-N9	5.31	112.45	108.20
3	0	1975	G	C5'-C4'-O4'	-5.31	102.72	109.10
3	0	2222	G	O4'-C1'-N9	5.31	112.45	108.20
3	0	193	U	O4'-C1'-N1	5.31	112.45	108.20
3	0	480	C	N3-C4-C5	-5.31	119.78	121.90
3	0	1237	C	N3-C4-C5	-5.31	119.78	121.90
3	0	1426	A	C5-C6-N1	-5.31	115.04	117.70
3	0	2057	C	N3-C4-C5	-5.31	119.78	121.90
1	f	240	PHE	C-N-CA	5.31	134.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	784	A	C5-C6-N1	-5.31	115.04	117.70
3	0	785	A	C5-C6-N1	-5.31	115.04	117.70
3	0	913	A	C5-C6-N1	-5.31	115.04	117.70
3	0	332	C	N3-C4-C5	-5.31	119.78	121.90
3	0	2205	A	C5-C6-N1	-5.31	115.05	117.70
2	1	12	G	O4'-C1'-N9	5.31	112.45	108.20
3	0	59	C	N3-C4-C5	-5.31	119.78	121.90
3	0	82	A	C5-C6-N1	-5.31	115.05	117.70
3	0	782	A	C5-C6-N1	-5.31	115.05	117.70
3	0	1303	C	N3-C4-C5	-5.31	119.78	121.90
3	0	1750	G	O4'-C1'-N9	5.31	112.45	108.20
3	0	1802	A	C5-C6-N1	-5.31	115.05	117.70
30	i	82	MET	C-N-CA	5.31	134.97	121.70
3	0	866	A	O4'-C1'-N9	5.31	112.44	108.20
3	0	2234	A	O4'-C1'-N9	5.31	112.44	108.20
47	8	369	PHE	C-N-CA	5.31	133.44	122.30
3	0	207	G	O4'-C1'-N9	5.30	112.44	108.20
3	0	523	A	C5-C6-N6	-5.30	119.46	123.70
3	0	655	A	C5-C6-N1	-5.30	115.05	117.70
3	0	761	G	C5-C6-O6	-5.30	125.42	128.60
3	0	1573	A	C5-C6-N1	-5.30	115.05	117.70
3	0	2265	A	C5-C6-N6	-5.30	119.46	123.70
3	0	216	A	C5-C6-N6	-5.30	119.46	123.70
3	0	1572	C	N3-C4-N4	5.30	121.71	118.00
3	0	2202	G	O4'-C1'-N9	5.30	112.44	108.20
3	0	55	A	C5-C6-N1	-5.30	115.05	117.70
3	0	548	C	N3-C4-C5	-5.30	119.78	121.90
3	0	501	A	O4'-C1'-N9	5.30	112.44	108.20
3	0	1823	A	C5-C6-N1	-5.30	115.05	117.70
1	f	150	PHE	CB-CG-CD2	-5.30	117.09	120.80
3	0	1338	A	O4'-C1'-N9	5.30	112.44	108.20
3	0	1667	A	C5-C6-N1	-5.30	115.05	117.70
3	0	1741	G	O4'-C1'-N9	5.30	112.44	108.20
3	0	2017	C	N3-C4-C5	-5.30	119.78	121.90
3	0	2194	A	C5-C6-N6	-5.30	119.46	123.70
3	0	181	A	C5-C6-N1	-5.30	115.05	117.70
3	0	369	C	N3-C4-C5	-5.30	119.78	121.90
3	0	694	A	C5-C6-N1	-5.30	115.05	117.70
3	0	1360	A	P-O3'-C3'	5.30	126.06	119.70
3	0	1901	C	N3-C4-C5	-5.30	119.78	121.90
3	0	2056	C	N3-C4-C5	-5.30	119.78	121.90
3	0	2243	A	O4'-C1'-N9	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	242	A	C5-C6-N1	-5.29	115.05	117.70
3	0	659	A	O4'-C1'-N9	5.29	112.44	108.20
3	0	2179	C	N3-C4-C5	-5.29	119.78	121.90
50	H	286	TYR	CB-CG-CD2	-5.29	117.82	121.00
3	0	351	A	C5-C6-N1	-5.29	115.05	117.70
3	0	1514	U	O4'-C1'-N1	5.29	112.44	108.20
3	0	2040	A	C5-C6-N1	-5.29	115.05	117.70
3	0	57	G	O4'-C1'-N9	5.29	112.43	108.20
3	0	78	A	O4'-C1'-N9	5.29	112.43	108.20
3	0	290	U	O4'-C1'-N1	5.29	112.43	108.20
3	0	425	A	O4'-C1'-N9	5.29	112.43	108.20
3	0	457	A	O4'-C1'-N9	5.29	112.43	108.20
3	0	1341	A	C5-C6-N1	-5.29	115.06	117.70
3	0	1342	G	O4'-C1'-N9	5.29	112.43	108.20
45	T	22	PHE	N-CA-CB	5.29	120.12	110.60
3	0	1390	A	C5-C6-N1	-5.29	115.06	117.70
3	0	1747	C	N3-C4-C5	-5.29	119.78	121.90
3	0	1867	C	N3-C4-C5	-5.29	119.78	121.90
2	1	41	A	O4'-C1'-N9	5.29	112.43	108.20
3	0	276	G	O4'-C1'-N9	5.29	112.43	108.20
3	0	653	A	C5-C6-N1	-5.29	115.06	117.70
3	0	766	C	N3-C4-C5	-5.29	119.78	121.90
3	0	916	A	C5-C6-N1	-5.29	115.06	117.70
3	0	1318	A	C5-C6-N1	-5.29	115.06	117.70
3	0	1517	A	C5-C6-N1	-5.29	115.06	117.70
3	0	2005	C	N3-C4-C5	-5.29	119.78	121.90
3	0	2288	A	C5-C6-N1	-5.29	115.06	117.70
1	f	1493	PRO	O-C-N	5.29	131.16	122.70
3	0	1681	A	C5-C6-N1	-5.29	115.06	117.70
3	0	2060	A	C5-C6-N1	-5.29	115.06	117.70
3	0	22	A	C5-C6-N1	-5.29	115.06	117.70
3	0	102	A	C5-C6-N1	-5.29	115.06	117.70
3	0	135	C	N3-C4-C5	-5.29	119.79	121.90
3	0	704	A	C5-C6-N1	-5.29	115.06	117.70
3	0	724	A	C5-C6-N6	-5.29	119.47	123.70
3	0	757	G	O4'-C1'-N9	5.29	112.43	108.20
3	0	1650	C	N3-C4-C5	-5.29	119.79	121.90
3	0	1817	A	C5-C6-N1	-5.29	115.06	117.70
3	0	1899	C	N3-C4-N4	5.29	121.70	118.00
3	0	69	C	N3-C4-C5	-5.28	119.79	121.90
3	0	294	G	O4'-C1'-N9	5.28	112.43	108.20
3	0	304	A	C5-C6-N1	-5.28	115.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	375	C	N3-C4-C5	-5.28	119.79	121.90
3	0	578	C	N3-C4-C5	-5.28	119.79	121.90
3	0	826	A	C5-C6-N1	-5.28	115.06	117.70
3	0	1287	C	N3-C4-C5	-5.28	119.79	121.90
3	0	1348	A	C5-C6-N1	-5.28	115.06	117.70
3	0	1976	C	N3-C4-C5	-5.28	119.79	121.90
3	0	300	A	O4'-C1'-N9	5.28	112.43	108.20
3	0	1290	C	N3-C4-C5	-5.28	119.79	121.90
3	0	467	A	C5-C6-N1	-5.28	115.06	117.70
3	0	814	C	N3-C4-C5	-5.28	119.79	121.90
3	0	1531	A	C5-C6-N1	-5.28	115.06	117.70
3	0	1657	A	C5-C6-N6	-5.28	119.47	123.70
3	0	655	A	C5-C6-N6	-5.28	119.48	123.70
3	0	935	A	C5-C6-N1	-5.28	115.06	117.70
3	0	2153	A	C5-C6-N1	-5.28	115.06	117.70
3	0	108	C	N3-C4-C5	-5.28	119.79	121.90
3	0	141	A	C5-C6-N1	-5.28	115.06	117.70
3	0	352	A	C5-C6-N1	-5.28	115.06	117.70
3	0	633	A	C5-C6-N1	-5.28	115.06	117.70
3	0	807	U	C2-N1-C1'	5.28	124.03	117.70
3	0	822	A	C5-C6-N1	-5.28	115.06	117.70
3	0	873	C	N3-C4-N4	5.28	121.69	118.00
3	0	1452	C	N3-C4-C5	-5.28	119.79	121.90
3	0	2320	A	O4'-C1'-N9	5.28	112.42	108.20
3	0	226	A	C5-C6-N1	-5.28	115.06	117.70
3	0	1080	G	O4'-C1'-N9	5.28	112.42	108.20
3	0	1978	A	C5-C6-N1	-5.27	115.06	117.70
3	0	19	A	C5-C6-N1	-5.27	115.06	117.70
3	0	184	A	C5-C6-N6	-5.27	119.48	123.70
3	0	577	A	C5-C6-N6	-5.27	119.48	123.70
3	0	681	C	N3-C4-C5	-5.27	119.79	121.90
3	0	889	A	O4'-C1'-N9	5.27	112.42	108.20
3	0	1246	A	O4'-C1'-N9	5.27	112.42	108.20
3	0	1368	C	N3-C4-C5	-5.27	119.79	121.90
3	0	2084	G	O4'-C1'-N9	5.27	112.42	108.20
3	0	186	C	N3-C4-C5	-5.27	119.79	121.90
3	0	1306	A	C5-C6-N1	-5.27	115.06	117.70
3	0	1553	C	N3-C4-N4	5.27	121.69	118.00
3	0	51	A	C5-C6-N1	-5.27	115.07	117.70
3	0	1911	C	N3-C4-N4	5.27	121.69	118.00
3	0	107	A	O4'-C1'-N9	5.27	112.41	108.20
3	0	203	C	N3-C4-C5	-5.27	119.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	987	G	O4'-C1'-N9	5.27	112.41	108.20
3	0	1383	A	C5-C6-N1	-5.27	115.07	117.70
3	0	1688	C	N3-C4-C5	-5.27	119.79	121.90
3	0	2125	A	O4'-C1'-N9	5.27	112.41	108.20
3	0	2147	C	N3-C4-C5	-5.27	119.79	121.90
2	1	73	C	N3-C4-N4	5.26	121.69	118.00
3	0	111	A	C5-C6-N1	-5.26	115.07	117.70
3	0	992	A	C5-C6-N1	-5.26	115.07	117.70
3	0	1525	A	C5-C6-N6	-5.26	119.49	123.70
3	0	2249	C	N3-C4-C5	-5.26	119.79	121.90
3	0	865	A	C5-C6-N1	-5.26	115.07	117.70
3	0	1497	U	O4'-C1'-N1	5.26	112.41	108.20
3	0	1603	G	N3-C2-N2	5.26	123.58	119.90
3	0	2042	A	C5-C6-N6	-5.26	119.49	123.70
3	0	1527	C	N3-C4-C5	-5.26	119.80	121.90
3	0	2020	U	P-O3'-C3'	5.26	126.01	119.70
3	0	2149	G	N3-C2-N2	5.26	123.58	119.90
3	0	2304	A	O4'-C1'-N9	5.26	112.41	108.20
3	0	400	G	N3-C2-N2	5.26	123.58	119.90
3	0	1314	A	O4'-C1'-N9	5.26	112.41	108.20
3	0	94	C	N3-C4-C5	-5.26	119.80	121.90
3	0	123	A	C5-C6-N1	-5.26	115.07	117.70
3	0	158	C	N3-C4-C5	-5.26	119.80	121.90
3	0	1066	C	N3-C4-C5	-5.26	119.80	121.90
3	0	1502	C	N3-C4-C5	-5.26	119.80	121.90
1	f	1851	ALA	N-CA-CB	5.25	117.46	110.10
3	0	875	A	C5-C6-N1	-5.25	115.07	117.70
3	0	1338	A	C5-C6-N1	-5.25	115.07	117.70
3	0	1708	C	N3-C4-N4	5.25	121.68	118.00
3	0	2269	A	O4'-C1'-N9	5.25	112.40	108.20
3	0	67	C	N3-C4-N4	5.25	121.68	118.00
3	0	379	G	O4'-C1'-N9	5.25	112.40	108.20
1	f	214	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	f	1245	ALA	N-CA-CB	5.25	117.45	110.10
3	0	151	A	C5-C6-N1	-5.25	115.07	117.70
3	0	831	A	C5-C6-N1	-5.25	115.07	117.70
3	0	1257	C	N3-C4-C5	-5.25	119.80	121.90
3	0	1961	C	N3-C4-C5	-5.25	119.80	121.90
3	0	1976	C	N3-C4-N4	5.25	121.68	118.00
3	0	2221	A	C5-C6-N1	-5.25	115.08	117.70
3	0	2320	A	C5-C6-N1	-5.25	115.08	117.70
3	0	121	A	C5-C6-N1	-5.25	115.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	653	A	O4'-C1'-N9	5.25	112.40	108.20
3	0	1747	C	O4'-C1'-N1	5.25	112.40	108.20
3	0	1958	G	O4'-C1'-N9	5.25	112.40	108.20
3	0	2009	A	C5-C6-N1	-5.25	115.08	117.70
2	1	5	C	N3-C4-C5	-5.25	119.80	121.90
3	0	402	C	N3-C4-C5	-5.25	119.80	121.90
3	0	990	A	O4'-C1'-N9	5.25	112.40	108.20
3	0	1181	A	C5-C6-N1	-5.25	115.08	117.70
3	0	1242	G	O4'-C1'-N9	5.25	112.40	108.20
3	0	1573	A	O4'-C1'-N9	5.25	112.40	108.20
2	1	4	A	C5-C6-N1	-5.25	115.08	117.70
2	1	59	A	C5-C6-N1	-5.25	115.08	117.70
3	0	229	G	O4'-C1'-N9	5.25	112.40	108.20
3	0	360	A	C5-C6-N1	-5.25	115.08	117.70
3	0	809	A	C5-C6-N1	-5.25	115.08	117.70
3	0	1317	A	C5-C6-N1	-5.25	115.08	117.70
3	0	1358	A	O4'-C1'-N9	5.25	112.40	108.20
3	0	2171	C	N3-C4-C5	-5.25	119.80	121.90
3	0	249	A	C5-C6-N1	-5.25	115.08	117.70
3	0	1449	C	N3-C4-C5	-5.25	119.80	121.90
2	1	61	C	N3-C4-C5	-5.24	119.80	121.90
3	0	161	A	C5-C6-N6	-5.24	119.51	123.70
3	0	475	A	C5-C6-N1	-5.24	115.08	117.70
3	0	268	C	N3-C4-C5	-5.24	119.80	121.90
3	0	922	C	N3-C4-N4	5.24	121.67	118.00
3	0	363	A	C5-C6-N1	-5.24	115.08	117.70
3	0	367	A	O4'-C1'-N9	5.24	112.39	108.20
3	0	1533	C	N3-C4-C5	-5.24	119.80	121.90
3	0	1921	C	N3-C4-C5	-5.24	119.80	121.90
3	0	1466	U	O4'-C1'-N1	5.24	112.39	108.20
3	0	1971	C	N3-C4-N4	5.24	121.67	118.00
3	0	2174	A	C5-C6-N1	-5.24	115.08	117.70
3	0	454	A	O4'-C1'-N9	5.24	112.39	108.20
3	0	972	A	C5-C6-N6	-5.24	119.51	123.70
3	0	1571	A	C5-C6-N1	-5.24	115.08	117.70
3	0	2004	A	C5-C6-N6	-5.24	119.51	123.70
3	0	2039	A	C5-C6-N1	-5.24	115.08	117.70
3	0	2056	C	N3-C4-N4	5.24	121.67	118.00
3	0	2135	C	N3-C4-C5	-5.24	119.81	121.90
1	f	242	SER	C-N-CA	5.23	134.78	121.70
3	0	1932	A	C5-C6-N1	-5.23	115.08	117.70
3	0	662	C	N3-C4-C5	-5.23	119.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1568	G	O4'-C1'-N9	5.23	112.39	108.20
3	0	1656	A	C5-C6-N1	-5.23	115.08	117.70
3	0	1941	A	C5-C6-N1	-5.23	115.08	117.70
2	1	46	A	C5-C6-N1	-5.23	115.08	117.70
3	0	176	C	N3-C4-C5	-5.23	119.81	121.90
3	0	374	G	O4'-C1'-N9	5.23	112.39	108.20
3	0	649	G	O4'-C1'-N9	5.23	112.39	108.20
3	0	2010	A	C5-C6-N1	-5.23	115.08	117.70
3	0	2286	A	O4'-C1'-N9	5.23	112.39	108.20
3	0	1980	A	C5-C6-N1	-5.23	115.08	117.70
1	f	1555	GLN	C-N-CA	5.23	134.77	121.70
3	0	1343	A	C5-C6-N1	-5.23	115.09	117.70
3	0	2081	A	C5-C6-N1	-5.23	115.09	117.70
3	0	2093	A	C5-C6-N6	-5.23	119.52	123.70
3	0	216	A	C5-C6-N1	-5.23	115.09	117.70
3	0	465	G	C4-N9-C1'	5.23	133.29	126.50
3	0	1757	U	O4'-C1'-N1	5.23	112.38	108.20
3	0	1947	A	C5-C6-N1	-5.23	115.09	117.70
3	0	250	A	C5-C6-N1	-5.22	115.09	117.70
3	0	658	A	C5-C6-N1	-5.22	115.09	117.70
3	0	1343	A	C5-C6-N6	-5.22	119.52	123.70
3	0	1419	G	O4'-C1'-N9	5.22	112.38	108.20
3	0	1668	C	N3-C4-C5	-5.22	119.81	121.90
3	0	1804	A	O4'-C1'-N9	5.22	112.38	108.20
3	0	2207	A	O4'-C1'-N9	5.22	112.38	108.20
3	0	425	A	C5-C6-N1	-5.22	115.09	117.70
3	0	723	C	N3-C4-C5	-5.22	119.81	121.90
3	0	877	A	C5-C6-N1	-5.22	115.09	117.70
3	0	1269	A	O4'-C1'-N9	5.22	112.38	108.20
3	0	1930	A	C5-C6-N1	-5.22	115.09	117.70
3	0	2115	A	O4'-C1'-N9	5.22	112.38	108.20
3	0	1545	C	N3-C4-C5	-5.22	119.81	121.90
3	0	1558	A	O4'-C1'-N9	5.22	112.38	108.20
3	0	1633	A	C5-C6-N1	-5.22	115.09	117.70
3	0	1820	A	C5-C6-N1	-5.22	115.09	117.70
50	H	46	SER	N-CA-CB	5.22	118.33	110.50
3	0	830	C	N3-C4-N4	5.22	121.65	118.00
3	0	2317	A	C5-C6-N6	-5.22	119.52	123.70
2	1	43	A	C5-C6-N1	-5.22	115.09	117.70
3	0	864	A	C5-C6-N1	-5.22	115.09	117.70
3	0	915	A	O4'-C1'-N9	5.22	112.37	108.20
3	0	1279	A	C4-C5-C6	5.22	119.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1347	C	N3-C4-C5	-5.22	119.81	121.90
43	G	136	TRP	CB-CG-CD2	5.22	133.38	126.60
3	0	336	C	N3-C4-C5	-5.22	119.81	121.90
3	0	1625	A	O4'-C1'-N9	5.22	112.37	108.20
3	0	2289	A	C5-C6-N1	-5.22	115.09	117.70
3	0	472	A	C5-C6-N1	-5.21	115.09	117.70
3	0	534	C	N3-C4-C5	-5.21	119.81	121.90
3	0	644	C	N3-C4-N4	5.21	121.65	118.00
3	0	884	A	C5-C6-N1	-5.21	115.09	117.70
3	0	1219	G	O4'-C1'-N9	5.21	112.37	108.20
1	f	305	TYR	CB-CA-C	-5.21	99.97	110.40
2	1	38	C	N3-C4-C5	-5.21	119.82	121.90
3	0	182	C	N3-C4-C5	-5.21	119.81	121.90
3	0	345	A	C5-C6-N1	-5.21	115.09	117.70
3	0	782	A	O4'-C1'-N9	5.21	112.37	108.20
3	0	1282	G	O4'-C1'-N9	5.21	112.37	108.20
3	0	1534	A	O4'-C1'-N9	5.21	112.37	108.20
3	0	1769	A	O4'-C1'-N9	5.21	112.37	108.20
3	0	522	A	O4'-C1'-N9	5.21	112.37	108.20
3	0	2115	A	C5-C6-N1	-5.21	115.09	117.70
3	0	432	A	C5-C6-N1	-5.21	115.10	117.70
3	0	1586	A	C5-C6-N1	-5.21	115.10	117.70
3	0	2194	A	C5-C6-N1	-5.21	115.10	117.70
3	0	1731	C	N3-C4-C5	-5.21	119.82	121.90
3	0	1866	A	C5-C6-N1	-5.21	115.10	117.70
3	0	26	A	C5-C6-N6	-5.21	119.54	123.70
3	0	536	A	C5-C6-N6	-5.21	119.54	123.70
3	0	710	A	O4'-C1'-N9	5.21	112.36	108.20
3	0	905	A	C5-C6-N1	-5.21	115.10	117.70
3	0	1220	A	C5-C6-N1	-5.21	115.10	117.70
3	0	659	A	C5-C6-N1	-5.20	115.10	117.70
3	0	1269	A	C5-C6-N1	-5.20	115.10	117.70
3	0	1279	A	O4'-C1'-N9	5.20	112.36	108.20
3	0	288	A	C5-C6-N1	-5.20	115.10	117.70
3	0	787	C	N3-C4-C5	-5.20	119.82	121.90
3	0	2074	A	C5-C6-N1	-5.20	115.10	117.70
1	f	1260	TYR	N-CA-CB	5.20	119.96	110.60
2	1	58	A	O4'-C1'-N9	5.20	112.36	108.20
3	0	167	A	C5-C6-N1	-5.20	115.10	117.70
3	0	531	A	C5-C6-N1	-5.20	115.10	117.70
3	0	597	C	N3-C4-C5	-5.20	119.82	121.90
3	0	830	C	N3-C4-C5	-5.20	119.82	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1316	C	N3-C4-C5	-5.20	119.82	121.90
3	0	1330	C	N3-C4-C5	-5.20	119.82	121.90
3	0	1512	C	N3-C4-C5	-5.20	119.82	121.90
3	0	2012	A	C4-C5-C6	5.20	119.60	117.00
5	s	164	ILE	C-N-CD	5.20	139.32	128.40
2	1	43	A	O4'-C1'-N9	5.20	112.36	108.20
3	0	55	A	O4'-C1'-N9	5.20	112.36	108.20
3	0	89	C	N3-C4-C5	-5.20	119.82	121.90
3	0	960	A	C5-C6-N1	-5.20	115.10	117.70
3	0	1738	A	C5-C6-N1	-5.20	115.10	117.70
3	0	1973	G	O4'-C1'-N9	5.20	112.36	108.20
10	u	100	THR	C-N-CA	5.20	134.69	121.70
3	0	1662	A	C5-C6-N1	-5.20	115.10	117.70
3	0	2299	A	C5-C6-N1	-5.20	115.10	117.70
3	0	916	A	O4'-C1'-N9	5.20	112.36	108.20
3	0	1360	A	C5-C6-N1	-5.20	115.10	117.70
3	0	1737	A	C5-C6-N1	-5.20	115.10	117.70
3	0	2005	C	N3-C4-N4	5.20	121.64	118.00
3	0	2139	A	C5-C6-N6	-5.20	119.54	123.70
3	0	125	A	C5-C6-N6	-5.19	119.55	123.70
3	0	2006	A	C5-C6-N1	-5.19	115.10	117.70
3	0	160	A	C5-C6-N1	-5.19	115.10	117.70
3	0	490	C	N3-C4-C5	-5.19	119.82	121.90
3	0	977	A	C5-C6-N1	-5.19	115.10	117.70
3	0	1707	A	C5-C6-N6	-5.19	119.55	123.70
9	r	139	SER	N-CA-CB	5.19	118.29	110.50
1	f	732	ALA	CB-CA-C	-5.19	102.31	110.10
3	0	535	G	O4'-C1'-N9	5.19	112.35	108.20
3	0	922	C	N3-C4-C5	-5.19	119.82	121.90
3	0	2275	C	N3-C4-C5	-5.19	119.82	121.90
3	0	890	C	N3-C4-C5	-5.19	119.82	121.90
3	0	1304	U	O4'-C1'-N1	5.19	112.35	108.20
1	f	1402	ALA	N-CA-CB	5.19	117.36	110.10
3	0	303	C	N3-C4-C5	-5.19	119.83	121.90
3	0	1694	A	C4-C5-C6	5.19	119.59	117.00
3	0	1861	G	O4'-C1'-N9	5.19	112.35	108.20
3	0	251	A	C5-C6-N1	-5.19	115.11	117.70
3	0	1503	G	O4'-C1'-N9	5.19	112.35	108.20
3	0	1604	A	O4'-C1'-N9	5.19	112.35	108.20
3	0	853	C	N3-C4-C5	-5.18	119.83	121.90
3	0	1644	A	O4'-C1'-N9	5.18	112.35	108.20
3	0	1752	C	N3-C4-C5	-5.18	119.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1857	G	O4'-C1'-N9	5.18	112.35	108.20
3	0	414	A	C5-C6-N1	-5.18	115.11	117.70
3	0	721	C	N3-C4-C5	-5.18	119.83	121.90
3	0	1192	C	N3-C4-C5	-5.18	119.83	121.90
3	0	1238	A	O4'-C1'-N9	5.18	112.35	108.20
3	0	1613	G	O4'-C1'-N9	5.18	112.35	108.20
3	0	1986	A	O4'-C1'-N9	5.18	112.35	108.20
3	0	381	A	C5-C6-N1	-5.18	115.11	117.70
2	1	16	U	P-O3'-C3'	5.18	125.92	119.70
2	1	65	C	N3-C4-C5	-5.18	119.83	121.90
3	0	127	C	N3-C4-C5	-5.18	119.83	121.90
3	0	225	C	N3-C4-C5	-5.18	119.83	121.90
3	0	1297	A	O4'-C1'-N9	5.18	112.34	108.20
3	0	1319	A	O4'-C1'-N9	5.18	112.34	108.20
3	0	1465	A	O4'-C1'-N9	5.18	112.34	108.20
3	0	1477	A	C5-C6-N1	-5.18	115.11	117.70
3	0	1557	A	C5-C6-N6	-5.18	119.56	123.70
44	K	26	PHE	CB-CG-CD2	-5.18	117.17	120.80
3	0	419	G	O4'-C1'-N9	5.18	112.34	108.20
2	1	37	A	C5-C6-N1	-5.18	115.11	117.70
3	0	406	A	C5-C6-N1	-5.18	115.11	117.70
3	0	1228	C	N3-C4-C5	-5.18	119.83	121.90
3	0	1307	A	C5-C6-N1	-5.18	115.11	117.70
3	0	1367	A	C5-C6-N1	-5.18	115.11	117.70
3	0	149	A	O4'-C1'-N9	5.17	112.34	108.20
3	0	185	A	O4'-C1'-N9	5.17	112.34	108.20
3	0	1630	A	C5-C6-N1	-5.17	115.11	117.70
3	0	2162	C	N3-C4-C5	-5.17	119.83	121.90
3	0	1423	A	C5-C6-N1	-5.17	115.11	117.70
3	0	16	G	N3-C2-N2	5.17	123.52	119.90
3	0	1327	G	O4'-C1'-N9	5.17	112.34	108.20
3	0	1363	G	O4'-C1'-N9	5.17	112.34	108.20
3	0	17	C	N3-C4-C5	-5.17	119.83	121.90
3	0	166	C	N3-C4-C5	-5.17	119.83	121.90
3	0	485	A	C5-C6-N6	-5.17	119.56	123.70
3	0	1373	A	C5-C6-N1	-5.17	115.11	117.70
3	0	1729	A	C5-C6-N6	-5.17	119.56	123.70
3	0	289	G	O4'-C1'-N9	5.17	112.33	108.20
3	0	711	A	C5-C6-N6	-5.17	119.56	123.70
3	0	2288	A	O4'-C1'-N9	5.17	112.33	108.20
3	0	417	A	C5-C6-N1	-5.17	115.12	117.70
28	5	88	ILE	N-CA-C	-5.17	97.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	62	A	C5-C6-N1	-5.17	115.12	117.70
3	0	746	A	O4'-C1'-N9	5.17	112.33	108.20
3	0	999	U	O4'-C1'-N1	5.17	112.33	108.20
3	0	1204	G	O4'-C1'-N9	5.17	112.33	108.20
3	0	887	C	N3-C4-C5	-5.16	119.83	121.90
3	0	2042	A	C5-C6-N1	-5.16	115.12	117.70
3	0	587	A	O4'-C1'-N9	5.16	112.33	108.20
3	0	1181	A	O4'-C1'-N9	5.16	112.33	108.20
3	0	1253	A	C5-C6-N1	-5.16	115.12	117.70
3	0	1409	G	O4'-C1'-N9	5.16	112.33	108.20
3	0	1420	A	O4'-C1'-N9	5.16	112.33	108.20
3	0	206	C	N3-C4-C5	-5.16	119.84	121.90
3	0	805	C	N3-C4-C5	-5.16	119.84	121.90
3	0	1279	A	C5-C6-N6	-5.16	119.57	123.70
3	0	2055	C	N3-C4-C5	-5.16	119.84	121.90
3	0	624	A	O4'-C1'-N9	5.16	112.33	108.20
3	0	1442	C	N3-C4-C5	-5.16	119.84	121.90
3	0	1970	U	C1'-O4'-C4'	-5.16	105.77	109.90
3	0	2032	C	N3-C4-C5	-5.16	119.84	121.90
2	1	34	A	C5-C6-N1	-5.16	115.12	117.70
3	0	447	A	C5-C6-N1	-5.16	115.12	117.70
3	0	966	C	N3-C4-C5	-5.16	119.84	121.90
3	0	1353	A	C5-C6-N1	-5.16	115.12	117.70
3	0	1372	G	O4'-C1'-N9	5.16	112.32	108.20
3	0	2181	G	O4'-C1'-N9	5.16	112.32	108.20
50	H	115	TYR	CB-CG-CD1	5.15	124.09	121.00
2	1	70	C	N3-C4-C5	-5.15	119.84	121.90
3	0	1390	A	O4'-C1'-N9	5.15	112.32	108.20
3	0	1606	A	C5-C6-N1	-5.15	115.12	117.70
3	0	1959	C	N3-C4-C5	-5.15	119.84	121.90
3	0	2172	A	C5-C6-N1	-5.15	115.12	117.70
46	C	612	TYR	N-CA-CB	5.15	119.88	110.60
3	0	440	C	N3-C4-C5	-5.15	119.84	121.90
3	0	1400	C	N3-C4-C5	-5.15	119.84	121.90
3	0	2048	G	O4'-C1'-N9	5.15	112.32	108.20
3	0	1454	A	C5-C6-N6	-5.15	119.58	123.70
3	0	2065	C	N3-C4-C5	-5.15	119.84	121.90
3	0	878	G	O4'-C1'-N9	5.15	112.32	108.20
3	0	898	A	O4'-C1'-N9	5.15	112.32	108.20
3	0	1616	A	C5-C6-N6	-5.15	119.58	123.70
3	0	1985	C	N3-C4-C5	-5.15	119.84	121.90
3	0	278	A	C5-C6-N1	-5.14	115.13	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	684	A	C5-C6-N1	-5.14	115.13	117.70
3	0	1268	G	O4'-C1'-N9	5.14	112.32	108.20
3	0	1376	C	N3-C4-C5	-5.14	119.84	121.90
3	0	1607	C	N3-C4-C5	-5.14	119.84	121.90
3	0	2168	G	O4'-C1'-N9	5.14	112.32	108.20
3	0	2291	G	P-O3'-C3'	5.14	125.87	119.70
3	0	68	A	C5-C6-N1	-5.14	115.13	117.70
3	0	1382	A	O4'-C1'-N9	5.14	112.31	108.20
3	0	1560	G	O4'-C1'-N9	5.14	112.31	108.20
2	1	62	A	O4'-C1'-N9	5.14	112.31	108.20
3	0	73	A	C5-C6-N1	-5.14	115.13	117.70
3	0	429	C	N3-C4-C5	-5.14	119.84	121.90
3	0	2001	A	C5-C6-N6	-5.14	119.59	123.70
3	0	1463	A	C5-C6-N1	-5.14	115.13	117.70
2	1	36	A	C5-C6-N1	-5.14	115.13	117.70
3	0	210	A	C5-C6-N1	-5.14	115.13	117.70
3	0	673	A	C5-C6-N1	-5.14	115.13	117.70
3	0	1646	C	N3-C4-C5	-5.14	119.85	121.90
2	1	2	G	O4'-C1'-N9	5.13	112.31	108.20
3	0	237	A	C5-C6-N1	-5.13	115.13	117.70
3	0	444	A	C5-C6-N1	-5.13	115.13	117.70
3	0	984	A	O4'-C1'-N9	5.13	112.31	108.20
3	0	1486	G	O4'-C1'-N9	5.13	112.31	108.20
3	0	1572	C	N3-C4-C5	-5.13	119.85	121.90
3	0	1647	G	O4'-C1'-N9	5.13	112.31	108.20
3	0	1991	A	C5-C6-N1	-5.13	115.13	117.70
3	0	2083	C	N3-C4-C5	-5.13	119.85	121.90
3	0	538	A	C5-C6-N6	-5.13	119.59	123.70
1	f	247	ALA	N-CA-CB	5.13	117.28	110.10
1	f	297	THR	CA-C-N	-5.13	105.91	117.20
3	0	852	A	O4'-C1'-N9	5.13	112.31	108.20
3	0	879	C	N3-C4-C5	-5.13	119.85	121.90
3	0	967	A	C5-C6-N6	-5.13	119.59	123.70
3	0	1579	A	C4'-C3'-C2'	-5.13	97.47	102.60
50	H	181	TYR	C-N-CA	5.13	134.53	121.70
3	0	427	U	O4'-C1'-N1	5.13	112.30	108.20
3	0	458	C	N3-C4-C5	-5.13	119.85	121.90
3	0	728	A	O4'-C1'-N9	5.13	112.30	108.20
3	0	1179	C	N3-C4-C5	-5.13	119.85	121.90
3	0	1612	A	O4'-C1'-N9	5.13	112.30	108.20
3	0	360	A	C5-C6-N6	-5.13	119.60	123.70
3	0	353	C	N3-C4-C5	-5.12	119.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1333	A	C5-C6-N1	-5.12	115.14	117.70
3	0	1353	A	C5-C6-N6	-5.12	119.60	123.70
3	0	149	A	C5-C6-N1	-5.12	115.14	117.70
3	0	260	A	C5-C6-N1	-5.12	115.14	117.70
3	0	349	A	C5-C6-N1	-5.12	115.14	117.70
3	0	1317	A	O4'-C1'-N9	5.12	112.30	108.20
3	0	1940	C	N3-C4-C5	-5.12	119.85	121.90
3	0	1991	A	O4'-C1'-N9	5.12	112.30	108.20
3	0	367	A	C5-C6-N1	-5.12	115.14	117.70
3	0	1263	A	O4'-C1'-N9	5.12	112.30	108.20
3	0	1693	C	N3-C4-C5	-5.12	119.85	121.90
3	0	2053	A	C5-C6-N1	-5.12	115.14	117.70
3	0	2148	C	N3-C4-C5	-5.12	119.85	121.90
3	0	658	A	O4'-C1'-N9	5.12	112.30	108.20
3	0	105	A	O4'-C1'-N9	5.12	112.30	108.20
3	0	259	C	N3-C4-C5	-5.12	119.85	121.90
3	0	397	G	O4'-C1'-N9	5.12	112.30	108.20
3	0	770	C	N3-C4-C5	-5.12	119.85	121.90
3	0	831	A	O4'-C1'-N9	5.12	112.30	108.20
3	0	1561	C	N3-C4-C5	-5.12	119.85	121.90
3	0	1778	U	O4'-C1'-N1	5.12	112.30	108.20
3	0	1373	A	O4'-C1'-N9	5.12	112.29	108.20
3	0	157	G	O4'-C1'-N9	5.12	112.29	108.20
3	0	464	C	N3-C4-N4	5.12	121.58	118.00
3	0	2311	A	C5-C6-N1	-5.12	115.14	117.70
3	0	627	C	N3-C4-C5	-5.11	119.85	121.90
3	0	1698	U	O4'-C1'-N1	5.11	112.29	108.20
3	0	1758	U	O4'-C1'-N1	5.11	112.29	108.20
2	1	72	A	C5-C6-N1	-5.11	115.14	117.70
3	0	97	A	C5-C6-N1	-5.11	115.14	117.70
3	0	504	A	O4'-C1'-N9	5.11	112.29	108.20
3	0	1725	C	N3-C4-C5	-5.11	119.86	121.90
40	Y	220	TYR	CB-CG-CD2	-5.11	117.93	121.00
3	0	448	A	O4'-C1'-N9	5.11	112.29	108.20
3	0	531	A	O4'-C1'-N9	5.11	112.29	108.20
3	0	1870	A	O4'-C1'-N9	5.11	112.29	108.20
3	0	2049	G	O4'-C1'-N9	5.11	112.29	108.20
3	0	1	G	O4'-C1'-N9	5.11	112.29	108.20
3	0	2224	C	N3-C4-C5	-5.11	119.86	121.90
3	0	179	G	O4'-C1'-N9	5.11	112.29	108.20
3	0	251	A	C5-C6-N6	-5.11	119.61	123.70
3	0	1585	G	N3-C2-N2	5.11	123.48	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	C	373	VAL	C-N-CA	5.11	134.47	121.70
3	0	579	C	N3-C4-C5	-5.11	119.86	121.90
3	0	579	C	N3-C4-N4	5.11	121.57	118.00
3	0	517	G	O4'-C1'-N9	5.10	112.28	108.20
3	0	2217	G	N3-C2-N2	5.10	123.47	119.90
3	0	190	A	O4'-C1'-N9	5.10	112.28	108.20
3	0	575	A	C5-C6-N6	-5.10	119.62	123.70
3	0	1247	A	C5-C6-N6	-5.10	119.62	123.70
3	0	1700	A	C5-C6-N1	-5.10	115.15	117.70
3	0	1816	C	N3-C4-C5	-5.10	119.86	121.90
3	0	2272	A	C5-C6-N1	-5.10	115.15	117.70
3	0	1375	A	C5-C6-N1	-5.10	115.15	117.70
3	0	371	A	O4'-C1'-N9	5.10	112.28	108.20
3	0	620	C	N3-C4-C5	-5.10	119.86	121.90
3	0	634	A	C5-C6-N6	-5.10	119.62	123.70
3	0	863	A	C5-C6-N1	-5.10	115.15	117.70
3	0	2121	U	O4'-C1'-N1	5.10	112.28	108.20
2	1	53	A	C5-C6-N1	-5.10	115.15	117.70
3	0	1200	G	O4'-C1'-N9	5.10	112.28	108.20
3	0	1595	G	N3-C2-N2	5.10	123.47	119.90
3	0	2118	G	O4'-C1'-N9	5.10	112.28	108.20
3	0	2303	G	P-O5'-C5'	-5.10	112.74	120.90
3	0	1202	A	C5-C6-N6	-5.10	119.62	123.70
3	0	1410	G	O4'-C1'-N9	5.09	112.28	108.20
1	f	240	PHE	CB-CG-CD2	-5.09	117.24	120.80
3	0	349	A	O4'-C1'-N9	5.09	112.27	108.20
3	0	521	A	O4'-C1'-N9	5.09	112.27	108.20
3	0	2173	C	N3-C4-C5	-5.09	119.86	121.90
1	f	233	VAL	CA-C-O	-5.09	109.41	120.10
1	f	1108	ALA	N-CA-C	5.09	124.74	111.00
3	0	512	A	C5-C6-N6	-5.09	119.63	123.70
3	0	608	C	N3-C4-C5	-5.09	119.86	121.90
3	0	684	A	O4'-C1'-N9	5.09	112.27	108.20
3	0	501	A	C5-C6-N1	-5.09	115.16	117.70
3	0	2004	A	C5-C6-N1	-5.09	115.16	117.70
51	A	302	ASN	C-N-CD	-5.09	109.41	120.60
3	0	1210	A	C5-C6-N1	-5.09	115.16	117.70
3	0	2054	C	N3-C4-C5	-5.09	119.86	121.90
3	0	2128	C	N3-C4-C5	-5.09	119.86	121.90
46	C	465	SER	N-CA-CB	5.09	118.13	110.50
1	f	1102	GLY	N-CA-C	-5.08	100.39	113.10
3	0	1594	C	N3-C4-C5	-5.08	119.87	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	273	G	O4'-C1'-N9	5.08	112.27	108.20
3	0	884	A	O4'-C1'-N9	5.08	112.27	108.20
3	0	1319	A	C5-C6-N1	-5.08	115.16	117.70
3	0	1964	C	N3-C4-C5	-5.08	119.87	121.90
3	0	396	C	N3-C4-C5	-5.08	119.87	121.90
3	0	1635	A	C5-C6-N1	-5.08	115.16	117.70
3	0	894	A	O4'-C1'-N9	5.08	112.26	108.20
3	0	902	A	O4'-C1'-N9	5.08	112.26	108.20
3	0	2136	A	C5-C6-N1	-5.08	115.16	117.70
3	0	2163	C	N3-C4-C5	-5.08	119.87	121.90
46	C	501	TYR	CB-CG-CD2	-5.08	117.95	121.00
3	0	1683	C	N3-C4-C5	-5.08	119.87	121.90
3	0	2051	A	C5-C6-N1	-5.08	115.16	117.70
2	1	64	C	N3-C4-C5	-5.08	119.87	121.90
3	0	852	A	C5-C6-N1	-5.08	115.16	117.70
3	0	1567	G	O4'-C1'-N9	5.08	112.26	108.20
3	0	1633	A	O4'-C1'-N9	5.08	112.26	108.20
44	K	88	TYR	CB-CG-CD1	-5.08	117.95	121.00
3	0	661	G	O4'-C1'-N9	5.07	112.26	108.20
3	0	883	C	N3-C4-C5	-5.07	119.87	121.90
3	0	1357	C	N3-C4-C5	-5.07	119.87	121.90
3	0	2263	C	N3-C4-C5	-5.07	119.87	121.90
50	H	58	ALA	N-CA-CB	5.07	117.20	110.10
19	v	57	ALA	N-CA-CB	5.07	117.20	110.10
3	0	168	A	O4'-C1'-N9	5.07	112.26	108.20
3	0	1292	A	O4'-C1'-N9	5.07	112.26	108.20
3	0	1951	C	N3-C4-C5	-5.07	119.87	121.90
46	C	468	ASN	C-N-CA	5.07	134.38	121.70
3	0	775	A	C5-C6-N1	-5.07	115.17	117.70
3	0	1552	A	C5-C6-N1	-5.07	115.17	117.70
3	0	96	C	O4'-C1'-N1	5.07	112.25	108.20
3	0	2191	C	N3-C4-C5	-5.07	119.87	121.90
3	0	861	A	C5-C6-N6	-5.07	119.65	123.70
3	0	1305	C	O4'-C1'-N1	5.07	112.25	108.20
3	0	1309	C	N3-C4-C5	-5.07	119.87	121.90
3	0	1238	A	C5-C6-N1	-5.06	115.17	117.70
3	0	1852	C	N3-C4-C5	-5.06	119.87	121.90
3	0	209	C	N3-C4-C5	-5.06	119.88	121.90
3	0	696	G	O4'-C1'-N9	5.06	112.25	108.20
3	0	904	C	N3-C4-C5	-5.06	119.88	121.90
3	0	924	G	C1'-O4'-C4'	-5.06	105.85	109.90
3	0	1999	U	O4'-C1'-N1	5.06	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	2052	A	O4'-C1'-N9	5.06	112.25	108.20
3	0	77	C	N3-C4-C5	-5.06	119.88	121.90
3	0	411	G	O4'-C1'-N9	5.06	112.25	108.20
3	0	1460	A	C5-C6-N1	-5.06	115.17	117.70
1	f	136	LEU	CB-CA-C	-5.06	100.59	110.20
3	0	620	C	N3-C4-N4	5.06	121.54	118.00
3	0	1899	C	N3-C4-C5	-5.06	119.88	121.90
46	C	475	GLN	C-N-CA	5.06	134.35	121.70
3	0	241	A	C5-C6-N1	-5.06	115.17	117.70
3	0	445	G	O4'-C1'-N9	5.06	112.25	108.20
3	0	1802	A	O4'-C1'-N9	5.06	112.25	108.20
3	0	2240	C	N3-C4-C5	-5.06	119.88	121.90
10	u	79	LYS	N-CA-CB	5.06	119.70	110.60
3	0	739	G	C5-C6-O6	-5.06	125.57	128.60
3	0	281	A	C5-C6-N6	-5.05	119.66	123.70
3	0	447	A	O4'-C1'-N9	5.05	112.24	108.20
3	0	756	G	O4'-C1'-N9	5.05	112.24	108.20
3	0	1193	C	C5-C4-N4	-5.05	116.66	120.20
3	0	1908	A	C5-C6-N1	-5.05	115.17	117.70
3	0	781	A	C5-C6-N1	-5.05	115.17	117.70
1	f	241	SER	O-C-N	-5.05	114.62	122.70
3	0	448	A	C5-C6-N1	-5.05	115.17	117.70
3	0	500	A	C5-C6-N1	-5.05	115.17	117.70
2	1	11	C	N3-C4-C5	-5.05	119.88	121.90
3	0	974	A	C5-C6-N1	-5.05	115.17	117.70
8	p	66	HIS	N-CA-CB	5.05	119.69	110.60
47	8	212	SER	N-CA-CB	5.05	118.07	110.50
3	0	576	A	C5-C6-N1	-5.05	115.18	117.70
3	0	838	G	O4'-C1'-N9	5.05	112.24	108.20
46	C	480	TYR	C-N-CA	5.05	134.32	121.70
3	0	542	C	N3-C4-C5	-5.05	119.88	121.90
3	0	450	A	C5-C6-N1	-5.04	115.18	117.70
3	0	506	A	O4'-C1'-N9	5.04	112.24	108.20
3	0	1332	A	C5-C6-N6	-5.04	119.66	123.70
2	1	71	U	C4'-C3'-C2'	-5.04	97.56	102.60
3	0	677	G	O4'-C1'-N9	5.04	112.23	108.20
3	0	1215	G	O4'-C1'-N9	5.04	112.23	108.20
3	0	561	A	C5-C6-N1	-5.04	115.18	117.70
3	0	776	G	N3-C2-N2	5.04	123.43	119.90
3	0	778	A	O4'-C1'-N9	5.04	112.23	108.20
3	0	965	C	N3-C4-C5	-5.04	119.88	121.90
3	0	1374	C	N3-C4-C5	-5.04	119.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1469	A	C5-C6-N1	-5.04	115.18	117.70
3	0	1589	A	C5-C6-N1	-5.04	115.18	117.70
3	0	1614	A	O4'-C1'-N9	5.04	112.23	108.20
3	0	1635	A	O4'-C1'-N9	5.04	112.23	108.20
3	0	1981	C	O4'-C1'-N1	5.04	112.23	108.20
2	1	26	A	C5-C6-N1	-5.04	115.18	117.70
3	0	829	C	N3-C4-C5	-5.04	119.89	121.90
3	0	2094	A	C5-C6-N6	-5.04	119.67	123.70
2	1	40	C	N3-C4-C5	-5.03	119.89	121.90
3	0	1270	A	O4'-C1'-N9	5.03	112.23	108.20
3	0	1436	C	N3-C4-C5	-5.03	119.89	121.90
3	0	1598	A	C5-C6-N6	-5.03	119.67	123.70
3	0	1611	A	O4'-C1'-N9	5.03	112.23	108.20
3	0	1909	U	O4'-C1'-N1	5.03	112.22	108.20
3	0	1989	A	C5-C6-N6	-5.03	119.67	123.70
3	0	990	A	C5-C6-N1	-5.03	115.19	117.70
3	0	1333	A	C5-C6-N6	-5.03	119.68	123.70
3	0	249	A	O4'-C1'-N9	5.03	112.22	108.20
3	0	299	A	O4'-C1'-N9	5.03	112.22	108.20
3	0	604	A	O4'-C1'-N9	5.03	112.22	108.20
3	0	880	A	C5-C6-N6	-5.03	119.68	123.70
3	0	1356	C	N3-C4-C5	-5.03	119.89	121.90
8	p	253	CYS	N-CA-CB	5.03	119.65	110.60
38	w	120	SER	N-CA-CB	5.03	118.04	110.50
3	0	365	C	N3-C4-C5	-5.03	119.89	121.90
3	0	408	C	N3-C4-C5	-5.03	119.89	121.90
3	0	2125	A	C5-C6-N6	-5.03	119.68	123.70
46	C	581	ASN	N-CA-CB	5.03	119.65	110.60
3	0	521	A	C5-C6-N1	-5.02	115.19	117.70
3	0	287	A	O4'-C1'-N9	5.02	112.22	108.20
3	0	350	C	N3-C4-C5	-5.02	119.89	121.90
3	0	577	A	O4'-C1'-N9	5.02	112.22	108.20
3	0	907	G	O4'-C1'-N9	5.02	112.22	108.20
3	0	1361	C	N3-C4-C5	-5.02	119.89	121.90
26	J	87	PHE	CB-CG-CD1	-5.02	117.28	120.80
3	0	31	C	N3-C4-C5	-5.02	119.89	121.90
3	0	221	C	N3-C4-C5	-5.02	119.89	121.90
3	0	764	A	O4'-C1'-N9	5.02	112.21	108.20
3	0	983	C	N3-C4-C5	-5.02	119.89	121.90
3	0	1531	A	C5-C6-N6	-5.02	119.69	123.70
2	1	14	A	C5-C6-N6	-5.01	119.69	123.70
3	0	751	C	N3-C4-C5	-5.01	119.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	0	1292	A	C5-C6-N1	-5.01	115.19	117.70
3	0	2285	A	C5-C6-N1	-5.01	115.19	117.70
3	0	694	A	O4'-C1'-N9	5.01	112.21	108.20
3	0	945	C	N3-C4-C5	-5.01	119.89	121.90
2	1	60	C	N3-C4-C5	-5.01	119.89	121.90
3	0	23	G	O4'-C1'-N9	5.01	112.21	108.20
3	0	461	C	N3-C4-C5	-5.01	119.90	121.90
3	0	512	A	C5-C6-N1	-5.01	115.19	117.70
3	0	744	C	N3-C4-C5	-5.01	119.89	121.90
3	0	1298	C	N3-C4-C5	-5.01	119.90	121.90
3	0	58	C	N3-C4-C5	-5.01	119.90	121.90
3	0	238	G	O4'-C1'-N9	5.01	112.21	108.20
3	0	515	C	N3-C4-C5	-5.01	119.90	121.90
3	0	541	G	O4'-C1'-N9	5.01	112.21	108.20
3	0	590	C	N3-C4-C5	-5.01	119.90	121.90
3	0	704	A	O4'-C1'-N9	5.01	112.21	108.20
3	0	2192	C	N3-C4-C5	-5.01	119.90	121.90
3	0	893	G	O4'-C1'-N9	5.01	112.21	108.20
3	0	2057	C	N3-C4-N4	5.01	121.51	118.00
3	0	22	A	O4'-C1'-N9	5.01	112.21	108.20
3	0	670	G	O4'-C1'-N9	5.01	112.20	108.20
3	0	41	G	O4'-C1'-N9	5.00	112.20	108.20
3	0	979	G	O4'-C1'-N9	5.00	112.20	108.20
3	0	1896	C	N3-C4-C5	-5.00	119.90	121.90
3	0	1979	C	C6-N1-C2	-5.00	118.30	120.30
3	0	2120	C	N3-C4-C5	-5.00	119.90	121.90
3	0	917	A	O4'-C1'-N9	5.00	112.20	108.20
3	0	1731	C	O4'-C1'-N1	5.00	112.20	108.20
3	0	1801	G	O4'-C1'-N9	5.00	112.20	108.20
3	0	25	C	N3-C4-C5	-5.00	119.90	121.90
3	0	705	G	O4'-C1'-N9	5.00	112.20	108.20
3	0	799	A	C5-C6-N1	-5.00	115.20	117.70
3	0	901	A	C5-C6-N1	-5.00	115.20	117.70

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	f	296	TYR	CA
1	f	305	TYR	CA
1	f	772	TYR	CA
3	0	974	A	C1'
3	0	1833	G	C1'

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Mol	Chain	Res	Type	Atom
39	E	281	TYR	CA
46	C	429	SER	CA
49	I	337	PRO	CA
49	I	350	TYR	CA

All (759) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	0	1185	A	Sidechain
3	0	1207	G	Sidechain
3	0	1254	G	Sidechain
3	0	1331	G	Sidechain
3	0	1418	U	Sidechain
3	0	1473	G	Sidechain
3	0	1485	U	Sidechain
3	0	1488	U	Sidechain
3	0	1518	C	Sidechain
3	0	152	A	Sidechain
3	0	1611	A	Sidechain
3	0	1666	A	Sidechain
3	0	1694	A	Sidechain
3	0	1702	G	Sidechain
3	0	1704	U	Sidechain
3	0	1779	U	Sidechain
3	0	1930	A	Sidechain
3	0	1970	U	Sidechain
3	0	1978	A	Sidechain
3	0	1997	A	Sidechain
3	0	2008	G	Sidechain
3	0	2011	A	Sidechain
3	0	2020	U	Sidechain
3	0	2078	G	Sidechain
3	0	2080	G	Sidechain
3	0	2086	G	Sidechain
3	0	2098	U	Sidechain
3	0	2102	U	Sidechain
3	0	2119	U	Sidechain
3	0	212	G	Sidechain
3	0	2120	C	Sidechain
3	0	2134	U	Sidechain
3	0	2136	A	Sidechain
3	0	2244	A	Sidechain

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Mol	Chain	Res	Type	Group
3	0	229	G	Sidechain
3	0	237	A	Sidechain
3	0	255	A	Sidechain
3	0	271	C	Sidechain
3	0	313	G	Sidechain
3	0	324	U	Sidechain
3	0	481	G	Sidechain
3	0	695	G	Sidechain
3	0	714	G	Sidechain
3	0	736	U	Sidechain
3	0	738	G	Sidechain
3	0	773	U	Sidechain
3	0	776	G	Sidechain
3	0	8	U	Sidechain
3	0	824	G	Sidechain
3	0	90	A	Sidechain
3	0	936	C	Sidechain
3	0	975	U	Sidechain
28	5	102	CYS	Peptide
28	5	233	ALA	Peptide
28	5	267	SER	Mainchain
28	5	271	ASN	Peptide
28	5	273	PRO	Peptide
28	5	278	ILE	Peptide
28	5	283	GLY	Peptide
28	5	411	LEU	Mainchain
28	5	412	GLN	Mainchain,Peptide
28	5	89	THR	Mainchain,Peptide
47	8	114	GLY	Peptide
47	8	115	GLU	Peptide
47	8	116	THR	Peptide
47	8	117	PRO	Peptide
47	8	118	SER	Peptide
47	8	127	LEU	Peptide
47	8	128	SER	Peptide
47	8	130	VAL	Peptide
47	8	132	PRO	Peptide
47	8	157	SER	Peptide
47	8	158	PHE	Peptide
47	8	161	ILE	Peptide
47	8	162	GLY	Peptide
47	8	186	ASN	Peptide

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Mol	Chain	Res	Type	Group
47	8	187	LEU	Peptide
47	8	189	ARG	Peptide
47	8	197	ALA	Mainchain
47	8	204	ARG	Peptide
47	8	207	LEU	Peptide
47	8	209	PRO	Peptide
47	8	210	ILE	Peptide
47	8	214	VAL	Peptide
47	8	22	ASN	Peptide
47	8	238	GLU	Peptide
47	8	240	PRO	Peptide
47	8	241	ASN	Peptide
47	8	256	LEU	Peptide
47	8	257	THR	Peptide
47	8	258	GLU	Peptide
47	8	259	MET	Peptide
47	8	261	SER	Peptide
47	8	262	TRP	Peptide
47	8	277	GLN	Peptide
47	8	279	ILE	Peptide
47	8	305	SER	Peptide
47	8	306	HIS	Peptide
47	8	322	GLY	Peptide
47	8	340	CYS	Peptide
47	8	345	ASN	Peptide
47	8	347	GLU	Peptide
47	8	349	ARG	Peptide
47	8	350	ASN	Peptide
47	8	368	LEU	Mainchain,Peptide
47	8	376	ALA	Peptide
47	8	388	GLN	Peptide
47	8	392	LYS	Peptide
47	8	393	ALA	Peptide
47	8	405	ARG	Peptide
47	8	424	ILE	Peptide
47	8	425	VAL	Peptide
47	8	435	GLU	Mainchain
47	8	467	ASN	Peptide
47	8	469	ALA	Peptide
47	8	470	SER	Peptide
47	8	473	VAL	Peptide
47	8	475	ILE	Peptide

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Mol	Chain	Res	Type	Group
47	8	492	ILE	Peptide
47	8	500	SER	Peptide
47	8	520	VAL	Peptide
47	8	521	ASP	Peptide
47	8	547	ILE	Peptide
47	8	56	PHE	Peptide
47	8	59	GLU	Peptide
47	8	60	GLN	Peptide
47	8	61	GLY	Peptide
47	8	62	ILE	Peptide
47	8	67	PHE	Peptide
47	8	74	ASN	Peptide
51	A	103	ARG	Peptide
51	A	17	GLY	Peptide
51	A	19	PRO	Peptide
51	A	2	GLY	Peptide
51	A	23	ILE	Peptide
51	A	24	GLU	Peptide
51	A	25	MET	Peptide
51	A	3	PHE	Peptide
51	A	4	GLU	Peptide
51	A	40	ALA	Peptide
51	A	57	GLN	Peptide
51	A	59	THR	Peptide
51	A	62	LYS	Peptide
51	A	64	GLU	Peptide
51	A	81	GLY	Peptide
51	A	97	PHE	Peptide
21	B	130	GLN	Peptide
21	B	159	ASP	Peptide
21	B	166	GLY	Peptide
21	B	81	ASP	Peptide
46	C	102	PRO	Peptide
46	C	108	CYS	Peptide
46	C	11	ASP	Peptide
46	C	113	PRO	Peptide
46	C	114	ASP	Peptide
46	C	12	GLU	Peptide
46	C	122	LYS	Peptide
46	C	123	GLU	Peptide
46	C	124	THR	Peptide
46	C	125	PHE	Peptide

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Mol	Chain	Res	Type	Group
46	C	126	LYS	Peptide
46	C	128	PRO	Peptide
46	C	14	LEU	Peptide
46	C	147	ILE	Peptide
46	C	157	ASP	Peptide
46	C	158	GLU	Peptide
46	C	159	GLU	Peptide
46	C	16	GLU	Peptide
46	C	160	SER	Peptide
46	C	162	GLU	Peptide
46	C	164	GLY	Peptide
46	C	166	ASP	Peptide
46	C	168	GLY	Peptide
46	C	169	GLN	Peptide
46	C	17	VAL	Peptide
46	C	170	GLY	Peptide
46	C	172	GLU	Peptide
46	C	175	GLU	Peptide
46	C	178	GLU	Peptide
46	C	179	GLU	Peptide
46	C	19	HIS	Peptide
46	C	194	LYS	Peptide
46	C	195	ARG	Peptide
46	C	196	ALA	Peptide
46	C	214	LEU	Peptide
46	C	22	GLU	Peptide
46	C	237	ALA	Peptide
46	C	256	THR	Peptide
46	C	258	ASN	Peptide
46	C	259	PRO	Peptide
46	C	260	ALA	Peptide
46	C	267	PHE	Peptide
46	C	268	SER	Peptide
46	C	271	LEU	Peptide
46	C	274	LYS	Peptide
46	C	281	GLY	Peptide
46	C	282	LEU	Peptide
46	C	283	CYS	Peptide
46	C	327	TYR	Peptide
46	C	328	TYR	Peptide
46	C	329	GLN	Peptide
46	C	332	LYS	Peptide

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Mol	Chain	Res	Type	Group
46	C	333	ARG	Peptide
46	C	344	GLU	Peptide
46	C	345	ILE	Peptide
46	C	348	SER	Peptide
46	C	350	ARG	Peptide
46	C	351	GLN	Peptide
46	C	352	GLN	Peptide
46	C	358	TYR	Peptide
46	C	361	MET	Peptide
46	C	362	THR	Peptide
46	C	363	ARG	Peptide
46	C	364	LEU	Peptide
46	C	365	THR	Peptide
46	C	374	ILE	Peptide
46	C	382	GLN	Peptide
46	C	386	VAL	Peptide
46	C	387	ILE	Peptide
46	C	388	GLY	Peptide
46	C	391	GLU	Peptide
46	C	394	CYS	Peptide
46	C	395	SER	Peptide
46	C	429	SER	Peptide
46	C	450	ALA	Peptide
46	C	453	VAL	Peptide
46	C	46	GLU	Peptide
46	C	464	TRP	Mainchain,Peptide
46	C	465	SER	Peptide
46	C	466	ASN	Peptide
46	C	467	ARG	Peptide
46	C	469	HIS	Peptide
46	C	471	VAL	Peptide
46	C	495	LEU	Peptide
46	C	501	TYR	Peptide
46	C	502	ILE	Peptide
46	C	504	HIS	Mainchain,Peptide
46	C	51	LEU	Peptide
46	C	522	LYS	Peptide
46	C	523	GLU	Peptide
46	C	524	ALA	Peptide
46	C	525	LYS	Peptide
46	C	526	LYS	Peptide
46	C	527	PRO	Peptide

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Mol	Chain	Res	Type	Group
46	C	528	TYR	Peptide
46	C	542	ASN	Peptide
46	C	544	MET	Peptide
46	C	545	ALA	Peptide
46	C	547	GLN	Peptide
46	C	548	PRO	Peptide
46	C	549	LEU	Peptide
46	C	553	PRO	Peptide
46	C	555	GLU	Peptide
46	C	568	LYS	Peptide
46	C	570	GLY	Peptide
46	C	571	ASP	Peptide
46	C	580	LYS	Peptide
46	C	581	ASN	Peptide
46	C	582	MET	Peptide
46	C	584	ALA	Peptide
46	C	585	TRP	Peptide
46	C	586	SER	Peptide
46	C	590	ASN	Peptide
46	C	591	GLY	Peptide
46	C	610	PHE	Peptide
46	C	612	TYR	Peptide
46	C	616	CYS	Peptide
46	C	617	ASN	Peptide
46	C	619	ALA	Peptide
46	C	621	ILE	Peptide
46	C	622	SER	Peptide
46	C	630	TYR	Sidechain
46	C	633	ASN	Peptide
46	C	634	GLU	Peptide
46	C	636	GLU	Peptide
46	C	647	GLU	Peptide
46	C	653	ILE	Peptide
46	C	654	ALA	Peptide
46	C	73	ASP	Peptide
46	C	75	GLU	Peptide
46	C	76	SER	Peptide
46	C	94	HIS	Peptide
46	C	95	LYS	Peptide
46	C	97	LYS	Peptide
46	C	99	LYS	Peptide
42	D	7	PRO	Peptide

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Mol	Chain	Res	Type	Group
39	E	105	VAL	Peptide
39	E	106	LEU	Peptide
39	E	107	GLU	Peptide
39	E	109	LYS	Peptide
39	E	111	ILE	Peptide
39	E	113	SER	Peptide
39	E	114	ASN	Peptide
39	E	115	VAL	Peptide
39	E	12	LEU	Peptide
39	E	126	TYR	Sidechain,Peptide
39	E	127	TYR	Peptide
39	E	128	ASP	Peptide
39	E	13	ASP	Peptide
39	E	131	ARG	Peptide
39	E	14	LYS	Peptide
39	E	147	GLY	Peptide
39	E	148	TYR	Peptide
39	E	15	HIS	Peptide
39	E	150	ILE	Peptide
39	E	190	GLU	Peptide
39	E	192	ILE	Peptide
39	E	194	ARG	Peptide
39	E	211	VAL	Peptide
39	E	216	PHE	Peptide
39	E	218	GLY	Peptide
39	E	221	GLN	Peptide
39	E	223	SER	Peptide
39	E	231	PHE	Peptide
39	E	233	ILE	Peptide
39	E	235	THR	Peptide
39	E	237	PHE	Peptide
39	E	244	GLU	Peptide
39	E	245	THR	Peptide
39	E	262	LYS	Peptide
39	E	263	GLN	Peptide
39	E	265	ARG	Peptide
39	E	266	SER	Peptide
39	E	283	ASP	Peptide
39	E	295	ARG	Peptide
39	E	297	SER	Peptide
39	E	30	ASP	Peptide
39	E	314	GLY	Peptide

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Mol	Chain	Res	Type	Group
39	E	315	ASP	Peptide
39	E	317	PHE	Peptide
39	E	318	LEU	Peptide
39	E	319	ILE	Peptide
39	E	32	ALA	Peptide
39	E	338	MET	Peptide
39	E	339	MET	Peptide
39	E	34	ALA	Peptide
39	E	340	THR	Peptide
39	E	345	SER	Peptide
39	E	35	LEU	Peptide
39	E	353	LEU	Peptide
39	E	38	VAL	Peptide
39	E	388	SER	Peptide
39	E	389	GLN	Peptide
39	E	390	ALA	Peptide
39	E	392	SER	Peptide
39	E	40	ALA	Peptide
39	E	41	THR	Peptide
39	E	42	THR	Peptide
39	E	43	ALA	Peptide
39	E	46	ALA	Peptide
39	E	47	GLU	Peptide
39	E	48	GLY	Peptide
39	E	62	ALA	Peptide
39	E	63	GLN	Peptide
39	E	64	ARG	Peptide
39	E	93	ASP	Peptide
39	E	94	ALA	Peptide
39	E	97	SER	Peptide
22	F	155	ALA	Peptide
22	F	191	THR	Peptide
22	F	198	TRP	Peptide
43	G	106	PRO	Peptide
43	G	111	SER	Peptide
43	G	112	LYS	Peptide
43	G	117	ASN	Peptide
43	G	118	GLN	Peptide
43	G	163	GLU	Peptide
43	G	179	LYS	Peptide
43	G	182	TYR	Peptide
43	G	185	SER	Peptide

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Mol	Chain	Res	Type	Group
43	G	188	TYR	Peptide
43	G	189	PRO	Peptide
43	G	194	THR	Peptide
43	G	195	ASN	Peptide
43	G	210	PHE	Peptide
43	G	212	ARG	Peptide
43	G	215	ASN	Peptide
43	G	217	ARG	Peptide
43	G	24	ARG	Peptide
43	G	250	GLY	Peptide
43	G	253	ASN	Peptide
43	G	254	LYS	Peptide
43	G	255	SER	Peptide
43	G	26	ARG	Peptide
43	G	268	TYR	Sidechain
43	G	278	GLN	Peptide
43	G	280	SER	Peptide
43	G	46	TYR	Sidechain
43	G	60	ARG	Peptide
43	G	75	CYS	Peptide
43	G	76	TYR	Peptide
43	G	79	SER	Peptide
43	G	89	ALA	Peptide
43	G	92	GLU	Peptide
43	G	93	PRO	Peptide
43	G	94	GLY	Peptide
43	G	95	LYS	Peptide
50	H	126	GLU	Peptide
50	H	127	LEU	Peptide
50	H	129	SER	Mainchain,Peptide
50	H	187	PRO	Peptide
50	H	188	THR	Peptide
50	H	190	GLU	Peptide
50	H	196	THR	Peptide
50	H	197	ARG	Peptide
50	H	202	ARG	Peptide
50	H	205	LEU	Peptide
50	H	221	VAL	Peptide
50	H	223	ARG	Peptide
50	H	241	GLY	Peptide
50	H	242	PHE	Peptide
50	H	243	ASN	Peptide

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Mol	Chain	Res	Type	Group
50	H	260	THR	Peptide
50	H	261	ASP	Peptide
50	H	269	SER	Peptide
50	H	293	SER	Peptide
50	H	294	TYR	Peptide
50	H	295	GLY	Peptide
50	H	299	GLN	Peptide
50	H	300	ARG	Peptide
50	H	92	PRO	Peptide
50	H	96	THR	Peptide
49	I	324	ASP	Peptide
49	I	342	ILE	Peptide
49	I	422	ASP	Peptide
49	I	429	ALA	Peptide
49	I	437	THR	Peptide
49	I	438	VAL	Peptide
26	J	107	PHE	Peptide
26	J	120	LEU	Peptide
26	J	139	THR	Peptide
26	J	147	ASN	Peptide
26	J	150	VAL	Peptide
26	J	154	SER	Peptide
26	J	155	PRO	Peptide
26	J	158	ARG	Peptide
26	J	159	ALA	Peptide
26	J	160	SER	Peptide
26	J	174	LYS	Peptide
26	J	179	ARG	Peptide
26	J	180	THR	Peptide
26	J	182	ARG	Peptide
26	J	183	ASN	Peptide
26	J	184	ASN	Peptide
26	J	203	LYS	Peptide
26	J	217	LEU	Peptide
26	J	71	TYR	Sidechain
26	J	77	GLN	Peptide
26	J	92	LYS	Peptide
44	K	178	LYS	Peptide
44	K	189	ASN	Peptide
31	L	103	ILE	Peptide
31	L	107	VAL	Peptide
31	L	35	GLU	Peptide

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Mol	Chain	Res	Type	Group
31	L	49	GLY	Peptide
31	L	51	VAL	Peptide
31	L	52	ARG	Peptide
31	L	93	GLU	Peptide
32	M	36	VAL	Peptide
32	M	7	LYS	Peptide
33	N	34	THR	Peptide
34	O	13	ARG	Sidechain
34	O	148	ALA	Peptide
34	O	49	ASN	Peptide
34	O	50	CYS	Peptide
34	O	70	TYR	Sidechain
34	O	95	ARG	Peptide
29	P	124	ILE	Peptide
29	P	163	ARG	Sidechain
29	P	219	ARG	Sidechain
29	P	44	ASP	Peptide
41	Q	11	GLN	Peptide
41	Q	42	GLN	Peptide
41	Q	48	ALA	Peptide
45	T	142	ALA	Peptide
48	W	136	THR	Peptide
48	W	99	LEU	Peptide
20	X	32	ASN	Peptide
20	X	33	SER	Mainchain,Peptide
20	X	35	ASN	Peptide
20	X	37	ASN	Peptide
20	X	40	HIS	Peptide
20	X	41	VAL	Peptide
20	X	42	ASN	Peptide
20	X	44	SER	Peptide
20	X	81	ILE	Peptide
40	Y	278	THR	Peptide
40	Y	318	PHE	Peptide
40	Y	355	ASP	Peptide
40	Y	365	ALA	Peptide
12	Z	205	GLU	Peptide
12	Z	67	TRP	Peptide
35	b	75	ILE	Peptide
36	c	12	GLY	Peptide
36	c	22	ALA	Peptide
36	c	33	ARG	Sidechain

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Mol	Chain	Res	Type	Group
23	d	203	VAL	Peptide
23	d	236	LEU	Peptide
23	d	38	GLU	Peptide
1	f	1010	GLU	Peptide
1	f	1024	ASN	Peptide
1	f	1038	GLY	Mainchain
1	f	1039	ARG	Mainchain
1	f	1044	VAL	Mainchain
1	f	1070	LYS	Mainchain,Peptide
1	f	1080	ALA	Peptide
1	f	1100	ASN	Peptide
1	f	1101	PRO	Peptide
1	f	1107	GLY	Peptide
1	f	1109	LEU	Peptide
1	f	1110	GLY	Mainchain,Peptide
1	f	1116	GLN	Peptide
1	f	1118	HIS	Peptide
1	f	112	ILE	Peptide
1	f	1121	CYS	Peptide
1	f	1122	GLN	Mainchain
1	f	1126	THR	Mainchain
1	f	1128	PRO	Mainchain
1	f	1148	ASP	Mainchain,Peptide
1	f	1153	ASP	Mainchain
1	f	1172	ALA	Peptide
1	f	1175	PRO	Mainchain
1	f	1176	CYS	Peptide
1	f	1212	LYS	Peptide
1	f	1214	ARG	Mainchain
1	f	1218	VAL	Mainchain
1	f	1219	HIS	Mainchain
1	f	1220	LEU	Peptide
1	f	1235	LYS	Mainchain
1	f	1250	LYS	Peptide
1	f	1251	LYS	Peptide
1	f	1258	ASN	Peptide
1	f	1259	CYS	Peptide
1	f	1264	LEU	Mainchain,Peptide
1	f	1265	HIS	Mainchain,Peptide
1	f	1266	PRO	Mainchain,Peptide
1	f	1267	LEU	Peptide
1	f	1268	SER	Peptide

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Mol	Chain	Res	Type	Group
1	f	1277	ARG	Peptide
1	f	1284	SER	Peptide
1	f	1306	TRP	Peptide
1	f	132	ALA	Peptide
1	f	1338	THR	Peptide
1	f	135	GLU	Mainchain,Peptide
1	f	1359	LEU	Peptide
1	f	136	LEU	Peptide
1	f	1361	HIS	Peptide
1	f	1369	ASN	Peptide
1	f	137	CYS	Mainchain,Peptide
1	f	1373	GLU	Peptide
1	f	1378	PHE	Peptide
1	f	1402	ALA	Peptide
1	f	143	LEU	Peptide
1	f	1439	GLN	Peptide
1	f	145	ALA	Peptide
1	f	1466	VAL	Peptide
1	f	1467	SER	Peptide
1	f	1470	GLY	Peptide
1	f	1474	PHE	Peptide
1	f	152	ASP	Mainchain,Peptide
1	f	1524	LYS	Peptide
1	f	1582	LEU	Peptide
1	f	1584	VAL	Peptide
1	f	1620	LEU	Peptide
1	f	1627	ARG	Mainchain
1	f	163	PRO	Peptide
1	f	1632	HIS	Peptide
1	f	164	GLN	Peptide
1	f	1654	GLY	Peptide
1	f	1702	LEU	Peptide
1	f	1723	MET	Peptide
1	f	1749	LEU	Peptide
1	f	1772	ASN	Peptide
1	f	1775	PHE	Peptide
1	f	1784	GLY	Peptide
1	f	1788	GLU	Peptide
1	f	1790	PHE	Peptide
1	f	1801	TYR	Peptide
1	f	1807	LEU	Peptide
1	f	1809	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	f	1814	SER	Peptide
1	f	1815	SER	Peptide
1	f	1836	GLY	Peptide
1	f	1849	ASP	Peptide
1	f	1854	SER	Peptide
1	f	1855	PRO	Peptide
1	f	189	CYS	Peptide
1	f	193	ARG	Mainchain,Peptide
1	f	194	PHE	Mainchain
1	f	195	HIS	Mainchain
1	f	198	PHE	Mainchain,Peptide
1	f	199	PHE	Mainchain
1	f	201	SER	Peptide
1	f	202	LEU	Peptide
1	f	206	TRP	Peptide
1	f	207	GLU	Peptide
1	f	227	SER	Peptide
1	f	234	GLY	Mainchain
1	f	235	LEU	Peptide
1	f	236	SER	Peptide
1	f	237	ILE	Peptide
1	f	238	SER	Peptide
1	f	239	ASN	Mainchain,Peptide
1	f	240	PHE	Mainchain,Peptide
1	f	241	SER	Mainchain
1	f	242	SER	Peptide
1	f	243	TYR	Peptide
1	f	257	PRO	Mainchain
1	f	258	GLU	Mainchain
1	f	259	PHE	Mainchain,Peptide
1	f	26	SER	Peptide
1	f	261	LEU	Peptide
1	f	262	MET	Mainchain
1	f	263	SER	Mainchain,Peptide
1	f	264	ASP	Peptide
1	f	267	GLN	Peptide
1	f	268	LEU	Peptide
1	f	269	GLY	Peptide
1	f	291	ARG	Mainchain
1	f	292	ARG	Sidechain,Peptide
1	f	294	ALA	Peptide
1	f	295	ASN	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	f	296	TYR	Mainchain,Sidechain,Peptide
1	f	297	THR	Peptide
1	f	298	ASP	Peptide
1	f	300	ASP	Peptide
1	f	301	GLU	Peptide
1	f	302	ALA	Mainchain,Peptide
1	f	304	PRO	Peptide
1	f	305	TYR	Peptide
1	f	306	ARG	Peptide
1	f	307	LEU	Mainchain,Peptide
1	f	38	SER	Peptide
1	f	46	SER	Peptide
1	f	55	VAL	Peptide
1	f	56	THR	Peptide
1	f	679	ASN	Peptide
1	f	681	THR	Peptide
1	f	682	ALA	Peptide
1	f	696	ASN	Peptide
1	f	700	ARG	Peptide
1	f	705	GLU	Peptide
1	f	718	THR	Peptide
1	f	719	VAL	Peptide
1	f	720	ALA	Peptide
1	f	721	GLU	Peptide
1	f	722	TRP	Peptide
1	f	723	HIS	Peptide
1	f	736	SER	Peptide
1	f	772	TYR	Mainchain,Peptide
1	f	773	THR	Peptide
1	f	775	GLY	Peptide
1	f	794	ALA	Peptide
1	f	795	ALA	Peptide
1	f	796	SER	Peptide
1	f	798	LEU	Peptide
1	f	800	GLU	Peptide
1	f	801	VAL	Peptide
1	f	802	GLU	Peptide
1	f	803	PHE	Peptide
1	f	824	SER	Peptide
1	f	832	TYR	Peptide
1	f	833	GLY	Peptide
1	f	834	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	f	849	ASN	Peptide
1	f	860	ALA	Peptide
1	f	874	ARG	Sidechain
1	f	89	VAL	Peptide
1	f	913	GLU	Peptide
1	f	934	VAL	Peptide
1	f	944	SER	Peptide
1	f	962	SER	Peptide
1	f	976	ASN	Peptide
1	f	981	THR	Peptide
1	f	987	LEU	Peptide
1	f	990	ASP	Peptide
1	f	996	THR	Peptide
24	g	36	ALA	Peptide
6	j	103	VAL	Peptide
6	j	82	LYS	Peptide
52	l	142	HIS	Peptide
52	l	143	ARG	Sidechain,Peptide
52	l	144	ILE	Peptide
52	l	145	ARG	Peptide
52	l	146	TYR	Peptide
52	l	147	PRO	Peptide
52	l	148	ASP	Peptide
52	l	149	PRO	Peptide
52	l	151	THR	Peptide
11	m	107	ARG	Peptide
11	m	124	LYS	Peptide
7	n	295	ASP	Peptide
13	o	151	ASN	Peptide
8	p	263	PHE	Peptide
8	p	42	ALA	Peptide
9	r	29	LYS	Peptide
9	r	42	VAL	Peptide
9	r	45	ILE	Peptide
9	r	76	ARG	Peptide
5	s	115	GLY	Peptide
5	s	272	ARG	Sidechain
5	s	299	VAL	Peptide
5	s	301	ASN	Peptide
5	s	312	MET	Peptide
5	s	333	PHE	Peptide
5	s	334	LYS	Peptide

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Mol	Chain	Res	Type	Group
5	s	335	ALA	Peptide
5	s	338	GLU	Peptide
5	s	339	PRO	Peptide
5	s	340	GLN	Peptide
5	s	343	ILE	Peptide
5	s	344	SER	Peptide
5	s	362	ARG	Peptide
5	s	392	GLY	Peptide
5	s	393	PRO	Peptide
5	s	395	ALA	Peptide
17	t	41	PHE	Peptide
10	u	48	LYS	Peptide
10	u	56	ARG	Sidechain
19	v	105	ALA	Peptide
19	v	92	ALA	Peptide
38	w	112	GLU	Peptide
38	w	119	ARG	Peptide
38	w	121	SER	Peptide
38	w	157	LYS	Peptide
38	w	52	GLU	Peptide
38	w	83	VAL	Peptide
4	y	73	GLY	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	f	1519/2174 (70%)	1094 (72%)	295 (19%)	130 (9%)	0 4
4	y	121/137 (88%)	109 (90%)	10 (8%)	2 (2%)	7 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	s	293/418 (70%)	207 (71%)	51 (17%)	35 (12%)	0	2
6	j	77/150 (51%)	68 (88%)	6 (8%)	3 (4%)	2	17
7	n	223/343 (65%)	179 (80%)	33 (15%)	11 (5%)	2	12
8	p	308/318 (97%)	268 (87%)	31 (10%)	9 (3%)	3	22
9	r	138/149 (93%)	101 (73%)	29 (21%)	8 (6%)	1	9
10	u	134/153 (88%)	87 (65%)	33 (25%)	14 (10%)	0	2
11	m	140/143 (98%)	120 (86%)	18 (13%)	2 (1%)	9	35
12	Z	171/221 (77%)	145 (85%)	20 (12%)	6 (4%)	3	19
13	o	188/190 (99%)	147 (78%)	33 (18%)	8 (4%)	2	15
14	q	198/211 (94%)	168 (85%)	28 (14%)	2 (1%)	13	43
15	R	139/151 (92%)	121 (87%)	15 (11%)	3 (2%)	5	27
16	S	80/86 (93%)	69 (86%)	9 (11%)	2 (2%)	4	25
17	t	102/112 (91%)	82 (80%)	19 (19%)	1 (1%)	13	43
18	U	66/91 (72%)	54 (82%)	10 (15%)	2 (3%)	3	22
19	v	133/144 (92%)	121 (91%)	10 (8%)	2 (2%)	8	34
20	X	146/173 (84%)	121 (83%)	20 (14%)	5 (3%)	3	19
21	B	177/190 (93%)	149 (84%)	23 (13%)	5 (3%)	4	23
22	F	205/245 (84%)	180 (88%)	23 (11%)	2 (1%)	13	43
23	d	221/263 (84%)	191 (86%)	28 (13%)	2 (1%)	14	44
24	g	81/247 (33%)	68 (84%)	12 (15%)	1 (1%)	11	39
25	a	68/110 (62%)	56 (82%)	12 (18%)	0	100	100
26	J	171/257 (66%)	132 (77%)	24 (14%)	15 (9%)	0	4
27	h	119/141 (84%)	96 (81%)	19 (16%)	4 (3%)	3	19
28	5	417/477 (87%)	325 (78%)	62 (15%)	30 (7%)	1	7
29	P	247/250 (99%)	219 (89%)	25 (10%)	3 (1%)	11	39
30	i	119/141 (84%)	91 (76%)	16 (13%)	12 (10%)	0	3
31	L	97/117 (83%)	75 (77%)	20 (21%)	2 (2%)	5	28
32	M	198/214 (92%)	160 (81%)	31 (16%)	7 (4%)	3	19
33	N	91/161 (56%)	78 (86%)	10 (11%)	3 (3%)	3	20
34	O	138/167 (83%)	103 (75%)	27 (20%)	8 (6%)	1	9
35	b	127/145 (88%)	108 (85%)	18 (14%)	1 (1%)	16	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	c	58/66 (88%)	47 (81%)	10 (17%)	1 (2%)	7 32
37	V	95/109 (87%)	70 (74%)	15 (16%)	10 (10%)	0 2
38	w	145/166 (87%)	105 (72%)	30 (21%)	10 (7%)	1 7
39	E	389/407 (96%)	288 (74%)	46 (12%)	55 (14%)	0 1
40	Y	172/379 (45%)	139 (81%)	27 (16%)	6 (4%)	3 19
41	Q	55/57 (96%)	40 (73%)	8 (14%)	7 (13%)	0 1
42	D	31/34 (91%)	25 (81%)	5 (16%)	1 (3%)	3 20
43	G	306/345 (89%)	254 (83%)	33 (11%)	19 (6%)	1 9
44	K	199/203 (98%)	185 (93%)	10 (5%)	4 (2%)	6 29
45	T	130/152 (86%)	100 (77%)	21 (16%)	9 (7%)	1 7
46	C	694/716 (97%)	490 (71%)	82 (12%)	122 (18%)	0 0
47	8	574/762 (75%)	462 (80%)	57 (10%)	55 (10%)	0 3
48	W	215/254 (85%)	181 (84%)	27 (13%)	7 (3%)	3 20
49	I	342/489 (70%)	302 (88%)	21 (6%)	19 (6%)	1 10
50	H	295/334 (88%)	231 (78%)	41 (14%)	23 (8%)	1 5
51	A	481/502 (96%)	341 (71%)	89 (18%)	51 (11%)	0 2
52	l	256/273 (94%)	216 (84%)	30 (12%)	10 (4%)	2 17
All	All	11089/13737 (81%)	8768 (79%)	1572 (14%)	749 (7%)	2 7

All (749) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	f	56	THR
1	f	91	ASP
1	f	190	ARG
1	f	203	LEU
1	f	235	LEU
1	f	241	SER
1	f	245	SER
1	f	247	ALA
1	f	295	ASN
1	f	297	THR
1	f	302	ALA
1	f	305	TYR
1	f	306	ARG
1	f	307	LEU

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Mol	Chain	Res	Type
1	f	680	LYS
1	f	706	ILE
1	f	713	ILE
1	f	721	GLU
1	f	732	ALA
1	f	772	TYR
1	f	803	PHE
1	f	834	PHE
1	f	861	LYS
1	f	982	LEU
1	f	1022	ALA
1	f	1039	ARG
1	f	1108	ALA
1	f	1109	LEU
1	f	1114	TYR
1	f	1117	PHE
1	f	1122	GLN
1	f	1149	TYR
1	f	1161	ASN
1	f	1221	LEU
1	f	1252	ILE
1	f	1259	CYS
1	f	1265	HIS
1	f	1267	LEU
1	f	1285	LEU
1	f	1305	VAL
1	f	1313	GLN
1	f	1333	ALA
1	f	1340	GLU
1	f	1403	LEU
1	f	1440	GLU
1	f	1468	PHE
1	f	1474	PHE
1	f	1559	THR
1	f	1587	ASP
1	f	1694	ALA
1	f	1723	MET
1	f	1816	LEU
1	f	1837	PHE
5	s	301	ASN
5	s	316	GLN
5	s	318	ASP

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Mol	Chain	Res	Type
5	s	357	ALA
5	s	363	GLU
7	n	207	ARG
7	n	323	SER
7	n	324	ALA
7	n	334	SER
8	p	66	HIS
8	p	176	ASN
10	u	57	ALA
10	u	103	MET
10	u	117	LYS
18	U	78	SER
26	J	94	VAL
26	J	155	PRO
26	J	160	SER
26	J	184	ASN
27	h	73	TYR
28	5	90	ILE
28	5	172	PHE
28	5	351	ASP
28	5	399	ALA
28	5	413	ILE
30	i	83	ASP
31	L	51	VAL
33	N	19	THR
33	N	93	ALA
36	c	53	GLU
37	V	96	ASN
37	V	99	THR
38	w	71	ARG
38	w	125	ASP
38	w	138	GLU
38	w	161	ASP
39	E	22	TYR
39	E	39	GLN
39	E	62	ALA
39	E	63	GLN
39	E	65	ALA
39	E	93	ASP
39	E	116	MET
39	E	126	TYR
39	E	150	ILE

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Mol	Chain	Res	Type
39	E	214	PRO
39	E	231	PHE
39	E	246	VAL
39	E	281	TYR
39	E	284	PRO
39	E	320	LEU
39	E	341	HIS
39	E	346	ILE
40	Y	288	ASP
40	Y	366	ALA
41	Q	10	ARG
41	Q	41	ARG
43	G	221	GLU
43	G	275	LYS
43	G	279	SER
44	K	183	ALA
46	C	4	PHE
46	C	5	PHE
46	C	10	SER
46	C	11	ASP
46	C	15	ASP
46	C	20	HIS
46	C	51	LEU
46	C	74	HIS
46	C	103	TRP
46	C	128	PRO
46	C	147	ILE
46	C	167	GLU
46	C	169	GLN
46	C	173	GLU
46	C	191	GLN
46	C	192	LYS
46	C	196	ALA
46	C	197	ALA
46	C	258	ASN
46	C	282	LEU
46	C	283	CYS
46	C	284	GLY
46	C	305	ASP
46	C	319	ASP
46	C	324	VAL
46	C	332	LYS

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Mol	Chain	Res	Type
46	C	346	LEU
46	C	353	ALA
46	C	358	TYR
46	C	369	VAL
46	C	375	GLU
46	C	394	CYS
46	C	396	ALA
46	C	454	ILE
46	C	469	HIS
46	C	476	ARG
46	C	489	LEU
46	C	501	TYR
46	C	504	HIS
46	C	505	ALA
46	C	526	LYS
46	C	529	GLU
46	C	542	ASN
46	C	546	TYR
46	C	556	PHE
46	C	572	TYR
46	C	581	ASN
46	C	582	MET
46	C	585	TRP
46	C	592	ASP
46	C	612	TYR
46	C	613	ASN
46	C	623	VAL
47	8	22	ASN
47	8	62	ILE
47	8	68	PHE
47	8	76	ASN
47	8	112	ALA
47	8	117	PRO
47	8	127	LEU
47	8	130	VAL
47	8	160	ALA
47	8	202	PHE
47	8	206	LEU
47	8	208	SER
47	8	279	ILE
47	8	283	PRO
47	8	306	HIS

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Mol	Chain	Res	Type
47	8	334	ALA
47	8	346	LYS
47	8	352	GLU
47	8	468	GLU
47	8	546	SER
49	I	175	SER
49	I	216	SER
49	I	219	LYS
49	I	303	TRP
49	I	351	LYS
49	I	430	VAL
50	H	46	SER
50	H	96	THR
50	H	171	PRO
50	H	182	LEU
50	H	199	THR
50	H	203	ASN
50	H	204	ILE
50	H	245	ALA
50	H	300	ARG
51	A	4	GLU
51	A	12	ALA
51	A	271	ILE
51	A	304	PHE
51	A	305	PRO
51	A	321	ALA
51	A	355	ASP
51	A	404	SER
51	A	451	MET
51	A	455	LYS
52	l	146	TYR
1	f	144	SER
1	f	165	SER
1	f	194	PHE
1	f	228	GLU
1	f	257	PRO
1	f	271	LEU
1	f	317	ASP
1	f	724	LYS
1	f	740	THR
1	f	802	GLU
1	f	977	MET

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Mol	Chain	Res	Type
1	f	1042	ALA
1	f	1071	VAL
1	f	1078	ALA
1	f	1101	PRO
1	f	1121	CYS
1	f	1175	PRO
1	f	1215	ASP
1	f	1284	SER
1	f	1368	GLU
1	f	1402	ALA
1	f	1439	GLN
1	f	1465	SER
1	f	1475	ILE
1	f	1628	GLY
5	s	124	VAL
5	s	239	ILE
5	s	305	THR
5	s	313	THR
5	s	317	CYS
5	s	335	ALA
5	s	362	ARG
6	j	76	LYS
7	n	165	SER
8	p	131	ASN
8	p	277	GLU
9	r	130	CYS
9	r	141	ARG
13	o	39	ALA
16	S	60	CYS
16	S	62	THR
19	v	40	MET
19	v	57	ALA
20	X	41	VAL
20	X	43	MET
21	B	131	ARG
26	J	75	TRP
26	J	110	ASN
26	J	164	LYS
26	J	183	ASN
26	J	204	ASN
27	h	70	ASP
28	5	223	GLY

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Mol	Chain	Res	Type
28	5	269	ASP
28	5	277	ASP
28	5	279	GLU
28	5	358	ASP
28	5	429	LYS
28	5	457	GLU
28	5	462	LEU
30	i	69	ILE
30	i	96	GLN
30	i	121	ALA
32	M	141	ILE
33	N	45	PRO
34	O	104	SER
35	b	79	PHE
37	V	18	GLN
37	V	35	GLY
38	w	167	PHE
39	E	13	ASP
39	E	46	ALA
39	E	47	GLU
39	E	92	ILE
39	E	107	GLU
39	E	132	TYR
39	E	211	VAL
39	E	216	PHE
39	E	233	ILE
39	E	279	TYR
39	E	319	ILE
39	E	389	GLN
39	E	393	VAL
41	Q	33	ARG
41	Q	40	CYS
43	G	75	CYS
43	G	93	PRO
43	G	149	SER
43	G	213	LYS
43	G	245	ALA
43	G	252	LYS
45	T	133	VAL
46	C	8	SER
46	C	12	GLU
46	C	27	LYS

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Mol	Chain	Res	Type
46	C	38	VAL
46	C	44	ALA
46	C	47	ARG
46	C	114	ASP
46	C	157	ASP
46	C	160	SER
46	C	174	LYS
46	C	230	ASP
46	C	234	PRO
46	C	243	ARG
46	C	259	PRO
46	C	261	ILE
46	C	280	ASP
46	C	298	GLN
46	C	318	VAL
46	C	334	GLY
46	C	351	GLN
46	C	373	VAL
46	C	389	ASN
46	C	410	TYR
46	C	429	SER
46	C	466	ASN
46	C	468	ASN
46	C	549	LEU
46	C	620	THR
47	8	21	GLY
47	8	60	GLN
47	8	67	PHE
47	8	115	GLU
47	8	188	LYS
47	8	191	ILE
47	8	213	ILE
47	8	322	GLY
47	8	369	PHE
47	8	476	HIS
47	8	486	SER
47	8	551	LEU
48	W	80	ASP
49	I	274	LYS
49	I	350	TYR
49	I	437	THR
50	H	130	TYR

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Mol	Chain	Res	Type
50	H	243	ASN
51	A	3	PHE
51	A	25	MET
51	A	39	ILE
51	A	63	ASP
51	A	73	LEU
51	A	117	ASP
51	A	170	GLU
51	A	200	THR
51	A	292	LYS
51	A	390	LEU
52	l	21	THR
52	l	38	CYS
1	f	94	GLU
1	f	177	ILE
1	f	697	LYS
1	f	722	TRP
1	f	774	LEU
1	f	918	ALA
1	f	981	THR
1	f	984	PRO
1	f	995	GLU
1	f	997	PRO
1	f	1049	SER
1	f	1128	PRO
1	f	1245	ALA
1	f	1250	LYS
1	f	1258	ASN
1	f	1467	SER
1	f	1535	ILE
1	f	1751	HIS
1	f	1851	ALA
5	s	149	SER
5	s	263	ASP
5	s	284	PRO
5	s	314	CYS
5	s	343	ILE
5	s	356	ARG
5	s	393	PRO
6	j	78	LYS
7	n	328	ALA
8	p	94	TRP

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Mol	Chain	Res	Type
8	p	253	CYS
8	p	306	ASP
10	u	11	GLN
10	u	35	LYS
10	u	75	PRO
10	u	79	LYS
12	Z	69	THR
12	Z	193	PRO
13	o	3	ALA
13	o	36	PRO
14	q	134	LEU
20	X	34	HIS
22	F	7	GLY
23	d	238	ALA
26	J	140	PRO
28	5	66	SER
28	5	120	ASP
28	5	173	PRO
28	5	268	PHE
28	5	270	ILE
28	5	314	GLY
28	5	350	LEU
30	i	18	GLU
30	i	80	ARG
30	i	87	GLU
32	M	147	LYS
32	M	187	ILE
32	M	196	GLU
37	V	22	GLU
37	V	24	GLN
37	V	62	TRP
37	V	74	ALA
38	w	136	VAL
39	E	15	HIS
39	E	94	ALA
39	E	110	GLY
39	E	148	TYR
39	E	217	LYS
39	E	232	ASP
39	E	265	ARG
39	E	266	SER
39	E	277	ASN

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Mol	Chain	Res	Type
39	E	296	GLN
39	E	391	ARG
40	Y	231	CYS
43	G	89	ALA
43	G	91	PRO
44	K	177	ALA
44	K	187	ASP
45	T	56	ALA
45	T	134	ILE
46	C	25	GLU
46	C	37	GLU
46	C	100	VAL
46	C	194	LYS
46	C	264	LYS
46	C	265	GLU
46	C	266	VAL
46	C	273	SER
46	C	274	LYS
46	C	303	ALA
46	C	331	ARG
46	C	465	SER
46	C	481	VAL
46	C	485	ASP
47	8	57	SER
47	8	77	LYS
47	8	132	PRO
47	8	214	VAL
47	8	216	THR
47	8	217	ASP
47	8	220	HIS
47	8	280	THR
47	8	409	SER
47	8	454	THR
48	W	77	GLN
48	W	159	LYS
49	I	298	PRO
49	I	301	LEU
49	I	337	PRO
50	H	58	ALA
50	H	59	THR
50	H	175	SER
50	H	206	ARG

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Mol	Chain	Res	Type
50	H	296	PRO
51	A	17	GLY
51	A	40	ALA
51	A	52	ALA
51	A	81	GLY
51	A	82	PRO
51	A	130	ALA
51	A	159	LYS
51	A	185	GLU
51	A	188	THR
51	A	262	GLU
51	A	337	ALA
51	A	339	GLN
51	A	363	LYS
51	A	379	ARG
52	l	150	ARG
52	l	168	ASP
52	l	169	LEU
1	f	230	ASP
1	f	232	LYS
1	f	769	ASP
1	f	800	GLU
1	f	860	ALA
1	f	1226	LYS
1	f	1233	ASP
1	f	1264	LEU
1	f	1525	THR
5	s	300	ARG
5	s	338	GLU
5	s	341	ILE
5	s	395	ALA
6	j	121	PRO
7	n	293	LYS
7	n	333	ARG
8	p	78	ASN
8	p	278	ALA
9	r	122	LEU
9	r	126	ASP
9	r	139	SER
10	u	43	TYR
10	u	84	PHE
10	u	91	PRO

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Mol	Chain	Res	Type
12	Z	59	ARG
12	Z	106	ALA
13	o	48	ARG
18	U	83	ARG
20	X	33	SER
24	g	47	ASN
26	J	161	THR
26	J	163	LYS
26	J	180	THR
27	h	71	GLU
28	5	310	ALA
28	5	352	PRO
28	5	353	THR
29	P	242	ALA
30	i	89	SER
30	i	92	ASP
31	L	85	LEU
32	M	113	GLN
34	O	77	ILE
34	O	81	VAL
34	O	99	LYS
37	V	63	GLY
37	V	100	GLU
38	w	147	ASP
38	w	156	ASN
39	E	14	LYS
39	E	97	SER
39	E	127	TYR
39	E	149	GLU
39	E	151	ASP
39	E	152	GLN
39	E	213	PHE
39	E	239	TYR
39	E	261	ASN
39	E	262	LYS
40	Y	339	ALA
40	Y	356	PRO
41	Q	31	VAL
43	G	76	TYR
43	G	247	LEU
43	G	254	LYS
45	T	22	PHE

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Mol	Chain	Res	Type
45	T	137	ARG
46	C	30	GLN
46	C	34	LYS
46	C	94	HIS
46	C	180	ASP
46	C	209	ARG
46	C	322	ASP
46	C	323	SER
46	C	329	GLN
46	C	330	GLN
46	C	364	LEU
46	C	383	GLU
46	C	568	LYS
46	C	665	VAL
47	8	58	GLN
47	8	187	LEU
47	8	210	ILE
47	8	257	THR
47	8	304	CYS
47	8	366	ALA
47	8	472	GLU
48	W	131	THR
49	I	423	LEU
50	H	84	PRO
50	H	95	GLU
51	A	58	PHE
51	A	79	ARG
51	A	138	ALA
51	A	426	LYS
51	A	472	SER
52	l	79	TYR
1	f	166	VAL
1	f	173	PRO
1	f	209	ALA
1	f	315	VAL
1	f	707	ARG
1	f	795	ALA
1	f	1079	ARG
1	f	1099	LYS
1	f	1103	ARG
1	f	1361	HIS
1	f	1750	ARG

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Mol	Chain	Res	Type
1	f	1772	ASN
1	f	1855	PRO
5	s	150	ALA
5	s	166	TYR
5	s	306	ILE
5	s	330	GLY
5	s	332	ARG
5	s	381	ALA
7	n	164	SER
10	u	17	LEU
10	u	53	VAL
11	m	97	ASN
12	Z	23	LYS
13	o	11	LYS
13	o	67	ARG
13	o	152	LEU
21	B	90	ASP
26	J	147	ASN
26	J	175	VAL
28	5	161	ALA
28	5	233	ALA
28	5	280	ASN
34	O	13	ARG
34	O	15	ILE
34	O	33	LYS
39	E	78	THR
39	E	87	LEU
39	E	131	ARG
41	Q	30	ALA
43	G	12	PRO
43	G	60	ARG
43	G	163	GLU
44	K	132	LYS
45	T	28	GLU
45	T	45	HIS
45	T	107	ARG
46	C	208	LYS
46	C	232	ARG
46	C	386	VAL
46	C	498	PRO
46	C	500	ALA
47	8	114	GLY

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Mol	Chain	Res	Type
47	8	347	GLU
48	W	56	ILE
48	W	119	TRP
49	I	215	LEU
49	I	275	PHE
49	I	325	GLU
49	I	343	PRO
49	I	346	THR
50	H	40	ARG
50	H	301	ILE
51	A	64	GLU
51	A	84	ARG
51	A	98	ALA
51	A	261	VAL
52	l	144	ILE
1	f	205	ILE
1	f	303	ASN
1	f	805	PHE
1	f	806	ALA
1	f	1046	ALA
1	f	1534	ARG
4	y	64	VAL
5	s	299	VAL
5	s	331	ARG
11	m	14	VAL
15	R	134	GLN
20	X	14	ASP
21	B	171	VAL
27	h	140	LEU
28	5	175	PRO
28	5	272	LYS
30	i	67	ARG
30	i	93	GLN
32	M	199	ILE
38	w	113	VAL
41	Q	21	HIS
42	D	3	THR
43	G	130	ALA
46	C	52	SER
46	C	96	GLU
46	C	165	GLY
46	C	548	PRO

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Mol	Chain	Res	Type
46	C	630	TYR
46	C	647	GLU
49	I	428	TYR
50	H	177	MET
50	H	191	TYR
50	H	205	LEU
51	A	174	SER
51	A	357	VAL
51	A	403	LEU
4	y	94	PRO
7	n	331	GLY
15	R	37	VAL
17	t	43	VAL
28	5	174	GLN
38	w	163	PRO
40	Y	358	VAL
43	G	177	ILE
46	C	113	PRO
46	C	547	GLN
47	8	80	GLY
47	8	284	ASP
48	W	142	ILE
51	A	8	ILE
51	A	30	VAL
52	l	44	ILE
52	l	45	ILE
1	f	1819	ILE
5	s	233	VAL
9	r	96	VAL
10	u	80	ILE
10	u	134	GLY
29	P	70	ALA
30	i	86	PRO
39	E	105	VAL
1	f	23	VAL
1	f	1782	VAL
9	r	61	VAL
12	Z	91	VAL
13	o	156	PRO
15	R	116	ILE
21	B	16	ARG
21	B	126	VAL

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Mol	Chain	Res	Type
28	5	125	PRO
32	M	92	VAL
51	A	308	GLN
51	A	329	ILE
1	f	1601	VAL
1	f	1605	VAL
5	s	229	ILE
5	s	348	VAL
7	n	330	VAL
9	r	106	VAL
14	q	51	VAL
23	d	203	VAL
46	C	477	MET
47	8	424	ILE
51	A	20	PRO
5	s	339	PRO
22	F	155	ALA
29	P	111	VAL
34	O	32	VAL
45	T	136	GLY
47	8	42	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	f	1318/1862 (71%)	1270 (96%)	48 (4%)	30 57
4	y	104/116 (90%)	104 (100%)	0	100 100
5	s	252/362 (70%)	239 (95%)	13 (5%)	19 48
6	j	69/123 (56%)	65 (94%)	4 (6%)	17 45
7	n	196/289 (68%)	181 (92%)	15 (8%)	10 34
8	p	262/268 (98%)	259 (99%)	3 (1%)	70 82
9	r	113/121 (93%)	113 (100%)	0	100 100
10	u	117/132 (89%)	111 (95%)	6 (5%)	20 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	m	116/117 (99%)	112 (97%)	4 (3%)	32 59
12	Z	143/184 (78%)	143 (100%)	0	100 100
13	o	160/160 (100%)	157 (98%)	3 (2%)	52 72
14	q	188/195 (96%)	187 (100%)	1 (0%)	86 91
15	R	125/132 (95%)	125 (100%)	0	100 100
16	S	70/73 (96%)	69 (99%)	1 (1%)	62 78
17	t	87/93 (94%)	87 (100%)	0	100 100
18	U	57/74 (77%)	50 (88%)	7 (12%)	4 16
19	v	103/112 (92%)	102 (99%)	1 (1%)	73 84
20	X	137/157 (87%)	135 (98%)	2 (2%)	60 77
21	B	159/165 (96%)	159 (100%)	0	100 100
22	F	182/212 (86%)	182 (100%)	0	100 100
23	d	187/208 (90%)	186 (100%)	1 (0%)	86 91
24	g	68/197 (34%)	67 (98%)	1 (2%)	60 77
25	a	64/96 (67%)	64 (100%)	0	100 100
26	J	138/191 (72%)	125 (91%)	13 (9%)	7 27
27	h	103/120 (86%)	102 (99%)	1 (1%)	73 84
28	5	358/408 (88%)	337 (94%)	21 (6%)	16 44
29	P	204/205 (100%)	202 (99%)	2 (1%)	73 84
30	i	110/124 (89%)	106 (96%)	4 (4%)	30 57
31	L	89/104 (86%)	89 (100%)	0	100 100
32	M	167/179 (93%)	161 (96%)	6 (4%)	30 57
33	N	84/125 (67%)	82 (98%)	2 (2%)	44 68
34	O	118/139 (85%)	117 (99%)	1 (1%)	79 87
35	b	110/123 (89%)	110 (100%)	0	100 100
36	c	49/53 (92%)	47 (96%)	2 (4%)	26 54
37	V	86/97 (89%)	71 (83%)	15 (17%)	1 7
38	w	125/137 (91%)	115 (92%)	10 (8%)	10 33
39	E	334/350 (95%)	322 (96%)	12 (4%)	30 57
40	Y	152/327 (46%)	145 (95%)	7 (5%)	23 52
41	Q	49/49 (100%)	46 (94%)	3 (6%)	15 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	D	30/31 (97%)	29 (97%)	1 (3%)	33 60
43	G	260/289 (90%)	256 (98%)	4 (2%)	60 77
44	K	176/178 (99%)	174 (99%)	2 (1%)	70 82
45	T	111/131 (85%)	108 (97%)	3 (3%)	40 65
46	C	616/628 (98%)	585 (95%)	31 (5%)	20 49
47	8	485/648 (75%)	465 (96%)	20 (4%)	26 54
48	W	194/217 (89%)	186 (96%)	8 (4%)	26 54
49	I	300/430 (70%)	295 (98%)	5 (2%)	56 75
50	H	266/299 (89%)	261 (98%)	5 (2%)	52 72
51	A	425/441 (96%)	380 (89%)	45 (11%)	5 22
52	l	217/230 (94%)	214 (99%)	3 (1%)	62 78
All	All	9633/11701 (82%)	9297 (96%)	336 (4%)	33 58

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	3	SER
1	f	88	ILE
1	f	89	VAL
1	f	93	GLU
1	f	137	CYS
1	f	138	ASP
1	f	206	TRP
1	f	240	PHE
1	f	259	PHE
1	f	303	ASN
1	f	305	TYR
1	f	316	GLU
1	f	722	TRP
1	f	743	ARG
1	f	772	TYR
1	f	785	LYS
1	f	789	TRP
1	f	855	ASP
1	f	906	GLU
1	f	941	ARG
1	f	1068	ASN
1	f	1101	PRO

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Mol	Chain	Res	Type
1	f	1115	HIS
1	f	1122	GLN
1	f	1217	GLU
1	f	1251	LYS
1	f	1260	TYR
1	f	1263	ASP
1	f	1264	LEU
1	f	1306	TRP
1	f	1327	PRO
1	f	1521	ARG
1	f	1525	THR
1	f	1530	LEU
1	f	1531	TYR
1	f	1532	LYS
1	f	1534	ARG
1	f	1545	ARG
1	f	1546	ARG
1	f	1549	ARG
1	f	1551	SER
1	f	1552	THR
1	f	1588	VAL
1	f	1598	LYS
1	f	1631	MET
1	f	1660	GLU
1	f	1705	LEU
1	f	1852	HIS
5	s	168	GLU
5	s	194	ILE
5	s	195	ASP
5	s	283	LEU
5	s	302	ASP
5	s	306	ILE
5	s	315	PHE
5	s	316	GLN
5	s	318	ASP
5	s	324	ARG
5	s	331	ARG
5	s	332	ARG
5	s	356	ARG
6	j	74	LYS
6	j	94	LYS
6	j	99	LYS

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Mol	Chain	Res	Type
6	j	133	GLN
7	n	125	LYS
7	n	198	ASN
7	n	208	ASN
7	n	209	ARG
7	n	255	ASN
7	n	267	GLU
7	n	287	LYS
7	n	291	CYS
7	n	293	LYS
7	n	300	LYS
7	n	309	CYS
7	n	326	TYR
7	n	333	ARG
7	n	335	LYS
7	n	341	MET
8	p	32	VAL
8	p	279	GLN
8	p	311	VAL
10	u	16	LEU
10	u	37	VAL
10	u	39	ILE
10	u	84	PHE
10	u	119	ARG
10	u	131	ARG
11	m	54	LYS
11	m	73	GLN
11	m	97	ASN
11	m	105	PHE
13	o	51	ARG
13	o	154	THR
13	o	177	LYS
14	q	122	THR
16	S	64	LEU
18	U	45	ASP
18	U	46	GLN
18	U	48	GLN
18	U	71	ARG
18	U	83	ARG
18	U	94	LYS
18	U	98	MET
19	v	131	ASP

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Mol	Chain	Res	Type
20	X	33	SER
20	X	35	ASN
23	d	217	PHE
24	g	86	LYS
26	J	94	VAL
26	J	102	ARG
26	J	103	TYR
26	J	105	ILE
26	J	107	PHE
26	J	150	VAL
26	J	152	PHE
26	J	162	THR
26	J	182	ARG
26	J	183	ASN
26	J	217	LEU
26	J	222	LEU
26	J	233	ARG
27	h	71	GLU
28	5	67	THR
28	5	76	LYS
28	5	88	ILE
28	5	146	ASP
28	5	170	GLU
28	5	209	ASP
28	5	234	GLN
28	5	266	ARG
28	5	275	GLU
28	5	281	LEU
28	5	321	LEU
28	5	349	THR
28	5	350	LEU
28	5	400	LYS
28	5	401	ARG
28	5	414	ASN
28	5	455	LEU
28	5	456	VAL
28	5	457	GLU
28	5	459	ASN
28	5	461	ARG
29	P	46	PHE
29	P	100	LEU
30	i	69	ILE

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Mol	Chain	Res	Type
30	i	71	LEU
30	i	76	GLU
30	i	116	VAL
32	M	60	GLU
32	M	80	GLU
32	M	141	ILE
32	M	147	LYS
32	M	149	MET
32	M	198	GLU
33	N	8	ARG
33	N	18	PHE
34	O	85	PRO
36	c	10	ARG
36	c	50	LYS
37	V	14	LYS
37	V	21	LEU
37	V	22	GLU
37	V	34	LYS
37	V	36	LYS
37	V	43	GLN
37	V	62	TRP
37	V	64	CYS
37	V	65	ASN
37	V	93	LEU
37	V	96	ASN
37	V	97	MET
37	V	100	GLU
37	V	101	GLN
37	V	102	ASN
38	w	34	GLN
38	w	74	TRP
38	w	86	ARG
38	w	125	ASP
38	w	130	HIS
38	w	133	TYR
38	w	135	PHE
38	w	164	LEU
38	w	166	THR
38	w	168	ASP
39	E	22	TYR
39	E	36	ARG
39	E	54	GLN

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Mol	Chain	Res	Type
39	E	71	GLU
39	E	83	TYR
39	E	148	TYR
39	E	202	ARG
39	E	244	GLU
39	E	279	TYR
39	E	316	TYR
39	E	374	ARG
39	E	378	ASP
40	Y	229	ARG
40	Y	230	ARG
40	Y	242	GLU
40	Y	288	ASP
40	Y	337	LYS
40	Y	354	VAL
40	Y	364	GLN
41	Q	7	TRP
41	Q	15	MET
41	Q	42	GLN
42	D	3	THR
43	G	85	TRP
43	G	136	TRP
43	G	160	VAL
43	G	289	TYR
44	K	26	PHE
44	K	194	ARG
45	T	78	GLU
45	T	91	VAL
45	T	137	ARG
46	C	1	MET
46	C	2	SER
46	C	4	PHE
46	C	6	ASP
46	C	27	LYS
46	C	30	GLN
46	C	31	ILE
46	C	37	GLU
46	C	47	ARG
46	C	52	SER
46	C	60	GLU
46	C	132	TYR
46	C	190	ILE

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Mol	Chain	Res	Type
46	C	191	GLN
46	C	207	LYS
46	C	209	ARG
46	C	211	LEU
46	C	232	ARG
46	C	233	LEU
46	C	274	LYS
46	C	287	GLN
46	C	307	TYR
46	C	331	ARG
46	C	359	HIS
46	C	434	ILE
46	C	435	LEU
46	C	464	TRP
46	C	482	LYS
46	C	486	GLU
46	C	538	PHE
46	C	549	LEU
47	8	8	ARG
47	8	10	CYS
47	8	18	ARG
47	8	33	LEU
47	8	35	GLU
47	8	43	MET
47	8	44	TYR
47	8	75	ARG
47	8	77	LYS
47	8	79	ARG
47	8	82	GLN
47	8	150	PHE
47	8	163	HIS
47	8	172	LEU
47	8	203	ARG
47	8	263	HIS
47	8	452	VAL
47	8	495	LYS
47	8	564	GLN
47	8	569	ARG
48	W	39	GLU
48	W	76	THR
48	W	77	GLN
48	W	121	THR

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Mol	Chain	Res	Type
48	W	161	ARG
48	W	165	TRP
48	W	192	ARG
48	W	207	VAL
49	I	144	ARG
49	I	337	PRO
49	I	338	LYS
49	I	412	ARG
49	I	434	ILE
50	H	194	PHE
50	H	255	HIS
50	H	259	MET
50	H	304	LEU
50	H	322	ASP
51	A	7	GLU
51	A	8	ILE
51	A	9	PHE
51	A	10	VAL
51	A	14	PHE
51	A	15	THR
51	A	28	MET
51	A	29	LYS
51	A	30	VAL
51	A	32	LEU
51	A	35	LYS
51	A	44	TRP
51	A	48	MET
51	A	50	ASP
51	A	100	LYS
51	A	114	VAL
51	A	149	ARG
51	A	151	LEU
51	A	207	THR
51	A	226	LEU
51	A	252	GLU
51	A	255	ASP
51	A	257	LEU
51	A	259	ARG
51	A	292	LYS
51	A	294	ARG
51	A	295	TYR
51	A	296	GLN

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Mol	Chain	Res	Type
51	A	297	MET
51	A	301	LYS
51	A	302	ASN
51	A	307	THR
51	A	351	GLU
51	A	352	GLN
51	A	368	GLN
51	A	371	LYS
51	A	378	ARG
51	A	383	LYS
51	A	403	LEU
51	A	425	THR
51	A	435	LEU
51	A	437	ILE
51	A	473	ILE
51	A	474	MET
51	A	479	MET
52	l	139	HIS
52	l	148	ASP
52	l	163	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	195	HIS
1	f	286	ASN
1	f	295	ASN
1	f	303	ASN
1	f	725	GLN
1	f	742	ASN
1	f	797	GLN
1	f	928	HIS
1	f	956	HIS
1	f	989	GLN
1	f	1007	HIS
1	f	1122	GLN
1	f	1351	ASN
1	f	1361	HIS
1	f	1542	GLN
1	f	1704	HIS
1	f	1852	HIS
5	s	307	HIS

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Mol	Chain	Res	Type
5	s	340	GLN
6	j	133	GLN
7	n	139	HIS
7	n	208	ASN
7	n	339	GLN
8	p	12	HIS
8	p	108	HIS
8	p	279	GLN
9	r	32	GLN
9	r	34	ASN
9	r	83	GLN
9	r	138	HIS
10	u	98	HIS
11	m	73	GLN
11	m	97	ASN
13	o	18	GLN
13	o	27	HIS
16	S	56	GLN
20	X	42	ASN
20	X	91	HIS
22	F	114	GLN
23	d	109	ASN
25	a	88	HIS
26	J	184	ASN
27	h	99	GLN
28	5	87	ASN
28	5	91	HIS
28	5	307	GLN
28	5	357	GLN
28	5	430	ASN
30	i	56	HIS
32	M	73	GLN
37	V	13	GLN
37	V	18	GLN
37	V	32	GLN
37	V	43	GLN
37	V	50	ASN
37	V	65	ASN
37	V	101	GLN
38	w	34	GLN
38	w	54	GLN
38	w	130	HIS

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Mol	Chain	Res	Type
39	E	209	HIS
39	E	240	GLN
39	E	373	GLN
40	Y	364	GLN
43	G	21	HIS
43	G	231	ASN
45	T	55	HIS
46	C	191	GLN
46	C	316	GLN
46	C	330	GLN
46	C	354	HIS
46	C	359	HIS
46	C	437	ASN
46	C	533	HIS
46	C	559	GLN
46	C	635	ASN
47	8	83	HIS
47	8	251	HIS
47	8	385	GLN
48	W	69	ASN
48	W	168	HIS
48	W	172	ASN
49	I	370	GLN
50	H	208	ASN
50	H	255	HIS
51	A	74	HIS
51	A	96	HIS
51	A	148	ASN
51	A	302	ASN
51	A	368	GLN
51	A	456	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	74/75 (98%)	11 (14%)	1 (1%)
3	0	2144/2319 (92%)	389 (18%)	28 (1%)
All	All	2218/2394 (92%)	400 (18%)	29 (1%)

All (400) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	16	U
2	1	17	G
2	1	20	A
2	1	25	G
2	1	32	U
2	1	45	G
2	1	47	C
2	1	55	C
2	1	72	A
2	1	73	C
2	1	74	C
3	0	2	A
3	0	3	U
3	0	4	C
3	0	25	C
3	0	26	A
3	0	34	G
3	0	42	G
3	0	45	U
3	0	63	G
3	0	65	A
3	0	68	A
3	0	75	U
3	0	82	A
3	0	83	U
3	0	90	A
3	0	99	U
3	0	101	C
3	0	113	U
3	0	123	A
3	0	127	C
3	0	136	U
3	0	155	U
3	0	157	G
3	0	170	C
3	0	189	G
3	0	194	U
3	0	196	U
3	0	197	C
3	0	200	U
3	0	201	U
3	0	202	C
3	0	204	G

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Mol	Chain	Res	Type
3	0	207	G
3	0	214	C
3	0	215	A
3	0	217	C
3	0	218	C
3	0	227	U
3	0	228	G
3	0	230	G
3	0	249	A
3	0	252	G
3	0	253	U
3	0	254	A
3	0	255	A
3	0	256	A
3	0	257	A
3	0	258	C
3	0	270	C
3	0	271	C
3	0	272	G
3	0	273	G
3	0	274	C
3	0	278	A
3	0	281	A
3	0	288	A
3	0	306	U
3	0	308	C
3	0	309	G
3	0	316	A
3	0	320	G
3	0	325	U
3	0	326	U
3	0	328	U
3	0	329	U
3	0	330	A
3	0	331	U
3	0	344	G
3	0	345	A
3	0	346	C
3	0	357	C
3	0	362	C
3	0	364	G
3	0	385	G

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Mol	Chain	Res	Type
3	0	386	A
3	0	400	G
3	0	408	C
3	0	425	A
3	0	447	A
3	0	448	A
3	0	451	G
3	0	464	C
3	0	471	C
3	0	473	G
3	0	486	U
3	0	488	G
3	0	491	C
3	0	492	A
3	0	501	A
3	0	505	A
3	0	506	A
3	0	507	A
3	0	511	G
3	0	512	A
3	0	520	A
3	0	527	A
3	0	528	U
3	0	545	U
3	0	546	U
3	0	547	G
3	0	555	G
3	0	556	U
3	0	557	U
3	0	558	U
3	0	571	A
3	0	585	A
3	0	586	A
3	0	592	A
3	0	596	A
3	0	599	A
3	0	600	U
3	0	605	G
3	0	611	G
3	0	648	A
3	0	665	U
3	0	673	A

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Mol	Chain	Res	Type
3	0	674	A
3	0	676	G
3	0	694	A
3	0	695	G
3	0	696	G
3	0	704	A
3	0	707	C
3	0	709	C
3	0	714	G
3	0	715	U
3	0	717	U
3	0	718	A
3	0	723	C
3	0	729	C
3	0	734	G
3	0	737	U
3	0	738	G
3	0	739	G
3	0	740	U
3	0	741	G
3	0	743	C
3	0	745	C
3	0	747	U
3	0	762	U
3	0	763	G
3	0	770	C
3	0	772	U
3	0	773	U
3	0	774	C
3	0	775	A
3	0	776	G
3	0	791	G
3	0	793	A
3	0	796	G
3	0	797	G
3	0	810	U
3	0	811	U
3	0	812	A
3	0	813	U
3	0	814	C
3	0	820	U
3	0	825	C

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Mol	Chain	Res	Type
3	0	826	A
3	0	830	C
3	0	834	G
3	0	846	U
3	0	847	U
3	0	848	U
3	0	849	U
3	0	861	A
3	0	871	G
3	0	872	A
3	0	874	C
3	0	881	G
3	0	885	U
3	0	887	C
3	0	888	G
3	0	889	A
3	0	891	U
3	0	892	U
3	0	895	A
3	0	919	G
3	0	923	A
3	0	924	G
3	0	925	C
3	0	935	A
3	0	938	G
3	0	940	U
3	0	941	U
3	0	942	C
3	0	946	U
3	0	976	U
3	0	977	A
3	0	984	A
3	0	985	G
3	0	987	G
3	0	991	C
3	0	999	U
3	0	1071	G
3	0	1077	U
3	0	1078	U
3	0	1183	U
3	0	1184	C
3	0	1190	A

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Mol	Chain	Res	Type
3	0	1191	U
3	0	1195	G
3	0	1196	G
3	0	1197	A
3	0	1199	U
3	0	1202	A
3	0	1212	U
3	0	1216	G
3	0	1226	U
3	0	1273	A
3	0	1275	A
3	0	1291	A
3	0	1300	U
3	0	1304	U
3	0	1306	A
3	0	1328	A
3	0	1344	G
3	0	1345	A
3	0	1361	C
3	0	1364	C
3	0	1365	A
3	0	1366	A
3	0	1367	A
3	0	1368	C
3	0	1394	U
3	0	1396	U
3	0	1397	G
3	0	1399	U
3	0	1400	C
3	0	1402	U
3	0	1411	U
3	0	1417	U
3	0	1418	U
3	0	1420	A
3	0	1423	A
3	0	1426	A
3	0	1427	U
3	0	1429	U
3	0	1430	U
3	0	1432	C
3	0	1433	A
3	0	1438	G

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Mol	Chain	Res	Type
3	0	1439	U
3	0	1440	U
3	0	1441	C
3	0	1451	C
3	0	1454	A
3	0	1456	G
3	0	1457	A
3	0	1459	U
3	0	1460	A
3	0	1461	U
3	0	1467	U
3	0	1468	U
3	0	1471	G
3	0	1477	A
3	0	1478	U
3	0	1481	U
3	0	1483	U
3	0	1485	U
3	0	1487	G
3	0	1491	U
3	0	1500	U
3	0	1502	C
3	0	1503	G
3	0	1512	C
3	0	1513	U
3	0	1514	U
3	0	1516	A
3	0	1521	G
3	0	1523	A
3	0	1525	A
3	0	1527	C
3	0	1528	C
3	0	1529	U
3	0	1530	C
3	0	1531	A
3	0	1532	G
3	0	1549	U
3	0	1550	U
3	0	1563	U
3	0	1564	U
3	0	1565	G
3	0	1570	U

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Mol	Chain	Res	Type
3	0	1580	G
3	0	1611	A
3	0	1623	G
3	0	1631	C
3	0	1633	A
3	0	1637	G
3	0	1658	U
3	0	1666	A
3	0	1669	A
3	0	1673	G
3	0	1674	G
3	0	1675	A
3	0	1676	A
3	0	1690	G
3	0	1691	G
3	0	1694	A
3	0	1695	G
3	0	1700	A
3	0	1702	G
3	0	1716	G
3	0	1718	G
3	0	1719	U
3	0	1728	G
3	0	1729	A
3	0	1731	C
3	0	1732	C
3	0	1773	A
3	0	1787	U
3	0	1788	U
3	0	1794	A
3	0	1819	U
3	0	1820	A
3	0	1833	G
3	0	1834	C
3	0	1835	C
3	0	1862	U
3	0	1863	U
3	0	1879	C
3	0	1880	G
3	0	1881	G
3	0	1882	U
3	0	1883	A

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Mol	Chain	Res	Type
3	0	1884	U
3	0	1888	C
3	0	1889	U
3	0	1890	U
3	0	1891	G
3	0	1908	A
3	0	1909	U
3	0	1914	U
3	0	1915	G
3	0	1935	U
3	0	1952	U
3	0	1955	G
3	0	1967	U
3	0	1971	C
3	0	1972	U
3	0	1975	G
3	0	1977	G
3	0	1978	A
3	0	1979	C
3	0	1980	A
3	0	1981	C
3	0	1982	G
3	0	1995	U
3	0	1996	C
3	0	1997	A
3	0	1998	G
3	0	1999	U
3	0	2013	A
3	0	2015	G
3	0	2016	A
3	0	2019	C
3	0	2021	U
3	0	2022	G
3	0	2028	C
3	0	2059	G
3	0	2075	C
3	0	2080	G
3	0	2095	U
3	0	2097	A
3	0	2099	U
3	0	2100	G
3	0	2103	C

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Mol	Chain	Res	Type
3	0	2107	C
3	0	2108	A
3	0	2112	A
3	0	2140	A
3	0	2158	C
3	0	2221	A
3	0	2232	U
3	0	2233	C
3	0	2279	A
3	0	2280	G
3	0	2283	G
3	0	2285	A
3	0	2288	A
3	0	2289	A
3	0	2292	U
3	0	2293	A
3	0	2315	G
3	0	2316	G
3	0	2317	A
3	0	2319	C
3	0	2322	U

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	73	C
3	0	68	A
3	0	122	A
3	0	200	U
3	0	217	C
3	0	251	A
3	0	325	U
3	0	693	G
3	0	785	A
3	0	812	A
3	0	923	A
3	0	945	C
3	0	975	U
3	0	1070	C
3	0	1196	G
3	0	1299	C
3	0	1393	U

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Mol	Chain	Res	Type
3	0	1450	G
3	0	1477	A
3	0	1528	C
3	0	1531	A
3	0	1579	A
3	0	1694	A
3	0	1977	G
3	0	1979	C
3	0	1980	A
3	0	1982	G
3	0	2073	C
3	0	2157	C

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	GNP	5	502	54	29,34,34	2.06	8 (27%)	33,54,54	2.39	9 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	GNP	5	502	54	-	6/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	5	502	GNP	PB-O3A	-7.46	1.49	1.59
55	5	502	GNP	C6-N1	3.87	1.39	1.33
55	5	502	GNP	PB-O2B	-3.60	1.47	1.56
55	5	502	GNP	PG-O3G	-2.43	1.50	1.56
55	5	502	GNP	C8-N7	-2.33	1.30	1.34
55	5	502	GNP	PG-N3B	-2.26	1.57	1.63
55	5	502	GNP	PG-O2G	-2.16	1.50	1.56
55	5	502	GNP	PB-N3B	-2.15	1.57	1.63

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	5	502	GNP	C5-C6-N1	-8.57	111.71	123.43
55	5	502	GNP	C2-N1-C6	5.52	124.69	115.93
55	5	502	GNP	O3G-PG-O1G	-3.59	104.44	113.45
55	5	502	GNP	PB-O3A-PA	-3.42	120.56	132.62
55	5	502	GNP	C3'-C2'-C1'	3.38	106.07	100.98
55	5	502	GNP	C2-N3-C4	-2.96	111.98	115.36
55	5	502	GNP	O2B-PB-O1B	2.79	115.76	109.92
55	5	502	GNP	N3-C2-N1	-2.23	124.25	127.22
55	5	502	GNP	O2G-PG-O3G	2.12	113.29	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	5	502	GNP	PG-N3B-PB-O1B
55	5	502	GNP	PG-N3B-PB-O3A
55	5	502	GNP	C5'-O5'-PA-O3A
55	5	502	GNP	O4'-C4'-C5'-O5'
55	5	502	GNP	C3'-C4'-C5'-O5'
55	5	502	GNP	C5'-O5'-PA-O1A

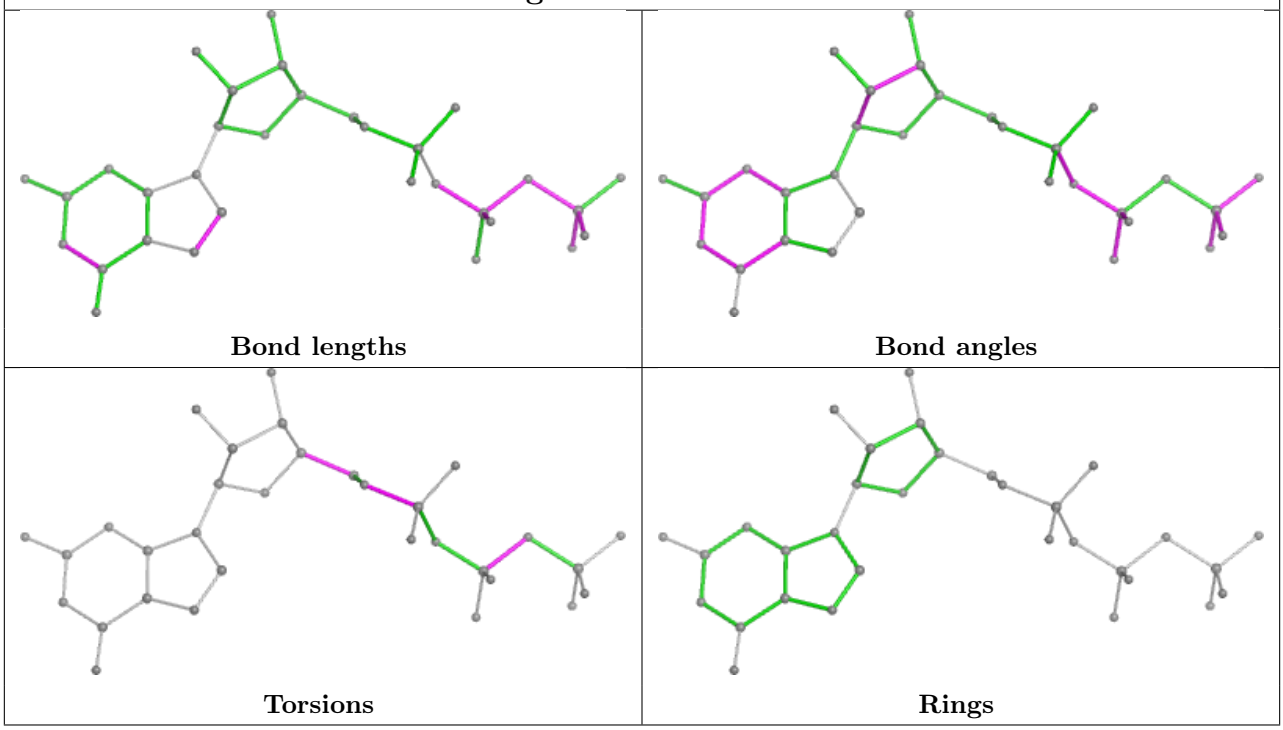
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP 5 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	f	20
28	5	2
46	C	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
48	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	282:ARG	C	283:GLY	N	2.09
1	f	1149:TYR	C	1150:VAL	N	1.72
1	f	1221:LEU	C	1222:PRO	N	1.71
1	f	1254:ALA	C	1255:GLN	N	1.68
1	C	53:ARG	C	54:ASN	N	1.67
1	f	774:LEU	C	775:GLY	N	1.66
1	f	1127:VAL	C	1128:PRO	N	1.66
1	f	307:LEU	C	308:ARG	N	1.65
1	f	301:GLU	C	302:ALA	N	1.62
1	f	1492:GLY	C	1493:PRO	N	1.61
1	f	132:ALA	C	133:ARG	N	1.19
1	f	296:TYR	C	297:THR	N	1.19
1	5	253:THR	C	254:ARG	N	1.19
1	f	263:SER	C	264:ASP	N	1.18
1	f	304:PRO	C	305:TYR	N	1.15
1	W	165:TRP	C	166:VAL	N	1.15
1	f	198:PHE	C	199:PHE	N	1.14
1	f	199:PHE	C	200:ASP	N	1.14
1	f	131:THR	C	132:ALA	N	1.13
1	f	1214:ARG	C	1215:ASP	N	1.13
1	f	195:HIS	C	196:VAL	N	1.12
1	f	139:MET	C	140:PHE	N	1.11
1	f	194:PHE	C	195:HIS	N	1.08
1	f	234:GLY	C	235:LEU	N	1.06

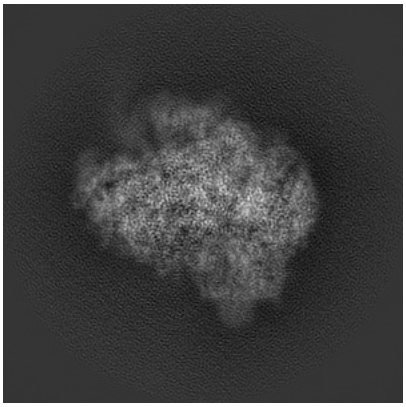
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11893. These allow visual inspection of the internal detail of the map and identification of artifacts.

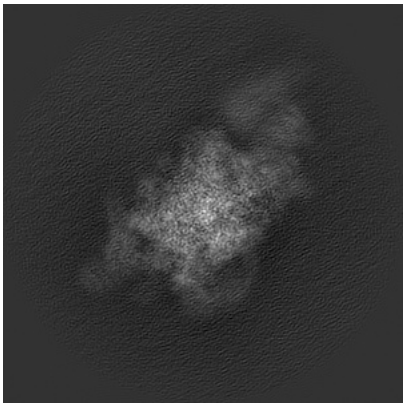
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

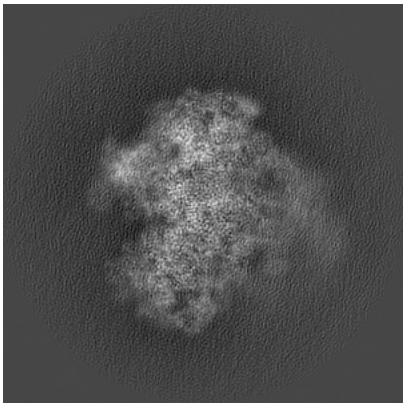
6.1.1 Primary map



X



Y

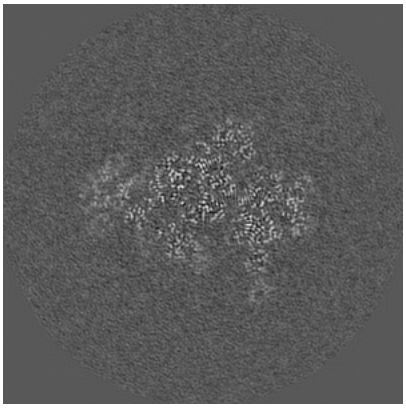


Z

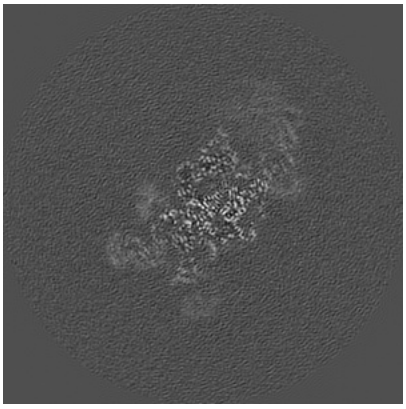
The images above show the map projected in three orthogonal directions.

6.2 Central slices

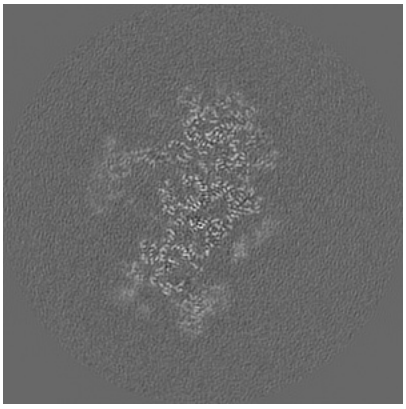
6.2.1 Primary map



X Index: 200



Y Index: 200

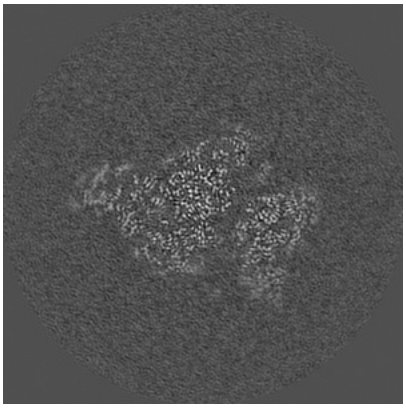


Z Index: 200

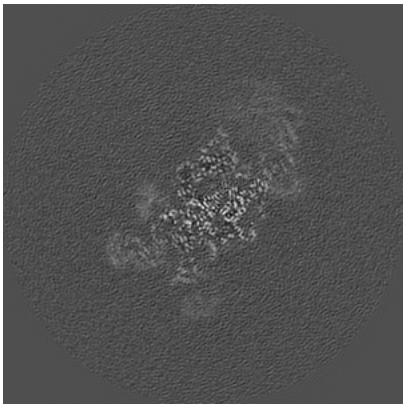
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

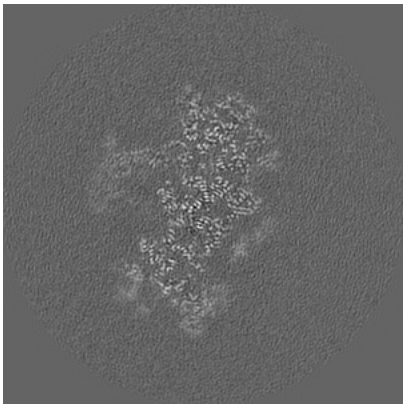
6.3.1 Primary map



X Index: 188



Y Index: 200

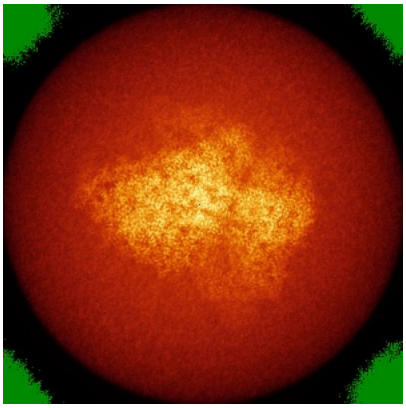


Z Index: 199

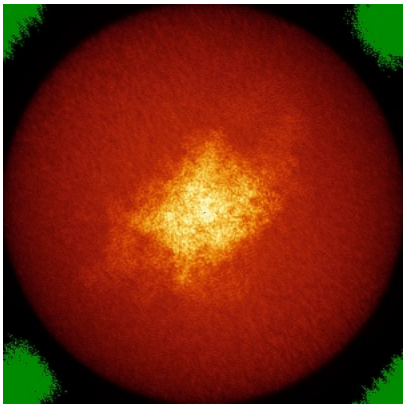
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

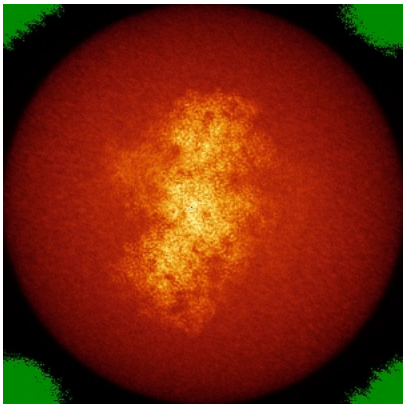
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0193. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

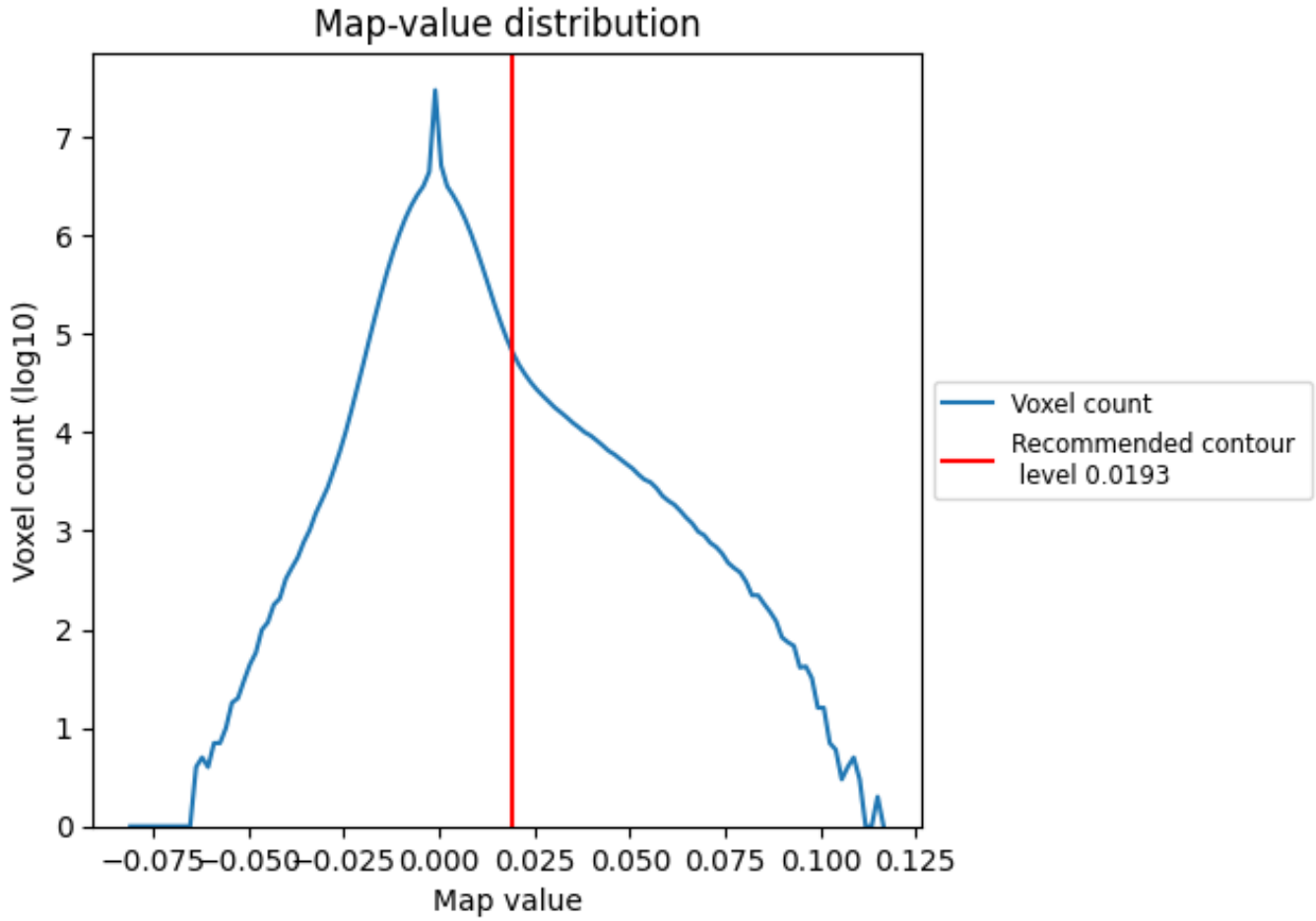
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

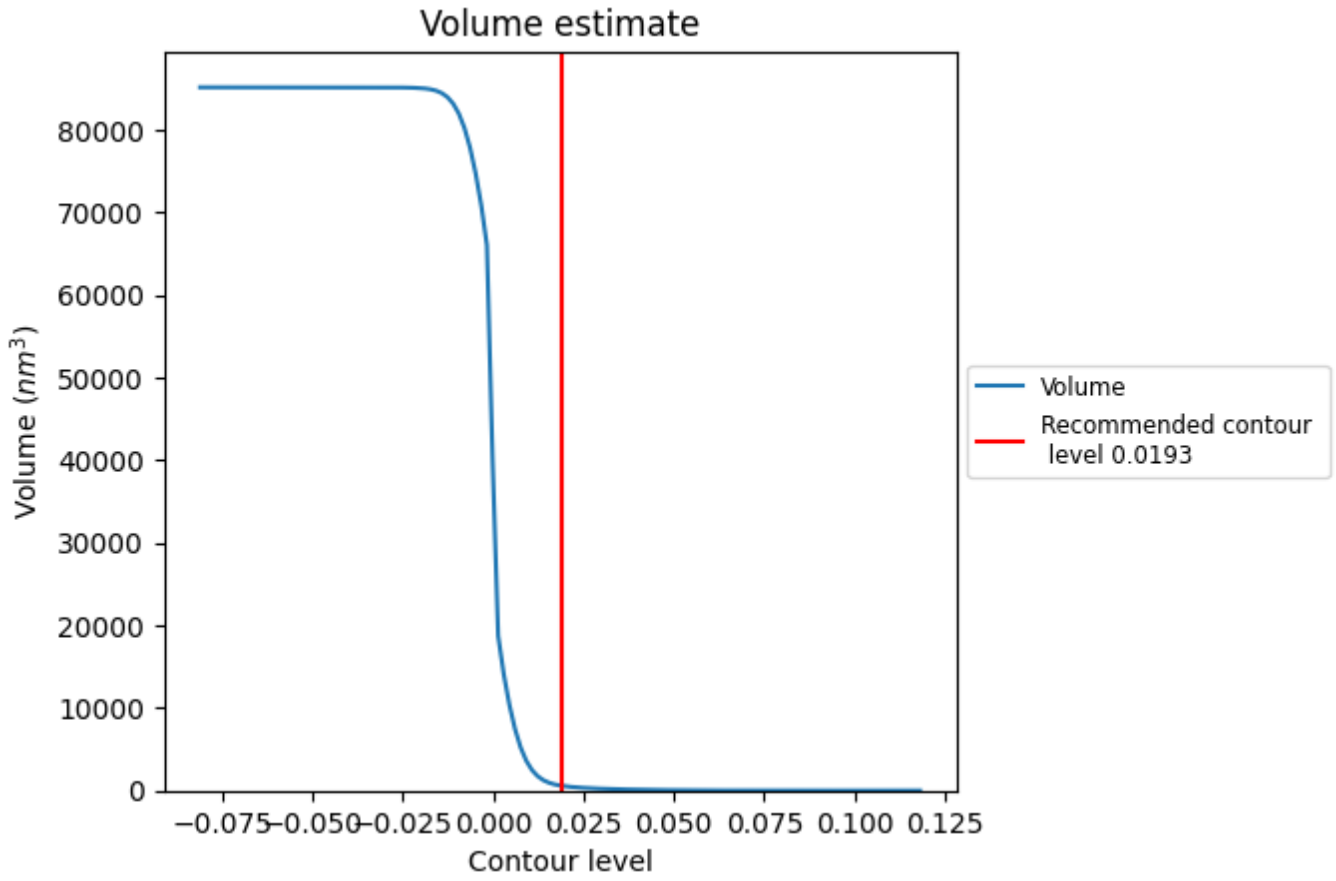
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

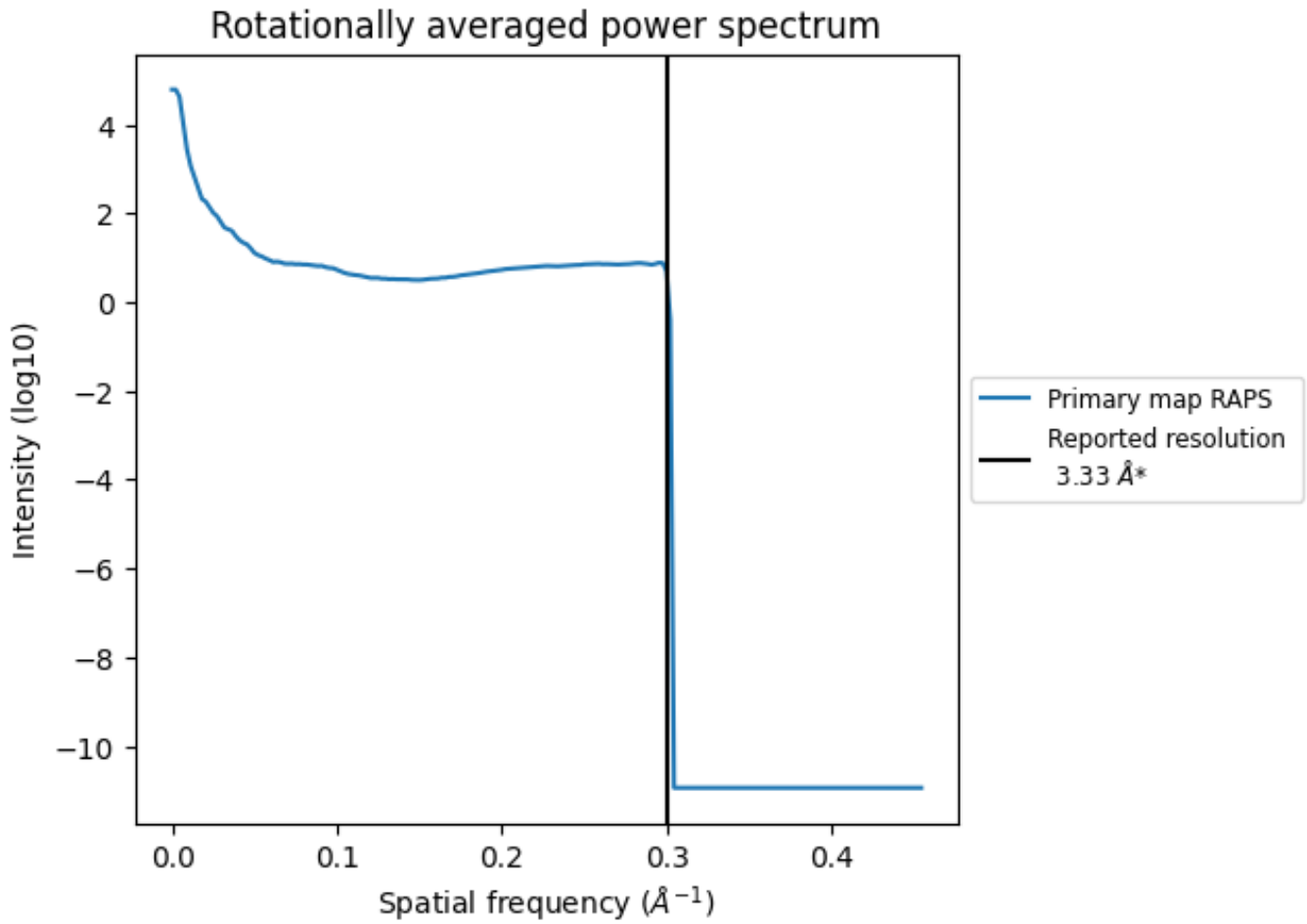
7.2 Volume estimate



The volume at the recommended contour level is 566 nm^3; this corresponds to an approximate mass of 511 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.300 Å^{-1}

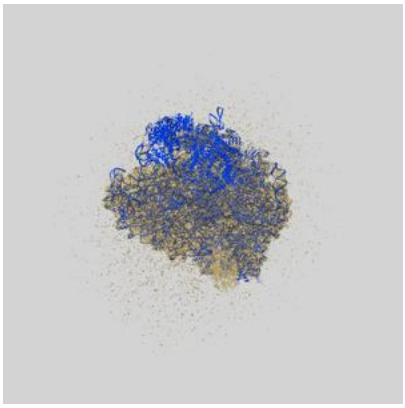
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

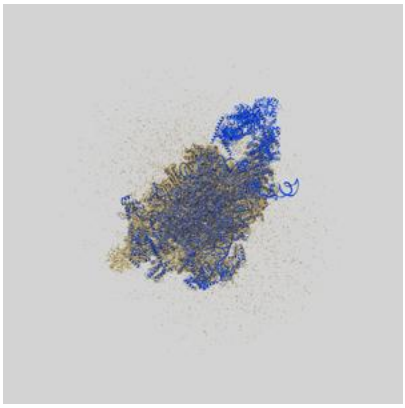
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11893 and PDB model 7ASE. Per-residue inclusion information can be found in section 3 on page 14.

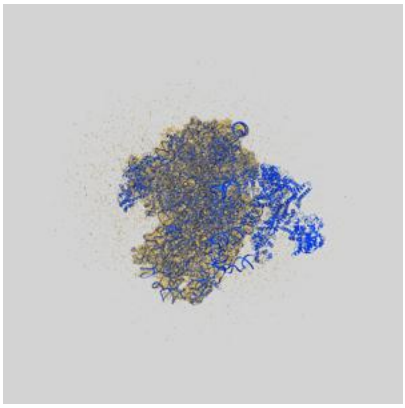
9.1 Map-model overlay



X



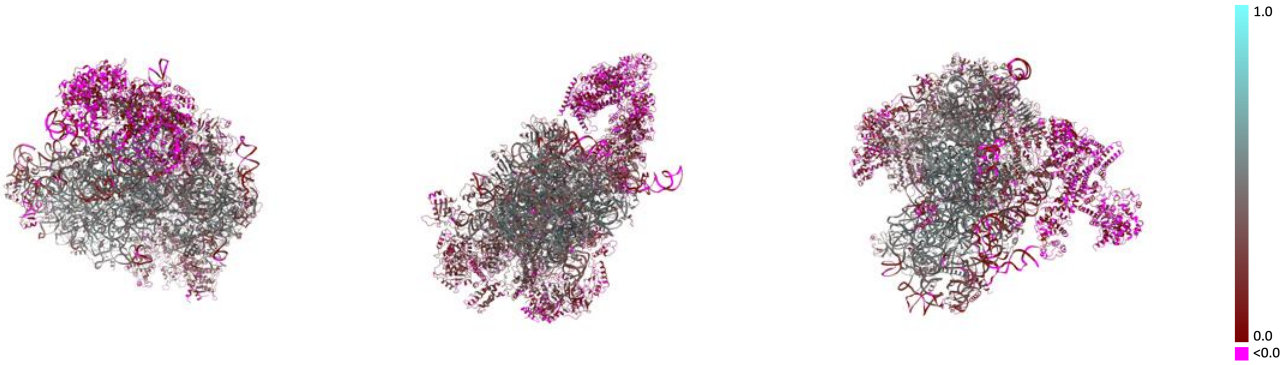
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

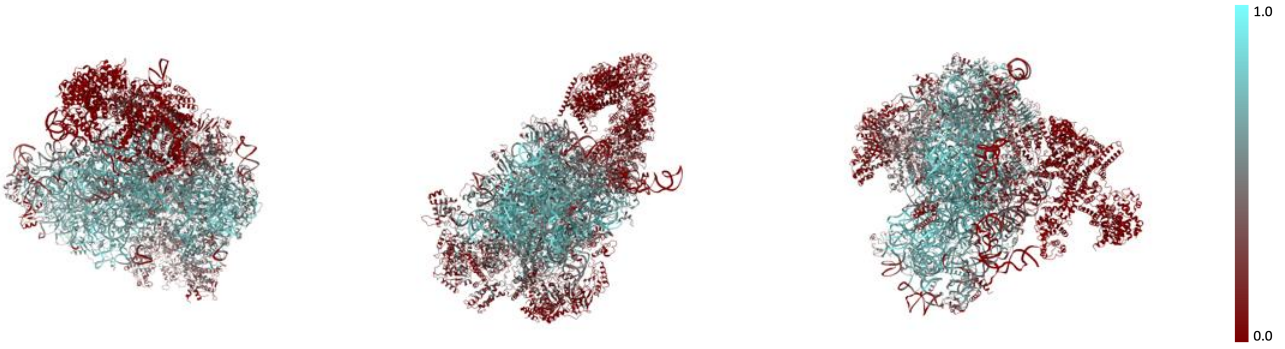
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

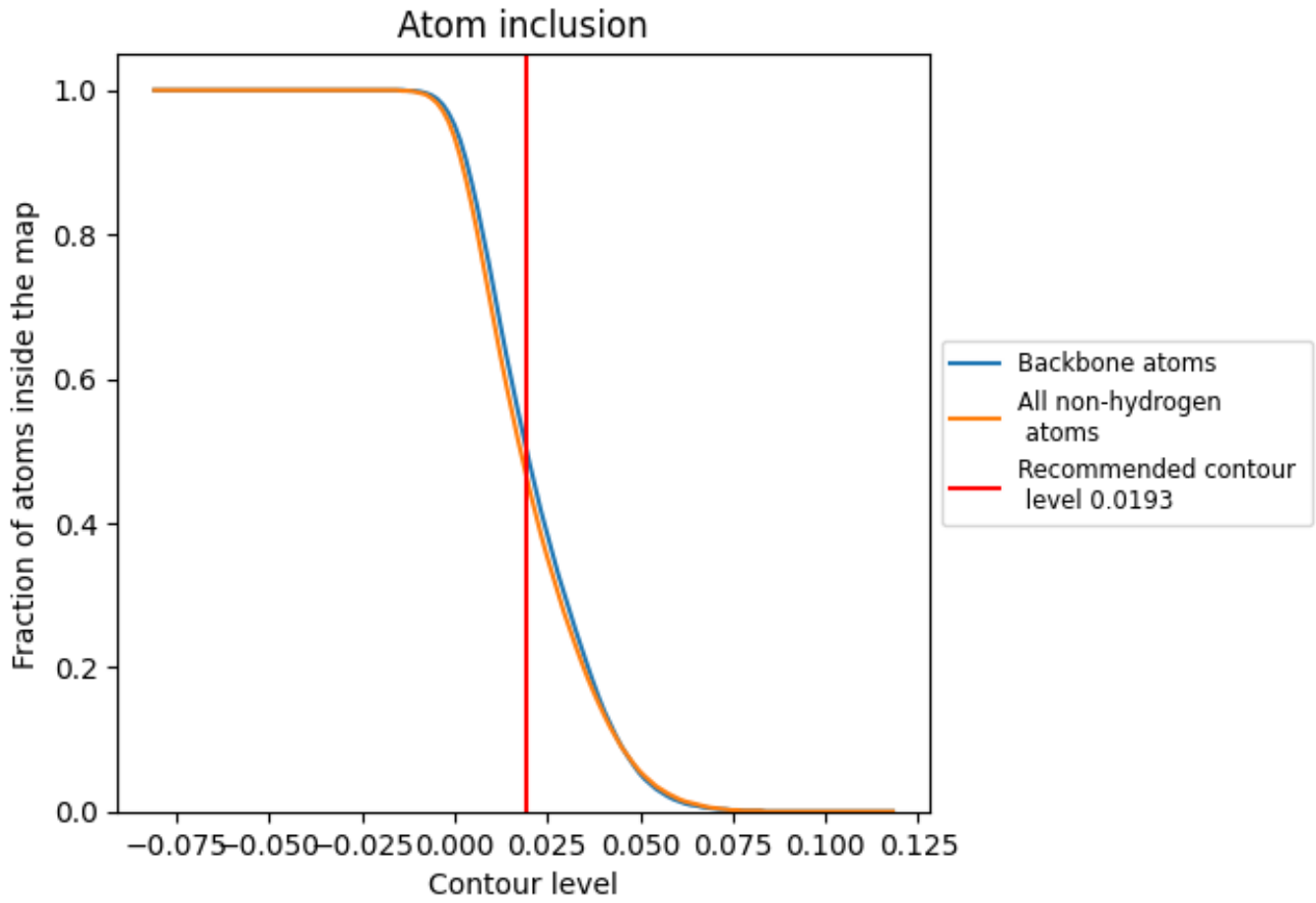
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0193).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4650	0.3140
0	0.6860	0.4100
1	0.6240	0.3900
5	0.1770	0.1970
8	0.1050	0.1110
A	0.1800	0.2290
B	0.6630	0.4450
C	0.1370	0.1530
D	0.6490	0.4030
E	0.0180	0.0580
F	0.6590	0.4440
G	0.0090	0.0310
H	0.0060	0.0140
I	0.0000	0.0270
J	0.2140	0.1620
K	0.0000	0.0090
L	0.5220	0.3740
M	0.5820	0.4010
N	0.5150	0.3200
O	0.5160	0.2710
P	0.5250	0.3680
Q	0.6170	0.3660
R	0.6710	0.4560
S	0.6560	0.4530
T	0.5680	0.3920
U	0.4510	0.3740
V	0.5590	0.4390
W	0.6410	0.4440
X	0.7030	0.4570
Y	0.0510	0.1140
Z	0.6630	0.4390
a	0.4440	0.3150
b	0.7230	0.4770
c	0.5110	0.3610
d	0.6770	0.4640

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Chain	Atom inclusion	Q-score
f	0.2540	0.2210
g	0.6680	0.4600
h	0.2370	0.1980
i	0.5450	0.3570
j	0.3190	0.2750
l	0.6780	0.4450
m	0.7000	0.4630
n	0.2780	0.2490
o	0.5770	0.3930
p	0.4880	0.3530
q	0.6080	0.4110
r	0.6470	0.4160
s	0.2070	0.1950
t	0.6920	0.4720
u	0.5260	0.3220
v	0.6550	0.4420
w	0.3930	0.3050
y	0.6420	0.4190