



Full wwPDB EM Validation Report ⓘ

Jul 13, 2026 – 12:36 pm BST

PDB ID : 9SRC / pdb_00009src
EMDB ID : EMD-55137
Title : Cryo-EM structure of P. abyssi 70S ribosome in complex with hibernation factor HibA in PTC conformation
Authors : Madru, C.M.; Bourgeois, G.B.; Mechulam, Y.M.; Schmitt, E.S.
Deposited on : 2025-09-24
Resolution : 2.10 Å(reported)
Based on initial model : .

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:

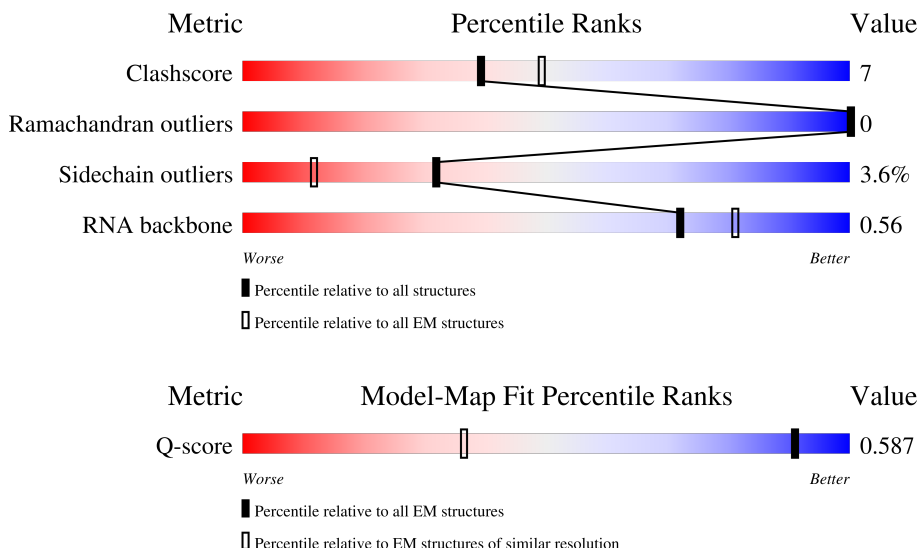
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2317 (1.60 - 2.60)

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 $\leq 5\%$. 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	1	3018	
2	2	1512	
3	3	128	

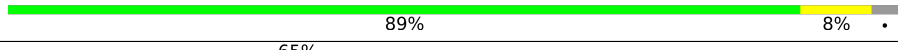
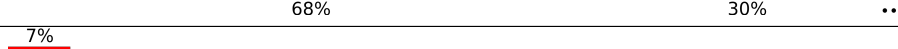
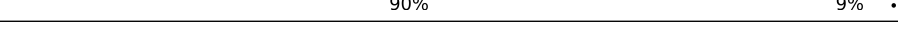
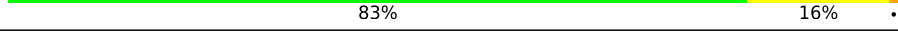
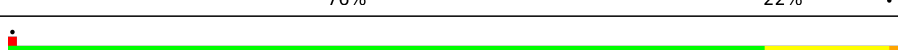
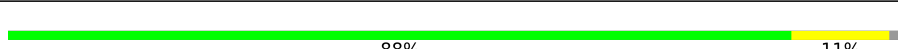
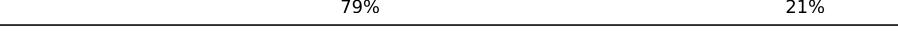
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Mol	Chain	Length	Quality of chain
4	H	392	
5	AA	199	
6	AB	202	
7	AC	63	
8	AD	180	
9	AE	243	
10	AF	236	
11	AG	125	
12	AH	215	
13	AI	130	
14	AJ	127	
15	AK	135	
16	AL	102	
17	AM	137	
18	AN	147	
19	AP	56	
20	AQ	158	
21	AR	113	
22	AS	67	
23	AU	150	
24	AV	99	
24	B6	99	
25	AW	65	
26	AX	71	
27	AY	51	

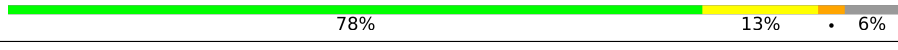
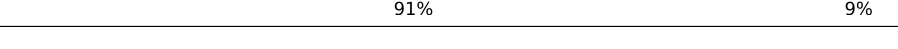
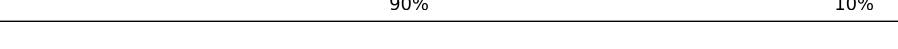
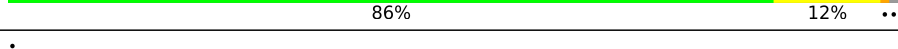
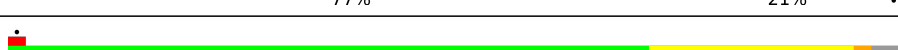
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Mol	Chain	Length	Quality of chain
28	AZ	210	
29	A0	37	
30	A3	123	
30	B4	123	
30	BG	123	
31	AT	132	
32	AO	148	
33	BB	239	
34	BY	155	
35	BO	203	
36	BC	361	
37	B5	82	
37	BK	82	
38	BL	147	
39	Bf	51	
40	BU	121	
41	Bb	130	
42	Be	62	
43	BE	188	
44	Ba	94	
45	BT	86	
46	BW	68	
47	Bi	83	
48	BI	142	
49	BR	97	

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Mol	Chain	Length	Quality of chain
50	BQ	151	
51	BV	67	
52	Bj	94	
53	BD	255	
54	BF	184	
55	BZ	99	
56	BP	120	
57	BM	194	
58	BS	155	
59	Bd	91	
60	BN	181	
61	Bg	51	
62	Bc	87	
63	BJ	141	
64	Bl	77	
65	Bk	65	

2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 170465 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 RNA chain called rRNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3018	Total	C	N	O	P	0	0
			65181	29055	12094	21014	3018		

- Molecule 2 is a RNA chain called rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1496	Total	C	N	O	P	0	0
			32291	14408	5957	10430	1496		

- Molecule 3 is a RNA chain called rRNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	126	Total	C	N	O	P	0	0
			2703	1203	498	876	126		

- Molecule 4 is a protein called Dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	386	Total	C	N	O	S	0	0
			3074	1962	535	567	10		

- Molecule 5 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	188	Total	C	N	O	S	0	0
			1531	993	268	266	4		

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 7 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	57	Total	C	N	O	S	0	0
			449	285	80	76	8		

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AD	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 9 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 11 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	214	Total	C	N	O	S	0	0
			1725	1095	323	300	7		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 14 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AJ	125	Total	C	N	O		
			986	612	205	169	0	0

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	AK	135	Total	C	N	O	S	
			1073	673	207	189	4	0

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	AL	100	Total	C	N	O	S	
			809	502	157	147	3	0

- Molecule 17 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AM	127	Total	C	N	O	S	
			955	591	190	172	2	0

- Molecule 18 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AN	146	Total	C	N	O	S	
			1148	727	224	194	3	0

- Molecule 19 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	AP	55	Total	C	N	O	S	
			455	288	95	67	5	0

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	AQ	157	Total	C	N	O	S	
			1305	833	249	219	4	0

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AR	107	Total	C	N	O	S	0	0
			884	562	172	147	3		

- Molecule 22 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AS	64	Total	C	N	O	S	0	0
			541	343	104	93	1		

- Molecule 23 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AU	149	Total	C	N	O	S	0	0
			1223	790	221	212			

- Molecule 24 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AV	96	Total	C	N	O	S	0	0
			808	528	129	148	3		
24	B6	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 25 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AW	61	Total	C	N	O	S	0	0
			470	294	91	80	5		

- Molecule 26 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AX	65	Total	C	N	O	S	0	0
			516	316	103	97			

- Molecule 27 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	49	Total	C	N	O	S	0	0
			400	257	76	62	5		

- Molecule 28 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AZ	196	Total	C	N	O	S	0	0
			1541	983	284	270	4		

- Molecule 29 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 30 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A3	122	Total	C	N	O	S	0	0
			933	594	156	180	3		
30	BG	122	Total	C	N	O	S	0	0
			932	594	156	179	3		
30	B4	122	Total	C	N	O	S	0	0
			933	594	156	180	3		

- Molecule 31 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AT	130	Total	C	N	O	S	0	0
			1057	675	201	174	7		

- Molecule 32 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AO	138	Total	C	N	O	S	0	0
			1116	700	221	190	5		

- Molecule 33 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BB	238	Total	C	N	O	S	0	0
			1838	1163	354	317	4		

- Molecule 34 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BY	154	Total	C	N	O	S	0	0
			1235	783	234	212	6		

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BO	198	Total	C	N	O	S	0	0
			1607	1024	302	279	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BC	360	Total	C	N	O	S	0	0
			2870	1843	522	494	11		

- Molecule 37 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B5	81	Total	C	N	O	S	0	0
			614	388	116	108	2		
37	BK	80	Total	C	N	O	S	0	0
			607	383	115	107	2		

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BL	147	Total	C	N	O	S	0	0
			1149	720	224	202	3		

- Molecule 39 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bf	50	Total	C	N	O	S	0	0
			435	275	99	60	1		

- Molecule 40 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BU	121	Total	C	N	O	S	0	0
			1011	638	198	170	5		

- Molecule 41 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bb	129	Total	C	N	O	S	0	0
			1095	702	221	171	1		

- Molecule 42 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Be	61	Total	C	N	O	S	0	0
			503	312	112	75	4		

- Molecule 43 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BE	185	Total	C	N	O	S	0	0
			1485	934	277	265	9		

- Molecule 44 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ba	94	Total	C	N	O	S	0	0
			778	503	147	127	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BT	86	Total	C	N	O	S	0	0
			696	451	118	126	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BW	68	Total	C	N	O	S	0	0
			565	349	111	99	6		

- Molecule 47 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bi	82	Total	C	N	O	S	0	0
			620	389	129	97	5		

- Molecule 48 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BI	142	Total	C	N	O	S	0	0
			1148	734	217	194	3		

- Molecule 49 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BR	96	Total	C	N	O	S	0	0
			797	507	164	125	1		

- Molecule 50 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BQ	150	Total	C	N	O	S	0	0
			1265	795	261	203	6		

- Molecule 51 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BV	63	Total	C	N	O	S	0	0
			532	339	103	84	6		

- Molecule 52 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bj	94	Total	C	N	O	S	0	0
			789	502	163	119	5		

- Molecule 53 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BD	255	Total	C	N	O	S	0	0
			2026	1290	388	343	5		

- Molecule 54 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BF	183	Total	C	N	O	S	0	0
			1456	943	251	261	1		

- Molecule 55 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BZ	98	Total	C	N	O		0	0
			749	486	122	141			

- Molecule 56 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BP	120	Total	C	N	O	S	0	0
			971	610	188	170	3		

- Molecule 57 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BM	193	Total	C	N	O	S	0	0
			1588	1014	318	251	5		

- Molecule 58 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BS	154	Total	C	N	O	S	0	0
			1247	786	246	211	4		

- Molecule 59 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bd	91	Total	C	N	O	S	0	0
			759	477	163	109	10		

- Molecule 60 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BN	178	Total	C	N	O	S	0	0
			1452	920	281	246	5		

- Molecule 61 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bg	48	Total	C	N	O	S	0	0
			387	243	80	60	4		

- Molecule 62 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bc	87	Total	C	N	O	S	0	0
			684	435	132	115	2		

- Molecule 63 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BJ	140	Total	C	N	O	S	0	0
			1066	664	214	185	3		

- Molecule 64 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bl	77	Total	C	N	O	S	0	0
			659	425	120	113	1		

- Molecule 65 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Bk	63	Total	C	N	O	S	0	0
			528	339	108	78	3		

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
66	1	166	Total	Mg	0
			166	166	
66	2	68	Total	Mg	0
			68	68	
66	3	1	Total	Mg	0
			1	1	
66	AK	1	Total	Mg	0
			1	1	
66	AN	1	Total	Mg	0
			1	1	
66	AR	1	Total	Mg	0
			1	1	
66	BB	2	Total	Mg	0
			2	2	
66	Bb	1	Total	Mg	0
			1	1	
66	BD	1	Total	Mg	0
			1	1	
66	BM	1	Total	Mg	0
			1	1	
66	BS	1	Total	Mg	0
			1	1	

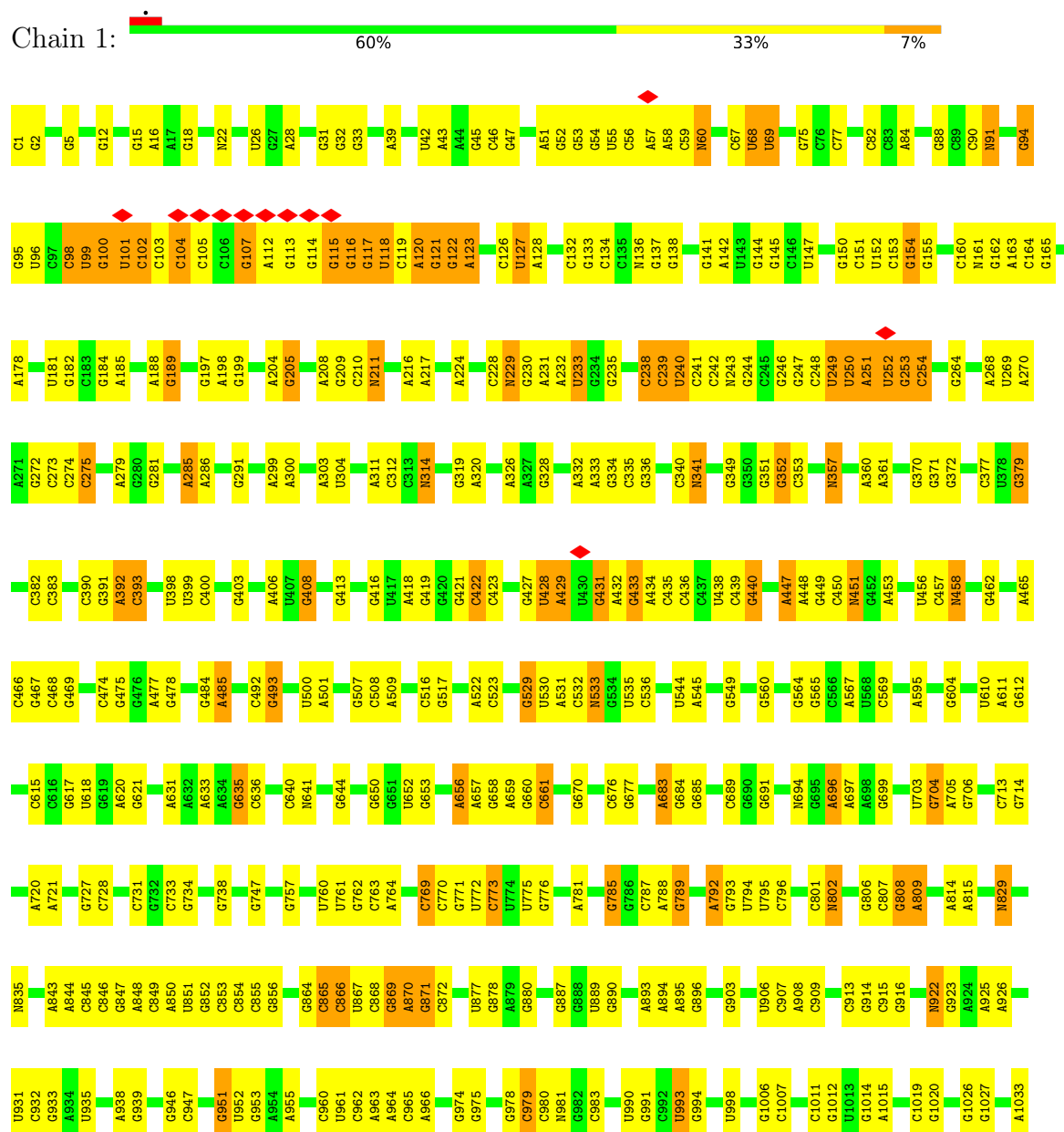
- Molecule 67 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
67	AC	2	Total 2	Zn 2	0
67	AF	1	Total 1	Zn 1	0
67	AP	1	Total 1	Zn 1	0
67	AR	1	Total 1	Zn 1	0
67	AW	1	Total 1	Zn 1	0
67	Be	1	Total 1	Zn 1	0
67	Bi	1	Total 1	Zn 1	0
67	BV	1	Total 1	Zn 1	0
67	Bj	1	Total 1	Zn 1	0
67	Bd	1	Total 1	Zn 1	0
67	Bg	1	Total 1	Zn 1	0
67	Bk	1	Total 1	Zn 1	0

3 Residue-property plots

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.

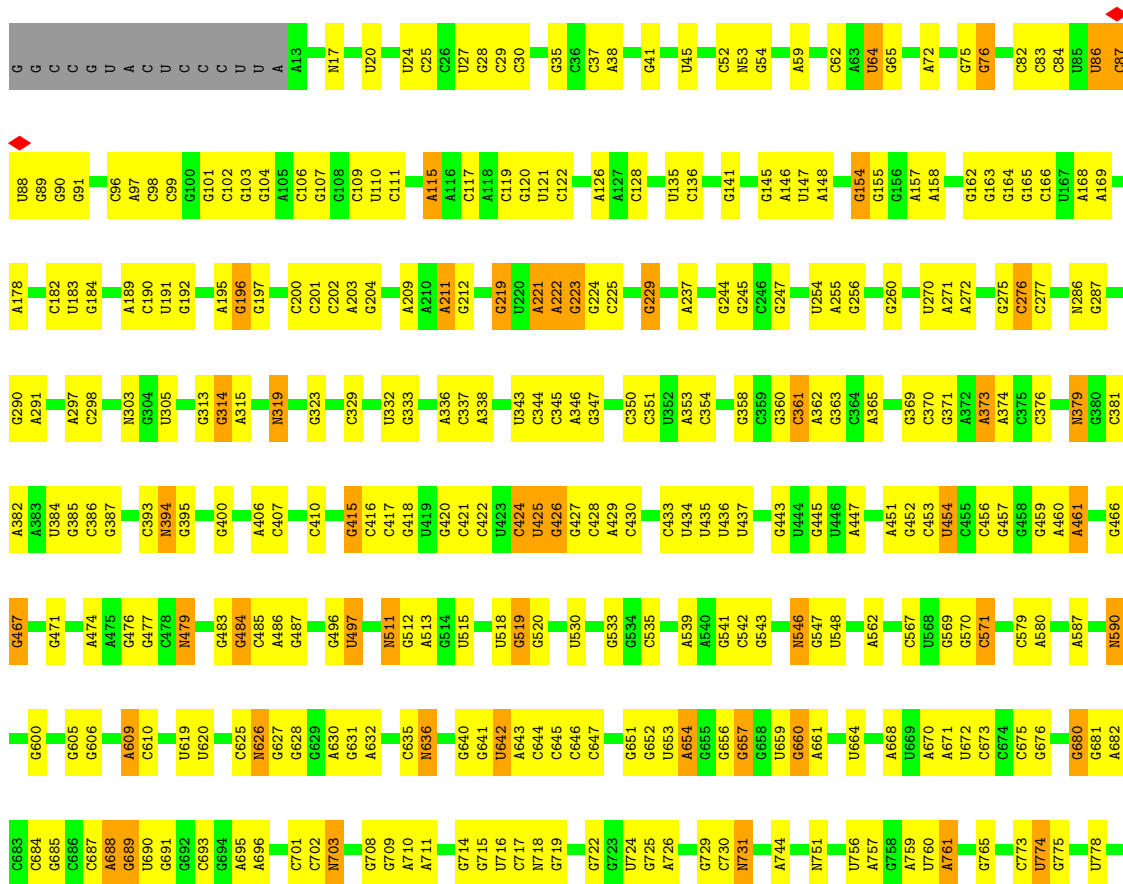
• Molecule 1: rRNA 23S

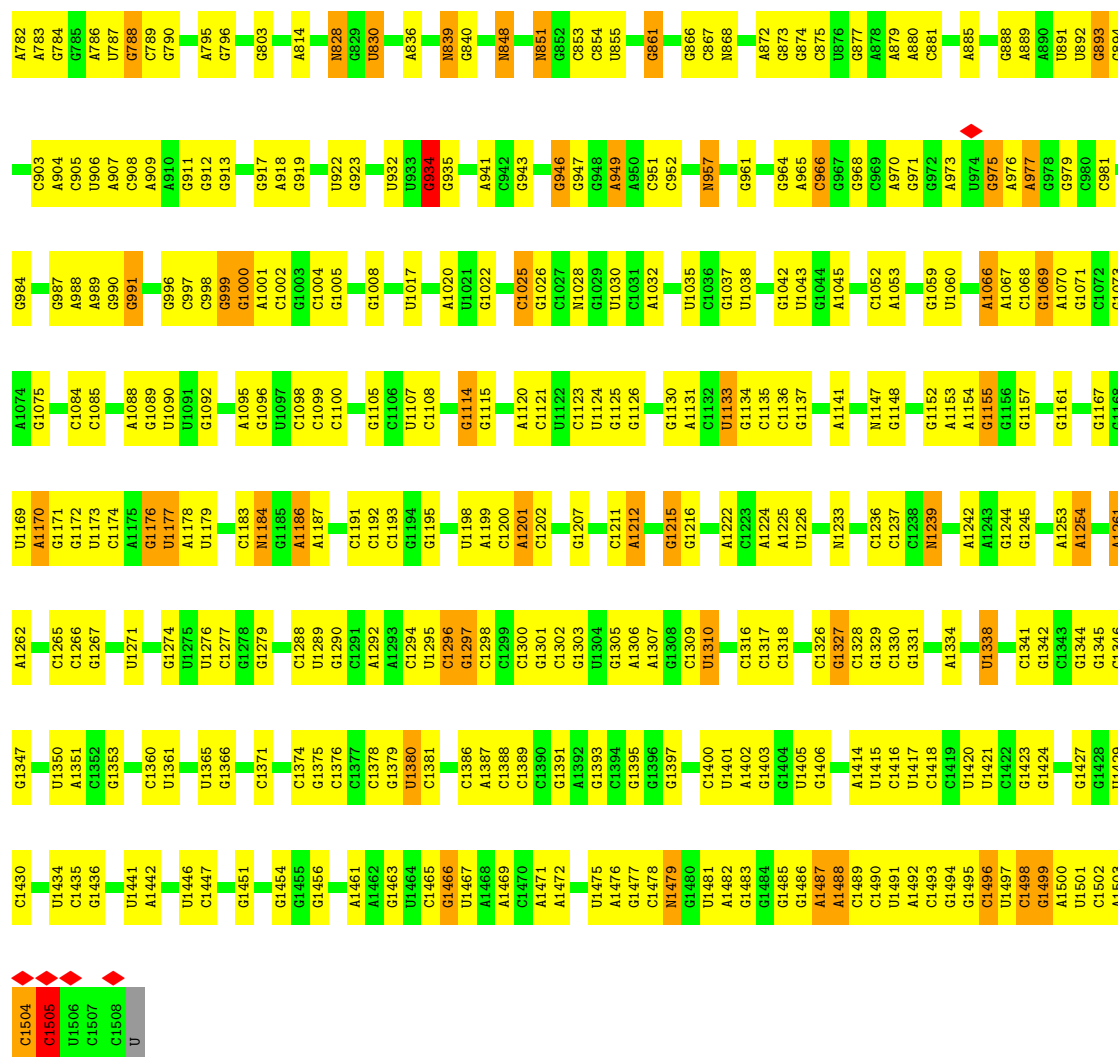




- Molecule 2: rRNA 16S

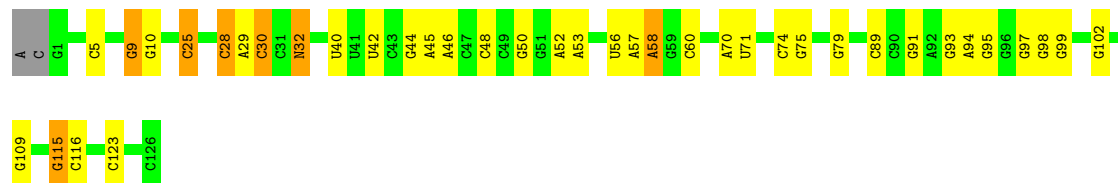
Chain 2: 55% 37% 6%





• Molecule 3: rRNA 5S

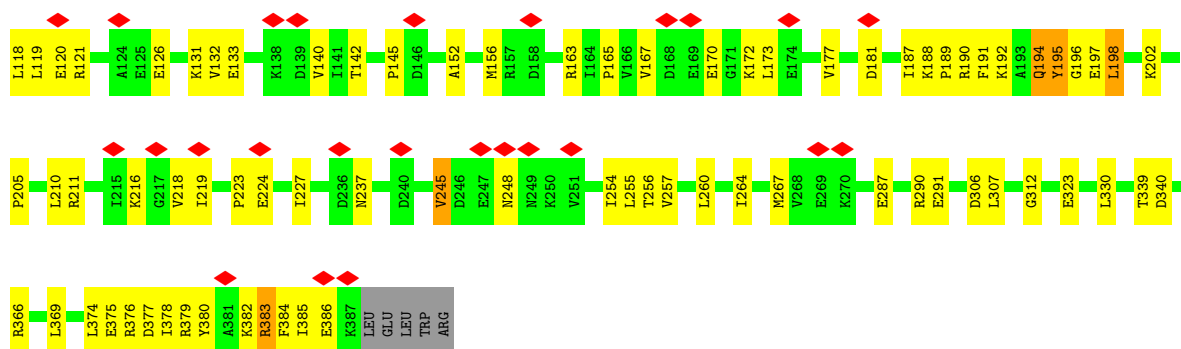
Chain 3: 68% 25% 5% •



• Molecule 4: Dehydrogenase

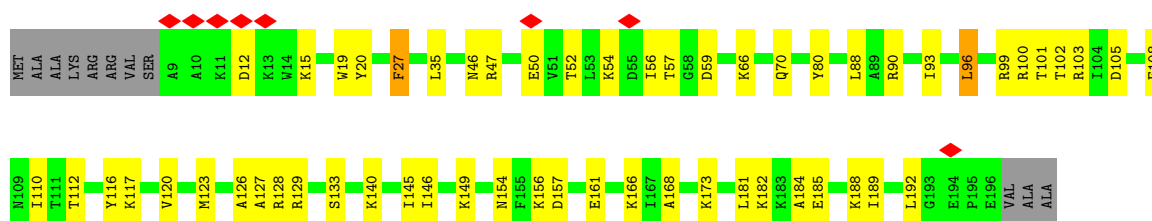
Chain H: 8% 71% 26% ••





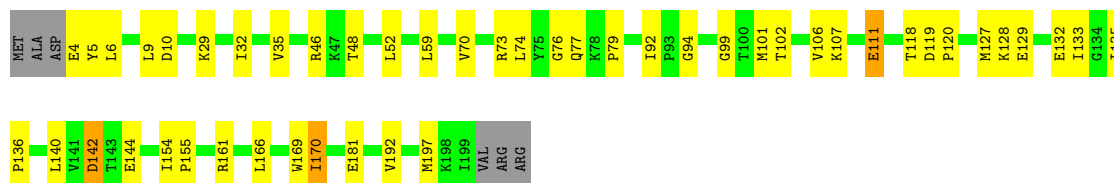
• Molecule 5: 30S ribosomal protein S3Ae

Chain AA: 66% 28% • 6%



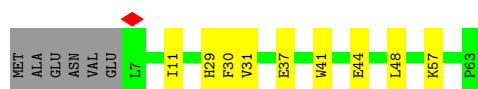
• Molecule 6: 30S ribosomal protein S2

Chain AB: 73% 22% • •



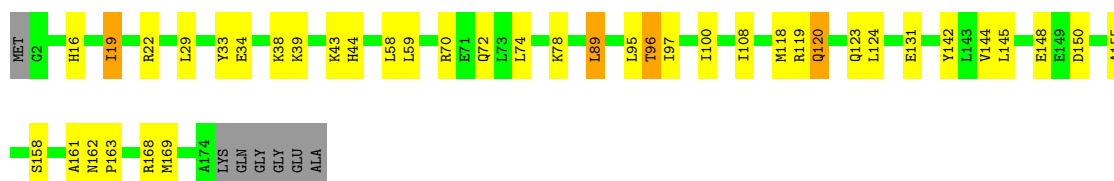
• Molecule 7: Zn-ribbon RNA-binding protein involved in translation

Chain AC: 76% 14% 10%

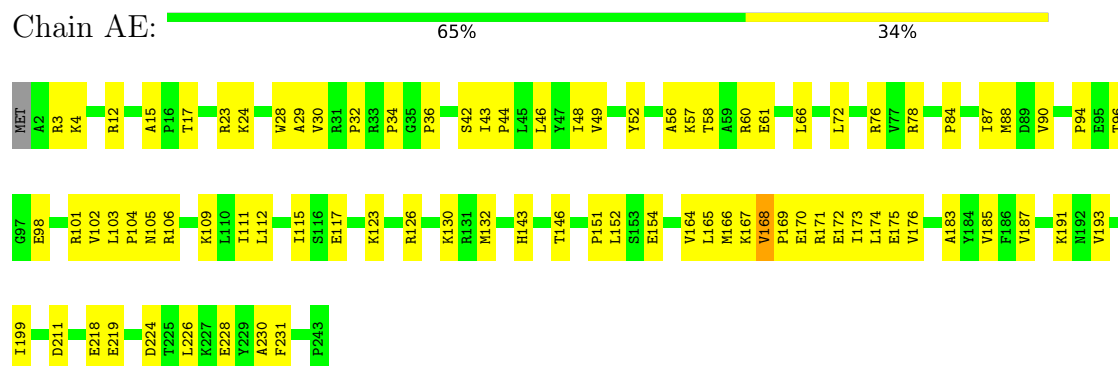


• Molecule 8: 30S ribosomal protein S4

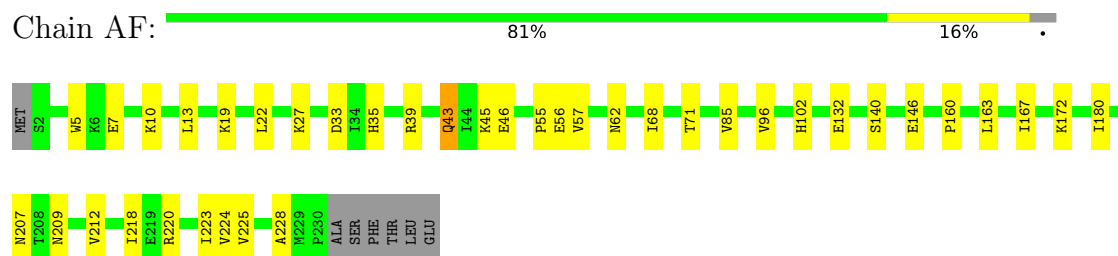
Chain AD: 74% 20% • •



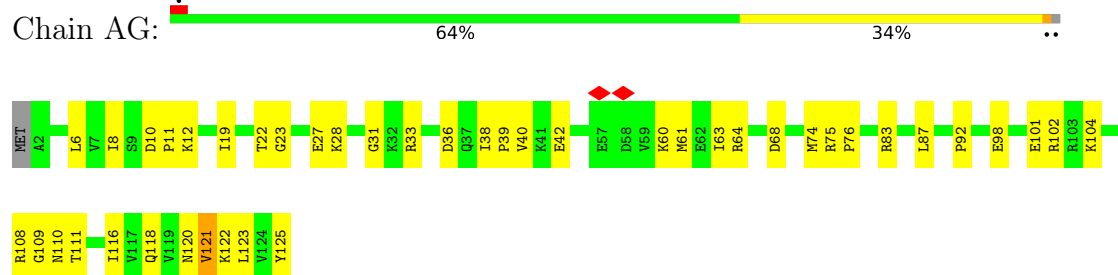
- Molecule 9: 30S ribosomal protein S4e



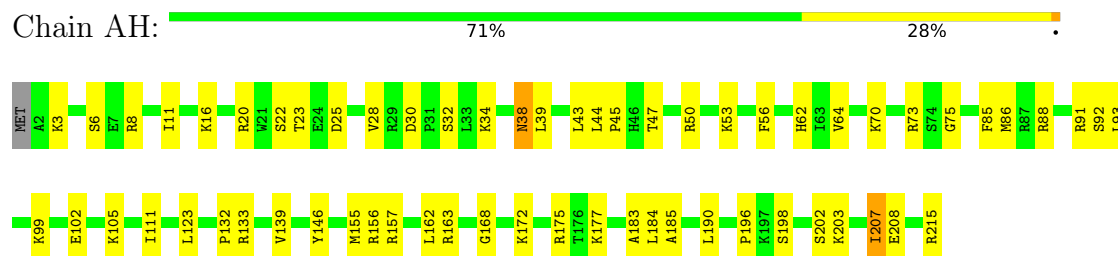
- Molecule 10: 30S ribosomal protein S5



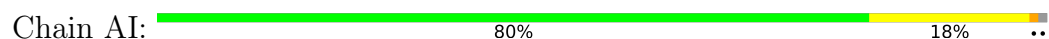
- Molecule 11: 30S ribosomal protein S6e

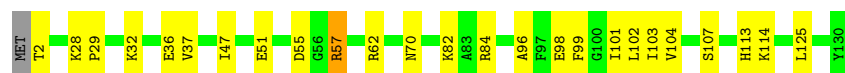


- Molecule 12: 30S ribosomal protein S7



- Molecule 13: 30S ribosomal protein S8





- Molecule 14: 30S ribosomal protein S8e

Chain AJ: 70% 28% ..



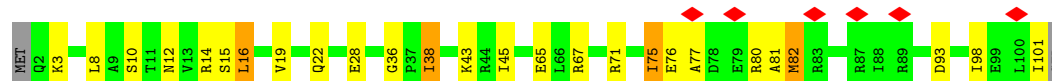
- Molecule 15: 30S ribosomal protein S9

Chain AK: 73% 27% .



- Molecule 16: 30S ribosomal protein S10

Chain AL: 6% 73% 22% . .



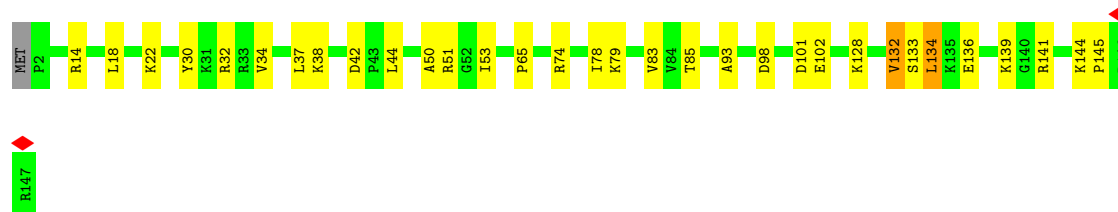
- Molecule 17: 30S ribosomal protein S11

Chain AM: 77% 15% 7% .



- Molecule 18: 30S ribosomal protein S12

Chain AN: 78% 20% ..



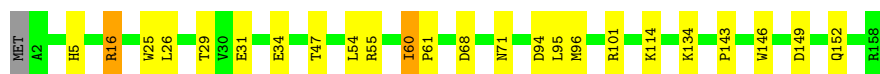
- Molecule 19: 30S ribosomal protein S14 type Z

Chain AP:  79% 18% ..



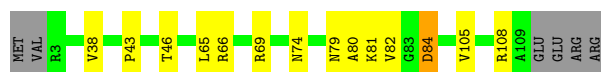
- Molecule 20: 30S ribosomal protein S15

Chain AQ:  84% 14% ..



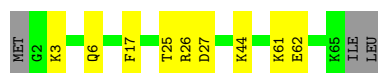
- Molecule 21: 30S ribosomal protein S17

Chain AR:  82% 12% 5%



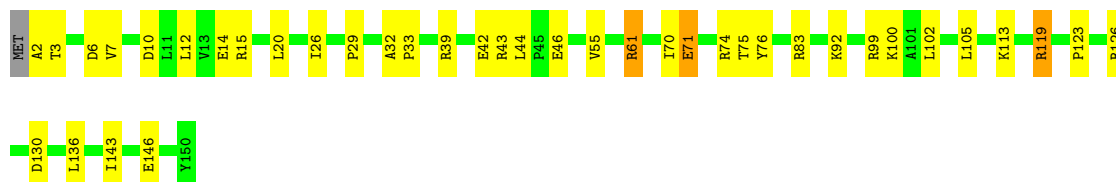
- Molecule 22: 30S ribosomal protein S17e

Chain AS:  82% 13% .



- Molecule 23: 30S ribosomal protein S19e

Chain AU:  73% 24% ..



- Molecule 24: 30S ribosomal protein S24e

Chain AV:  70% 23% . .

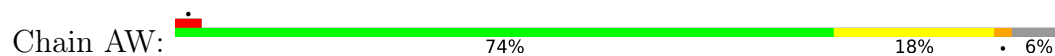


- Molecule 24: 30S ribosomal protein S24e

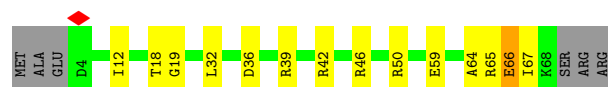
Chain B6:  72% 23% 5%



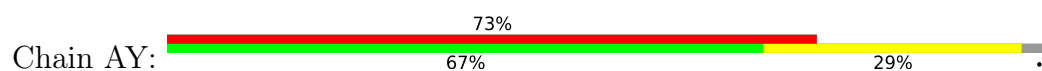
- Molecule 25: 30S ribosomal protein S27e



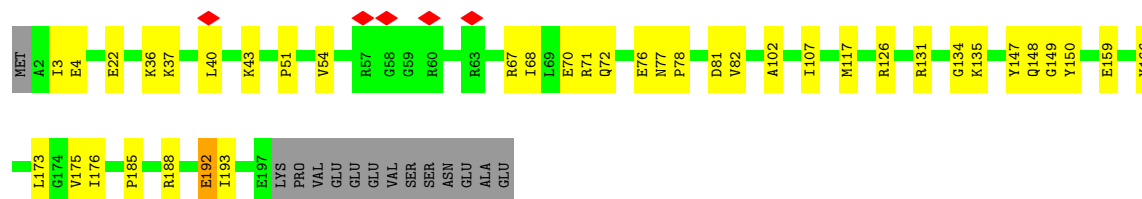
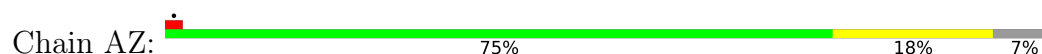
- Molecule 26: 30S ribosomal protein S28e



- Molecule 27: 30S ribosomal protein S27ae



- Molecule 28: 30S ribosomal protein S3



- Molecule 29: Small ribosomal subunit protein eS32



- Molecule 30: 50S ribosomal protein L7Ae





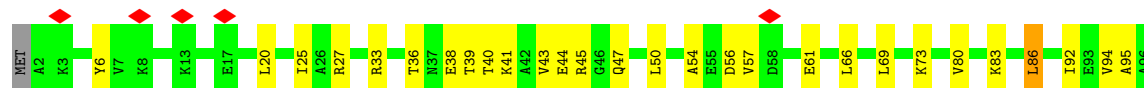
- Molecule 30: 50S ribosomal protein L7Ae

Chain BG: 80% 19%



- Molecule 30: 50S ribosomal protein L7Ae

Chain B4: 7% 64% 33%



- Molecule 31: 30S ribosomal protein S19

Chain AT: 5% 67% 30%



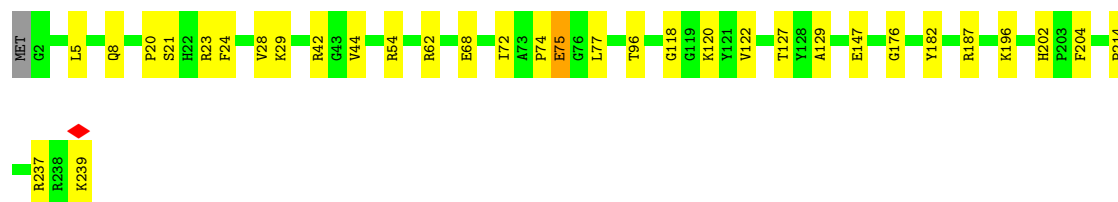
- Molecule 32: 30S ribosomal protein S13

Chain AO: 63% 28% 7%



- Molecule 33: Large ribosomal subunit protein uL2

Chain BB: 86% 13%



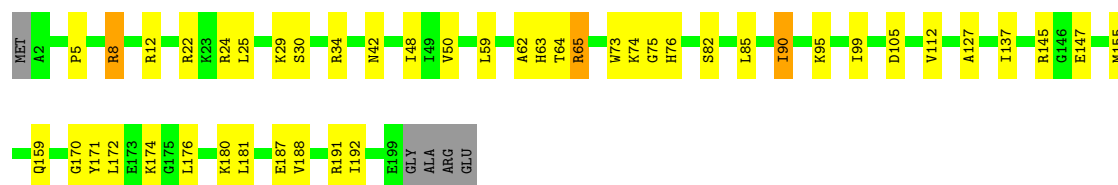
- Molecule 34: Large ribosomal subunit protein uL30

Chain BY: 90% 9% .



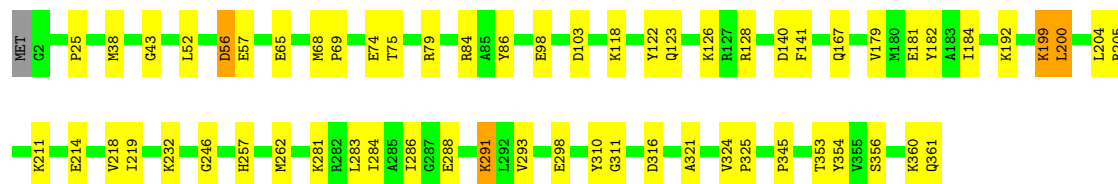
- Molecule 35: Large ribosomal subunit protein uL18

Chain BO: 75% 21% ..



- Molecule 36: Large ribosomal subunit protein uL3

Chain BC: 83% 16% .



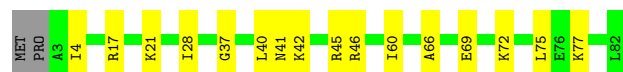
- Molecule 37: Large ribosomal subunit protein eL14

Chain B5: 76% 20% ..



- Molecule 37: Large ribosomal subunit protein eL14

Chain BK: 78% 20% .



- Molecule 38: Large ribosomal subunit protein uL15

Chain BL:  83% 16%



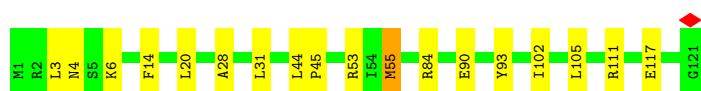
- Molecule 39: Large ribosomal subunit protein eL39

Chain Bf:  76% 22%



- Molecule 40: Large ribosomal subunit protein uL24

Chain BU:  85% 14%



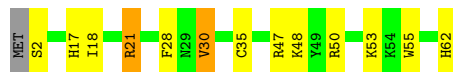
- Molecule 41: Large ribosomal subunit protein eL32

Chain Bb:  88% 11%



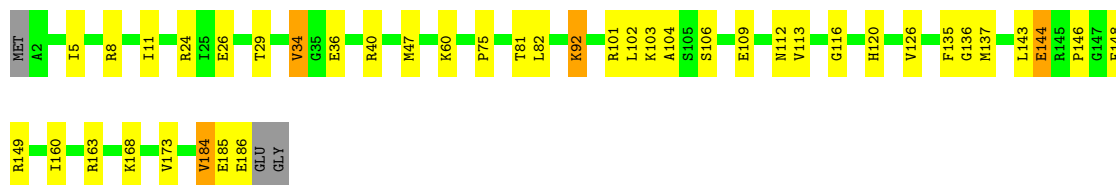
- Molecule 42: Large ribosomal subunit protein eL37

Chain Be:  77% 18%



- Molecule 43: Large ribosomal subunit protein uL5

Chain BE:  77% 20%



- Molecule 44: Large ribosomal subunit protein eL31

Chain Ba:  79% 21%



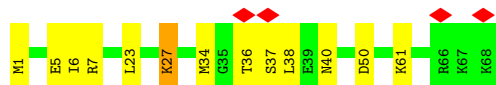
- Molecule 45: Large ribosomal subunit protein uL23

Chain BT:  92% 7%



- Molecule 46: Large ribosomal subunit protein uL29

Chain BW:  6% 81% 18%



- Molecule 47: Large ribosomal subunit protein eL43

Chain Bi:  88% 11%



- Molecule 48: Large ribosomal subunit protein uL13

Chain BI:  78% 21%



- Molecule 49: Large ribosomal subunit protein eL21

Chain BR:  87% 12%



- Molecule 50: Large ribosomal subunit protein eL19

Chain BQ:  83% 15%



- Molecule 51: Large ribosomal subunit protein eL24

Chain BV:  78% 13% 6%



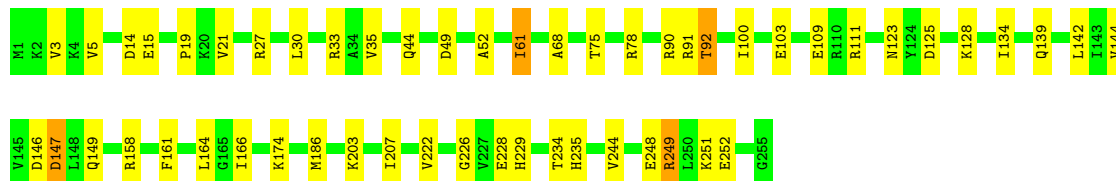
- Molecule 52: Large ribosomal subunit protein eL42

Chain Bj:  91% 9%



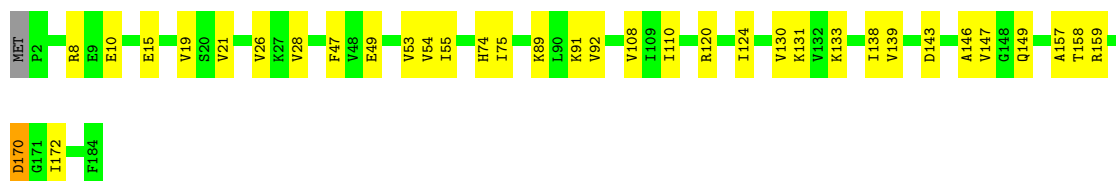
- Molecule 53: Large ribosomal subunit protein uL4

Chain BD:  79% 19%



- Molecule 54: Large ribosomal subunit protein uL6

Chain BF:  80% 18%



- Molecule 55: Large ribosomal subunit protein eL30

Chain BZ:  77% 21%



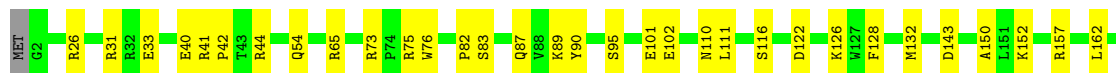
- Molecule 56: Large ribosomal subunit protein eL18

Chain BP:  81% 19%



- Molecule 57: Large ribosomal subunit protein eL15

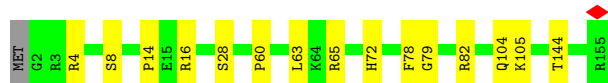
Chain BM:  82% 17%



K194

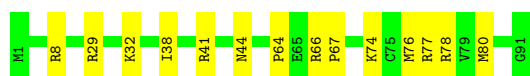
- Molecule 58: Large ribosomal subunit protein uL22

Chain BS:  90% 10%



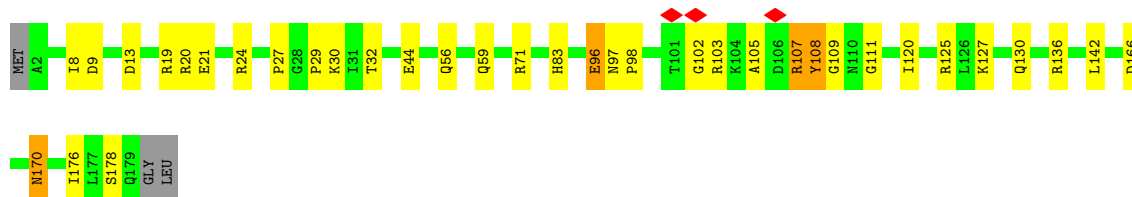
- Molecule 59: Large ribosomal subunit protein eL34

Chain Bd:  85% 15%



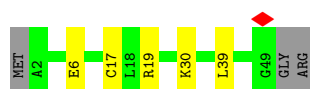
- Molecule 60: Large ribosomal subunit protein uL16

Chain BN:  78% 18%



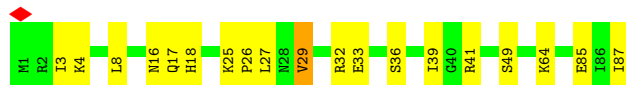
- Molecule 61: Large ribosomal subunit protein eL40

Chain Bg:  84% 10% 6%



- Molecule 62: Large ribosomal subunit protein eL33

Chain Bc:  78% 21%



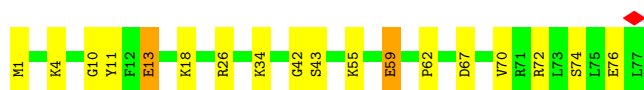
- Molecule 63: Large ribosomal subunit protein uL14

Chain BJ:  86% 12%



- Molecule 64: Large ribosomal subunit protein eL20

Chain Bl:  77% 21% .



- Molecule 65: C2H2-type domain-containing protein

Chain Bk:  72% 23% . .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00095	Depositor
Map size (Å)	302.04, 302.04, 302.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83900005, 0.83900005, 0.83900005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OMG, OMC, MG, LHH, 6MZ, 5MC, MA6, A2M, UR3, OMU, 4AC, B8H

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	1	0.22	1/70601 (0.0%)	0.31	0/110066
2	2	0.18	0/34435	0.27	0/53681
3	3	0.17	0/2995	0.27	0/4669
4	H	0.19	0/3120	0.44	2/4209 (0.0%)
5	AA	0.12	0/1557	0.28	0/2087
6	AB	0.12	0/1602	0.27	0/2165
7	AC	0.12	0/463	0.26	0/628
8	AD	0.14	0/1476	0.25	0/1980
9	AE	0.17	0/2032	0.32	0/2742
10	AF	0.15	0/1838	0.28	0/2478
11	AG	0.13	0/993	0.31	0/1329
12	AH	0.13	0/1762	0.29	0/2366
13	AI	0.16	0/1055	0.27	0/1415
14	AJ	0.13	0/995	0.25	0/1327
15	AK	0.15	0/1089	0.29	0/1459
16	AL	0.15	0/817	0.29	0/1097
17	AM	0.14	0/973	0.30	0/1311
18	AN	0.15	0/1165	0.27	0/1547
19	AP	0.13	0/465	0.26	0/613
20	AQ	0.12	0/1333	0.27	0/1791
21	AR	0.13	0/907	0.27	0/1225
22	AS	0.12	0/548	0.22	0/725
23	AU	0.14	0/1253	0.28	0/1689
24	AV	0.14	0/826	0.27	0/1108
24	B6	0.11	0/808	0.27	0/1086
25	AW	0.11	0/476	0.23	0/641
26	AX	0.12	0/518	0.29	0/694
27	AY	0.11	0/412	0.30	0/549
28	AZ	0.13	0/1563	0.29	0/2099
29	A0	0.17	0/349	0.32	0/451
30	A3	0.12	0/945	0.33	0/1274
30	B4	0.13	0/945	0.32	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	BG	0.13	0/944	0.27	0/1274
31	AT	0.20	0/1077	0.33	0/1439
32	AO	0.13	0/1135	0.34	0/1526
33	BB	0.19	0/1882	0.30	0/2538
34	BY	0.17	0/1254	0.27	0/1677
35	BO	0.15	0/1645	0.26	0/2209
36	BC	0.18	0/2933	0.29	0/3943
37	B5	0.14	0/619	0.27	0/830
37	BK	0.13	0/611	0.36	0/819
38	BL	0.16	0/1167	0.28	0/1552
39	Bf	0.18	0/443	0.27	0/589
40	BU	0.29	0/1027	0.38	0/1368
41	Bb	0.17	0/1120	0.27	0/1494
42	Be	0.19	0/514	0.28	0/676
43	BE	0.13	0/1509	0.28	0/2022
44	Ba	0.16	0/793	0.26	0/1064
45	BT	0.16	0/705	0.26	0/945
46	BW	0.13	0/566	0.25	0/747
47	Bi	0.16	0/630	0.32	0/839
48	BI	0.17	0/1166	0.26	0/1559
49	BR	0.18	0/819	0.26	0/1098
50	BQ	0.17	0/1281	0.27	0/1689
51	BV	0.18	0/547	0.27	0/729
52	Bj	0.16	0/807	0.24	0/1070
53	BD	0.17	0/2069	0.29	0/2787
54	BF	0.15	0/1485	0.25	0/2003
55	BZ	0.15	0/759	0.30	0/1023
56	BP	0.16	0/984	0.27	0/1314
57	BM	0.19	0/1627	0.29	0/2170
58	BS	0.18	0/1275	0.31	0/1715
59	Bd	0.17	0/778	0.27	0/1036
60	BN	0.16	0/1483	0.26	0/1992
61	Bg	0.14	0/396	0.24	0/526
62	Bc	0.17	0/693	0.31	0/926
63	BJ	0.18	0/1080	0.28	0/1456
64	Bl	0.14	0/669	0.27	0/886
65	Bk	0.18	0/538	0.27	0/709
All	All	0.19	1/179346 (0.0%)	0.30	2/264014 (0.0%)

All (1) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	96	U	C1'-N1	5.75	1.57	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	377	ASP	O-C-N	-11.25	107.35	122.43
4	H	383	ARG	N-CA-C	6.29	120.56	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	65181	0	32949	726	0
2	2	32291	0	16342	429	0
3	3	2703	0	1375	29	0
4	H	3074	0	3190	83	0
5	AA	1531	0	1623	38	0
6	AB	1571	0	1630	30	0
7	AC	449	0	435	4	0
8	AD	1452	0	1521	29	0
9	AE	1983	0	2060	55	0
10	AF	1808	0	1879	26	0
11	AG	977	0	1037	29	0
12	AH	1725	0	1780	45	0
13	AI	1034	0	1069	18	0
14	AJ	986	0	1070	24	0
15	AK	1073	0	1133	28	0
16	AL	809	0	859	20	0
17	AM	955	0	981	24	0
18	AN	1148	0	1248	20	0
19	AP	455	0	475	10	0
20	AQ	1305	0	1388	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AR	884	0	906	10	0
22	AS	541	0	573	8	0
23	AU	1223	0	1263	22	0
24	AV	808	0	832	17	0
24	B6	790	0	806	13	0
25	AW	470	0	495	9	0
26	AX	516	0	544	13	0
27	AY	400	0	401	11	0
28	AZ	1541	0	1624	22	0
29	A0	343	0	407	2	0
30	A3	933	0	982	27	0
30	B4	933	0	982	28	0
30	BG	932	0	982	14	0
31	AT	1057	0	1131	30	0
32	AO	1116	0	1152	26	0
33	BB	1838	0	1903	23	0
34	BY	1235	0	1314	10	0
35	BO	1607	0	1638	31	0
36	BC	2870	0	3020	38	0
37	B5	614	0	671	15	0
37	BK	607	0	663	11	0
38	BL	1149	0	1218	22	0
39	Bf	435	0	494	9	0
40	BU	1011	0	1078	13	0
41	Bb	1095	0	1190	10	0
42	Be	503	0	533	12	0
43	BE	1485	0	1539	27	0
44	Ba	778	0	851	12	0
45	BT	696	0	758	5	0
46	BW	565	0	628	9	0
47	Bi	620	0	668	6	0
48	BI	1148	0	1237	20	0
49	BR	797	0	835	10	0
50	BQ	1265	0	1392	21	0
51	BV	532	0	523	10	0
52	Bj	789	0	842	3	0
53	BD	2026	0	2131	37	0
54	BF	1456	0	1514	21	0
55	BZ	749	0	796	14	0
56	BP	971	0	1039	13	0
57	BM	1588	0	1683	21	0
58	BS	1247	0	1280	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	Bd	759	0	825	10	0
60	BN	1452	0	1491	27	0
61	Bg	387	0	397	4	0
62	Bc	684	0	748	12	0
63	BJ	1066	0	1133	12	0
64	Bl	659	0	702	12	0
65	Bk	528	0	575	12	0
66	1	166	0	0	0	0
66	2	68	0	0	0	0
66	3	1	0	0	0	0
66	AK	1	0	0	0	0
66	AN	1	0	0	0	0
66	AR	1	0	0	0	0
66	BB	2	0	0	0	0
66	BD	1	0	0	0	0
66	BM	1	0	0	0	0
66	BS	1	0	0	0	0
66	Bb	1	0	0	0	0
67	AC	2	0	0	0	0
67	AF	1	0	0	0	0
67	AP	1	0	0	0	0
67	AR	1	0	0	0	0
67	AW	1	0	0	0	0
67	BV	1	0	0	0	0
67	Bd	1	0	0	0	0
67	Be	1	0	0	0	0
67	Bg	1	0	0	0	0
67	Bi	1	0	0	0	0
67	Bj	1	0	0	0	0
67	Bk	1	0	0	0	0
All	All	170465	0	124433	2098	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2098) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:384:PHE:CZ	26:AX:65:ARG:NH1	1.74	1.45
1:1:107:G:N2	1:1:112:A:N7	1.85	1.20
1:1:107:G:N2	1:1:112:A:C8	2.14	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:100:G:N2	1:1:119:C:O2	1.82	1.12
1:1:117:G:O2'	1:1:118:U:OP1	1.67	1.12
1:1:2585:4AC:H5	1:1:2597:G:H1	1.18	1.06
4:H:382:LYS:HB2	17:AM:52:ARG:CG	1.80	1.05
1:1:2608:4AC:H5	1:1:2613:G:H1	1.22	1.01
1:1:102:C:N4	1:1:117:G:O6	1.97	0.97
1:1:2346:G:N2	1:1:2423:C:O2	2.05	0.90
4:H:382:LYS:CB	17:AM:52:ARG:HG2	2.03	0.89
1:1:235:G:H1	1:1:242:C:H5	1.22	0.88
2:2:631:G:H22	2:2:708:G:H1	1.18	0.87
1:1:163:A:H2	1:1:233:U:H3	1.23	0.87
4:H:383:ARG:HG2	17:AM:55:PRO:HG3	1.56	0.87
4:H:384:PHE:HZ	26:AX:65:ARG:NH1	1.35	0.86
4:H:384:PHE:CE2	26:AX:65:ARG:NH1	2.26	0.86
4:H:382:LYS:HB2	17:AM:52:ARG:HG3	1.57	0.86
1:1:1713:G:H21	1:1:1787:A:H8	1.20	0.84
4:H:382:LYS:CB	17:AM:52:ARG:CG	2.48	0.84
27:AY:25:CYS:HB3	30:A3:45:ARG:HH22	1.40	0.84
2:2:977:A:H62	2:2:999:G:H21	1.24	0.83
1:1:2431:C:H2'	1:1:2432:G:C8	2.14	0.82
54:BF:158:THR:HG21	54:BF:172:ILE:H	1.45	0.82
2:2:651:G:H21	17:AM:38:THR:HG21	1.45	0.82
2:2:323:G:N7	9:AE:3:ARG:NH1	2.26	0.81
1:1:793:G:OP2	38:BL:12:ARG:NH2	2.13	0.80
2:2:484:G:N2	18:AN:65:PRO:O	2.15	0.78
30:B4:33:ARG:HG2	30:B4:102:ILE:HD11	1.64	0.78
2:2:1271:U:O2'	12:AH:177:LYS:NZ	2.17	0.78
2:2:1095:A:H2'	2:2:1096:G:H8	1.49	0.77
38:BL:1:MET:HE1	53:BD:30:LEU:HD12	1.63	0.77
1:1:438:U:O2'	1:1:440:G:N7	2.17	0.77
1:1:2585:4AC:H5	1:1:2597:G:N1	1.99	0.76
1:1:2536:U:H5''	43:BE:116:GLY:HA3	1.68	0.76
2:2:1379:G:H2'	2:2:1380:OMU:H6	1.68	0.76
13:AI:102:LEU:H	13:AI:113:HIS:HD2	1.31	0.76
1:1:2242:C:O2'	44:Ba:24:ARG:NH2	2.19	0.75
1:1:2346:G:N1	1:1:2423:C:N3	2.33	0.75
2:2:660:G:OP2	4:H:383:ARG:NH2	2.20	0.75
1:1:1310:G:O2'	1:1:1339:A:N6	2.20	0.75
1:1:205:G:N7	39:Bf:34:ARG:NH2	2.35	0.74
37:BK:45:ARG:NH2	37:BK:66:ALA:O	2.20	0.74
1:1:3021:U:H3'	1:1:3021:U:OP2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2057:U:OP2	33:BB:120:LYS:NZ	2.20	0.74
1:1:2377:C:H42	1:1:2394:G:H1	1.35	0.74
27:AY:24:ARG:NH1	27:AY:24:ARG:O	2.21	0.74
1:1:792:A:H62	1:1:1509:C:H5	1.34	0.73
1:1:1601:U:O4	45:BT:15:LYS:NZ	2.20	0.73
1:1:103:C:H2'	1:1:104:C:C6	2.23	0.73
4:H:119:LEU:HD11	4:H:257:VAL:HG13	1.69	0.73
37:BK:21:LYS:O	37:BK:41:ASN:ND2	2.21	0.73
1:1:2036:A:HO2'	42:Be:2:SER:N	1.86	0.73
5:AA:12:ASP:HA	5:AA:15:LYS:HE2	1.70	0.73
16:AL:77:ALA:HA	16:AL:82:MET:HE3	1.71	0.73
2:2:415:G:H21	8:AD:123:GLN:HE22	1.37	0.73
10:AF:212:VAL:H	13:AI:70:ASN:HD21	1.35	0.73
1:1:117:G:O2'	1:1:118:U:P	2.47	0.72
35:BO:95:LYS:NZ	35:BO:127:ALA:O	2.23	0.72
35:BO:187:GLU:OE2	35:BO:191:ARG:NH2	2.22	0.72
5:AA:127:ALA:HB2	5:AA:182:LYS:HD3	1.70	0.72
1:1:102:C:C4	1:1:103:C:C4	2.78	0.72
5:AA:120:VAL:HG21	5:AA:146:ILE:HG21	1.71	0.72
1:1:103:C:H2'	1:1:104:C:H6	1.55	0.72
1:1:117:G:HO2'	1:1:118:U:P	2.12	0.71
2:2:1491:U:H2'	2:2:1492:A:H8	1.55	0.71
2:2:778:U:O2'	2:2:872:A:N1	2.23	0.71
9:AE:126:ARG:HG2	9:AE:143:HIS:HB3	1.70	0.71
1:1:102:C:N4	1:1:103:C:N4	2.38	0.71
2:2:636:4AC:HM73	2:2:703:4AC:HM73	1.73	0.71
60:BN:20:ARG:NH2	60:BN:27:PRO:O	2.23	0.71
30:B4:83:LYS:HG2	30:B4:95:ALA:HB1	1.72	0.71
1:1:112:A:H3'	1:1:113:G:C8	2.26	0.71
37:BK:45:ARG:NH1	64:BI:1:MET:O	2.23	0.70
30:B4:118:VAL:HG13	30:B4:119:ARG:HH11	1.56	0.70
3:3:97:G:H2'	3:3:98:G:H8	1.55	0.70
5:AA:103:ARG:NH1	5:AA:105:ASP:OD2	2.25	0.70
2:2:1130:G:N7	22:AS:44:LYS:NZ	2.35	0.70
8:AD:19:ILE:HG22	8:AD:22:ARG:H	1.56	0.70
48:BI:29:VAL:HG22	48:BI:98:LYS:HB2	1.73	0.70
1:1:1734:G:H2'	1:1:1735:G:H8	1.56	0.70
32:AO:81:ARG:HD3	32:AO:93:LEU:HD13	1.73	0.70
1:1:2426:C:H2'	1:1:2427:G:C8	2.27	0.70
1:1:2887:A:HO2'	63:BJ:2:ALA:N	1.90	0.69
22:AS:25:THR:HG23	22:AS:27:ASP:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AH:215:ARG:NH1	26:AX:59:GLU:OE2	2.25	0.69
36:BC:205:ARG:NH2	36:BC:288:GLU:OE1	2.26	0.69
1:1:2430:G:H3'	1:1:2431:C:H6	1.57	0.69
13:AI:96:ALA:HB3	13:AI:99:PHE:HB2	1.73	0.69
18:AN:14:ARG:NH2	21:AR:65:LEU:O	2.25	0.69
41:Bb:97:ARG:NH2	24:B6:2:GLU:OE1	2.25	0.69
1:1:2388:G:H2'	1:1:2389:G:H8	1.58	0.69
5:AA:19:TRP:HD1	5:AA:35:LEU:HB3	1.57	0.69
63:BJ:36:LYS:HE3	63:BJ:69:GLY:HA2	1.73	0.69
2:2:918:A:H2'	2:2:919:G:C8	2.28	0.69
4:H:172:LYS:NZ	4:H:248:ASN:O	2.25	0.69
15:AK:37:GLU:HG2	15:AK:38:PRO:HA	1.73	0.69
4:H:384:PHE:HZ	26:AX:65:ARG:HH11	1.40	0.69
1:1:653:G:N1	1:1:656:A:OP2	2.26	0.69
1:1:1905:G:N1	1:1:1908:A:OP2	2.24	0.69
4:H:142:THR:HG22	4:H:165:PRO:HG2	1.74	0.69
1:1:1806:G:OP2	1:1:1806:G:N2	2.21	0.68
15:AK:26:VAL:HG13	15:AK:62:ILE:HB	1.76	0.68
27:AY:37:ARG:HH21	27:AY:39:ALA:HA	1.58	0.68
30:B4:116:MET:HE3	30:B4:117:LYS:HG2	1.75	0.68
1:1:2367:G:H21	1:1:2413:A:H1'	1.58	0.68
2:2:247:G:OP1	21:AR:66:ARG:NH1	2.27	0.68
1:1:2426:C:H2'	1:1:2427:G:H8	1.58	0.68
9:AE:87:ILE:HD12	9:AE:104:PRO:HG3	1.76	0.68
43:BE:60:LYS:HA	43:BE:75:PRO:HA	1.75	0.68
1:1:102:C:C4	1:1:103:C:C5	2.81	0.68
4:H:219:ILE:HG13	4:H:237:ASN:HD22	1.59	0.68
4:H:378:ILE:HG13	4:H:378:ILE:O	1.93	0.68
2:2:1022:G:HO2'	28:AZ:166:TYR:HH	1.27	0.68
15:AK:1:MET:HE3	15:AK:3:ILE:HD11	1.76	0.67
33:BB:122:VAL:HG13	33:BB:127:THR:HG22	1.76	0.67
1:1:2001:4AC:OP2	50:BQ:76:ARG:NH1	2.27	0.67
12:AH:75:GLY:HA3	12:AH:86:MET:HE3	1.76	0.67
30:B4:101:ILE:HD11	30:B4:104:PRO:HA	1.75	0.67
1:1:117:G:C2	1:1:118:U:C6	2.83	0.67
3:3:10:G:O6	35:BO:12:ARG:NH1	2.27	0.67
1:1:894:A:H2'	1:1:895:A:C8	2.30	0.67
21:AR:79:ASN:OD1	21:AR:81:LYS:NZ	2.27	0.67
30:A3:3:LYS:HG2	30:A3:6:TYR:HB2	1.76	0.67
1:1:3007:A:H2	1:1:3009:A:H62	1.39	0.67
2:2:912:G:OP1	12:AH:73:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1262:U:O4	48:BI:16:SER:OG	2.12	0.67
2:2:975:G:N2	2:2:1000:G:O2'	2.28	0.67
1:1:113:G:H2'	1:1:114:G:H8	1.59	0.67
30:B4:92:ILE:HG22	30:B4:94:VAL:H	1.60	0.67
1:1:955:A:OP2	47:Bi:2:SER:N	2.28	0.67
2:2:1191:C:OP1	19:AP:9:ARG:NH2	2.28	0.67
18:AN:51:ARG:NH1	18:AN:102:GLU:OE2	2.27	0.67
1:1:595:A:H5''	40:BU:6:LYS:HE2	1.77	0.67
1:1:2109:A:H2'	1:1:2110:A:C8	2.30	0.67
2:2:853:C:OP2	18:AN:22:LYS:NZ	2.27	0.67
5:AA:57:THR:HG23	5:AA:59:ASP:H	1.60	0.67
30:A3:31:LYS:HB3	30:A3:102:ILE:HG22	1.76	0.67
10:AF:7:GLU:HA	10:AF:10:LYS:HE3	1.77	0.66
37:B5:67:SER:OG	37:B5:70:GLU:OE1	2.12	0.66
53:BD:33:ARG:NH1	53:BD:109:GLU:OE2	2.28	0.66
1:1:1810:G:OP2	50:BQ:43:ARG:NH1	2.28	0.66
47:Bi:82:VAL:HG12	47:Bi:83:GLU:HG3	1.77	0.66
1:1:869:G:O2'	1:1:870:A:O5'	2.14	0.66
1:1:2683:A:O2'	4:H:198:LEU:O	2.13	0.66
1:1:2701:A:N6	1:1:2713:G:O2'	2.28	0.66
2:2:386:C:H2'	2:2:387:G:H8	1.58	0.66
2:2:386:C:H2'	2:2:387:G:C8	2.30	0.66
2:2:661:A:H5''	17:AM:52:ARG:HD3	1.77	0.66
44:Ba:16:ARG:HA	44:Ba:19:LYS:HG3	1.77	0.66
2:2:1200:C:N4	32:AO:132:ARG:HD2	2.11	0.66
4:H:382:LYS:HB2	17:AM:52:ARG:HG2	1.61	0.66
38:BL:79:LYS:HB3	38:BL:116:GLY:HA3	1.77	0.66
2:2:41:G:OP1	18:AN:128:LYS:NZ	2.28	0.66
5:AA:50:GLU:OE1	17:AM:82:ARG:NH2	2.28	0.66
21:AR:43:PRO:HB2	21:AR:46:THR:HB	1.76	0.66
1:1:916:G:OP2	38:BL:31:LYS:NZ	2.28	0.66
1:1:418:A:H2'	1:1:419:G:C8	2.31	0.66
1:1:433:G:O2'	65:Bk:47:ARG:NH1	2.29	0.66
24:B6:25:HIS:HB2	24:B6:28:GLU:HB2	1.78	0.66
3:3:74:C:O2	3:3:109:G:N2	2.18	0.65
4:H:19:ILE:HG12	4:H:70:ARG:HD2	1.78	0.65
9:AE:58:THR:HG22	9:AE:60:ARG:H	1.61	0.65
2:2:417:C:H5'	8:AD:120:GLN:HG3	1.78	0.65
30:B4:39:THR:HG23	30:B4:100:ALA:HB2	1.77	0.65
1:1:2311:A:H2'	1:1:2312:G:C8	2.32	0.65
28:AZ:68:ILE:HG12	28:AZ:72:GLN:HE22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:189:G:H22	1:1:224:A:H2	1.45	0.65
1:1:764:A:O2'	62:Bc:17:GLN:NE2	2.28	0.65
1:1:931:U:H3	1:1:1046:G:H1	1.43	0.65
1:1:2698:G:OP1	61:Bg:19:ARG:NH1	2.27	0.65
2:2:702:C:H2'	2:2:703:4AC:H6	1.78	0.65
2:2:1089:G:N2	2:2:1090:U:O4	2.27	0.65
1:1:848:A:O2'	1:1:887:G:O2'	2.12	0.65
2:2:541:G:N2	2:2:851:4AC:O2	2.27	0.65
21:AR:84:ASP:OD1	21:AR:84:ASP:N	2.28	0.65
1:1:2955:U:OP1	36:BC:232:LYS:NZ	2.30	0.65
2:2:1176:G:N2	19:AP:45:GLU:OE2	2.23	0.65
2:2:627:G:H2'	2:2:628:G:C8	2.31	0.65
2:2:790:G:HO2'	13:AI:2:THR:N	1.95	0.65
1:1:848:A:HO2'	1:1:887:G:HO2'	1.41	0.65
1:1:2960:4AC:O2'	36:BC:281:LYS:NZ	2.28	0.65
2:2:1310:U:O4	12:AH:91:ARG:NH2	2.27	0.65
8:AD:97:ILE:HD12	8:AD:100:ILE:HD11	1.78	0.65
16:AL:43:LYS:HD2	28:AZ:3:ILE:HD11	1.79	0.65
1:1:720:A:H2'	1:1:721:A:H8	1.61	0.64
1:1:2608:4AC:H5	1:1:2613:G:N1	2.05	0.64
2:2:570:G:H4'	9:AE:226:LEU:HD11	1.78	0.64
2:2:918:A:H2'	2:2:919:G:H8	1.62	0.64
2:2:987:G:OP2	31:AT:64:ARG:NH1	2.31	0.64
1:1:116:G:H2'	1:1:117:G:H8	1.62	0.64
1:1:1283:A:H2'	1:1:1284:A:C8	2.33	0.64
1:1:2951:C:O2'	36:BC:361:GLN:O	2.16	0.64
12:AH:196:PRO:O	12:AH:202:SER:OG	2.15	0.64
33:BB:5:LEU:H	33:BB:8:GLN:HE21	1.44	0.64
1:1:102:C:C2	1:1:103:C:C6	2.86	0.64
1:1:163:A:H2	1:1:233:U:N3	1.94	0.64
35:BO:145:ARG:NH1	35:BO:147:GLU:OE2	2.31	0.64
1:1:31:G:H4'	44:Ba:14:PRO:HG3	1.79	0.64
1:1:772:U:O2'	38:BL:22:LYS:NZ	2.31	0.64
11:AG:40:VAL:HG22	11:AG:61:MET:HE3	1.80	0.64
56:BP:57:LYS:NZ	56:BP:60:ASP:OD1	2.31	0.64
1:1:1653:U:OP2	50:BQ:42:ARG:NH2	2.31	0.64
1:1:2344:G:H1	1:1:2425:U:H3	1.45	0.64
1:1:2388:G:H2'	1:1:2389:G:C8	2.32	0.64
2:2:1499:G:H2'	2:2:1500:A:C8	2.33	0.63
4:H:382:LYS:N	4:H:382:LYS:HD2	2.12	0.63
32:AO:58:GLN:HA	32:AO:61:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AI:102:LEU:H	13:AI:113:HIS:CD2	2.14	0.63
1:1:352:G:H5'	1:1:353:C:H5''	1.79	0.63
2:2:977:A:H62	2:2:999:G:N2	1.93	0.63
9:AE:168:VAL:HG22	9:AE:169:PRO:HA	1.80	0.63
10:AF:146:GLU:O	10:AF:207:ASN:ND2	2.29	0.63
2:2:1037:G:H2'	2:2:1038:U:C6	2.32	0.63
49:BR:45:ILE:H	49:BR:59:HIS:HD2	1.45	0.63
6:AB:161:ARG:NH1	6:AB:197:MET:O	2.31	0.63
28:AZ:67:ARG:HE	28:AZ:71:ARG:HG3	1.63	0.63
1:1:1421:C:H2'	1:1:1422:A:C8	2.33	0.63
2:2:28:G:H2'	2:2:29:C:C6	2.34	0.63
5:AA:19:TRP:CD1	5:AA:35:LEU:HB3	2.34	0.63
28:AZ:135:LYS:NZ	28:AZ:173:LEU:O	2.30	0.63
2:2:1211:C:OP2	12:AH:91:ARG:NH1	2.30	0.63
2:2:415:G:H21	8:AD:123:GLN:NE2	1.97	0.63
4:H:384:PHE:CE2	26:AX:65:ARG:CZ	2.81	0.63
1:1:1715:U:H5	1:1:1824:A:N7	1.97	0.62
1:1:2808:G:O2'	1:1:2811:C:OP2	2.17	0.62
32:AO:10:VAL:HG12	32:AO:59:VAL:HG13	1.80	0.62
1:1:112:A:H3'	1:1:113:G:H8	1.63	0.62
2:2:659:U:O4	4:H:383:ARG:HD3	1.98	0.62
2:2:987:G:P	31:AT:64:ARG:HH12	2.22	0.62
48:BI:88:ASP:OD2	48:BI:92:LYS:NZ	2.31	0.62
44:Ba:25:TRP:HA	44:Ba:64:GLU:HG2	1.81	0.62
1:1:850:A:N6	38:BL:117:LYS:O	2.26	0.62
65:Bk:34:ILE:O	65:Bk:38:ASN:ND2	2.32	0.62
16:AL:45:ILE:HD11	28:AZ:4:GLU:HB3	1.82	0.62
2:2:681:G:H2'	2:2:682:A:H8	1.64	0.62
10:AF:5:TRP:HB3	10:AF:55:PRO:HB2	1.82	0.62
11:AG:39:PRO:HG2	11:AG:42:GLU:HB3	1.81	0.62
1:1:809:A:N7	1:1:903:G:O2'	2.31	0.62
2:2:75:G:H2'	2:2:76:G:C8	2.34	0.61
30:BG:43:VAL:HG13	30:BG:75:ILE:HD12	1.82	0.61
60:BN:97:ASN:HD22	60:BN:98:PRO:HD2	1.65	0.61
4:H:384:PHE:CE2	26:AX:65:ARG:NH2	2.68	0.61
53:BD:5:VAL:N	53:BD:14:ASP:O	2.30	0.61
1:1:1146:C:H2'	1:1:1147:C:C6	2.35	0.61
1:1:2035:U:OP2	1:1:2040:A:N6	2.25	0.61
2:2:1123:C:OP1	15:AK:9:LYS:NZ	2.33	0.61
18:AN:53:ILE:HD13	18:AN:78:ILE:HD11	1.82	0.61
27:AY:3:GLN:HE21	30:A3:61:GLU:HG3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2108:G:N1	1:1:2130:A:OP2	2.33	0.61
1:1:2990:G:H21	54:BF:149:GLN:HE22	1.48	0.61
1:1:162:G:H21	1:1:163:A:H62	1.47	0.61
1:1:2559:A:H2'	1:1:2560:G:C8	2.35	0.61
2:2:965:A:H5''	2:2:966:C:H5	1.66	0.61
18:AN:101:ASP:OD2	18:AN:144:LYS:NZ	2.31	0.61
21:AR:105:VAL:HG11	21:AR:108:ARG:HG2	1.82	0.61
1:1:26:U:O2	36:BC:123:GLN:NE2	2.33	0.61
2:2:135:U:OP1	9:AE:78:ARG:NH2	2.34	0.61
20:AQ:26:LEU:HD11	20:AQ:60:ILE:HG22	1.81	0.61
30:A3:33:ARG:HH22	30:A3:42:ALA:HB2	1.65	0.61
1:1:2358:U:H3	1:1:2388:G:H1'	1.65	0.61
1:1:2498:A:H2	1:1:2503:U:H3	1.48	0.61
2:2:680:OMG:H2'	2:2:681:G:C8	2.36	0.61
40:BU:53:ARG:HD2	40:BU:55:MET:HE3	1.83	0.61
2:2:115:A:OP2	2:2:297:A:N6	2.30	0.60
54:BF:139:VAL:HG12	54:BF:147:VAL:HG13	1.83	0.60
30:BG:39:THR:HG23	30:BG:100:ALA:HB2	1.82	0.60
2:2:162:G:H2'	2:2:163:G:H8	1.65	0.60
1:1:1676:A:N1	1:1:1692:G:O2'	2.33	0.60
2:2:687:C:OP2	2:2:688:A:O2'	2.19	0.60
2:2:1095:A:H2'	2:2:1096:G:C8	2.34	0.60
9:AE:48:ILE:HA	9:AE:52:TYR:HB2	1.83	0.60
32:AO:14:ASP:OD1	32:AO:15:LEU:N	2.34	0.60
56:BP:99:GLU:OE2	56:BP:109:ARG:NH1	2.27	0.60
1:1:2304:C:H2'	1:1:2305:C:C6	2.36	0.60
1:1:2422:U:H2'	1:1:2423:C:C6	2.37	0.60
5:AA:117:LYS:HG2	5:AA:192:LEU:HB2	1.83	0.60
11:AG:27:GLU:OE1	11:AG:27:GLU:N	2.35	0.60
2:2:435:U:O2'	2:2:437:U:O4	2.17	0.60
9:AE:90:VAL:HG22	9:AE:101:ARG:HE	1.66	0.60
64:Bl:13:GLU:HG2	64:Bl:18:LYS:HD3	1.82	0.60
12:AH:38:ASN:HB3	12:AH:62:HIS:HA	1.83	0.60
53:BD:49:ASP:HB3	53:BD:52:ALA:HB2	1.82	0.60
62:Bc:33:GLU:N	62:Bc:33:GLU:OE1	2.34	0.60
1:1:113:G:H2'	1:1:114:G:C8	2.36	0.60
1:1:1742:A:H2'	1:1:1743:A:C8	2.37	0.60
1:1:253:G:H2'	1:1:254:C:C6	2.37	0.60
9:AE:105:ASN:N	9:AE:109:LYS:O	2.35	0.60
53:BD:249:ARG:HH21	53:BD:252:GLU:HG3	1.66	0.60
2:2:709:G:OP1	20:AQ:101:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:977:A:N6	2:2:999:G:H21	1.97	0.60
2:2:1174:C:O2'	2:2:1179:U:O4	2.20	0.60
2:2:1302:C:OP1	32:AO:34:ASN:ND2	2.34	0.60
1:1:279:A:O2'	57:BM:110:ASN:ND2	2.35	0.59
2:2:1095:A:C4	2:2:1096:G:C8	2.90	0.59
3:3:97:G:H2'	3:3:98:G:C8	2.37	0.59
2:2:1338:U:OP2	23:AU:83:ARG:NH2	2.35	0.59
4:H:113:ILE:HD11	4:H:118:LEU:HD12	1.84	0.59
6:AB:111:GLU:OE2	10:AF:43:GLN:NE2	2.30	0.59
48:BI:56:ARG:HA	48:BI:65:PRO:HD2	1.84	0.59
54:BF:91:LYS:HD3	61:Bg:6:GLU:HG2	1.83	0.59
1:1:230:G:OP1	42:Be:21:ARG:NH1	2.35	0.59
1:1:314:4AC:O7	42:Be:50:ARG:NH2	2.36	0.59
1:1:2430:G:H3'	1:1:2431:C:C6	2.37	0.59
4:H:131:LYS:NZ	4:H:224:GLU:O	2.35	0.59
31:AT:9:ARG:HG3	32:AO:88:GLY:HA2	1.84	0.59
31:AT:11:TYR:HE2	31:AT:27:LEU:HD11	1.67	0.59
1:1:785:G:H5''	1:1:2259:U:H5''	1.84	0.59
1:1:2878:G:OP2	1:1:2962:C:O2'	2.19	0.59
15:AK:55:GLU:HG2	15:AK:56:ILE:HG23	1.85	0.59
1:1:447:A:N7	1:1:500:U:O2'	2.35	0.59
1:1:2305:C:H2'	1:1:2306:C:H6	1.68	0.59
4:H:152:ALA:HB2	4:H:210:LEU:HD11	1.85	0.59
12:AH:11:ILE:HD13	15:AK:34:GLU:HG3	1.84	0.59
1:1:772:U:H2'	1:1:773:C:C6	2.36	0.59
2:2:1380:OMU:HM22	2:2:1381:C:H5'	1.85	0.59
56:BP:19:ARG:NH2	56:BP:38:GLU:OE1	2.25	0.59
1:1:2944:C:O2'	1:1:2946:C:OP2	2.15	0.59
21:AR:74:ASN:HD21	21:AR:80:ALA:H	1.49	0.59
28:AZ:36:LYS:HB2	28:AZ:43:LYS:HB3	1.84	0.59
35:BO:34:ARG:NH1	35:BO:105:ASP:OD2	2.35	0.59
1:1:913:C:H2'	1:1:914:G:H8	1.68	0.59
1:1:1116:G:H2'	1:1:1117:C:C6	2.37	0.59
1:1:2340:G:H1'	1:1:2341:G:C8	2.38	0.59
1:1:2963:A:O2'	1:1:2964:G:O4'	2.20	0.59
4:H:384:PHE:HD1	17:AM:96:PRO:HG3	1.68	0.59
6:AB:166:LEU:O	6:AB:170:ILE:HG12	2.03	0.59
55:BZ:40:ASN:HB2	55:BZ:66:THR:HA	1.83	0.59
2:2:1075:G:O2'	22:AS:6:GLN:NE2	2.36	0.58
18:AN:74:ARG:NH1	18:AN:85:THR:OG1	2.36	0.58
1:1:209:G:O2'	46:BW:40:ASN:ND2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1577:A:H62	50:BQ:36:ILE:HG21	1.67	0.58
2:2:511:4AC:O2'	2:2:515:U:OP1	2.21	0.58
4:H:177:VAL:HG21	4:H:210:LEU:HD22	1.85	0.58
1:1:340:C:H2'	1:1:341:4AC:H6	1.84	0.58
2:2:1242:A:N3	2:2:1300:C:O2'	2.35	0.58
5:AA:27:PHE:HB3	5:AA:156:LYS:HD3	1.86	0.58
56:BP:36:ARG:NH1	56:BP:120:GLU:OE2	2.26	0.58
1:1:1146:C:H2'	1:1:1147:C:H6	1.68	0.58
2:2:609:A:N7	13:AI:107:SER:HA	2.18	0.58
2:2:757:A:C8	4:H:307:LEU:HD11	2.39	0.58
38:BL:77:THR:HB	38:BL:115:THR:HG23	1.86	0.58
1:1:1710:C:H2'	1:1:1711:G:H8	1.69	0.58
1:1:2272:C:OP1	1:1:2686:G:O2'	2.22	0.58
1:1:2377:C:N4	1:1:2394:G:H1	1.99	0.58
1:1:2823:C:H2'	1:1:2824:G:C8	2.38	0.58
1:1:2455:A:H4'	1:1:2456:C:O5'	2.04	0.58
10:AF:218:ILE:HA	10:AF:223:ILE:HG12	1.86	0.58
46:BW:1:MET:N	46:BW:50:ASP:OD2	2.33	0.58
1:1:418:A:H2'	1:1:419:G:H8	1.66	0.58
1:1:2504:A:O5'	49:BR:2:VAL:N	2.37	0.58
2:2:681:G:H2'	2:2:682:A:C8	2.38	0.58
37:B5:45:ARG:NH2	37:B5:66:ALA:O	2.37	0.58
2:2:1265:C:O2'	15:AK:37:GLU:OE2	2.15	0.58
12:AH:44:LEU:HD11	15:AK:40:ILE:HG13	1.86	0.58
36:BC:291:LYS:HG2	36:BC:298:GLU:HG2	1.86	0.58
38:BL:38:GLY:HA2	38:BL:43:ASN:HB3	1.85	0.58
30:B4:6:TYR:OH	30:B4:54:ALA:O	2.22	0.58
30:B4:61:GLU:OE1	30:B4:61:GLU:N	2.37	0.58
1:1:1317:G:H2'	1:1:1318:G:H8	1.69	0.58
1:1:1550:4AC:OP1	50:BQ:8:ARG:NH1	2.36	0.58
1:1:2827:G:N2	1:1:2830:A:OP2	2.29	0.58
1:1:2373:G:N2	1:1:2397:G:N3	2.52	0.57
9:AE:36:PRO:HD2	9:AE:84:PRO:HG2	1.85	0.57
43:BE:11:ILE:HG21	43:BE:173:VAL:HG11	1.86	0.57
1:1:1842:A:H2'	1:1:1843:A:C8	2.39	0.57
2:2:951:C:O2	19:AP:12:ARG:NH1	2.37	0.57
1:1:1703:G:OP2	59:Bd:32:LYS:NZ	2.37	0.57
2:2:203:A:H2'	2:2:204:G:C8	2.39	0.57
2:2:907:A:H2'	2:2:908:C:H6	1.68	0.57
2:2:1499:G:H2'	2:2:1500:A:H8	1.68	0.57
1:1:116:G:H2'	1:1:117:G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:520:G:OP1	18:AN:38:LYS:NZ	2.36	0.57
20:AQ:25:TRP:CE2	25:AW:64:LEU:HD21	2.40	0.57
3:3:42:U:H3	43:BE:81:THR:HG22	1.69	0.57
11:AG:10:ASP:HB3	11:AG:123:LEU:HD12	1.85	0.57
12:AH:6:SER:HB3	23:AU:143:ILE:HD11	1.86	0.57
14:AJ:83:ASN:ND2	14:AJ:96:THR:OG1	2.36	0.57
25:AW:59:LYS:NZ	25:AW:60:ILE:O	2.37	0.57
2:2:1042:G:N2	2:2:1045:A:OP2	2.31	0.57
35:BO:75:GLY:HA2	35:BO:171:TYR:HE1	1.69	0.57
65:Bk:49:LYS:HG3	65:Bk:50:PRO:HD2	1.87	0.57
30:BG:40:THR:HG22	30:BG:66:LEU:HD21	1.87	0.57
2:2:1289:U:O2'	2:2:1334:A:N3	2.35	0.57
39:Bf:9:LYS:NZ	39:Bf:51:GLU:OXT	2.37	0.57
2:2:162:G:O2'	11:AG:120:ASN:ND2	2.38	0.57
14:AJ:67:ASP:HB3	14:AJ:124:LEU:HD12	1.87	0.57
1:1:889:U:H2'	1:1:890:G:C8	2.40	0.57
1:1:1441:A:OP1	34:BY:114:LYS:NZ	2.38	0.57
2:2:1177:OMU:HM22	2:2:1178:A:H5'	1.86	0.57
9:AE:185:VAL:HG21	9:AE:230:ALA:HB1	1.85	0.57
1:1:532:C:H2'	1:1:533:4AC:H6	1.87	0.56
1:1:1667:4AC:H2'	1:1:1668:G:H8	1.70	0.56
9:AE:88:MET:N	9:AE:102:VAL:O	2.38	0.56
24:AV:72:TYR:CE1	24:AV:81:ILE:HD11	2.39	0.56
27:AY:38:TRP:HE1	27:AY:49:LYS:HB3	1.69	0.56
33:BB:202:HIS:HD2	33:BB:204:PHE:H	1.52	0.56
1:1:349:G:N2	1:1:357:4AC:O2	2.30	0.56
1:1:1612:A:H2'	1:1:1613:A:C8	2.40	0.56
2:2:1052:C:H2'	2:2:1053:A:H8	1.70	0.56
4:H:312:GLY:HA3	4:H:339:THR:HG22	1.87	0.56
4:H:385:ILE:O	4:H:385:ILE:HG13	2.05	0.56
43:BE:47:MET:HE1	43:BE:137:MET:HE1	1.87	0.56
1:1:100:G:O2'	1:1:101:U:H5'	2.05	0.56
1:1:229:4AC:O2'	42:Be:21:ARG:HG2	2.04	0.56
2:2:145:G:H2'	2:2:146:A:C8	2.40	0.56
9:AE:106:ARG:NE	9:AE:193:VAL:O	2.37	0.56
24:AV:19:ILE:HD11	24:AV:40:LEU:HD13	1.88	0.56
47:Bi:31:LYS:HG2	47:Bi:69:LEU:HD21	1.85	0.56
1:1:908:A:H2'	1:1:909:C:C6	2.41	0.56
1:1:1943:G:O2'	1:1:2232:U:O4	2.20	0.56
2:2:1375:G:N7	4:H:366:ARG:NH2	2.46	0.56
1:1:705:A:H2'	1:1:706:G:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1416:C:H2'	2:2:1417:U:C6	2.40	0.56
2:2:1491:U:H2'	2:2:1492:A:C8	2.38	0.56
43:BE:185:GLU:HG3	43:BE:186:GLU:HG2	1.88	0.56
1:1:720:A:H2'	1:1:721:A:C8	2.40	0.56
1:1:1266:G:N2	64:BI:43:SER:HB2	2.21	0.56
9:AE:15:ALA:O	9:AE:23:ARG:NH2	2.38	0.56
30:A3:83:LYS:HE2	30:A3:95:ALA:HB1	1.88	0.56
2:2:270:U:OP1	14:AJ:30:ARG:NH1	2.30	0.56
35:BO:48:ILE:HG21	35:BO:99:ILE:HD13	1.87	0.56
14:AJ:42:LYS:HB3	14:AJ:59:ALA:HB3	1.88	0.56
40:BU:84:ARG:NE	40:BU:90:GLU:OE2	2.38	0.56
1:1:457:C:H2'	1:1:458:4AC:H6	1.87	0.56
6:AB:48:THR:OG1	6:AB:155:PRO:O	2.24	0.56
14:AJ:103:THR:OG1	14:AJ:106:GLY:O	2.23	0.56
24:AV:72:TYR:OH	24:AV:82:GLU:OE1	2.23	0.56
1:1:431:G:OP2	1:1:431:G:H8	1.89	0.56
2:2:1069:OMG:HM22	2:2:1070:A:H5'	1.88	0.56
12:AH:16:LYS:HE2	12:AH:22:SER:HB2	1.88	0.56
36:BC:74:GLU:OE1	36:BC:310:TYR:OH	2.17	0.56
2:2:1201:A:H4'	32:AO:139:GLN:HA	1.88	0.55
32:AO:65:ILE:HG12	32:AO:72:HIS:ND1	2.20	0.55
60:BN:83:HIS:HD2	60:BN:136:ARG:HE	1.54	0.55
1:1:1739:G:HO2'	1:1:1816:U:HO2'	1.47	0.55
14:AJ:63:ALA:HB2	14:AJ:77:ILE:HD11	1.87	0.55
6:AB:120:PRO:HB3	6:AB:127:MET:HE1	1.86	0.55
1:1:1415:C:OP2	34:BY:118:ARG:NH2	2.40	0.55
1:1:1734:G:H2'	1:1:1735:G:C8	2.41	0.55
1:1:1998:A:OP2	50:BQ:71:LYS:HE2	2.06	0.55
2:2:684:C:O2'	2:2:701:C:O4'	2.20	0.55
4:H:121:ARG:NH1	4:H:121:ARG:O	2.37	0.55
50:BQ:43:ARG:O	50:BQ:47:GLU:HG2	2.07	0.55
1:1:107:G:N2	1:1:112:A:H8	1.93	0.55
2:2:1292:A:O2'	31:AT:69:ASP:OD2	2.16	0.55
9:AE:117:GLU:OE1	9:AE:117:GLU:N	2.33	0.55
31:AT:26:LYS:HA	31:AT:33:ARG:HD3	1.87	0.55
43:BE:120:HIS:HD2	43:BE:135:PHE:H	1.53	0.55
1:1:776:G:H2'	1:1:2270:C:C5	2.41	0.55
2:2:1415:U:H4'	51:BV:62:GLN:O	2.05	0.55
1:1:462:G:H21	1:1:485:A:H62	1.55	0.55
1:1:1015:A:H5'	33:BB:176:GLY:HA2	1.89	0.55
1:1:1575:A:H2'	1:1:1576:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1942:G:OP1	63:BJ:86:ARG:NH1	2.38	0.55
1:1:2314:U:H2'	1:1:2315:U:C6	2.41	0.55
1:1:2533:G:O2'	43:BE:109:GLU:OE1	2.18	0.55
3:3:91:G:N2	3:3:94:A:OP2	2.37	0.55
12:AH:70:LYS:HG3	12:AH:162:LEU:HB3	1.87	0.55
37:B5:69:GLU:OE1	37:B5:69:GLU:N	2.37	0.55
12:AH:8:ARG:NH2	23:AU:10:ASP:OD2	2.37	0.55
34:BY:75:ILE:HD12	34:BY:112:ASN:HD22	1.72	0.55
51:BV:46:ASN:HD22	51:BV:47:PRO:HD2	1.71	0.55
2:2:121:U:H2'	2:2:122:C:C6	2.42	0.55
30:BG:36:THR:O	30:BG:40:THR:HG23	2.06	0.55
53:BD:226:GLY:H	53:BD:229:HIS:HD2	1.54	0.55
2:2:183:U:H2'	2:2:184:G:H8	1.71	0.55
2:2:908:C:C2	2:2:909:A:C8	2.95	0.55
2:2:1152:G:N2	2:2:1155:G:OP2	2.40	0.55
8:AD:58:LEU:HD13	8:AD:70:ARG:HA	1.89	0.55
57:BM:41:ARG:HD3	57:BM:42:PRO:HD2	1.89	0.55
1:1:360:A:H2'	1:1:361:A:C8	2.41	0.54
1:1:1006:G:H2'	1:1:1007:C:C6	2.42	0.54
1:1:2073:G:OP1	33:BB:54:ARG:NH2	2.37	0.54
6:AB:102:THR:OG1	10:AF:45:LYS:NZ	2.40	0.54
1:1:493:G:H4'	40:BU:3:LEU:HD12	1.88	0.54
1:1:801:C:H2'	1:1:802:4AC:H6	1.90	0.54
1:1:1348:G:N1	1:1:1349:U:O4	2.40	0.54
1:1:2166:U:H4'	4:H:75:PRO:HB2	1.89	0.54
3:3:98:G:H2'	3:3:99:G:H8	1.72	0.54
4:H:287:GLU:OE1	4:H:290:ARG:NH2	2.41	0.54
8:AD:142:TYR:OH	8:AD:148:GLU:OE2	2.19	0.54
46:BW:1:MET:HG3	46:BW:6:ILE:HD11	1.89	0.54
55:BZ:61:TYR:OH	55:BZ:64:GLU:OE2	2.25	0.54
1:1:102:C:N3	1:1:103:C:C5	2.74	0.54
1:1:529:G:OP2	57:BM:44:ARG:NH1	2.39	0.54
1:1:829:4AC:OP2	53:BD:111:ARG:NH2	2.40	0.54
1:1:670:G:OP1	58:BS:65:ARG:NH1	2.39	0.54
2:2:579:C:O2'	8:AD:72:GLN:NE2	2.40	0.54
5:AA:93:ILE:HG23	5:AA:123:MET:HE1	1.88	0.54
9:AE:154:GLU:OE1	9:AE:154:GLU:N	2.41	0.54
27:AY:6:LYS:HG3	27:AY:7:LEU:HG	1.88	0.54
52:Bj:2:LYS:HG2	52:Bj:92:VAL:HG21	1.89	0.54
1:1:2363:G:H2'	1:1:2364:G:H8	1.73	0.54
2:2:37:C:H2'	2:2:38:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:30:C:H5'	43:BE:149:ARG:HD3	1.90	0.54
9:AE:87:ILE:HG23	9:AE:104:PRO:HD3	1.89	0.54
10:AF:224:VAL:HG11	10:AF:228:ALA:HA	1.88	0.54
31:AT:72:VAL:HG11	31:AT:98:MET:HB3	1.88	0.54
1:1:351:G:OP2	1:1:353:C:N4	2.39	0.54
28:AZ:70:GLU:OE2	28:AZ:77:ASN:N	2.40	0.54
30:A3:70:CYS:HA	30:A3:75:ILE:HD12	1.89	0.54
50:BQ:7:GLN:OE1	50:BQ:7:GLN:N	2.40	0.54
1:1:32:G:H2'	1:1:33:G:H8	1.71	0.54
1:1:252:U:O2'	45:BT:2:ASP:N	2.41	0.54
2:2:907:A:H2'	2:2:908:C:C6	2.42	0.54
2:2:1365:U:H2'	2:2:1366:G:C8	2.43	0.54
4:H:196:GLY:O	4:H:202:LYS:NZ	2.41	0.54
6:AB:4:GLU:HG3	6:AB:5:TYR:CD1	2.42	0.54
41:Bb:67:SER:O	41:Bb:72:ARG:NH1	2.40	0.54
2:2:687:C:H3'	2:2:688:A:H2'	1.90	0.54
32:AO:110:ARG:HD2	32:AO:121:GLU:HG2	1.90	0.54
40:BU:28:ALA:HA	40:BU:45:PRO:HA	1.89	0.54
1:1:757:G:O2'	1:1:1478:G:OP1	2.26	0.54
1:1:1574:C:H2'	1:1:1575:A:C8	2.43	0.54
1:1:2305:C:H2'	1:1:2306:C:C6	2.42	0.54
1:1:2377:C:N3	1:1:2394:G:N2	2.55	0.54
23:AU:33:PRO:HB3	32:AO:41:ARG:HG2	1.89	0.54
1:1:952:U:H2'	1:1:953:G:O4'	2.08	0.54
2:2:1183:C:H2'	2:2:1184:4AC:H6	1.90	0.54
31:AT:98:MET:HG3	31:AT:106:PHE:CZ	2.43	0.54
1:1:1421:C:H2'	1:1:1422:A:H8	1.70	0.53
1:1:1769:A:N1	1:1:1831:G:O2'	2.40	0.53
1:1:2351:C:H5''	1:1:2387:G:N2	2.23	0.53
2:2:874:G:OP1	29:A0:24:ARG:NH2	2.40	0.53
2:2:893:G:H2'	2:2:894:G:C8	2.43	0.53
4:H:380:TYR:HD1	12:AH:146:TYR:HA	1.73	0.53
28:AZ:117:MET:HB3	28:AZ:148:GLN:NE2	2.23	0.53
60:BN:21:GLU:OE1	60:BN:21:GLU:N	2.35	0.53
1:1:1227:G:H5''	41:Bb:55:LYS:HB2	1.90	0.53
1:1:1481:G:N2	1:1:1484:A:OP2	2.36	0.53
1:1:1842:A:H2'	1:1:1843:A:H8	1.73	0.53
28:AZ:188:ARG:HG3	28:AZ:192:GLU:HG3	1.89	0.53
57:BM:76:TRP:CD1	57:BM:76:TRP:H	2.25	0.53
60:BN:102:GLY:H	60:BN:105:ALA:HB2	1.73	0.53
1:1:3014:C:H2'	1:1:3015:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:416:C:H5''	8:AD:119:ARG:HD2	1.90	0.53
1:1:32:G:H2'	1:1:33:G:C8	2.43	0.53
1:1:197:G:O6	40:BU:111:ARG:NH1	2.41	0.53
9:AE:174:LEU:HD12	9:AE:175:GLU:HB2	1.90	0.53
28:AZ:134:GLY:HA3	28:AZ:176:ILE:HG12	1.90	0.53
43:BE:5:ILE:HB	43:BE:8:ARG:HB2	1.90	0.53
1:1:964:A:O2'	1:1:966:A:OP2	2.25	0.53
2:2:24:U:H2'	2:2:25:C:C6	2.43	0.53
2:2:433:C:H2'	2:2:434:U:C6	2.43	0.53
2:2:695:A:H2'	2:2:696:A:C8	2.43	0.53
2:2:1415:U:H2'	2:2:1416:C:C6	2.44	0.53
2:2:1416:C:H2'	2:2:1417:U:H6	1.74	0.53
3:3:48:C:H4'	35:BO:112:VAL:HG21	1.89	0.53
13:AI:28:LYS:HB3	13:AI:29:PRO:HD3	1.90	0.53
1:1:567:A:H1'	1:1:2121:A:C2	2.43	0.53
1:1:1413:C:H2'	1:1:1414:C:H6	1.73	0.53
2:2:154:G:H21	11:AG:118:GLN:HE22	1.57	0.53
2:2:688:A:H4'	2:2:689:G:O5'	2.08	0.53
39:Bf:20:ASN:HD21	39:Bf:42:ARG:H	1.56	0.53
9:AE:32:PRO:HG3	9:AE:44:PRO:HD3	1.91	0.53
27:AY:22:CYS:HB2	27:AY:25:CYS:HB2	1.91	0.53
31:AT:64:ARG:HG2	31:AT:82:TYR:HB2	1.90	0.53
54:BF:110:ILE:HB	54:BF:120:ARG:HB2	1.90	0.53
60:BN:56:GLN:HE21	60:BN:125:ARG:HE	1.56	0.53
63:BJ:84:ARG:NH1	63:BJ:121:PRO:O	2.37	0.53
1:1:102:C:C2	1:1:103:C:C5	2.97	0.53
1:1:398:U:H2'	1:1:399:U:H6	1.74	0.53
1:1:855:C:H2'	1:1:856:G:O4'	2.09	0.53
1:1:2650:G:H2'	1:1:2651:C:H6	1.74	0.53
2:2:443:G:O2'	24:AV:30:THR:O	2.26	0.53
1:1:569:C:O2'	1:1:2119:A:N6	2.42	0.53
1:1:2535:G:H22	1:1:2543:U:H3	1.57	0.53
2:2:970:A:H3'	2:2:971:G:H8	1.73	0.53
8:AD:59:LEU:HG	8:AD:89:LEU:HD12	1.91	0.53
9:AE:172:GLU:N	9:AE:172:GLU:OE1	2.42	0.53
49:BR:89:HIS:HD2	49:BR:91:VAL:H	1.56	0.53
1:1:2281:G:OP1	48:BI:77:ARG:NH2	2.37	0.53
1:1:2353:C:H2'	1:1:2354:A:H8	1.74	0.53
2:2:630:A:OP1	5:AA:133:SER:OG	2.14	0.53
30:A3:18:LYS:NZ	30:A3:113:GLU:OE2	2.42	0.53
32:AO:93:LEU:HD23	32:AO:97:LYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BC:57:GLU:HG2	36:BC:345:PRO:HG3	1.91	0.53
48:BI:6:ALA:HA	48:BI:9:LEU:HD12	1.91	0.53
58:BS:14:PRO:O	58:BS:105:LYS:NZ	2.29	0.53
1:1:1111:G:O2'	1:1:1168:G:O6	2.23	0.52
1:1:1847:C:H2'	1:1:1848:U:H6	1.73	0.52
1:1:2471:A:H2'	1:1:2472:G:C8	2.44	0.52
1:1:2635:G:O2'	1:1:2636:C:O5'	2.28	0.52
2:2:964:G:H22	2:2:1186:A:P	2.31	0.52
20:AQ:149:ASP:HB3	20:AQ:152:GLN:HG3	1.90	0.52
36:BC:86:TYR:OH	36:BC:181:GLU:OE2	2.19	0.52
1:1:2402:G:H5''	1:1:2411:A:C6	2.44	0.52
1:1:2522:U:H2'	1:1:2523:C:C6	2.44	0.52
3:3:98:G:H2'	3:3:99:G:C8	2.44	0.52
33:BB:122:VAL:HG21	33:BB:129:ALA:HB2	1.91	0.52
37:B5:18:ALA:HB3	59:Bd:67:PRO:HG2	1.91	0.52
49:BR:45:ILE:H	49:BR:59:HIS:CD2	2.27	0.52
55:BZ:28:LYS:HE3	55:BZ:52:TYR:CZ	2.45	0.52
1:1:2130:A:H2'	1:1:2131:A:C8	2.44	0.52
2:2:163:G:H2'	2:2:164:G:H8	1.74	0.52
14:AJ:81:ILE:HG22	14:AJ:82:GLU:HG2	1.91	0.52
37:B5:8:ARG:NH1	37:B5:56:LEU:O	2.38	0.52
53:BD:19:PRO:HB2	53:BD:21:VAL:HG12	1.90	0.52
2:2:976:A:N6	2:2:1001:A:O4'	2.43	0.52
24:AV:50:THR:O	24:AV:50:THR:OG1	2.27	0.52
34:BY:69:ARG:NH2	34:BY:94:GLU:OE2	2.38	0.52
1:1:379:G:O6	30:BG:37:ASN:ND2	2.42	0.52
1:1:1331:C:H2'	1:1:1332:A:C8	2.45	0.52
1:1:2827:G:H4'	4:H:66:LYS:HD3	1.91	0.52
2:2:1341:C:OP1	15:AK:120:ASN:N	2.42	0.52
4:H:189:PRO:HB2	4:H:192:LYS:HE3	1.91	0.52
9:AE:164:VAL:HG22	9:AE:176:VAL:HG12	1.92	0.52
28:AZ:126:ARG:HG3	28:AZ:185:PRO:HA	1.92	0.52
1:1:67:C:OP2	1:1:68:U:O2'	2.26	0.52
1:1:1140:G:O2'	1:1:1143:A:N7	2.41	0.52
1:1:2559:A:H2'	1:1:2560:G:H8	1.75	0.52
2:2:1045:A:OP1	10:AF:102:HIS:NE2	2.38	0.52
2:2:1309:C:O2'	12:AH:175:ARG:NH1	2.42	0.52
2:2:1434:U:H2'	2:2:1435:C:C6	2.44	0.52
33:BB:74:PRO:HG2	33:BB:77:LEU:HB2	1.91	0.52
54:BF:55:ILE:HD11	54:BF:75:ILE:HD12	1.91	0.52
57:BM:31:ARG:NH1	57:BM:122:ASP:OD2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:187:ILE:O	4:H:190:ARG:HG2	2.09	0.52
5:AA:52:THR:HG22	5:AA:54:LYS:H	1.73	0.52
15:AK:34:GLU:HG2	23:AU:146:GLU:HB2	1.92	0.52
16:AL:3:LYS:HB2	16:AL:101:ILE:HD11	1.91	0.52
28:AZ:37:LYS:NZ	28:AZ:76:GLU:OE2	2.34	0.52
34:BY:59:ILE:HA	34:BY:148:ASN:HD21	1.75	0.52
1:1:2367:G:H2'	1:1:2368:G:H8	1.75	0.52
9:AE:106:ARG:NH2	9:AE:191:LYS:O	2.42	0.52
11:AG:76:PRO:C	11:AG:110:ASN:HD21	2.17	0.52
16:AL:3:LYS:HA	16:AL:76:GLU:HA	1.91	0.52
26:AX:36:ASP:OD2	26:AX:39:ARG:NH1	2.43	0.52
1:1:1077:C:H5'	1:1:2662:A:O2'	2.10	0.52
1:1:1166:C:H4'	35:BO:5:PRO:HB2	1.92	0.52
1:1:1283:A:H2'	1:1:1284:A:H8	1.74	0.52
1:1:2347:G:N2	1:1:2422:U:O2	2.42	0.52
2:2:223:G:H2'	2:2:224:G:H8	1.75	0.52
20:AQ:54:LEU:HD13	20:AQ:60:ILE:HD11	1.92	0.52
1:1:2050:U:H2'	1:1:2051:C:H6	1.75	0.52
1:1:2823:C:H2'	1:1:2824:G:H8	1.75	0.52
2:2:37:C:H2'	2:2:38:A:C8	2.45	0.52
2:2:579:C:H2'	2:2:580:A:C8	2.44	0.52
2:2:1501:U:H2'	2:2:1502:C:C6	2.44	0.52
5:AA:50:GLU:OE2	5:AA:66:LYS:NZ	2.42	0.52
32:AO:46:ASP:HB3	32:AO:49:MET:HB2	1.92	0.52
36:BC:68:MET:HE3	36:BC:69:PRO:HD2	1.92	0.52
1:1:90:C:H2'	1:1:91:4AC:H6	1.93	0.51
1:1:617:G:N2	1:1:620:A:OP2	2.33	0.51
1:1:795:U:H2'	1:1:796:C:C6	2.45	0.51
1:1:2858:U:H3	1:1:3007:A:H62	1.58	0.51
2:2:204:G:O2'	14:AJ:64:ASN:ND2	2.42	0.51
2:2:836:A:H5'	2:2:1043:U:C5	2.44	0.51
2:2:1296:C:OP1	31:AT:110:ARG:NH2	2.40	0.51
2:2:1476:A:H2'	2:2:1477:G:C8	2.46	0.51
56:BP:72:GLY:O	56:BP:92:LYS:NZ	2.35	0.51
1:1:508:C:H2'	1:1:509:A:C8	2.45	0.51
1:1:1848:U:H2'	1:1:1849:C:C6	2.44	0.51
1:1:1848:U:H2'	1:1:1849:C:H6	1.74	0.51
1:1:2193:A:C6	63:BJ:41:ILE:HG13	2.44	0.51
1:1:2338:G:H2'	1:1:2339:C:C6	2.45	0.51
14:AJ:21:ARG:NH2	14:AJ:27:GLU:OE2	2.43	0.51
64:BL:67:ASP:HB3	64:BL:70:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:763:C:H2'	1:1:764:A:C8	2.46	0.51
1:1:1841:A:H2'	1:1:1842:A:C8	2.45	0.51
2:2:62:C:H2'	2:2:361:C:H41	1.75	0.51
2:2:136:C:OP1	9:AE:76:ARG:NH2	2.43	0.51
2:2:687:C:O2'	5:AA:101:THR:O	2.27	0.51
2:2:783:A:OP1	2:2:1495:G:O2'	2.27	0.51
2:2:861:G:O2'	2:2:877:G:O6	2.24	0.51
2:2:1167:G:OP2	28:AZ:131:ARG:NH2	2.43	0.51
2:2:1386:C:H2'	2:2:1387:A:C8	2.45	0.51
6:AB:73:ARG:NH1	6:AB:119:ASP:OD2	2.38	0.51
9:AE:126:ARG:HB3	9:AE:231:PHE:CE2	2.45	0.51
23:AU:26:ILE:O	23:AU:26:ILE:HG13	2.09	0.51
37:B5:31:ASN:HD21	55:BZ:25:ARG:HH11	1.57	0.51
2:2:1492:A:H2'	2:2:1493:C:C6	2.46	0.51
57:BM:33:GLU:O	57:BM:65:ARG:NH2	2.44	0.51
64:BL:4:LYS:HB3	64:BL:59:GLU:OE2	2.11	0.51
1:1:299:A:H5''	38:BL:37:ALA:HB2	1.91	0.51
1:1:806:G:OP1	53:BD:27:ARG:NH2	2.44	0.51
1:1:2816:U:O2'	4:H:197:GLU:HA	2.10	0.51
2:2:730:C:H2'	2:2:731:4AC:H6	1.91	0.51
53:BD:146:ASP:O	53:BD:149:GLN:HG2	2.10	0.51
1:1:2416:G:H2'	1:1:2417:C:C6	2.45	0.51
4:H:50:LEU:HG	4:H:55:ILE:HD11	1.92	0.51
10:AF:13:LEU:O	10:AF:27:LYS:NZ	2.36	0.51
36:BC:65:GLU:OE1	36:BC:353:THR:OG1	2.24	0.51
1:1:122:G:H2'	1:1:123:A:C8	2.45	0.51
1:1:210:C:H5'	46:BW:40:ASN:HD21	1.75	0.51
1:1:960:C:H2'	1:1:961:U:C6	2.45	0.51
1:1:1278:C:OP1	1:1:1281:C:N4	2.44	0.51
1:1:2351:C:H5''	1:1:2387:G:H21	1.75	0.51
1:1:2399:G:C2	1:1:2400:C:C5	2.99	0.51
2:2:1266:C:H2'	2:2:1267:G:H8	1.75	0.51
6:AB:70:VAL:HG12	6:AB:92:ILE:HB	1.92	0.51
12:AH:168:GLY:O	12:AH:172:LYS:HG2	2.10	0.51
24:AV:14:ILE:HD11	24:AV:81:ILE:HD13	1.92	0.51
30:A3:36:THR:O	30:A3:40:THR:OG1	2.22	0.51
60:BN:107:ARG:NH1	60:BN:108:TYR:OH	2.43	0.51
1:1:115:G:N3	1:1:115:G:H2'	2.26	0.51
1:1:431:G:H2'	1:1:432:A:H8	1.76	0.51
1:1:1011:C:H2'	1:1:1012:G:O4'	2.11	0.51
1:1:1939:G:O2'	1:1:2919:G:H4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:988:A:OP1	31:AT:50:LYS:NZ	2.37	0.51
2:2:1212:A:H2	2:2:1215:G:N3	2.08	0.51
35:BO:8:ARG:NH1	49:BR:23:ARG:O	2.44	0.51
1:1:2357:G:H1	1:1:2410:G:H1	1.56	0.51
2:2:483:G:H4'	2:2:485:C:C2	2.46	0.51
30:A3:107:ALA:H	30:A3:108:ARG:HE	1.58	0.51
30:A3:107:ALA:H	30:A3:108:ARG:HH21	1.59	0.51
40:BU:4:ASN:N	40:BU:4:ASN:OD1	2.44	0.51
1:1:250:U:H4'	1:1:251:A:OP1	2.11	0.51
1:1:2363:G:H2'	1:1:2364:G:C8	2.45	0.51
2:2:1375:G:H2'	2:2:1376:OMC:O4'	2.11	0.51
6:AB:181:GLU:OE1	6:AB:181:GLU:N	2.42	0.51
17:AM:31:THR:OG1	17:AM:37:GLU:O	2.19	0.51
33:BB:29:LYS:HG3	33:BB:118:GLY:HA3	1.93	0.51
48:BI:68:PRO:HB3	48:BI:73:GLU:HB3	1.93	0.51
1:1:595:A:O2'	53:BD:44:GLN:NE2	2.42	0.50
1:1:1706:G:H2'	1:1:1707:C:C6	2.46	0.50
2:2:96:C:H2'	2:2:97:A:C8	2.46	0.50
2:2:332:U:H2'	2:2:333:G:O4'	2.11	0.50
4:H:383:ARG:HD2	17:AM:24:ASN:HD22	1.75	0.50
35:BO:63:HIS:HD2	35:BO:65:ARG:HB2	1.76	0.50
1:1:1324:A:H4'	1:1:1325:A:H5''	1.93	0.50
1:1:1363:U:O2'	1:1:1364:C:OP1	2.28	0.50
2:2:122:C:OP1	2:2:571:C:O2'	2.29	0.50
2:2:343:U:H2'	2:2:344:C:H6	1.76	0.50
2:2:661:A:O3'	17:AM:52:ARG:NH1	2.44	0.50
2:2:1096:G:OP1	15:AK:20:ARG:NH2	2.43	0.50
2:2:1301:G:H2'	2:2:1302:C:C6	2.46	0.50
6:AB:99:GLY:HA2	6:AB:102:THR:HG22	1.93	0.50
6:AB:136:PRO:HG3	7:AC:30:PHE:HB3	1.92	0.50
20:AQ:68:ASP:HB3	20:AQ:71:ASN:O	2.11	0.50
31:AT:70:MET:HB3	31:AT:103:LEU:HD12	1.93	0.50
2:2:384:U:O2'	9:AE:28:TRP:O	2.28	0.50
2:2:891:U:H2'	2:2:892:U:C6	2.46	0.50
9:AE:96:THR:HB	9:AE:98:GLU:HG2	1.94	0.50
1:1:787:C:H2'	1:1:788:A:C8	2.47	0.50
1:1:2473:U:H2'	1:1:2474:U:C6	2.46	0.50
2:2:190:C:H2'	2:2:191:U:C6	2.46	0.50
2:2:1088:A:H4'	16:AL:36:GLY:HA3	1.94	0.50
7:AC:11:ILE:HG23	10:AF:39:ARG:HD3	1.93	0.50
1:1:703:U:OP1	30:B4:97:ALA:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:28:C:H2'	3:3:29:A:O4'	2.11	0.50
9:AE:57:LYS:NZ	24:AV:18:GLU:OE2	2.35	0.50
10:AF:140:SER:HA	10:AF:180:ILE:HG23	1.93	0.50
33:BB:42:ARG:HH12	33:BB:44:VAL:HG13	1.76	0.50
57:BM:101:GLU:OE2	57:BM:116:SER:OG	2.27	0.50
1:1:431:G:H2'	1:1:432:A:C8	2.47	0.50
1:1:1035:G:H5'	1:1:1036:G:OP1	2.11	0.50
1:1:1301:A:H4'	1:1:1302:G:H5'	1.93	0.50
1:1:1847:C:H2'	1:1:1848:U:C6	2.47	0.50
11:AG:87:LEU:HD11	11:AG:102:ARG:HB3	1.93	0.50
18:AN:32:ARG:HG2	18:AN:37:LEU:HD12	1.92	0.50
30:A3:32:ILE:HD11	30:A3:90:ALA:HB1	1.92	0.50
57:BM:157:ARG:HB2	57:BM:162:LEU:HB2	1.93	0.50
64:Bl:10:GLY:HA2	64:Bl:55:LYS:HG3	1.93	0.50
1:1:978:G:O2'	1:1:1014:G:H4'	2.11	0.50
1:1:2367:G:H2'	1:1:2368:G:C8	2.46	0.50
30:A3:66:LEU:O	30:A3:70:CYS:N	2.45	0.50
32:AO:5:ARG:NH2	32:AO:54:LEU:O	2.38	0.50
30:BG:61:GLU:OE2	57:BM:26:ARG:NH2	2.41	0.50
54:BF:92:VAL:HG22	54:BF:172:ILE:HG12	1.94	0.50
1:1:84:A:OP1	44:Ba:2:PRO:HD2	2.12	0.50
1:1:435:C:H2'	1:1:436:C:H6	1.77	0.50
1:1:2477:G:H2'	1:1:2478:C:H6	1.77	0.50
2:2:1123:C:H2'	2:2:1124:U:C6	2.46	0.50
4:H:115:ASP:O	4:H:119:LEU:HG	2.11	0.50
5:AA:46:ASN:HA	5:AA:70:GLN:HE21	1.77	0.50
13:AI:104:VAL:HG22	13:AI:125:LEU:HD23	1.94	0.50
17:AM:18:HIS:HB2	17:AM:29:HIS:HB3	1.93	0.50
17:AM:28:ILE:HD11	17:AM:101:ALA:HB1	1.94	0.50
22:AS:17:PHE:HZ	22:AS:61:LYS:HD3	1.77	0.50
25:AW:36:ARG:HA	25:AW:49:PRO:HD3	1.94	0.50
1:1:118:U:H2'	1:1:118:U:O2	2.12	0.50
1:1:264:G:OP1	1:1:403:G:O2'	2.27	0.50
1:1:478:G:H21	53:BD:174:LYS:HD3	1.77	0.50
1:1:1756:G:OP1	59:Bd:77:ARG:NH1	2.23	0.50
1:1:2311:A:H2'	1:1:2312:G:H8	1.73	0.50
11:AG:31:GLY:HA2	11:AG:111:THR:HG23	1.92	0.50
12:AH:156:ARG:NH2	26:AX:46:ARG:HH21	2.10	0.50
2:2:135:U:H2'	2:2:136:C:C6	2.46	0.49
2:2:1487:MA6:H93	2:2:1488:MA6:H92	1.93	0.49
4:H:95:THR:HG21	4:H:100:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:52:LEU:HD12	6:AB:154:ILE:HD13	1.94	0.49
10:AF:212:VAL:N	13:AI:70:ASN:HD21	2.06	0.49
1:1:107:G:C2	1:1:112:A:N7	2.75	0.49
1:1:787:C:H2'	1:1:788:A:H8	1.76	0.49
1:1:792:A:N1	1:1:1060:G:O2'	2.38	0.49
1:1:2304:C:H2'	1:1:2305:C:H6	1.75	0.49
1:1:2326:U:H2'	1:1:2327:G:H8	1.77	0.49
2:2:1207:G:H4'	15:AK:121:ARG:HH22	1.76	0.49
14:AJ:31:GLU:H	14:AJ:31:GLU:CD	2.20	0.49
26:AX:42:ARG:CZ	26:AX:66:GLU:HG2	2.42	0.49
33:BB:62:ARG:NH1	33:BB:68:GLU:OE1	2.45	0.49
30:B4:40:THR:HG22	30:B4:66:LEU:HD21	1.94	0.49
1:1:434:A:H2'	1:1:435:C:C6	2.46	0.49
1:1:658:G:H5''	1:1:661:C:H1'	1.94	0.49
1:1:788:A:H2'	1:1:789:OMG:H8	1.77	0.49
1:1:1210:U:H4'	60:BN:8:ILE:HG23	1.93	0.49
8:AD:155:ALA:HB3	8:AD:158:SER:HB2	1.94	0.49
12:AH:32:SER:OG	12:AH:157:ARG:NH2	2.39	0.49
38:BL:83:GLU:HA	56:BP:73:LYS:HD2	1.93	0.49
1:1:659:A:H5''	1:1:660:G:H3'	1.95	0.49
1:1:705:A:H2'	1:1:706:G:H8	1.77	0.49
1:1:1055:A2M:HM'2	1:1:1057:C:C6	2.47	0.49
1:1:1314:G:H2'	1:1:1315:U:C5	2.48	0.49
1:1:2382:C:H2'	1:1:2383:C:C6	2.47	0.49
2:2:157:A:H2'	2:2:158:A:O4'	2.13	0.49
2:2:1089:G:O4'	16:AL:38:ILE:HD11	2.12	0.49
4:H:37:LEU:HD11	4:H:49:VAL:HB	1.95	0.49
9:AE:3:ARG:HG3	9:AE:4:LYS:HG2	1.94	0.49
9:AE:30:VAL:HG21	9:AE:46:LEU:HD23	1.93	0.49
15:AK:97:GLU:HA	15:AK:100:ILE:HB	1.94	0.49
17:AM:39:ILE:HG21	17:AM:71:ALA:HA	1.93	0.49
36:BC:218:VAL:HG11	36:BC:324:VAL:HG13	1.94	0.49
1:1:133:G:H2'	1:1:134:C:C6	2.48	0.49
1:1:535:U:H2'	1:1:536:C:C6	2.47	0.49
1:1:889:U:H2'	1:1:890:G:H8	1.74	0.49
1:1:1998:A:H2'	1:1:1999:C:C6	2.48	0.49
1:1:2723:C:H5'	1:1:2802:G:H5''	1.94	0.49
30:A3:12:PRO:HB2	30:A3:15:LEU:HD13	1.94	0.49
43:BE:24:ARG:HH11	43:BE:146:PRO:HG3	1.77	0.49
43:BE:120:HIS:CD2	43:BE:135:PHE:H	2.30	0.49
45:BT:21:GLU:OE1	45:BT:21:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BK:69:GLU:HA	37:BK:72:LYS:HB3	1.94	0.49
1:1:1295:G:N2	60:BN:178:SER:OG	2.41	0.49
1:1:2128:U:H2'	1:1:2129:G:O4'	2.13	0.49
2:2:98:C:H2'	2:2:99:C:H6	1.76	0.49
2:2:223:G:H2'	2:2:224:G:C8	2.47	0.49
2:2:343:U:H2'	2:2:344:C:C6	2.47	0.49
12:AH:56:PHE:HB3	26:AX:50:ARG:HH21	1.77	0.49
13:AI:51:GLU:OE2	13:AI:62:ARG:NH1	2.44	0.49
13:AI:57:ARG:NH1	25:AW:9:PRO:HD2	2.28	0.49
23:AU:71:GLU:HA	23:AU:74:ARG:HB2	1.95	0.49
39:Bf:21:ARG:O	39:Bf:38:HIS:HE1	1.94	0.49
1:1:2265:U:H2'	1:1:2266:G:C8	2.47	0.49
1:1:2522:U:OP1	1:1:2614:G:O2'	2.30	0.49
1:1:2931:U:H2'	1:1:2932:C:C6	2.47	0.49
1:1:398:U:H2'	1:1:399:U:C6	2.47	0.49
1:1:1574:C:H2'	1:1:1575:A:H8	1.77	0.49
1:1:2050:U:H2'	1:1:2051:C:C6	2.48	0.49
1:1:2611:A:H2'	1:1:2612:A:C8	2.48	0.49
1:1:2693:C:H2'	1:1:2694:U:C6	2.48	0.49
2:2:428:C:H2'	2:2:429:A:H8	1.77	0.49
2:2:659:U:C4	4:H:383:ARG:HD3	2.47	0.49
2:2:1052:C:H2'	2:2:1053:A:C8	2.46	0.49
2:2:1420:U:O2'	2:2:1423:G:O6	2.16	0.49
12:AH:23:THR:HG21	12:AH:39:LEU:HD22	1.95	0.49
1:1:133:G:OP1	41:Bb:35:LYS:NZ	2.41	0.49
2:2:219:G:H21	2:2:222:A:H8	1.60	0.49
2:2:379:4AC:O2	2:2:400:G:N2	2.33	0.49
2:2:1415:U:H2'	2:2:1416:C:H6	1.78	0.49
22:AS:26:ARG:NH2	22:AS:62:GLU:OE2	2.39	0.49
23:AU:61:ARG:NH1	23:AU:76:TYR:OH	2.46	0.49
31:AT:28:LEU:O	31:AT:33:ARG:NH1	2.46	0.49
37:B5:9:ILE:HD13	37:B5:80:ILE:HG21	1.95	0.49
54:BF:8:ARG:NH1	54:BF:10:GLU:OE2	2.46	0.49
24:B6:40:LEU:HD12	24:B6:43:MET:HE2	1.95	0.49
60:BN:96:GLU:HG2	60:BN:120:ILE:HG21	1.95	0.49
30:B4:80:VAL:HG11	30:B4:86:LEU:HB2	1.95	0.49
1:1:2702:G:OP1	60:BN:71:ARG:NH2	2.46	0.49
2:2:109:C:O2	2:2:362:A:O2'	2.28	0.49
2:2:196:G:H2'	2:2:196:G:N3	2.28	0.49
2:2:1092:G:H5'	2:2:1254:A:O2'	2.12	0.49
8:AD:74:LEU:HD12	8:AD:78:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AF:132:GLU:HG3	10:AF:160:PRO:HG3	1.95	0.49
12:AH:44:LEU:HD12	12:AH:45:PRO:HD2	1.93	0.49
24:AV:23:ILE:HG23	24:AV:65:SER:HB2	1.95	0.49
35:BO:62:ALA:HB3	35:BO:90:ILE:HG12	1.95	0.49
60:BN:127:LYS:H	60:BN:130:GLN:NE2	2.11	0.49
1:1:796:C:H5''	53:BD:100:ILE:HG12	1.95	0.48
40:BU:44:LEU:HD21	40:BU:105:LEU:HD21	1.95	0.48
53:BD:35:VAL:HB	53:BD:234:THR:HG22	1.95	0.48
58:BS:60:PRO:HG2	58:BS:78:PHE:CZ	2.48	0.48
63:BJ:116:THR:C	63:BJ:136:ILE:HD11	2.37	0.48
1:1:2277:C:H2'	1:1:2278:A:C8	2.48	0.48
1:1:2850:A:H2'	1:1:2851:C:C6	2.47	0.48
2:2:183:U:H2'	2:2:184:G:C8	2.48	0.48
2:2:344:C:H2'	2:2:345:C:H6	1.78	0.48
2:2:1493:C:H2'	2:2:1494:G:C8	2.48	0.48
10:AF:167:ILE:O	10:AF:172:LYS:NZ	2.33	0.48
14:AJ:100:ILE:HD12	14:AJ:125:LEU:HD11	1.95	0.48
30:A3:53:ILE:HD11	30:A3:66:LEU:HD23	1.95	0.48
53:BD:149:GLN:NE2	53:BD:203:LYS:HG2	2.28	0.48
1:1:154:G:C5	1:1:155:G:C8	3.01	0.48
1:1:238:C:H4'	1:1:239:C:O5'	2.12	0.48
1:1:794:U:H2'	1:1:795:U:C6	2.47	0.48
1:1:1401:C:O2'	64:Bl:42:GLY:O	2.31	0.48
1:1:2356:C:N4	1:1:2357:G:O6	2.46	0.48
1:1:2375:A:N6	1:1:2396:G:O2'	2.46	0.48
2:2:344:C:H2'	2:2:345:C:C6	2.48	0.48
2:2:710:A:H2'	2:2:711:A:H8	1.78	0.48
4:H:119:LEU:HD13	4:H:260:LEU:HD11	1.95	0.48
10:AF:33:ASP:OD2	10:AF:35:HIS:ND1	2.36	0.48
1:1:228:C:HO2'	1:1:240:U:HO2'	1.60	0.48
1:1:895:A:H2'	1:1:896:G:O4'	2.13	0.48
1:1:1054:U:H2'	1:1:1055:A2M:H8	1.94	0.48
2:2:619:U:O4	2:2:719:G:O2'	2.25	0.48
63:BJ:33:SER:HB3	63:BJ:114:ARG:O	2.14	0.48
1:1:371:G:O2'	65:Bk:23:CYS:SG	2.65	0.48
1:1:788:A:H2'	1:1:789:OMG:C8	2.48	0.48
1:1:2066:A:H2'	1:1:2067:G:O4'	2.13	0.48
2:2:1025:5MC:H2'	2:2:1026:G:H8	1.77	0.48
2:2:1095:A:N3	2:2:1096:G:C8	2.82	0.48
2:2:1261:A:H2'	2:2:1262:A:C8	2.48	0.48
9:AE:164:VAL:HG13	9:AE:173:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AG:28:LYS:H	11:AG:28:LYS:HD3	1.78	0.48
12:AH:203:LYS:O	12:AH:207:ILE:HG22	2.13	0.48
36:BC:84:ARG:NE	36:BC:98:GLU:OE1	2.40	0.48
1:1:69:U:OP2	51:BV:51:LYS:NZ	2.35	0.48
1:1:382:C:H2'	1:1:383:C:H6	1.77	0.48
1:1:1317:G:H2'	1:1:1318:G:C8	2.48	0.48
1:1:2326:U:H2'	1:1:2327:G:C8	2.48	0.48
1:1:2416:G:H2'	1:1:2417:C:H6	1.79	0.48
6:AB:169:TRP:CD2	6:AB:192:VAL:HG22	2.48	0.48
16:AL:8:LEU:HB2	16:AL:71:ARG:HB2	1.96	0.48
23:AU:3:THR:OG1	23:AU:6:ASP:OD1	2.30	0.48
32:AO:68:ASP:OD1	32:AO:71:ALA:HB3	2.14	0.48
33:BB:28:VAL:HG11	33:BB:72:ILE:HG13	1.96	0.48
37:B5:70:GLU:OE1	37:B5:70:GLU:N	2.46	0.48
49:BR:18:LYS:HD3	49:BR:47:PRO:HD2	1.96	0.48
53:BD:125:ASP:OD2	24:B6:54:GLN:NE2	2.45	0.48
1:1:492:C:H2'	1:1:493:G:O4'	2.13	0.48
1:1:870:A:H62	56:BP:31:LYS:NZ	2.12	0.48
1:1:1110:G:N3	1:1:2499:A:H2'	2.28	0.48
1:1:1755:4AC:O7	1:1:1755:4AC:H5	2.14	0.48
1:1:2792:C:H2'	1:1:2793:A:C8	2.49	0.48
2:2:221:A:H8	2:2:221:A:OP2	1.97	0.48
2:2:426:G:H2'	2:2:427:G:C8	2.49	0.48
2:2:1133:U:H5''	22:AS:3:LYS:HD3	1.96	0.48
2:2:1417:U:O3'	11:AG:33:ARG:NH2	2.46	0.48
12:AH:88:ARG:O	12:AH:92:SER:HB3	2.14	0.48
1:1:117:G:N3	1:1:118:U:C6	2.82	0.48
1:1:360:A:H2'	1:1:361:A:H8	1.79	0.48
1:1:1667:4AC:H2'	1:1:1668:G:C8	2.47	0.48
1:1:1706:G:H2'	1:1:1707:C:H6	1.78	0.48
2:2:579:C:H2'	2:2:580:A:H8	1.79	0.48
2:2:911:G:OP1	12:AH:163:ARG:NH1	2.45	0.48
1:1:1577:A:N3	1:1:1577:A:H2'	2.29	0.48
1:1:2072:U:OP1	33:BB:21:SER:OG	2.23	0.48
2:2:287:G:OP2	21:AR:69:ARG:NH2	2.46	0.48
2:2:459:G:O2'	2:2:461:A:H1'	2.14	0.48
2:2:1121:C:O2	15:AK:16:ARG:NH1	2.47	0.48
4:H:24:SER:O	4:H:27:ILE:HG13	2.14	0.48
4:H:167:VAL:HG12	4:H:173:LEU:HA	1.96	0.48
5:AA:103:ARG:HE	5:AA:123:MET:HE2	1.79	0.48
15:AK:117:HIS:ND1	15:AK:122:SER:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BB:20:PRO:HG3	33:BB:23:ARG:HH21	1.79	0.48
30:BG:29:THR:HG21	30:BG:106:LYS:HB2	1.96	0.48
1:1:98:C:H6	1:1:98:C:H5''	1.78	0.48
1:1:304:U:OP1	57:BM:82:PRO:HG2	2.14	0.48
1:1:931:U:O2'	42:Be:47:ARG:NH2	2.45	0.48
1:1:1049:G:OP1	42:Be:53:LYS:NZ	2.47	0.48
1:1:1164:C:OP1	60:BN:19:ARG:NH1	2.46	0.48
1:1:2462:U:H2'	1:1:2463:A:C8	2.49	0.48
1:1:2534:G:O3'	43:BE:106:SER:HA	2.13	0.48
2:2:888:G:H2'	2:2:889:A:C8	2.49	0.48
9:AE:3:ARG:HE	9:AE:3:ARG:HB2	1.43	0.48
17:AM:39:ILE:HG23	17:AM:74:LYS:HD2	1.95	0.48
31:AT:5:GLU:CD	31:AT:5:GLU:H	2.22	0.48
37:B5:26:ASP:O	37:B5:33:VAL:HG22	2.13	0.48
64:Bl:72:ARG:HA	64:Bl:76:GLU:HB2	1.96	0.48
1:1:102:C:C4	1:1:103:C:N4	2.81	0.47
1:1:102:C:N3	1:1:103:C:C4	2.81	0.47
1:1:429:A:H1'	1:1:431:G:C8	2.48	0.47
1:1:1303:A:H1'	1:1:1304:C:H5'	1.95	0.47
1:1:2986:U:H1'	1:1:2987:A:H5''	1.95	0.47
2:2:724:U:H2'	2:2:725:G:O4'	2.13	0.47
4:H:63:ASP:OD2	4:H:65:THR:OG1	2.24	0.47
9:AE:166:MET:SD	9:AE:171:ARG:HA	2.54	0.47
12:AH:88:ARG:HB3	12:AH:91:ARG:HG3	1.95	0.47
14:AJ:91:ARG:HA	14:AJ:91:ARG:HH11	1.79	0.47
54:BF:108:VAL:HG23	54:BF:124:ILE:HD11	1.95	0.47
1:1:382:C:H2'	1:1:383:C:C6	2.48	0.47
1:1:1826:C:OP1	59:Bd:8:ARG:NH2	2.34	0.47
1:1:2591:A:H5''	49:BR:82:LYS:HE3	1.95	0.47
2:2:83:C:H2'	2:2:84:C:C6	2.48	0.47
2:2:645:C:H2'	2:2:646:C:H6	1.79	0.47
2:2:879:A:H2'	2:2:880:A:C8	2.49	0.47
3:3:9:G:OP1	35:BO:24:ARG:NH1	2.47	0.47
11:AG:12:LYS:HD3	11:AG:12:LYS:H	1.78	0.47
12:AH:172:LYS:HB2	12:AH:183:ALA:HB1	1.96	0.47
16:AL:93:ASP:OD1	16:AL:93:ASP:N	2.48	0.47
30:A3:12:PRO:HD2	30:A3:15:LEU:HD22	1.96	0.47
30:BG:82:SER:HB3	30:BG:85:GLU:HB2	1.95	0.47
1:1:285:A:OP2	42:Be:48:LYS:NZ	2.46	0.47
1:1:353:C:OP2	1:1:2628:C:O2'	2.27	0.47
1:1:564:G:H2'	1:1:2641:C:H5	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:683:A:O2'	1:1:769:C:H5''	2.14	0.47
1:1:696:A:H2'	1:1:697:A:C8	2.49	0.47
1:1:2504:A:H2'	1:1:2505:U:C6	2.49	0.47
2:2:119:C:H2'	2:2:120:G:H8	1.79	0.47
2:2:422:C:H3'	2:2:424:C:H42	1.79	0.47
2:2:1434:U:H2'	2:2:1435:C:H6	1.78	0.47
2:2:1485:G:N1	2:2:1488:MA6:OP2	2.44	0.47
4:H:156:MET:HE1	4:H:177:VAL:HG12	1.96	0.47
53:BD:128:LYS:HB2	53:BD:134:ILE:HD11	1.95	0.47
1:1:147:U:OP2	53:BD:186:MET:HG2	2.14	0.47
1:1:549:G:H5''	57:BM:95:SER:HB3	1.95	0.47
1:1:703:U:H5'	30:B4:36:THR:HG22	1.96	0.47
1:1:960:C:H2'	1:1:961:U:H6	1.79	0.47
1:1:1064:C:H2'	1:1:1065:4AC:H6	1.96	0.47
1:1:2001:4AC:O7	1:1:2001:4AC:H5	2.14	0.47
2:2:714:G:O2'	20:AQ:55:ARG:NH1	2.47	0.47
3:3:74:C:H2'	3:3:75:G:H8	1.79	0.47
6:AB:5:TYR:OH	6:AB:46:ARG:HG3	2.13	0.47
11:AG:63:ILE:HD13	11:AG:121:VAL:HG23	1.96	0.47
31:AT:52:ARG:O	31:AT:56:LYS:HG2	2.14	0.47
32:AO:20:GLN:NE2	32:AO:22:ARG:HE	2.11	0.47
62:Bc:8:LEU:HD11	62:Bc:25:LYS:HB2	1.96	0.47
1:1:113:G:C4	1:1:114:G:C8	3.03	0.47
1:1:845:C:H2'	1:1:846:C:C6	2.49	0.47
1:1:1303:A:O2'	1:1:1304:C:H6	1.96	0.47
1:1:2449:G:H2'	1:1:2450:G:H8	1.80	0.47
1:1:2758:C:OP1	54:BF:159:ARG:NH2	2.38	0.47
2:2:162:G:H2'	2:2:163:G:C8	2.49	0.47
2:2:445:G:OP2	24:AV:33:ARG:NH1	2.48	0.47
20:AQ:143:PRO:HG2	20:AQ:146:TRP:HB2	1.96	0.47
43:BE:34:VAL:HG23	43:BE:36:GLU:H	1.80	0.47
55:BZ:9:LYS:O	55:BZ:13:THR:OG1	2.30	0.47
1:1:102:C:OP2	1:1:102:C:H6	1.96	0.47
1:1:691:G:OP1	62:Bc:49:SER:OG	2.28	0.47
1:1:1735:G:H2'	1:1:1736:C:H6	1.79	0.47
1:1:2833:C:H5''	4:H:194:GLN:CB	2.44	0.47
2:2:567:C:OP1	13:AI:84:ARG:NH2	2.43	0.47
5:AA:88:LEU:HD11	5:AA:185:GLU:HG3	1.97	0.47
6:AB:52:LEU:HD21	6:AB:170:ILE:HG13	1.96	0.47
12:AH:62:HIS:ND1	12:AH:64:VAL:HG22	2.29	0.47
14:AJ:62:TYR:HE1	14:AJ:76:ARG:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AZ:54:VAL:HG11	28:AZ:82:VAL:HG21	1.97	0.47
44:Ba:43:ALA:O	44:Ba:87:ARG:NH2	2.46	0.47
50:BQ:100:ARG:O	50:BQ:104:LYS:HG3	2.14	0.47
1:1:117:G:C5	1:1:118:U:C5	3.02	0.47
1:1:422:C:H2'	1:1:423:C:H6	1.80	0.47
1:1:1173:C:H2'	1:1:1174:A:H8	1.80	0.47
1:1:1287:G:O3'	61:Bg:30:LYS:NZ	2.48	0.47
1:1:2804:A:OP2	1:1:2804:A:H8	1.98	0.47
1:1:2907:C:H2'	1:1:2908:4AC:H6	1.97	0.47
2:2:195:A:O2'	2:2:197:G:N7	2.44	0.47
2:2:382:A:H1'	2:2:447:A:H5'	1.97	0.47
2:2:908:C:H2'	2:2:909:A:H8	1.80	0.47
2:2:1345:G:O3'	15:AK:70:GLY:HA3	2.14	0.47
2:2:1350:U:H2'	2:2:1351:A:H8	1.79	0.47
2:2:1378:C:H2'	2:2:1379:G:C8	2.50	0.47
3:3:58:A:OP1	43:BE:163:ARG:NH1	2.48	0.47
3:3:115:G:H2'	3:3:116:C:C6	2.49	0.47
37:B5:2:PRO:HB3	55:BZ:30:GLY:HA3	1.95	0.47
56:BP:22:SER:OG	56:BP:27:VAL:O	2.31	0.47
57:BM:152:LYS:HG3	65:Bk:12:ARG:HA	1.96	0.47
1:1:618:U:O2'	42:Be:17:HIS:HD2	1.98	0.47
1:1:1152:C:H2'	1:1:1153:C:H6	1.79	0.47
2:2:190:C:O3'	9:AE:130:LYS:NZ	2.48	0.47
2:2:191:U:H2'	2:2:192:G:O4'	2.15	0.47
2:2:271:A:H2'	2:2:272:A:H8	1.79	0.47
2:2:485:C:H2'	2:2:486:A:O4'	2.14	0.47
2:2:1066:A:H4'	2:2:1067:A:O5'	2.15	0.47
2:2:1310:U:O2'	12:AH:85:PHE:O	2.30	0.47
18:AN:98:ASP:OD2	18:AN:144:LYS:NZ	2.47	0.47
37:B5:9:ILE:HD12	37:B5:58:GLU:HB2	1.97	0.47
38:BL:3:ARG:NH2	53:BD:103:GLU:OE2	2.48	0.47
1:1:45:G:H2'	1:1:46:C:C6	2.49	0.47
1:1:53:G:OP1	14:AJ:91:ARG:NH1	2.47	0.47
1:1:120:A:H5''	1:1:120:A:C8	2.49	0.47
1:1:1498:C:H2'	1:1:1499:G:H8	1.80	0.47
1:1:1525:U:H2'	1:1:1526:A:H8	1.79	0.47
1:1:2164:U:H2'	1:1:2165:C:C6	2.49	0.47
1:1:2712:C:H2'	1:1:2713:G:O4'	2.14	0.47
2:2:82:C:H2'	2:2:83:C:C6	2.50	0.47
2:2:548:U:OP1	20:AQ:134:LYS:NZ	2.48	0.47
11:AG:83:ARG:HG3	11:AG:108:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AJ:33:SER:HB3	14:AJ:56:ARG:HD3	1.97	0.47
50:BQ:105:GLU:OE2	50:BQ:139:TYR:OH	2.28	0.47
1:1:16:A:N1	1:1:2287:4AC:O2'	2.46	0.47
1:1:676:C:H2'	1:1:677:G:O4'	2.15	0.47
1:1:814:A:H2'	1:1:815:A:C8	2.49	0.47
1:1:1616:C:H2'	1:1:1617:4AC:H6	1.97	0.47
2:2:410:C:O2'	2:2:587:A:N3	2.46	0.47
2:2:1360:C:H2'	2:2:1361:U:H6	1.79	0.47
24:AV:33:ARG:NH2	24:AV:53:ILE:O	2.47	0.47
62:Bc:41:ARG:HE	62:Bc:87:ILE:C	2.23	0.47
63:BJ:85:GLN:HA	63:BJ:102:ASN:HD22	1.79	0.47
30:B4:36:THR:O	30:B4:40:THR:HG23	2.14	0.47
2:2:369:G:H2'	2:2:370:C:C6	2.50	0.46
8:AD:131:GLU:HG3	8:AD:155:ALA:HA	1.97	0.46
12:AH:111:ILE:HG13	12:AH:185:ALA:HB1	1.97	0.46
31:AT:48:LEU:O	31:AT:52:ARG:HG2	2.15	0.46
30:BG:31:LYS:HE2	30:BG:31:LYS:HB3	1.80	0.46
57:BM:111:LEU:HB2	57:BM:132:MET:HE2	1.96	0.46
63:BJ:93:ASP:OD1	63:BJ:93:ASP:N	2.37	0.46
1:1:1940:A:H61	1:1:2237:C:H42	1.63	0.46
1:1:2480:G:O2'	1:1:2728:U:OP1	2.25	0.46
1:1:2593:A:H2	1:1:2662:A:H61	1.63	0.46
2:2:90:G:H2'	2:2:91:G:C8	2.51	0.46
2:2:628:G:N2	2:2:803:G:H4'	2.29	0.46
48:BI:2:ARG:NH1	48:BI:113:GLU:OE1	2.48	0.46
1:1:102:C:N3	1:1:117:G:N1	2.37	0.46
1:1:2164:U:H2'	1:1:2165:C:H6	1.79	0.46
2:2:1326:C:H2'	2:2:1327:G:C8	2.51	0.46
6:AB:29:LYS:HA	6:AB:32:ILE:HG13	1.96	0.46
11:AG:74:MET:HG2	11:AG:109:GLY:O	2.14	0.46
23:AU:55:VAL:HG13	23:AU:105:LEU:HD21	1.98	0.46
23:AU:70:ILE:HD12	23:AU:99:ARG:HA	1.97	0.46
30:A3:3:LYS:HD2	30:A3:60:GLU:HG2	1.97	0.46
46:BW:38:LEU:HD23	46:BW:38:LEU:H	1.80	0.46
1:1:877:U:H2'	1:1:878:G:O4'	2.15	0.46
1:1:1302:G:H1'	1:1:1303:A:C2	2.50	0.46
1:1:1310:G:C2	1:1:1311:G:H1'	2.51	0.46
1:1:1580:C:C5	1:1:1589:U:H5''	2.51	0.46
1:1:2206:C:H3'	1:1:2207:A:H2'	1.98	0.46
2:2:729:G:H2'	2:2:730:C:C6	2.51	0.46
2:2:998:C:H1'	27:AY:42:ARG:HE	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1328:C:H2'	2:2:1329:G:H8	1.80	0.46
2:2:1329:G:H2'	2:2:1330:C:C6	2.50	0.46
4:H:30:ILE:HG21	4:H:52:GLN:OE1	2.15	0.46
6:AB:118:THR:HA	6:AB:140:LEU:HD23	1.98	0.46
8:AD:96:THR:OG1	8:AD:97:ILE:N	2.48	0.46
9:AE:167:LYS:HB2	9:AE:174:LEU:HD23	1.97	0.46
36:BC:43:GLY:HA3	36:BC:75:THR:HG22	1.96	0.46
1:1:1780:4AC:O7	1:1:1780:4AC:H5	2.14	0.46
1:1:1805:C:H3'	1:1:1806:G:H21	1.80	0.46
1:1:2065:A:H2'	1:1:2066:A:C8	2.51	0.46
1:1:2725:U:H4'	60:BN:103:ARG:HG2	1.98	0.46
2:2:385:G:H2'	2:2:386:C:C6	2.51	0.46
2:2:1201:A:C8	31:AT:123:THR:HA	2.50	0.46
5:AA:20:TYR:O	5:AA:35:LEU:HD13	2.16	0.46
33:BB:182:TYR:HB3	33:BB:187:ARG:HB2	1.97	0.46
34:BY:3:LYS:HD3	34:BY:3:LYS:HA	1.79	0.46
42:Be:28:PHE:HA	42:Be:35:CYS:HA	1.96	0.46
1:1:120:A:C8	1:1:120:A:C5'	2.98	0.46
1:1:450:C:H2'	1:1:451:4AC:H6	1.97	0.46
1:1:703:U:H3'	1:1:704:G:H5'	1.97	0.46
1:1:990:U:H2'	1:1:991:G:C8	2.51	0.46
1:1:993:U:N3	1:1:2841:A:OP1	2.47	0.46
1:1:1303:A:N6	1:1:1367:G:H1'	2.31	0.46
1:1:2058:A:H2'	1:1:2059:G:C8	2.50	0.46
2:2:35:G:O2'	2:2:305:U:OP1	2.34	0.46
10:AF:56:GLU:O	10:AF:62:ASN:ND2	2.48	0.46
15:AK:33:VAL:O	15:AK:36:VAL:HG22	2.16	0.46
43:BE:102:LEU:HD13	43:BE:113:VAL:HG21	1.97	0.46
55:BZ:9:LYS:HD2	55:BZ:91:SER:HA	1.98	0.46
55:BZ:20:SER:HA	55:BZ:23:THR:HG22	1.98	0.46
1:1:107:G:C2	1:1:113:G:C6	3.04	0.46
1:1:631:A:N3	40:BU:93:TYR:OH	2.42	0.46
1:1:2110:A:H2'	1:1:2111:G:O4'	2.15	0.46
1:1:2255:A:H2'	1:1:2256:A:C8	2.51	0.46
2:2:255:A:C2	2:2:291:A:C5	3.03	0.46
2:2:635:C:H2'	2:2:636:4AC:H6	1.98	0.46
2:2:645:C:H2'	2:2:646:C:C6	2.50	0.46
3:3:93:G:H2'	3:3:94:A:C8	2.51	0.46
31:AT:49:ARG:O	31:AT:53:LEU:HD23	2.16	0.46
41:Bb:103:ALA:HB3	41:Bb:106:VAL:HG23	1.98	0.46
62:Bc:4:LYS:NZ	62:Bc:85:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:704:G:H8	1:1:704:G:OP2	1.98	0.46
1:1:761:U:H2'	1:1:762:G:H8	1.81	0.46
2:2:333:G:N1	2:2:336:A:OP2	2.49	0.46
4:H:383:ARG:CZ	4:H:383:ARG:HB2	2.44	0.46
9:AE:132:MET:HE1	9:AE:152:LEU:HD21	1.98	0.46
11:AG:74:MET:HE2	11:AG:116:ILE:HD13	1.97	0.46
13:AI:32:LYS:O	13:AI:36:GLU:N	2.37	0.46
48:BI:117:GLU:OE1	48:BI:117:GLU:N	2.35	0.46
30:B4:33:ARG:HB3	30:B4:38:GLU:HG3	1.97	0.46
1:1:117:G:C6	1:1:118:U:C5	3.04	0.46
1:1:1428:C:O2'	24:B6:56:ILE:O	2.31	0.46
1:1:1710:C:H2'	1:1:1711:G:C8	2.49	0.46
1:1:1933:C:H5''	36:BC:246:GLY:HA3	1.97	0.46
2:2:168:A:H2'	2:2:169:A:C8	2.50	0.46
4:H:384:PHE:CD1	17:AM:96:PRO:HG3	2.51	0.46
5:AA:140:LYS:HE3	5:AA:140:LYS:HB3	1.83	0.46
9:AE:165:LEU:HD23	9:AE:165:LEU:HA	1.82	0.46
16:AL:16:LEU:HD23	16:AL:71:ARG:HG2	1.98	0.46
23:AU:42:GLU:HG2	23:AU:43:ARG:HG3	1.98	0.46
24:AV:75:LYS:HE3	24:AV:75:LYS:HB3	1.60	0.46
31:AT:8:TYR:HE2	31:AT:28:LEU:HD23	1.79	0.46
37:B5:62:ILE:HD13	37:B5:62:ILE:HA	1.86	0.46
54:BF:120:ARG:NH1	54:BF:157:ALA:O	2.47	0.46
1:1:880:G:H22	1:1:1096:G:P	2.39	0.46
1:1:1327:C:H42	1:1:1353:A:P	2.39	0.46
1:1:1739:G:O2'	1:1:1816:U:O2'	2.21	0.46
1:1:1763:G:H2'	1:1:1764:C:C6	2.51	0.46
1:1:2419:C:C2	1:1:2420:A:N7	2.84	0.46
2:2:155:G:O4'	11:AG:118:GLN:NE2	2.49	0.46
8:AD:162:ASN:OD1	8:AD:162:ASN:N	2.48	0.46
33:BB:28:VAL:O	33:BB:29:LYS:HD2	2.16	0.46
1:1:392:A:O2'	1:1:393:C:H5''	2.16	0.45
1:1:1220:A:O2'	34:BY:14:ASN:ND2	2.41	0.45
1:1:1687:C:OP1	59:Bd:44:ASN:HB2	2.15	0.45
1:1:2558:A:H2'	1:1:2559:A:C8	2.51	0.45
2:2:1071:G:H5''	28:AZ:150:TYR:CZ	2.51	0.45
2:2:1225:A:H2'	2:2:1226:U:C6	2.51	0.45
3:3:74:C:N3	3:3:109:G:N1	2.39	0.45
12:AH:28:VAL:HB	12:AH:34:LYS:HG2	1.98	0.45
12:AH:30:ASP:OD1	12:AH:32:SER:OG	2.28	0.45
24:AV:1:MET:HE2	24:AV:25:HIS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AY:38:TRP:NE1	27:AY:49:LYS:HB3	2.32	0.45
28:AZ:102:ALA:O	28:AZ:107:ILE:HG22	2.16	0.45
35:BO:74:LYS:HD3	35:BO:174:LYS:HB3	1.99	0.45
1:1:932:C:H2'	1:1:933:G:C8	2.52	0.45
1:1:1090:U:H2'	1:1:1091:C:C6	2.50	0.45
1:1:2103:U:O2'	1:1:2104:A:N7	2.47	0.45
1:1:2462:U:H2'	1:1:2463:A:H8	1.81	0.45
2:2:271:A:H2'	2:2:272:A:C8	2.51	0.45
2:2:547:G:N1	2:2:726:A:OP2	2.38	0.45
2:2:625:C:H2'	2:2:626:4AC:H6	1.98	0.45
2:2:654:A:O2'	2:2:668:A:N6	2.49	0.45
2:2:688:A:OP2	5:AA:129:ARG:NH2	2.49	0.45
2:2:1244:G:C2	2:2:1245:G:C8	3.04	0.45
2:2:1301:G:H2'	2:2:1302:C:H6	1.80	0.45
4:H:132:VAL:HG13	4:H:255:LEU:HG	1.97	0.45
11:AG:68:ASP:HA	11:AG:116:ILE:HA	1.98	0.45
38:BL:47:TRP:CH2	38:BL:51:ILE:HD11	2.51	0.45
1:1:807:C:H2'	1:1:808:G:O4'	2.16	0.45
1:1:1170:A:H5''	3:3:102:G:O2'	2.16	0.45
1:1:1489:C:H2'	1:1:1490:G:H8	1.81	0.45
1:1:1625:A:H2'	1:1:1626:C:C6	2.51	0.45
1:1:1668:G:H2'	1:1:1669:C:C6	2.52	0.45
1:1:1687:C:OP2	59:Bd:66:ARG:NE	2.40	0.45
1:1:1986:U:H2'	1:1:1987:G:O4'	2.16	0.45
1:1:2153:A:O2'	2:2:1463:G:O2'	2.30	0.45
2:2:345:C:H2'	2:2:346:A:H8	1.82	0.45
2:2:1084:C:H2'	2:2:1085:C:H6	1.82	0.45
4:H:71:ASP:OD1	4:H:71:ASP:N	2.50	0.45
14:AJ:108:ALA:HB1	14:AJ:122:ALA:HB1	1.99	0.45
23:AU:75:THR:HB	23:AU:92:LYS:HE2	1.98	0.45
30:A3:84:LYS:HD3	30:A3:95:ALA:HB2	1.98	0.45
37:B5:31:ASN:HD21	55:BZ:25:ARG:NH1	2.12	0.45
41:Bb:52:LEU:HD23	41:Bb:52:LEU:HA	1.81	0.45
48:BI:108:LYS:HB3	48:BI:108:LYS:HE2	1.79	0.45
50:BQ:56:LYS:O	50:BQ:56:LYS:HG2	2.17	0.45
24:B6:17:LYS:HB3	24:B6:71:TYR:HB3	1.99	0.45
1:1:1347:C:H2'	1:1:1348:G:O4'	2.15	0.45
1:1:2302:A:H2'	1:1:2303:C:H5'	1.98	0.45
1:1:2537:C:OP2	1:1:2538:A:O2'	2.26	0.45
2:2:109:C:H2'	2:2:110:U:C6	2.52	0.45
2:2:393:C:H2'	2:2:394:4AC:H6	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:689:G:O5'	5:AA:99:ARG:NH2	2.49	0.45
23:AU:123:PRO:HA	23:AU:126:ARG:HB3	1.99	0.45
32:AO:64:GLU:HG2	32:AO:72:HIS:CE1	2.51	0.45
43:BE:137:MET:HE2	43:BE:137:MET:HB3	1.91	0.45
50:BQ:40:ASP:OD1	50:BQ:40:ASP:N	2.50	0.45
1:1:806:G:H2'	1:1:807:C:C6	2.51	0.45
1:1:1877:C:O2'	1:1:1883:A:N1	2.47	0.45
1:1:1993:G:N2	1:1:1995:G:H3'	2.31	0.45
2:2:903:C:H2'	2:2:904:A:C8	2.51	0.45
2:2:961:G:H4'	2:2:991:G:H1'	1.97	0.45
4:H:340:ASP:OD1	4:H:340:ASP:N	2.50	0.45
36:BC:284:ILE:HD11	36:BC:321:ALA:HB2	1.98	0.45
37:BK:28:ILE:O	64:Bl:26:ARG:NH1	2.48	0.45
24:B6:37:LYS:HB2	24:B6:53:ILE:HD11	1.98	0.45
58:BS:72:HIS:HA	58:BS:79:GLY:O	2.16	0.45
1:1:659:A:OP2	58:BS:4:ARG:NH1	2.46	0.45
1:1:2498:A:N3	1:1:2498:A:H2'	2.32	0.45
2:2:1288:C:H2'	2:2:1289:U:C6	2.51	0.45
6:AB:10:ASP:OD1	6:AB:10:ASP:N	2.50	0.45
9:AE:17:THR:HA	9:AE:23:ARG:HH21	1.81	0.45
12:AH:99:LYS:O	12:AH:102:GLU:HG2	2.17	0.45
32:AO:103:ARG:O	32:AO:107:MET:HG2	2.16	0.45
30:B4:41:LYS:O	30:B4:44:GLU:HG2	2.16	0.45
1:1:1161:A:H2'	1:1:1164:C:C5	2.51	0.45
1:1:1431:U:O2	56:BP:7:THR:HG23	2.16	0.45
1:1:2376:G:H1	1:1:2395:U:H3	1.63	0.45
2:2:424:C:H4'	2:2:425:U:C5	2.51	0.45
2:2:541:G:O2'	2:2:788:G:H5'	2.17	0.45
2:2:687:C:OP1	5:AA:99:ARG:NH1	2.50	0.45
2:2:1099:C:H2'	2:2:1100:C:H6	1.82	0.45
2:2:1154:A:P	15:AK:104:ARG:HH22	2.40	0.45
5:AA:173:LYS:O	5:AA:173:LYS:NZ	2.34	0.45
8:AD:39:LYS:O	8:AD:43:LYS:HG3	2.16	0.45
9:AE:42:SER:OG	9:AE:43:ILE:N	2.50	0.45
23:AU:100:LYS:HE3	23:AU:100:LYS:HB3	1.83	0.45
36:BC:283:LEU:HD21	36:BC:286:ILE:HD11	1.98	0.45
44:Ba:73:LYS:HE3	44:Ba:94:ALA:C	2.42	0.45
53:BD:144:VAL:HG11	53:BD:164:LEU:HD21	1.99	0.45
55:BZ:98:LYS:HG3	55:BZ:99:ARG:HD2	1.98	0.45
24:B6:33:ARG:HG3	24:B6:53:ILE:HD13	1.99	0.45
64:Bl:62:PRO:HB3	64:Bl:74:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:908:A:H2'	1:1:909:C:H6	1.82	0.45
1:1:915:C:H2'	1:1:916:G:C8	2.52	0.45
1:1:1524:G:N7	58:BS:28:SER:OG	2.42	0.45
1:1:1715:U:H2'	1:1:1716:A:H8	1.82	0.45
1:1:2247:C:H2'	1:1:2248:C:C6	2.52	0.45
1:1:2463:A:OP2	57:BM:89:LYS:NZ	2.50	0.45
2:2:98:C:H2'	2:2:99:C:C6	2.52	0.45
2:2:244:G:H2'	2:2:245:G:C8	2.52	0.45
2:2:757:A:H62	4:H:369:LEU:HD21	1.81	0.45
11:AG:87:LEU:HA	11:AG:104:LYS:HA	1.97	0.45
11:AG:98:GLU:HB2	11:AG:101:GLU:OE1	2.17	0.45
27:AY:3:GLN:NE2	30:A3:61:GLU:HG3	2.31	0.45
32:AO:50:LYS:HE2	32:AO:50:LYS:HB2	1.84	0.45
36:BC:356:SER:OG	51:BV:15:GLU:OE2	2.18	0.45
37:BK:77:LYS:HE3	37:BK:77:LYS:HB3	1.77	0.45
53:BD:35:VAL:HG13	53:BD:228:GLU:HG2	1.99	0.45
53:BD:91:ARG:HA	53:BD:91:ARG:HD2	1.90	0.45
65:Bk:4:LEU:HD13	65:Bk:37:VAL:HG13	1.98	0.45
1:1:475:G:O6	53:BD:158:ARG:NH1	2.42	0.45
1:1:1591:A:H2'	1:1:1593:C:C5	2.52	0.45
1:1:1806:G:C8	1:1:1809:A:C8	3.04	0.45
1:1:2344:G:O6	1:1:2426:C:N4	2.50	0.45
2:2:200:C:H2'	2:2:201:C:H6	1.81	0.45
2:2:1346:C:H2'	2:2:1347:G:O4'	2.17	0.45
4:H:195:TYR:HD1	4:H:195:TYR:HA	1.67	0.45
12:AH:190:LEU:HB2	12:AH:198:SER:HB3	1.99	0.45
16:AL:19:VAL:O	16:AL:22:GLN:HG2	2.17	0.45
33:BB:202:HIS:CD2	33:BB:204:PHE:H	2.32	0.45
57:BM:73:ARG:HD2	57:BM:90:TYR:CD1	2.52	0.45
65:Bk:8:ILE:HG23	65:Bk:16:GLU:HG3	1.98	0.45
1:1:530:U:H2'	1:1:531:A:H8	1.82	0.45
1:1:728:C:H5''	37:BK:46:ARG:NH2	2.31	0.45
1:1:770:C:H2'	1:1:771:G:H8	1.82	0.45
1:1:946:G:H2'	1:1:947:C:C6	2.52	0.45
1:1:1250:A:H2'	1:1:1251:A:C8	2.52	0.45
1:1:1779:C:H2'	1:1:1780:4AC:H6	1.98	0.45
1:1:2010:C:N3	1:1:2947:C:O2'	2.47	0.45
1:1:2393:G:H2'	1:1:2394:G:C8	2.51	0.45
1:1:2593:A:H4'	38:BL:51:ILE:HG22	1.98	0.45
1:1:2916:C:H4'	51:BV:18:THR:HG22	1.98	0.45
1:1:2963:A:H2'	1:1:2963:A:N3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:178:A:H1'	2:2:209:A:N6	2.31	0.45
2:2:1095:A:C8	2:2:1120:A:N1	2.85	0.45
4:H:384:PHE:CD1	4:H:384:PHE:O	2.69	0.45
9:AE:175:GLU:OE1	9:AE:176:VAL:N	2.50	0.45
59:Bd:41:ARG:NH1	59:Bd:74:LYS:HD2	2.32	0.45
30:B4:83:LYS:HB3	30:B4:83:LYS:HE2	1.74	0.45
1:1:274:C:HO2'	1:1:275:C:H6	1.64	0.44
1:1:1590:C:OP1	50:BQ:1:MET:N	2.42	0.44
1:1:2564:A:H5''	35:BO:22:ARG:NH2	2.32	0.44
2:2:148:A:OP2	2:2:166:C:N4	2.50	0.44
2:2:456:C:H2'	2:2:457:G:H8	1.82	0.44
2:2:724:U:OP1	2:2:789:C:O2'	2.33	0.44
2:2:965:A:H5''	2:2:966:C:C5	2.49	0.44
12:AH:47:THR:O	12:AH:50:ARG:HG2	2.17	0.44
16:AL:38:ILE:HD13	16:AL:38:ILE:HA	1.73	0.44
20:AQ:29:THR:HG23	20:AQ:31:GLU:H	1.81	0.44
47:Bi:50:SER:HB3	47:Bi:53:ILE:HD12	1.99	0.44
37:BK:41:ASN:O	37:BK:42:LYS:HG3	2.17	0.44
53:BD:244:VAL:O	53:BD:248:GLU:HG2	2.17	0.44
60:BN:166:ASP:OD2	60:BN:170:ASN:ND2	2.49	0.44
1:1:1228:G:H5''	62:Bc:16:ASN:HD22	1.82	0.44
1:1:1362:G:O2'	1:1:1363:U:H5'	2.18	0.44
1:1:2197:G:H3'	1:1:2198:5MC:HM53	1.99	0.44
1:1:2456:C:H2'	1:1:2457:A:O4'	2.18	0.44
2:2:270:U:OP2	14:AJ:56:ARG:NH2	2.37	0.44
2:2:643:A:H5''	17:AM:120:PRO:HB2	1.99	0.44
2:2:830:OMU:OP2	2:2:840:G:N1	2.39	0.44
2:2:1153:A:H2'	2:2:1154:A:O4'	2.16	0.44
2:2:1493:C:H2'	2:2:1494:G:H8	1.80	0.44
56:BP:119:MET:HE2	56:BP:119:MET:HB3	1.91	0.44
60:BN:9:ASP:O	60:BN:56:GLN:HB2	2.17	0.44
1:1:127:U:H2'	1:1:128:A:H8	1.81	0.44
1:1:769:C:OP2	41:Bb:49:LYS:HE2	2.18	0.44
1:1:1549:C:H2'	1:1:1550:4AC:H6	2.00	0.44
1:1:1755:4AC:HM73	1:1:1780:4AC:HM73	1.99	0.44
1:1:2609:G:N2	1:1:2612:A:OP2	2.36	0.44
1:1:2630:C:H2'	1:1:2631:C:H6	1.82	0.44
2:2:373:A2M:HM'2	2:2:374:A:C5	2.53	0.44
2:2:653:U:O4	2:2:670:A:H1'	2.18	0.44
3:3:52:A:H5''	35:BO:170:GLY:H	1.82	0.44
4:H:205:PRO:HA	60:BN:107:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AL:65:GLU:HB3	19:AP:55:TYR:HD2	1.82	0.44
19:AP:13:LYS:HD3	19:AP:13:LYS:H	1.82	0.44
31:AT:32:GLN:OE1	31:AT:32:GLN:N	2.47	0.44
37:B5:61:ASP:OD1	37:B5:61:ASP:N	2.50	0.44
42:Be:48:LYS:HE2	42:Be:55:TRP:CE3	2.52	0.44
54:BF:47:PHE:HE2	54:BF:49:GLU:HG2	1.82	0.44
59:Bd:76:MET:HE2	59:Bd:80:MET:HE3	2.00	0.44
1:1:633:A:N3	1:1:635:G:H5''	2.32	0.44
1:1:864:G:H2'	1:1:865:C:O4'	2.18	0.44
1:1:2353:C:N4	1:1:2359:A:H62	2.16	0.44
1:1:2400:C:H2'	1:1:2401:C:C6	2.51	0.44
1:1:2871:A:H2'	1:1:2872:G:O4'	2.17	0.44
2:2:641:G:H2'	2:2:642:U:C6	2.53	0.44
2:2:1095:A:C4	2:2:1096:G:N7	2.85	0.44
2:2:1290:G:N2	2:2:1292:A:H3'	2.32	0.44
2:2:1465:C:H2'	2:2:1466:G:O4'	2.17	0.44
24:AV:26:PRO:HA	24:AV:63:TYR:HB3	1.99	0.44
25:AW:19:LYS:NZ	25:AW:24:GLY:O	2.50	0.44
30:A3:74:GLU:HG2	30:A3:76:PRO:HD3	1.98	0.44
43:BE:103:LYS:HG2	43:BE:184:VAL:HG22	2.00	0.44
62:Bc:36:SER:HA	62:Bc:39:ILE:HD13	1.99	0.44
30:B4:25:ILE:HG23	30:B4:107:ALA:HB2	1.98	0.44
1:1:703:U:O4	30:B4:83:LYS:NZ	2.46	0.44
1:1:846:C:H2'	1:1:847:G:O4'	2.17	0.44
1:1:951:G:OP1	50:BQ:86:THR:HG23	2.17	0.44
1:1:2058:A:H2'	1:1:2059:G:H8	1.83	0.44
2:2:590:4AC:H5''	9:AE:24:LYS:HD2	1.99	0.44
2:2:756:U:H5''	4:H:376:ARG:HD3	2.00	0.44
2:2:774:OMU:HM22	2:2:775:G:H5'	1.99	0.44
2:2:922:U:H2'	2:2:923:G:C8	2.53	0.44
2:2:1236:C:H2'	2:2:1237:C:H6	1.83	0.44
4:H:117:ALA:O	4:H:120:GLU:HG3	2.17	0.44
5:AA:102:THR:HB	5:AA:126:ALA:HB3	1.99	0.44
8:AD:155:ALA:O	8:AD:161:ALA:HB2	2.18	0.44
13:AI:37:VAL:HG22	13:AI:103:ILE:HG21	1.99	0.44
40:BU:117:GLU:HA	40:BU:117:GLU:OE1	2.18	0.44
50:BQ:123:LEU:HD11	50:BQ:142:LEU:HD21	2.00	0.44
54:BF:21:VAL:HG22	54:BF:26:VAL:HG22	1.98	0.44
1:1:15:G:H2'	1:1:16:A:H5''	1.99	0.44
1:1:120:A:C5'	1:1:120:A:H8	2.31	0.44
1:1:422:C:H2'	1:1:423:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2719:G:H2'	1:1:2720:A:H8	1.83	0.44
2:2:86:U:H3'	2:2:87:C:H5''	2.00	0.44
2:2:211:A:N1	2:2:229:G:O2'	2.46	0.44
2:2:420:G:H2'	2:2:421:C:C6	2.52	0.44
2:2:774:OMU:OP1	20:AQ:114:LYS:NZ	2.50	0.44
2:2:1095:A:C5	2:2:1096:G:N7	2.86	0.44
2:2:1224:A:H2'	2:2:1225:A:C8	2.52	0.44
8:AD:16:HIS:HB3	8:AD:19:ILE:CD1	2.48	0.44
28:AZ:147:TYR:OH	28:AZ:149:GLY:O	2.36	0.44
34:BY:60:ASN:H	34:BY:148:ASN:HD21	1.64	0.44
36:BC:211:LYS:HB2	36:BC:211:LYS:HE3	1.84	0.44
48:BI:5:ASN:HB2	48:BI:112:LEU:HB3	1.99	0.44
60:BN:30:LYS:H	60:BN:59:GLN:NE2	2.16	0.44
1:1:1133:A:O2'	1:1:1134:G:H5'	2.18	0.44
1:1:1392:G:OP1	48:BI:52:ARG:NH2	2.51	0.44
1:1:2701:A:H2'	1:1:2702:G:O4'	2.18	0.44
1:1:2799:G:H2'	1:1:2800:G:C8	2.52	0.44
2:2:646:C:H2'	2:2:647:C:C6	2.53	0.44
2:2:1318:C:OP1	15:AK:129:LYS:HE2	2.17	0.44
2:2:1496:5MC:H2'	2:2:1497:U:C6	2.53	0.44
5:AA:145:ILE:O	5:AA:149:LYS:HG2	2.17	0.44
11:AG:75:ARG:HD3	11:AG:107:VAL:HG21	1.99	0.44
30:B4:45:ARG:O	30:B4:47:GLN:NE2	2.51	0.44
1:1:871:G:H2'	1:1:872:C:C6	2.52	0.44
1:1:2187:U:H2'	1:1:2188:C:C6	2.52	0.44
2:2:237:A:N3	9:AE:34:PRO:HB3	2.32	0.44
2:2:1172:G:H2'	2:2:1173:U:C6	2.53	0.44
5:AA:154:ASN:N	5:AA:157:ASP:OD1	2.51	0.44
6:AB:4:GLU:HG3	6:AB:5:TYR:HD1	1.80	0.44
9:AE:218:GLU:H	9:AE:218:GLU:CD	2.26	0.44
12:AH:20:ARG:NH2	15:AK:39:GLU:OE1	2.51	0.44
13:AI:101:ILE:HG22	13:AI:114:LYS:HE3	1.99	0.44
31:AT:12:THR:O	31:AT:16:LEU:HD23	2.17	0.44
43:BE:26:GLU:HB2	43:BE:144:GLU:HG2	2.00	0.44
45:BT:12:ILE:HG13	46:BW:34:MET:HB3	2.00	0.44
60:BN:24:ARG:HA	60:BN:24:ARG:HD3	1.82	0.44
1:1:1:C:H2'	1:1:2:G:O4'	2.18	0.44
1:1:102:C:OP2	1:1:102:C:C6	2.71	0.44
1:1:132:C:O2'	1:1:760:U:OP1	2.32	0.44
1:1:406:A:H5''	1:1:408:G:O4'	2.18	0.44
1:1:1019:C:H2'	1:1:1020:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1877:C:H2'	1:1:1878:4AC:H6	2.00	0.44
1:1:2988:A:N1	54:BF:74:HIS:HE1	2.16	0.44
2:2:989:A:H2'	2:2:991:G:N7	2.32	0.44
2:2:1045:A:H5''	10:AF:71:THR:HG21	1.99	0.44
2:2:1098:C:H2'	2:2:1099:C:C6	2.53	0.44
5:AA:188:LYS:HG3	5:AA:189:ILE:N	2.33	0.44
15:AK:51:LEU:HD23	15:AK:51:LEU:HA	1.88	0.44
16:AL:80:ARG:HG3	16:AL:81:ALA:N	2.33	0.44
30:A3:3:LYS:HG3	30:A3:5:SER:H	1.83	0.44
36:BC:38:MET:HE3	36:BC:182:TYR:CG	2.53	0.44
46:BW:7:ARG:HA	46:BW:61:LYS:HZ2	1.83	0.44
1:1:1211:A:H2'	1:1:1212:A:C8	2.53	0.43
1:1:1687:C:H5''	59:Bd:64:PRO:HB3	2.00	0.43
1:1:2727:C:H5''	60:BN:111:GLY:HA2	2.00	0.43
1:1:2850:A:H2'	1:1:2851:C:H6	1.82	0.43
2:2:451:A:C4	2:2:452:G:C8	3.05	0.43
6:AB:77:GLN:HE22	6:AB:94:GLY:HA2	1.83	0.43
8:AD:44:HIS:HB3	8:AD:100:ILE:CD1	2.48	0.43
18:AN:74:ARG:HH21	18:AN:83:VAL:HG12	1.82	0.43
22:AS:61:LYS:HB3	22:AS:61:LYS:HE2	1.80	0.43
55:BZ:69:GLU:H	55:BZ:69:GLU:HG2	1.62	0.43
57:BM:126:LYS:HG2	57:BM:128:PHE:CE2	2.53	0.43
61:Bg:17:CYS:HA	61:Bg:39:LEU:HD13	2.00	0.43
65:Bk:15:GLU:OE1	65:Bk:16:GLU:N	2.51	0.43
1:1:94:G:C2	1:1:3020:U:C6	3.06	0.43
1:1:141:G:O2'	1:1:142:A:OP2	2.34	0.43
1:1:285:A:H2'	1:1:286:A:C8	2.53	0.43
1:1:636:C:O2'	1:1:650:G:N2	2.49	0.43
1:1:853:C:H2'	1:1:854:C:H6	1.83	0.43
1:1:1575:A:H2'	1:1:1576:C:H6	1.81	0.43
1:1:2077:U:H2'	1:1:2078:G:C8	2.53	0.43
1:1:2678:OMG:HM21	1:1:2680:A:H2'	2.00	0.43
2:2:146:A:H2'	2:2:147:U:C6	2.53	0.43
2:2:447:A:H5''	24:AV:85:TYR:CE1	2.53	0.43
2:2:1136:C:H2'	2:2:1137:G:H8	1.83	0.43
3:3:29:A:N3	3:3:58:A:N6	2.65	0.43
3:3:70:A:H2'	3:3:71:U:O4'	2.19	0.43
10:AF:160:PRO:HD2	10:AF:163:LEU:HD22	2.01	0.43
13:AI:57:ARG:HH12	25:AW:9:PRO:HD2	1.83	0.43
30:A3:117:LYS:HE3	30:A3:117:LYS:HB3	1.81	0.43
41:Bb:103:ALA:O	41:Bb:111:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BE:104:ALA:O	43:BE:168:LYS:NZ	2.51	0.43
58:BS:63:LEU:HD11	58:BS:82:ARG:HB2	1.99	0.43
1:1:372:G:H4'	65:Bk:25:MET:HE1	2.01	0.43
1:1:1305:A:C6	1:1:1306:G:C6	3.07	0.43
1:1:2477:G:H2'	1:1:2478:C:C6	2.53	0.43
2:2:271:A:C8	14:AJ:49:TYR:CD2	3.06	0.43
2:2:854:C:O2'	2:2:855:U:H5'	2.17	0.43
4:H:3:GLY:H	4:H:4:ILE:HD12	1.83	0.43
6:AB:76:GLY:C	6:AB:79:PRO:HD2	2.42	0.43
28:AZ:40:LEU:HD23	28:AZ:40:LEU:H	1.84	0.43
28:AZ:51:PRO:HA	28:AZ:54:VAL:HG12	1.99	0.43
38:BL:47:TRP:CZ2	38:BL:51:ILE:HD11	2.53	0.43
1:1:99:U:O4	1:1:120:A:N1	2.51	0.43
1:1:2044:C:H5'	33:BB:196:LYS:HE2	2.00	0.43
1:1:2046:C:H2'	1:1:2047:A:C8	2.54	0.43
2:2:646:C:H2'	2:2:647:C:H6	1.84	0.43
2:2:973:A:C5	30:A3:34:LYS:HE3	2.53	0.43
2:2:1095:A:N7	2:2:1120:A:C6	2.87	0.43
2:2:1212:A:H5'	12:AH:175:ARG:HG2	1.99	0.43
4:H:132:VAL:HG22	4:H:227:ILE:HG22	1.99	0.43
4:H:223:PRO:HD3	4:H:245:VAL:O	2.18	0.43
6:AB:133:ILE:HG13	6:AB:135:ILE:HG23	1.99	0.43
10:AF:68:ILE:HG12	10:AF:85:VAL:HG22	2.00	0.43
11:AG:75:ARG:NH1	11:AG:92:PRO:O	2.51	0.43
17:AM:32:ASP:OD1	17:AM:34:THR:OG1	2.28	0.43
32:AO:82:PRO:HA	32:AO:90:ASP:HB3	2.01	0.43
43:BE:148:PHE:HA	43:BE:160:ILE:HD11	2.00	0.43
44:Ba:22:VAL:HG11	44:Ba:30:ARG:HG2	2.01	0.43
56:BP:84:LYS:HD2	56:BP:85:PHE:N	2.33	0.43
30:B4:66:LEU:HD23	30:B4:66:LEU:HA	1.75	0.43
1:1:60:4AC:O7	1:1:60:4AC:H5	2.19	0.43
1:1:114:G:N3	1:1:115:G:C8	2.86	0.43
1:1:249:U:H2'	1:1:251:A:N1	2.33	0.43
1:1:713:C:H2'	1:1:714:G:O4'	2.19	0.43
1:1:1142:A:H4'	1:1:1143:A:C8	2.54	0.43
2:2:1068:C:O3'	6:AB:107:LYS:NZ	2.50	0.43
2:2:1134:G:C2	2:2:1135:C:C6	3.07	0.43
2:2:1417:U:H2'	2:2:1418:C:C6	2.52	0.43
35:BO:42:ASN:HD22	35:BO:76:HIS:HE1	1.65	0.43
62:Bc:4:LYS:HB2	62:Bc:4:LYS:HE2	1.83	0.43
1:1:1318:G:H2'	1:1:1319:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1662:4AC:O7	1:1:1662:4AC:H5	2.18	0.43
1:1:2216:G:H2'	1:1:2217:U:O4'	2.18	0.43
1:1:2341:G:O2'	1:1:2342:C:H6	2.02	0.43
1:1:2367:G:HO2'	1:1:2368:G:P	2.41	0.43
2:2:605:G:C2	2:2:606:G:C8	3.06	0.43
2:2:717:C:H4'	20:AQ:47:THR:HG22	2.00	0.43
2:2:759:A:O2'	2:2:761:A:N7	2.38	0.43
2:2:946:G:H5''	19:AP:29:PRO:HB3	2.00	0.43
3:3:32:4AC:O2	3:3:50:G:N2	2.38	0.43
3:3:52:A:H62	35:BO:42:ASN:HD21	1.67	0.43
25:AW:16:LEU:HB3	25:AW:60:ILE:HD13	2.00	0.43
40:BU:31:LEU:HD23	40:BU:102:ILE:HB	2.00	0.43
41:Bb:127:ASN:OD1	41:Bb:127:ASN:N	2.51	0.43
51:BV:54:LYS:HD2	51:BV:54:LYS:HA	1.72	0.43
53:BD:142:LEU:HD12	53:BD:142:LEU:HA	1.85	0.43
1:1:1757:G:OP2	37:B5:51:LYS:NZ	2.51	0.43
2:2:1309:C:HO2'	12:AH:175:ARG:NH1	2.17	0.43
5:AA:47:ARG:NH2	17:AM:37:GLU:OE2	2.43	0.43
9:AE:56:ALA:HB1	9:AE:61:GLU:HG3	2.00	0.43
21:AR:84:ASP:HB3	21:AR:108:ARG:HA	1.99	0.43
1:1:99:U:H3	1:1:120:A:H2	1.66	0.43
1:1:117:G:N2	1:1:118:U:H1'	2.34	0.43
1:1:217:A:C2	40:BU:20:LEU:HB3	2.54	0.43
1:1:291:G:OP1	57:BM:194:LYS:NZ	2.50	0.43
1:1:1410:A:OP1	62:Bc:18:HIS:HE1	2.02	0.43
1:1:1525:U:H2'	1:1:1526:A:C8	2.54	0.43
1:1:1730:A:H2'	1:1:1732:G:N2	2.33	0.43
1:1:2130:A:H2'	1:1:2131:A:H8	1.83	0.43
1:1:2329:4AC:O7	1:1:2329:4AC:H5	2.18	0.43
1:1:2418:C:H2'	1:1:2419:C:H6	1.83	0.43
1:1:2916:C:O2	63:BJ:96:ARG:NH1	2.51	0.43
2:2:625:C:H2'	2:2:626:4AC:C6	2.48	0.43
2:2:1215:G:H2'	2:2:1216:G:H8	1.84	0.43
36:BC:65:GLU:OE2	51:BV:2:ALA:HB2	2.19	0.43
38:BL:1:MET:HE2	53:BD:33:ARG:HD2	2.00	0.43
53:BD:61:ILE:HD11	53:BD:68:ALA:O	2.19	0.43
1:1:204:A:H1'	39:Bf:30:LYS:HE2	2.01	0.43
1:1:2418:C:C2	1:1:2419:C:C5	3.07	0.43
1:1:2584:C:H2'	1:1:2585:4AC:O2	2.19	0.43
2:2:164:G:C2	2:2:165:G:C8	3.07	0.43
2:2:1388:C:H2'	2:2:1389:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1405:U:H2'	2:2:1406:G:O4'	2.19	0.43
3:3:74:C:H2'	3:3:75:G:C8	2.54	0.43
5:AA:168:ALA:HB1	5:AA:184:ALA:O	2.19	0.43
12:AH:105:LYS:HB3	12:AH:105:LYS:HE2	1.86	0.43
31:AT:21:LEU:HD12	31:AT:21:LEU:HA	1.85	0.43
56:BP:15:ILE:HD13	56:BP:38:GLU:HG3	2.00	0.43
30:B4:56:ASP:OD1	30:B4:56:ASP:N	2.52	0.43
1:1:434:A:H2'	1:1:435:C:H6	1.84	0.43
1:1:612:G:N7	42:Be:62:HIS:NE2	2.63	0.43
1:1:1019:C:H2'	1:1:1020:G:H8	1.84	0.43
1:1:1065:4AC:O7	1:1:1065:4AC:H5	2.19	0.43
1:1:1631:C:C2	1:1:1632:G:C8	3.07	0.43
1:1:1806:G:H1'	1:1:1809:A:C4	2.54	0.43
1:1:2517:U:H4'	1:1:2518:A:O4'	2.19	0.43
1:1:2684:C:C2	1:1:2685:A:C8	3.07	0.43
2:2:145:G:H2'	2:2:146:A:H8	1.83	0.43
2:2:979:G:OP1	19:AP:3:LYS:N	2.46	0.43
3:3:40:U:N3	3:3:44:G:OP2	2.44	0.43
4:H:165:PRO:O	4:H:167:VAL:HG13	2.19	0.43
9:AE:72:LEU:HD23	9:AE:94:PRO:HD3	2.01	0.43
10:AF:132:GLU:H	10:AF:132:GLU:HG2	1.71	0.43
27:AY:26:GLY:H	30:A3:45:ARG:NH1	2.16	0.43
31:AT:26:LYS:HB2	31:AT:26:LYS:HE2	1.82	0.43
35:BO:42:ASN:HD22	35:BO:76:HIS:CE1	2.37	0.43
55:BZ:34:LEU:HD22	55:BZ:97:ALA:HB2	2.01	0.43
1:1:42:U:C4	51:BV:51:LYS:HB2	2.54	0.42
1:1:453:A:N3	1:1:474:C:O2'	2.51	0.42
1:1:979:C:H2'	1:1:980:C:H6	1.83	0.42
1:1:1254:C:H2'	1:1:1261:G:C8	2.54	0.42
1:1:1327:C:N4	1:1:1352:C:O3'	2.50	0.42
1:1:1393:G:H5'	48:BI:78:THR:HG23	2.00	0.42
1:1:2913:C:H5'	36:BC:325:PRO:HA	2.00	0.42
2:2:716:U:P	20:AQ:16:ARG:HH21	2.42	0.42
2:2:917:G:C2	2:2:918:A:C8	3.06	0.42
2:2:1099:C:H2'	2:2:1100:C:C6	2.54	0.42
2:2:1401:U:H2'	2:2:1402:A:C8	2.54	0.42
4:H:287:GLU:O	4:H:291:GLU:HG2	2.18	0.42
5:AA:96:LEU:HD13	5:AA:96:LEU:HA	1.80	0.42
5:AA:161:GLU:OE1	5:AA:166:LYS:HB3	2.18	0.42
9:AE:183:ALA:HB3	9:AE:199:ILE:HD13	2.01	0.42
9:AE:219:GLU:N	9:AE:219:GLU:OE1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AG:63:ILE:HA	11:AG:121:VAL:HG23	2.01	0.42
16:AL:3:LYS:H	16:AL:101:ILE:HD11	1.84	0.42
16:AL:65:GLU:OE2	16:AL:67:ARG:NE	2.37	0.42
18:AN:38:LYS:O	18:AN:42:ASP:HB2	2.19	0.42
18:AN:139:LYS:HB3	18:AN:141:ARG:HE	1.83	0.42
20:AQ:60:ILE:HD12	20:AQ:61:PRO:O	2.20	0.42
26:AX:42:ARG:NE	26:AX:64:ALA:O	2.51	0.42
31:AT:95:LYS:HB2	31:AT:98:MET:SD	2.59	0.42
36:BC:25:PRO:HB2	36:BC:219:ILE:HG22	2.01	0.42
38:BL:4:ARG:HE	38:BL:4:ARG:HB3	1.65	0.42
47:Bi:69:LEU:HD23	47:Bi:69:LEU:HA	1.87	0.42
57:BM:75:ARG:HE	57:BM:87:GLN:HE22	1.66	0.42
60:BN:83:HIS:CD2	60:BN:136:ARG:HE	2.34	0.42
60:BN:176:ILE:HD13	60:BN:176:ILE:HA	1.90	0.42
1:1:427:G:N1	1:1:428:U:O4	2.52	0.42
1:1:436:C:O2'	65:Bk:30:ARG:HD3	2.19	0.42
1:1:1283:A:N3	1:1:2718:4AC:O2'	2.46	0.42
1:1:1371:C:H2'	1:1:1372:G:C8	2.54	0.42
1:1:1617:4AC:H2'	1:1:1618:G:H8	1.83	0.42
1:1:1735:G:H2'	1:1:1736:C:C6	2.54	0.42
1:1:1740:C:O2'	1:1:1741:U:H5'	2.19	0.42
1:1:1742:A:H2'	1:1:1743:A:H8	1.83	0.42
1:1:1787:A:H1'	1:1:1828:C:H1'	2.02	0.42
1:1:3014:C:H2'	1:1:3015:G:H8	1.82	0.42
2:2:345:C:C2	2:2:346:A:C8	3.07	0.42
2:2:703:4AC:O7	2:2:703:4AC:H5	2.19	0.42
2:2:1306:A:H2'	2:2:1307:A:C8	2.54	0.42
2:2:1342:G:OP2	15:AK:122:SER:OG	2.25	0.42
2:2:1487:MA6:H2'	2:2:1488:MA6:C8	2.49	0.42
3:3:52:A:N6	35:BO:42:ASN:HD21	2.17	0.42
10:AF:218:ILE:HA	10:AF:223:ILE:CG1	2.49	0.42
14:AJ:81:ILE:CD1	14:AJ:102:GLU:HB2	2.49	0.42
30:A3:74:GLU:HG2	30:A3:75:ILE:N	2.33	0.42
35:BO:63:HIS:CD2	35:BO:65:ARG:HB2	2.54	0.42
60:BN:56:GLN:NE2	60:BN:125:ARG:HH21	2.16	0.42
1:1:103:C:C2	1:1:117:G:C2	3.08	0.42
1:1:1333:U:H4'	1:1:1334:C:C6	2.55	0.42
1:1:1434:G:H2'	1:1:1435:U:C6	2.55	0.42
1:1:1487:U:H2'	1:1:1488:C:C6	2.54	0.42
1:1:1806:G:H2'	1:1:1807:U:H5''	2.02	0.42
1:1:2081:G:OP1	33:BB:202:HIS:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2612:A:O3'	35:BO:30:SER:HB3	2.19	0.42
1:1:2699:C:H2'	1:1:2700:G:O4'	2.18	0.42
1:1:3022:C:O2	1:1:3022:C:H2'	2.18	0.42
4:H:51:THR:O	4:H:55:ILE:HG12	2.20	0.42
6:AB:9:LEU:H	6:AB:9:LEU:HD22	1.84	0.42
9:AE:90:VAL:HG13	9:AE:115:ILE:HD11	2.02	0.42
14:AJ:86:ASN:HB3	14:AJ:89:PHE:CG	2.54	0.42
16:AL:14:ARG:HA	16:AL:14:ARG:HD3	1.85	0.42
18:AN:132:VAL:HG21	18:AN:145:PRO:HD3	2.01	0.42
32:AO:125:PRO:HB3	32:AO:129:GLN:OE1	2.19	0.42
44:Ba:1:MET:HG2	44:Ba:44:LYS:HG3	2.01	0.42
53:BD:14:ASP:OD1	53:BD:15:GLU:N	2.52	0.42
1:1:210:C:H2'	1:1:211:4AC:H6	2.01	0.42
1:1:379:G:N2	1:1:408:G:N3	2.68	0.42
1:1:1731:U:H4'	1:1:1732:G:O5'	2.19	0.42
1:1:1733:A:C2	1:1:1734:G:H1'	2.54	0.42
2:2:29:C:H2'	2:2:30:C:C6	2.55	0.42
2:2:270:U:P	14:AJ:56:ARG:HH22	2.40	0.42
2:2:675:C:H2'	2:2:676:G:H8	1.84	0.42
2:2:848:4AC:O7	2:2:848:4AC:H5	2.20	0.42
2:2:1212:A:C8	2:2:1277:C:H1'	2.54	0.42
4:H:140:VAL:HG11	4:H:254:ILE:HG12	2.00	0.42
6:AB:142:ASP:HB3	6:AB:144:GLU:OE1	2.19	0.42
6:AB:170:ILE:HG12	6:AB:170:ILE:H	1.63	0.42
9:AE:66:LEU:HD23	9:AE:66:LEU:HA	1.89	0.42
29:A0:32:LYS:HD3	29:A0:32:LYS:HA	1.70	0.42
36:BC:262:MET:HG2	48:BI:59:THR:HG22	2.00	0.42
1:1:151:C:H2'	1:1:152:U:C6	2.55	0.42
1:1:1462:G:O2'	53:BD:235:HIS:HD2	2.02	0.42
1:1:1805:C:H3'	1:1:1806:G:N2	2.34	0.42
1:1:1878:4AC:O7	1:1:1878:4AC:H5	2.18	0.42
1:1:2368:G:H1'	1:1:2413:A:O2'	2.20	0.42
1:1:2719:G:H2'	1:1:2720:A:C8	2.54	0.42
2:2:244:G:H2'	2:2:245:G:H8	1.85	0.42
4:H:323:GLU:OE1	4:H:330:LEU:HD22	2.19	0.42
5:AA:90:ARG:NH2	17:AM:119:THR:O	2.43	0.42
18:AN:44:LEU:HG	18:AN:50:ALA:HB2	2.01	0.42
49:BR:19:HIS:CD2	49:BR:22:ARG:HH21	2.37	0.42
53:BD:75:THR:O	53:BD:78:ARG:HG2	2.19	0.42
54:BF:131:LYS:HG3	54:BF:133:LYS:HE3	2.01	0.42
24:B6:41:VAL:HG11	24:B6:48:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B4:115:ALA:O	30:B4:118:VAL:HG12	2.19	0.42
1:1:922:4AC:O7	1:1:922:4AC:H5	2.19	0.42
1:1:1408:C:H2'	1:1:1409:G:O4'	2.19	0.42
1:1:1715:U:H2'	1:1:1716:A:C8	2.55	0.42
1:1:2570:4AC:H5	1:1:2570:4AC:O7	2.19	0.42
2:2:319:4AC:O7	2:2:319:4AC:H5	2.20	0.42
2:2:609:A:H2'	2:2:610:C:H6	1.83	0.42
2:2:1114:G:H2'	2:2:1115:G:C8	2.55	0.42
4:H:59:HIS:CD2	4:H:188:LYS:HD3	2.54	0.42
18:AN:93:ALA:HB1	18:AN:134:LEU:HD11	2.01	0.42
24:AV:95:LYS:HE3	24:AV:95:LYS:HB3	1.80	0.42
35:BO:73:TRP:NE1	35:BO:82:SER:OG	2.50	0.42
36:BC:360:LYS:HD3	36:BC:360:LYS:HA	1.84	0.42
50:BQ:3:THR:HG22	50:BQ:5:LYS:HG3	2.01	0.42
1:1:208:A:H2'	1:1:209:G:O4'	2.19	0.42
1:1:311:A:H2'	1:1:312:C:O4'	2.20	0.42
1:1:475:G:H4'	1:1:477:A:N7	2.33	0.42
1:1:1809:A:C5	1:1:1810:G:H1'	2.53	0.42
2:2:313:G:H2'	2:2:314:G:O4'	2.20	0.42
2:2:1161:G:O2'	19:AP:56:GLU:OXT	2.30	0.42
2:2:1331:G:H5''	19:AP:33:ILE:HD11	2.01	0.42
2:2:1429:U:H2'	2:2:1430:C:C6	2.55	0.42
2:2:1490:C:H2'	2:2:1491:U:H6	1.85	0.42
4:H:374:LEU:HD23	4:H:374:LEU:HA	1.90	0.42
5:AA:161:GLU:OE2	5:AA:166:LYS:HD2	2.20	0.42
8:AD:43:LYS:HE3	8:AD:43:LYS:HB2	1.76	0.42
28:AZ:70:GLU:OE2	28:AZ:78:PRO:HD3	2.20	0.42
36:BC:128:ARG:HG2	36:BC:179:VAL:HG23	2.02	0.42
43:BE:112:ASN:ND2	43:BE:143:LEU:H	2.17	0.42
53:BD:149:GLN:HA	53:BD:207:ILE:HB	2.02	0.42
30:B4:118:VAL:HG13	30:B4:119:ARG:HD2	2.00	0.42
1:1:2488:A:C4	1:1:2506:C:H5'	2.55	0.42
2:2:880:A:H2'	2:2:881:C:O4'	2.19	0.42
9:AE:146:THR:HB	9:AE:171:ARG:HH22	1.85	0.42
16:AL:3:LYS:HD3	16:AL:75:ILE:O	2.20	0.42
20:AQ:94:ASP:OD1	20:AQ:95:LEU:N	2.52	0.42
23:AU:15:ARG:NH1	23:AU:136:LEU:HD23	2.35	0.42
31:AT:45:LYS:O	31:AT:49:ARG:N	2.38	0.42
35:BO:50:VAL:HB	35:BO:59:LEU:HD21	2.02	0.42
35:BO:63:HIS:HD2	35:BO:65:ARG:H	1.67	0.42
35:BO:180:LYS:HB3	35:BO:180:LYS:HE2	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BC:56:ASP:OD1	36:BC:56:ASP:C	2.63	0.42
36:BC:126:LYS:HB3	36:BC:126:LYS:HE2	1.74	0.42
36:BC:316:ASP:OD1	36:BC:316:ASP:N	2.51	0.42
43:BE:109:GLU:OE1	43:BE:109:GLU:N	2.52	0.42
48:BI:1:MET:HB2	48:BI:1:MET:HE2	1.82	0.42
48:BI:72:ASP:OD1	48:BI:72:ASP:N	2.53	0.42
24:B6:7:GLU:HB3	24:B6:20:TYR:HB2	2.01	0.42
1:1:198:A:C2	1:1:216:A:C5	3.07	0.42
1:1:399:U:H2'	1:1:400:C:H6	1.85	0.42
1:1:1153:C:H2'	1:1:1154:C:H6	1.83	0.42
1:1:1413:C:H2'	1:1:1414:C:C6	2.52	0.42
1:1:1934:4AC:O7	1:1:1934:4AC:H5	2.20	0.42
1:1:2098:G:H1'	33:BB:214:PRO:HG2	2.02	0.42
1:1:2718:4AC:O7	1:1:2718:4AC:H5	2.19	0.42
1:1:2833:C:H5''	4:H:194:GLN:HB2	2.01	0.42
1:1:2925:4AC:O7	1:1:2925:4AC:H5	2.20	0.42
1:1:3004:4AC:H2'	1:1:3005:G:O4'	2.19	0.42
2:2:417:C:H2'	2:2:418:G:H8	1.83	0.42
2:2:479:4AC:O7	2:2:479:4AC:H5	2.20	0.42
2:2:644:C:H2'	2:2:645:C:C6	2.55	0.42
2:2:672:U:C5	2:2:673:C:C5	3.08	0.42
2:2:1017:U:O2'	2:2:1020:A:OP2	2.27	0.42
2:2:1105:G:N7	23:AU:2:ALA:N	2.68	0.42
2:2:1401:U:OP1	14:AJ:16:ARG:NH2	2.53	0.42
3:3:25:C:O2	3:3:123:C:O2'	2.36	0.42
4:H:197:GLU:OE1	4:H:198:LEU:HD22	2.19	0.42
8:AD:33:TYR:HA	8:AD:118:MET:SD	2.60	0.42
8:AD:108:ILE:HD12	8:AD:144:VAL:HB	2.01	0.42
11:AG:64:ARG:HD2	11:AG:122:LYS:HE2	2.02	0.42
12:AH:53:LYS:HB2	12:AH:53:LYS:HE3	1.88	0.42
15:AK:52:ALA:HB1	15:AK:56:ILE:HD11	2.02	0.42
53:BD:3:VAL:HB	53:BD:139:GLN:HE22	1.84	0.42
1:1:468:C:H2'	1:1:469:G:C8	2.55	0.42
1:1:727:G:N7	37:BK:17:ARG:NH2	2.64	0.42
1:1:802:4AC:O7	1:1:802:4AC:H5	2.20	0.42
1:1:1695:4AC:H5	1:1:1695:4AC:O7	2.20	0.42
1:1:1847:C:OP1	1:1:1862:U:H5	2.03	0.42
1:1:1901:G:H22	50:BQ:58:GLN:NE2	2.17	0.42
1:1:2287:4AC:O7	1:1:2287:4AC:H5	2.19	0.42
1:1:2449:G:H2'	1:1:2450:G:C8	2.54	0.42
1:1:2590:C:H5''	49:BR:82:LYS:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:453:C:H2'	2:2:454:U:C6	2.55	0.42
2:2:1481:U:H2'	2:2:1482:A:C8	2.55	0.42
5:AA:112:THR:OG1	5:AA:116:TYR:HB2	2.20	0.42
8:AD:169:MET:HB3	8:AD:169:MET:HE2	1.78	0.42
10:AF:220:ARG:HD3	13:AI:98:GLU:HB2	2.01	0.42
46:BW:27:LYS:HE3	46:BW:27:LYS:HB3	1.77	0.42
59:Bd:38:ILE:HG21	59:Bd:78:ARG:NH2	2.35	0.42
1:1:137:G:H1'	58:BS:8:SER:HB3	2.02	0.41
1:1:335:C:H2'	1:1:336:G:O4'	2.19	0.41
1:1:1966:A:H2'	1:1:1967:C:O4'	2.20	0.41
1:1:2102:G:H2'	1:1:2103:U:O4'	2.19	0.41
1:1:2849:U:C2	1:1:2850:A:C8	3.08	0.41
2:2:424:C:H4'	2:2:425:U:H5	1.85	0.41
2:2:433:C:H2'	2:2:434:U:H6	1.83	0.41
2:2:795:A:H2'	2:2:796:G:O4'	2.20	0.41
2:2:1125:G:C2	2:2:1126:G:C5	3.08	0.41
2:2:1302:C:H2'	2:2:1303:G:O4'	2.20	0.41
2:2:1417:U:H2'	2:2:1418:C:H6	1.85	0.41
8:AD:145:LEU:HB2	8:AD:148:GLU:HG2	2.00	0.41
15:AK:51:LEU:HD11	15:AK:102:TYR:CG	2.55	0.41
24:AV:46:LEU:HD22	24:AV:71:TYR:CE2	2.54	0.41
24:AV:84:GLU:O	24:AV:88:ILE:HG22	2.19	0.41
31:AT:56:LYS:HB2	31:AT:58:LYS:HG2	2.02	0.41
32:AO:79:VAL:HB	32:AO:92:HIS:HB2	2.00	0.41
30:BG:118:VAL:O	30:BG:122:MET:HG2	2.19	0.41
53:BD:251:LYS:HE3	53:BD:251:LYS:HB2	1.87	0.41
30:B4:108:ARG:NH1	30:B4:108:ARG:O	2.53	0.41
1:1:150:G:N3	1:1:604:G:O2'	2.54	0.41
1:1:1615:C:H2'	1:1:1616:C:H6	1.85	0.41
1:1:2136:4AC:H5	1:1:2136:4AC:O7	2.20	0.41
1:1:2183:5MC:OP2	1:1:2184:U:O2'	2.28	0.41
1:1:3022:C:O2	1:1:3022:C:C2'	2.69	0.41
2:2:202:C:C2	2:2:203:A:C8	3.09	0.41
2:2:379:4AC:O7	2:2:379:4AC:H5	2.20	0.41
2:2:934:OMG:HM22	2:2:935:G:H5'	2.02	0.41
2:2:1032:A:N1	2:2:1073:G:O2'	2.47	0.41
15:AK:47:GLU:OE2	15:AK:102:TYR:OH	2.35	0.41
16:AL:101:ILE:H	16:AL:101:ILE:HG13	1.61	0.41
48:BI:1:MET:HE1	48:BI:29:VAL:HG23	2.01	0.41
24:B6:44:LEU:HB3	24:B6:46:LEU:HD21	2.01	0.41
1:1:144:G:H2'	1:1:145:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:776:G:H2'	1:1:2270:C:C4	2.55	0.41
1:1:906:U:H2'	1:1:907:C:C6	2.55	0.41
1:1:994:G:O2'	1:1:1935:G:OP1	2.37	0.41
1:1:1202:U:C2	1:1:1203:G:C8	3.08	0.41
1:1:1320:U:H2'	1:1:1321:U:O4'	2.20	0.41
1:1:1765:4AC:O7	1:1:1765:4AC:H5	2.20	0.41
1:1:1909:A:H2'	1:1:1910:G:C8	2.56	0.41
1:1:2992:4AC:CM7	1:1:2992:4AC:H5	2.49	0.41
2:2:64:OMU:HM22	2:2:65:G:O4'	2.20	0.41
2:2:1169:U:H5''	2:2:1170:A:OP2	2.20	0.41
2:2:1192:C:H2'	2:2:1193:C:C6	2.54	0.41
2:2:1237:C:O3'	23:AU:113:LYS:NZ	2.46	0.41
4:H:264:ILE:HA	4:H:267:MET:HG2	2.02	0.41
5:AA:110:ILE:HG21	5:AA:146:ILE:HG22	2.02	0.41
23:AU:46:GLU:HB2	32:AO:48:PHE:CE1	2.56	0.41
31:AT:62:PRO:HB3	31:AT:82:TYR:CE2	2.55	0.41
32:AO:63:GLU:O	32:AO:67:GLN:HG2	2.20	0.41
33:BB:237:ARG:HB3	33:BB:239:LYS:HG2	2.01	0.41
36:BC:52:LEU:HB2	36:BC:354:TYR:HB3	2.02	0.41
36:BC:79:ARG:HH21	36:BC:167:GLN:HE22	1.69	0.41
36:BC:199:LYS:HE2	36:BC:204:LEU:HD13	2.01	0.41
42:Be:18:ILE:HG12	42:Be:30:VAL:HG22	2.01	0.41
43:BE:92:LYS:HE2	43:BE:92:LYS:HB2	1.85	0.41
30:BG:116:MET:N	30:BG:116:MET:SD	2.92	0.41
1:1:2302:A:H2	1:1:2735:C:H42	1.68	0.41
1:1:3020:U:H3'	1:1:3021:U:H2'	2.02	0.41
2:2:182:C:H2'	2:2:183:U:C6	2.55	0.41
2:2:394:4AC:H2'	2:2:395:G:C8	2.55	0.41
11:AG:8:ILE:HD11	11:AG:19:ILE:HG22	2.03	0.41
43:BE:36:GLU:OE2	43:BE:40:ARG:HD3	2.21	0.41
43:BE:101:ARG:HE	43:BE:184:VAL:HG12	1.85	0.41
44:Ba:33:LYS:HE3	44:Ba:33:LYS:HB2	1.88	0.41
37:BK:37:GLY:HA3	37:BK:41:ASN:OD1	2.21	0.41
1:1:46:C:H2'	1:1:47:G:H8	1.86	0.41
1:1:77:C:H4'	36:BC:311:GLY:HA2	2.02	0.41
1:1:377:C:O2'	1:1:422:C:H5''	2.21	0.41
1:1:761:U:H2'	1:1:762:G:C8	2.55	0.41
1:1:961:U:H2'	1:1:962:C:C6	2.55	0.41
1:1:1056:G:H5'	38:BL:29:GLY:HA3	2.02	0.41
1:1:1065:4AC:HM72	38:BL:10:LYS:HE3	2.01	0.41
1:1:2087:G:H2'	1:1:2088:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2423:C:H2'	1:1:2424:C:C6	2.55	0.41
1:1:2817:U:H2'	4:H:197:GLU:HB2	2.02	0.41
2:2:29:C:H2'	2:2:30:C:H6	1.86	0.41
2:2:165:G:H5'	11:AG:11:PRO:HA	2.03	0.41
2:2:866:G:H2'	2:2:867:C:C6	2.56	0.41
3:3:45:A:C4	3:3:46:A:C8	3.08	0.41
8:AD:95:LEU:HD12	8:AD:95:LEU:HA	1.94	0.41
12:AH:133:ARG:NE	12:AH:208:GLU:OE2	2.40	0.41
15:AK:104:ARG:O	15:AK:108:VAL:HG22	2.21	0.41
35:BO:25:LEU:O	35:BO:29:LYS:HG3	2.21	0.41
38:BL:44:LYS:HG3	38:BL:47:TRP:CB	2.50	0.41
53:BD:90:ARG:NH1	53:BD:92:THR:HA	2.35	0.41
1:1:113:G:H8	1:1:113:G:O5'	2.03	0.41
1:1:652:U:H2'	1:1:653:G:O4'	2.20	0.41
1:1:1173:C:H2'	1:1:1174:A:C8	2.56	0.41
1:1:1598:G:O2'	1:1:1655:A:N1	2.46	0.41
1:1:2394:G:H2'	1:1:2395:U:H6	1.85	0.41
2:2:952:C:O2	19:AP:17:GLY:N	2.44	0.41
2:2:1195:G:H5'	2:2:1295:U:O2	2.21	0.41
2:2:1360:C:H2'	2:2:1361:U:C6	2.56	0.41
2:2:1446:U:H2'	2:2:1447:C:C6	2.54	0.41
2:2:1482:A:H2'	2:2:1483:G:C8	2.54	0.41
4:H:93:LEU:HA	4:H:93:LEU:HD12	1.79	0.41
7:AC:29:HIS:HB3	7:AC:41:TRP:CE3	2.56	0.41
8:AD:169:MET:H	8:AD:169:MET:HG2	1.71	0.41
13:AI:55:ASP:OD1	13:AI:55:ASP:N	2.53	0.41
15:AK:48:PRO:HG3	15:AK:106:MET:HE2	2.02	0.41
28:AZ:43:LYS:NZ	28:AZ:81:ASP:HB2	2.35	0.41
33:BB:75:GLU:OE2	47:Bi:72:THR:OG1	2.33	0.41
34:BY:33:HIS:CE1	34:BY:118:ARG:HG2	2.54	0.41
34:BY:145:GLU:N	34:BY:145:GLU:OE1	2.53	0.41
38:BL:47:TRP:O	38:BL:51:ILE:HG12	2.21	0.41
53:BD:19:PRO:HG3	53:BD:251:LYS:HE2	2.02	0.41
54:BF:89:LYS:HG3	54:BF:138:ILE:HD13	2.01	0.41
55:BZ:11:LEU:HD12	55:BZ:11:LEU:HA	1.92	0.41
63:BJ:92:LEU:HD23	63:BJ:92:LEU:HA	1.86	0.41
30:B4:44:GLU:O	30:B4:73:LYS:NZ	2.51	0.41
1:1:1335:C:H2'	1:1:1336:U:C6	2.55	0.41
1:1:1867:4AC:O7	1:1:1867:4AC:H5	2.21	0.41
1:1:2804:A:OP2	36:BC:257:HIS:HD2	2.03	0.41
2:2:276:C:H2'	2:2:277:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:839:4AC:H2'	2:2:840:G:O4'	2.21	0.41
2:2:957:4AC:O7	2:2:957:4AC:H5	2.21	0.41
2:2:1098:C:H2'	2:2:1099:C:H6	1.84	0.41
2:2:1266:C:H2'	2:2:1267:G:C8	2.56	0.41
8:AD:38:LYS:HA	8:AD:38:LYS:HD2	1.92	0.41
9:AE:211:ASP:N	9:AE:211:ASP:OD1	2.52	0.41
11:AG:22:THR:OG1	11:AG:23:GLY:N	2.54	0.41
12:AH:132:PRO:O	12:AH:157:ARG:HD2	2.20	0.41
12:AH:139:VAL:HG23	26:AX:19:GLY:HA2	2.03	0.41
35:BO:176:LEU:HD21	35:BO:181:LEU:HD13	2.02	0.41
52:Bj:26:LYS:NZ	52:Bj:28:ARG:HH22	2.18	0.41
30:BG:62:ILE:HG22	30:BG:63:VAL:HG13	2.03	0.41
30:B4:113:GLU:O	30:B4:117:LYS:HG3	2.20	0.41
1:1:103:C:O2'	1:1:104:C:H5'	2.21	0.41
1:1:640:C:H1'	58:BS:104:GLN:NE2	2.36	0.41
1:1:866:C:H2'	1:1:866:C:OP2	2.20	0.41
1:1:1293:4AC:H5	1:1:1293:4AC:O7	2.20	0.41
1:1:1489:C:H2'	1:1:1490:G:C8	2.56	0.41
1:1:1653:U:P	50:BQ:42:ARG:HH22	2.43	0.41
1:1:1689:C:H2'	1:1:1691:A:H62	1.86	0.41
1:1:2949:G:OP1	51:BV:39:ARG:HD3	2.21	0.41
2:2:640:G:H2'	2:2:641:G:H8	1.86	0.41
2:2:671:A:C5	2:2:672:U:C5	3.09	0.41
2:2:949:A:N6	2:2:1198:U:O5'	2.53	0.41
2:2:1391:G:N2	2:2:1451:G:H2'	2.36	0.41
2:2:1435:C:H2'	2:2:1436:G:O4'	2.20	0.41
4:H:38:ILE:HB	4:H:50:LEU:HB3	2.02	0.41
4:H:60:LEU:HD23	4:H:187:ILE:HG12	2.02	0.41
6:AB:59:LEU:HD23	6:AB:59:LEU:HA	1.90	0.41
6:AB:101:MET:HE3	6:AB:129:GLU:HB2	2.02	0.41
6:AB:128:LYS:O	6:AB:132:GLU:HG3	2.21	0.41
23:AU:20:LEU:HB3	23:AU:26:ILE:HD11	2.02	0.41
30:A3:13:LYS:O	30:A3:17:GLU:HG2	2.21	0.41
30:A3:66:LEU:HB3	30:A3:67:PRO:HD3	2.01	0.41
35:BO:188:VAL:O	35:BO:192:ILE:HG12	2.20	0.41
41:Bb:29:TRP:CD1	41:Bb:29:TRP:H	2.38	0.41
48:BI:130:THR:HG1	48:BI:133:GLU:HG3	1.86	0.41
49:BR:19:HIS:HB3	49:BR:22:ARG:HE	1.86	0.41
57:BM:150:ALA:O	65:Bk:11:ASP:HB2	2.21	0.41
1:1:120:A:H2'	1:1:121:G:C8	2.56	0.41
1:1:399:U:H2'	1:1:400:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:829:4AC:O7	1:1:829:4AC:H5	2.21	0.41
1:1:1587:C:H2'	1:1:1588:G:O4'	2.20	0.41
1:1:1882:A:H1'	39:Bf:45:ARG:HH22	1.86	0.41
1:1:2367:G:C6	1:1:2402:G:N1	2.89	0.41
1:1:2370:G:O2'	1:1:2373:G:O2'	2.34	0.41
1:1:2419:C:H2'	1:1:2420:A:H8	1.85	0.41
1:1:2818:U:H2'	1:1:2819:A:O4'	2.21	0.41
2:2:103:G:H2'	2:2:104:G:O4'	2.21	0.41
2:2:109:C:H2'	2:2:110:U:H6	1.85	0.41
2:2:518:U:H2'	2:2:519:OMG:C8	2.56	0.41
2:2:569:G:H5'	9:AE:224:ASP:HB2	2.03	0.41
2:2:626:4AC:O7	2:2:626:4AC:H5	2.20	0.41
2:2:731:4AC:O7	2:2:731:4AC:H5	2.21	0.41
2:2:828:4AC:O7	2:2:828:4AC:H5	2.21	0.41
2:2:1297:G:H2'	2:2:1298:C:C6	2.56	0.41
2:2:1316:C:H2'	2:2:1317:C:C6	2.56	0.41
2:2:1402:A:H2'	2:2:1403:G:C8	2.56	0.41
2:2:1494:G:OP2	17:AM:132:ARG:NH1	2.46	0.41
8:AD:34:GLU:HG2	8:AD:119:ARG:HB2	2.03	0.41
10:AF:39:ARG:HH22	10:AF:209:ASN:ND2	2.18	0.41
11:AG:33:ARG:NH1	11:AG:36:ASP:OD1	2.53	0.41
22:AS:17:PHE:CZ	22:AS:61:LYS:HD3	2.55	0.41
31:AT:7:ARG:NH1	31:AT:10:GLY:O	2.53	0.41
32:AO:60:LYS:HB3	32:AO:60:LYS:HE3	1.87	0.41
35:BO:155:MET:O	35:BO:159:GLN:HG2	2.20	0.41
38:BL:10:LYS:HE2	38:BL:10:LYS:HB3	1.89	0.41
39:Bf:9:LYS:NZ	39:Bf:51:GLU:HG3	2.36	0.41
39:Bf:38:HIS:HD2	39:Bf:40:LYS:H	1.68	0.41
45:BT:11:VAL:HB	45:BT:27:THR:HG23	2.03	0.41
37:BK:40:LEU:HD22	37:BK:72:LYS:HD3	2.03	0.41
50:BQ:64:ARG:O	50:BQ:68:GLU:HG2	2.20	0.41
30:BG:115:ALA:O	30:BG:119:ARG:HG3	2.21	0.41
54:BF:170:ASP:OD1	54:BF:170:ASP:N	2.53	0.41
57:BM:54:GLN:NE2	57:BM:143:ASP:OD2	2.50	0.41
60:BN:142:LEU:HD12	60:BN:142:LEU:HA	1.84	0.41
1:1:117:G:C4	1:1:118:U:C6	3.09	0.41
1:1:163:A:H5''	1:1:165:G:O4'	2.21	0.41
1:1:181:U:C2	1:1:182:G:C8	3.09	0.41
1:1:1550:4AC:O7	1:1:1550:4AC:H5	2.20	0.41
1:1:1574:C:O2'	1:1:1654:A:N3	2.50	0.41
1:1:1933:C:H2'	1:1:1934:4AC:H6	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2242:C:HO2'	44:Ba:24:ARG:NH2	2.16	0.41
1:1:2466:U:H2'	1:1:2467:G:O4'	2.21	0.41
1:1:2536:U:C2	43:BE:136:GLY:HA3	2.56	0.41
1:1:2539:G:N3	1:1:2539:G:H2'	2.35	0.41
2:2:190:C:H2'	2:2:191:U:H6	1.86	0.41
2:2:546:4AC:H5''	20:AQ:5:HIS:CD2	2.56	0.41
2:2:1267:G:OP1	12:AH:3:LYS:N	2.54	0.41
4:H:145:PRO:HB2	4:H:211:ARG:HB2	2.03	0.41
7:AC:37:GLU:O	7:AC:57:LYS:NZ	2.47	0.41
10:AF:13:LEU:HD11	10:AF:27:LYS:HA	2.03	0.41
10:AF:19:LYS:N	10:AF:46:GLU:OE2	2.31	0.41
16:AL:12:ASN:ND2	16:AL:15:SER:OG	2.54	0.41
18:AN:133:SER:HB3	18:AN:136:GLU:HG2	2.03	0.41
31:AT:68:ARG:HB3	31:AT:104:GLY:HA3	2.03	0.41
36:BC:141:PHE:HZ	36:BC:200:LEU:HD13	1.86	0.41
36:BC:211:LYS:O	36:BC:214:GLU:HG2	2.21	0.41
44:Ba:25:TRP:CZ2	44:Ba:26:LYS:HD3	2.56	0.41
53:BD:161:PHE:CD1	53:BD:166:ILE:HD11	2.56	0.41
30:B4:119:ARG:NH2	30:B4:123:LYS:HD3	2.35	0.41
1:1:465:A:C4	1:1:467:G:C8	3.09	0.40
1:1:1084:A:N6	1:1:1198:A:H2	2.18	0.40
1:1:1093:C:H2'	1:1:1094:C:H6	1.86	0.40
1:1:1303:A:O2'	1:1:1304:C:O5'	2.28	0.40
1:1:2009:G:N2	1:1:2012:G:OP2	2.48	0.40
1:1:2027:4AC:O7	1:1:2027:4AC:H5	2.21	0.40
2:2:110:U:H2'	2:2:111:C:C6	2.56	0.40
2:2:466:G:H2'	2:2:467:OMG:C8	2.56	0.40
2:2:656:G:H2'	2:2:657:OMG:O4'	2.21	0.40
2:2:664:U:O2	2:2:765:G:H1'	2.21	0.40
2:2:1504:C:H3'	2:2:1505:5MC:HM53	2.01	0.40
14:AJ:4:TRP:CG	14:AJ:23:LYS:HD3	2.56	0.40
32:AO:64:GLU:OE1	32:AO:64:GLU:N	2.35	0.40
46:BW:36:THR:OG1	46:BW:37:SER:N	2.54	0.40
51:BV:5:ASN:HB2	51:BV:14:PHE:CZ	2.57	0.40
30:BG:110:LEU:HD23	30:BG:110:LEU:HA	1.90	0.40
54:BF:10:GLU:OE1	54:BF:54:VAL:HG22	2.21	0.40
54:BF:143:ASP:HB3	54:BF:146:ALA:HB3	2.02	0.40
55:BZ:34:LEU:HD12	55:BZ:35:ILE:H	1.85	0.40
60:BN:29:PRO:HA	60:BN:59:GLN:HE22	1.86	0.40
64:Bl:34:LYS:HB2	64:Bl:34:LYS:HE2	1.92	0.40
1:1:18:G:H8	1:1:2855:G:H4'	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:843:A:H2'	1:1:844:A:C8	2.56	0.40
1:1:1209:G:N2	1:1:1211:A:H3'	2.37	0.40
1:1:1783:G:H2'	1:1:1784:U:C6	2.56	0.40
1:1:2118:U:N3	1:1:2121:A:OP2	2.34	0.40
1:1:2564:A:H5''	35:BO:22:ARG:HH22	1.86	0.40
1:1:2931:U:H2'	1:1:2932:C:H6	1.86	0.40
2:2:106:C:H2'	2:2:107:G:O4'	2.21	0.40
2:2:350:C:H2'	2:2:351:C:C6	2.57	0.40
2:2:685:G:H5'	17:AM:124:ASP:CG	2.46	0.40
2:2:1239:4AC:O7	2:2:1239:4AC:H5	2.21	0.40
2:2:1489:C:H2'	2:2:1490:C:H6	1.85	0.40
3:3:32:4AC:O7	3:3:32:4AC:H5	2.21	0.40
4:H:237:ASN:OD1	4:H:237:ASN:N	2.55	0.40
12:AH:16:LYS:O	12:AH:43:LEU:HA	2.21	0.40
15:AK:46:LEU:HD23	15:AK:49:LEU:HD12	2.02	0.40
18:AN:30:TYR:O	18:AN:34:VAL:HG22	2.21	0.40
23:AU:29:PRO:HD2	23:AU:32:ALA:HB2	2.02	0.40
25:AW:5:ARG:HB2	25:AW:6:ASN:H	1.68	0.40
36:BC:103:ASP:HB2	36:BC:122:TYR:CD2	2.55	0.40
36:BC:184:ILE:O	36:BC:192:LYS:HE3	2.22	0.40
52:Bj:48:GLY:HA2	57:BM:83:SER:HA	2.02	0.40
54:BF:19:VAL:HG22	54:BF:28:VAL:HG22	2.04	0.40
1:1:2344:G:H2'	1:1:2345:G:C8	2.55	0.40
1:1:2587:U:OP2	1:1:2588:A:O2'	2.32	0.40
2:2:27:U:H2'	2:2:28:G:O4'	2.22	0.40
2:2:101:G:H2'	2:2:102:C:C6	2.56	0.40
2:2:163:G:H2'	2:2:164:G:C8	2.56	0.40
2:2:1037:G:C5	2:2:1038:U:C4	3.09	0.40
2:2:1184:4AC:O7	2:2:1184:4AC:H5	2.21	0.40
2:2:1215:G:H2'	2:2:1216:G:C8	2.56	0.40
8:AD:163:PRO:HA	8:AD:168:ARG:HD2	2.02	0.40
23:AU:102:LEU:HD13	23:AU:119:ARG:HD3	2.02	0.40
25:AW:18:VAL:HG12	25:AW:60:ILE:HA	2.03	0.40
40:BU:3:LEU:HD21	40:BU:14:PHE:CD2	2.56	0.40
48:BI:7:GLU:HA	48:BI:35:LYS:HB2	2.03	0.40
50:BQ:3:THR:HG21	50:BQ:5:LYS:HE2	2.04	0.40
53:BD:147:ASP:OD1	53:BD:147:ASP:N	2.52	0.40
54:BF:130:VAL:HG22	54:BF:139:VAL:HG22	2.04	0.40
24:B6:21:PHE:CE2	24:B6:67:GLY:HA3	2.56	0.40
24:B6:46:LEU:HD22	24:B6:71:TYR:CD2	2.57	0.40
56:BP:26:LYS:HB3	56:BP:26:LYS:HE3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:BJ:86:ARG:H	63:BJ:102:ASN:ND2	2.20	0.40
64:BL:11:TYR:CE2	64:BL:18:LYS:HD2	2.56	0.40
1:1:390:C:H2'	1:1:391:G:O4'	2.21	0.40
1:1:869:G:H4'	1:1:870:A:OP1	2.21	0.40
1:1:938:A:H2'	1:1:939:G:C8	2.56	0.40
1:1:1296:G:H1'	60:BN:178:SER:CB	2.51	0.40
1:1:1529:A:N3	1:1:2244:G:O2'	2.49	0.40
1:1:1594:4AC:O7	1:1:1594:4AC:H5	2.22	0.40
1:1:1953:A:H2'	1:1:1954:A:C8	2.57	0.40
1:1:2187:U:H2'	1:1:2188:C:H6	1.86	0.40
2:2:154:G:H21	11:AG:118:GLN:NE2	2.18	0.40
2:2:497:U:H6	2:2:497:U:H2'	1.67	0.40
2:2:1441:U:H2'	2:2:1442:A:C8	2.56	0.40
2:2:1478:C:H2'	2:2:1479:4AC:H6	2.03	0.40
9:AE:12:ARG:HG2	9:AE:29:ALA:HB2	2.03	0.40
9:AE:170:GLU:OE1	9:AE:170:GLU:N	2.50	0.40
14:AJ:44:LYS:HE2	14:AJ:44:LYS:HB3	1.82	0.40
21:AR:74:ASN:ND2	21:AR:80:ALA:H	2.15	0.40
31:AT:46:LYS:HE2	31:AT:46:LYS:HB3	1.83	0.40
38:BL:106:THR:HG22	38:BL:127:ARG:HD2	2.03	0.40
39:Bf:20:ASN:ND2	39:Bf:42:ARG:H	2.19	0.40
1:1:152:U:H2'	1:1:153:C:C6	2.55	0.40
1:1:189:G:H2'	1:1:189:G:N3	2.37	0.40
1:1:435:C:H2'	1:1:436:C:C6	2.56	0.40
1:1:733:C:H2'	1:1:734:G:H8	1.86	0.40
1:1:775:U:O2'	1:1:1234:A:N1	2.52	0.40
1:1:974:G:OP1	1:1:1768:A:O2'	2.36	0.40
1:1:1953:A:H2'	1:1:1954:A:H8	1.87	0.40
1:1:2017:U:H2'	1:1:2018:A:O4'	2.22	0.40
1:1:2371:U:H5'	1:1:2373:G:O4'	2.21	0.40
1:1:2380:G:C2	1:1:2381:G:C5	3.09	0.40
1:1:2933:C:OP2	50:BQ:62:ARG:NH2	2.51	0.40
2:2:373:A2M:O5'	2:2:373:A2M:H8	2.22	0.40
2:2:511:4AC:H2'	2:2:512:G:O4'	2.22	0.40
2:2:976:A:H2	2:2:1000:G:N3	2.20	0.40
5:AA:108:PHE:HD2	5:AA:120:VAL:HG23	1.86	0.40
5:AA:182:LYS:HA	5:AA:182:LYS:HD2	1.94	0.40
9:AE:151:PRO:HG2	9:AE:154:GLU:OE1	2.22	0.40
18:AN:79:LYS:HB2	18:AN:79:LYS:HE3	1.94	0.40
33:BB:21:SER:HA	33:BB:24:PHE:CD2	2.57	0.40
48:BI:17:ARG:O	48:BI:21:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:BN:105:ALA:O	60:BN:109:GLY:N	2.46	0.40
62:Bc:26:PRO:HB2	62:Bc:29:VAL:HG13	2.03	0.40
62:Bc:64:LYS:HA	62:Bc:64:LYS:HD3	1.73	0.40
65:Bk:25:MET:HE3	65:Bk:36:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

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	
4	H	384/392 (98%)	369 (96%)	15 (4%)	0	100	100
5	AA	186/199 (94%)	181 (97%)	5 (3%)	0	100	100
6	AB	194/202 (96%)	194 (100%)	0	0	100	100
7	AC	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
8	AD	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
9	AE	240/243 (99%)	233 (97%)	7 (3%)	0	100	100
10	AF	227/236 (96%)	221 (97%)	6 (3%)	0	100	100
11	AG	122/125 (98%)	116 (95%)	6 (5%)	0	100	100
12	AH	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
13	AI	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
14	AJ	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
15	AK	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
16	AL	98/102 (96%)	96 (98%)	2 (2%)	0	100	100
17	AM	125/137 (91%)	120 (96%)	5 (4%)	0	100	100
18	AN	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
19	AP	53/56 (95%)	52 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AQ	155/158 (98%)	151 (97%)	4 (3%)	0	100	100
21	AR	105/113 (93%)	101 (96%)	4 (4%)	0	100	100
22	AS	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
23	AU	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
24	AV	94/99 (95%)	93 (99%)	1 (1%)	0	100	100
24	B6	92/99 (93%)	92 (100%)	0	0	100	100
25	AW	59/65 (91%)	57 (97%)	2 (3%)	0	100	100
26	AX	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
27	AY	47/51 (92%)	42 (89%)	5 (11%)	0	100	100
28	AZ	194/210 (92%)	189 (97%)	5 (3%)	0	100	100
29	A0	34/37 (92%)	34 (100%)	0	0	100	100
30	A3	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
30	B4	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
30	BG	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
31	AT	128/132 (97%)	126 (98%)	2 (2%)	0	100	100
32	AO	136/148 (92%)	127 (93%)	9 (7%)	0	100	100
33	BB	236/239 (99%)	227 (96%)	9 (4%)	0	100	100
34	BY	152/155 (98%)	151 (99%)	1 (1%)	0	100	100
35	BO	196/203 (97%)	193 (98%)	3 (2%)	0	100	100
36	BC	358/361 (99%)	348 (97%)	10 (3%)	0	100	100
37	B5	79/82 (96%)	77 (98%)	2 (2%)	0	100	100
37	BK	78/82 (95%)	74 (95%)	4 (5%)	0	100	100
38	BL	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
39	Bf	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
40	BU	119/121 (98%)	119 (100%)	0	0	100	100
41	Bb	127/130 (98%)	127 (100%)	0	0	100	100
42	Be	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
43	BE	183/188 (97%)	182 (100%)	1 (0%)	0	100	100
44	Ba	92/94 (98%)	92 (100%)	0	0	100	100
45	BT	84/86 (98%)	84 (100%)	0	0	100	100
46	BW	66/68 (97%)	65 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	Bi	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
48	BI	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
49	BR	94/97 (97%)	94 (100%)	0	0	100	100
50	BQ	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
51	BV	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
52	Bj	92/94 (98%)	92 (100%)	0	0	100	100
53	BD	253/255 (99%)	249 (98%)	4 (2%)	0	100	100
54	BF	181/184 (98%)	181 (100%)	0	0	100	100
55	BZ	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
56	BP	118/120 (98%)	118 (100%)	0	0	100	100
57	BM	191/194 (98%)	189 (99%)	2 (1%)	0	100	100
58	BS	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
59	Bd	89/91 (98%)	89 (100%)	0	0	100	100
60	BN	176/181 (97%)	169 (96%)	7 (4%)	0	100	100
61	Bg	46/51 (90%)	46 (100%)	0	0	100	100
62	Bc	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
63	BJ	138/141 (98%)	138 (100%)	0	0	100	100
64	Bl	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
65	Bk	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
All	All	8568/8861 (97%)	8378 (98%)	190 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	
4	H	332/338 (98%)	312 (94%)	20 (6%)	17	15
5	AA	160/167 (96%)	153 (96%)	7 (4%)	25	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AB	168/173 (97%)	161 (96%)	7 (4%)	26	28
7	AC	50/55 (91%)	47 (94%)	3 (6%)	17	15
8	AD	156/160 (98%)	149 (96%)	7 (4%)	24	25
9	AE	213/214 (100%)	205 (96%)	8 (4%)	29	32
10	AF	192/198 (97%)	187 (97%)	5 (3%)	40	46
11	AG	107/108 (99%)	102 (95%)	5 (5%)	23	24
12	AH	183/184 (100%)	176 (96%)	7 (4%)	29	32
13	AI	106/107 (99%)	103 (97%)	3 (3%)	38	43
14	AJ	101/103 (98%)	98 (97%)	3 (3%)	36	41
15	AK	111/111 (100%)	107 (96%)	4 (4%)	31	34
16	AL	89/91 (98%)	82 (92%)	7 (8%)	11	9
17	AM	94/104 (90%)	93 (99%)	1 (1%)	65	74
18	AN	120/121 (99%)	117 (98%)	3 (2%)	42	48
19	AP	45/46 (98%)	43 (96%)	2 (4%)	25	26
20	AQ	142/143 (99%)	138 (97%)	4 (3%)	38	43
21	AR	96/102 (94%)	93 (97%)	3 (3%)	35	39
22	AS	58/61 (95%)	58 (100%)	0	100	100
23	AU	126/127 (99%)	117 (93%)	9 (7%)	13	11
24	AV	88/90 (98%)	81 (92%)	7 (8%)	11	8
24	B6	86/90 (96%)	83 (96%)	3 (4%)	32	35
25	AW	53/56 (95%)	51 (96%)	2 (4%)	29	32
26	AX	55/60 (92%)	50 (91%)	5 (9%)	9	6
27	AY	40/42 (95%)	37 (92%)	3 (8%)	12	10
28	AZ	155/168 (92%)	150 (97%)	5 (3%)	34	38
29	A0	34/35 (97%)	33 (97%)	1 (3%)	37	42
30	A3	98/99 (99%)	93 (95%)	5 (5%)	21	21
30	B4	98/99 (99%)	88 (90%)	10 (10%)	7	4
30	BG	98/99 (99%)	97 (99%)	1 (1%)	68	76
31	AT	113/114 (99%)	107 (95%)	6 (5%)	20	19
32	AO	115/123 (94%)	107 (93%)	8 (7%)	14	11
33	BB	188/189 (100%)	185 (98%)	3 (2%)	55	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	BY	132/133 (99%)	131 (99%)	1 (1%)	73	81
35	BO	167/170 (98%)	160 (96%)	7 (4%)	26	28
36	BC	306/307 (100%)	299 (98%)	7 (2%)	44	51
37	B5	65/66 (98%)	61 (94%)	4 (6%)	16	14
37	BK	64/66 (97%)	61 (95%)	3 (5%)	23	24
38	BL	118/118 (100%)	114 (97%)	4 (3%)	32	35
39	Bf	46/47 (98%)	45 (98%)	1 (2%)	45	53
40	BU	109/109 (100%)	108 (99%)	1 (1%)	70	78
41	Bb	117/118 (99%)	115 (98%)	2 (2%)	53	62
42	Be	52/53 (98%)	50 (96%)	2 (4%)	29	32
43	BE	158/160 (99%)	151 (96%)	7 (4%)	25	26
44	Ba	84/84 (100%)	81 (96%)	3 (4%)	31	34
45	BT	77/77 (100%)	75 (97%)	2 (3%)	40	46
46	BW	63/63 (100%)	60 (95%)	3 (5%)	23	23
47	Bi	61/62 (98%)	60 (98%)	1 (2%)	55	64
48	BI	122/122 (100%)	119 (98%)	3 (2%)	42	48
49	BR	86/87 (99%)	85 (99%)	1 (1%)	63	72
50	BQ	132/133 (99%)	129 (98%)	3 (2%)	44	51
51	BV	54/58 (93%)	52 (96%)	2 (4%)	30	33
52	Bj	83/84 (99%)	80 (96%)	3 (4%)	31	34
53	BD	212/212 (100%)	206 (97%)	6 (3%)	38	43
54	BF	156/157 (99%)	153 (98%)	3 (2%)	50	58
55	BZ	79/80 (99%)	76 (96%)	3 (4%)	29	32
56	BP	102/102 (100%)	99 (97%)	3 (3%)	37	42
57	BM	160/161 (99%)	158 (99%)	2 (1%)	61	69
58	BS	130/131 (99%)	128 (98%)	2 (2%)	57	65
59	Bd	82/82 (100%)	81 (99%)	1 (1%)	63	72
60	BN	149/151 (99%)	142 (95%)	7 (5%)	23	24
61	Bg	37/39 (95%)	37 (100%)	0	100	100
62	Bc	74/74 (100%)	70 (95%)	4 (5%)	20	18
63	BJ	108/109 (99%)	103 (95%)	5 (5%)	24	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	Bl	72/72 (100%)	70 (97%)	2 (3%)	38	43
65	Bk	55/57 (96%)	54 (98%)	1 (2%)	51	60
All	All	7382/7521 (98%)	7116 (96%)	266 (4%)	32	34

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	42	ASP
4	H	85	LEU
4	H	90	LYS
4	H	126	GLU
4	H	133	GLU
4	H	163	ARG
4	H	170	GLU
4	H	181	ASP
4	H	191	PHE
4	H	194	GLN
4	H	195	TYR
4	H	198	LEU
4	H	216	LYS
4	H	218	VAL
4	H	245	VAL
4	H	256	THR
4	H	306	ASP
4	H	375	GLU
4	H	379	ARG
4	H	386	GLU
5	AA	27	PHE
5	AA	56	ILE
5	AA	80	TYR
5	AA	96	LEU
5	AA	100	ARG
5	AA	128	ARG
5	AA	181	LEU
6	AB	6	LEU
6	AB	35	VAL
6	AB	74	LEU
6	AB	106	VAL
6	AB	111	GLU
6	AB	142	ASP
6	AB	170	ILE

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Mol	Chain	Res	Type
7	AC	31	VAL
7	AC	44	GLU
7	AC	48	LEU
8	AD	19	ILE
8	AD	29	LEU
8	AD	89	LEU
8	AD	96	THR
8	AD	120	GLN
8	AD	124	LEU
8	AD	150	ASP
9	AE	49	VAL
9	AE	103	LEU
9	AE	111	ILE
9	AE	112	LEU
9	AE	123	LYS
9	AE	168	VAL
9	AE	187	VAL
9	AE	228	GLU
10	AF	22	LEU
10	AF	43	GLN
10	AF	57	VAL
10	AF	96	VAL
10	AF	225	VAL
11	AG	6	LEU
11	AG	38	ILE
11	AG	60	LYS
11	AG	121	VAL
11	AG	125	TYR
12	AH	25	ASP
12	AH	38	ASN
12	AH	93	LEU
12	AH	123	LEU
12	AH	155	MET
12	AH	184	LEU
12	AH	207	ILE
13	AI	47	ILE
13	AI	57	ARG
13	AI	82	LYS
14	AJ	18	VAL
14	AJ	96	THR
14	AJ	126	GLU
15	AK	37	GLU

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Mol	Chain	Res	Type
15	AK	67	GLN
15	AK	76	GLU
15	AK	82	ILE
16	AL	10	SER
16	AL	16	LEU
16	AL	28	GLU
16	AL	38	ILE
16	AL	75	ILE
16	AL	82	MET
16	AL	98	ILE
17	AM	38	THR
18	AN	18	LEU
18	AN	132	VAL
18	AN	134	LEU
19	AP	13	LYS
19	AP	22	ILE
20	AQ	16	ARG
20	AQ	34	GLU
20	AQ	60	ILE
20	AQ	96	MET
21	AR	38	VAL
21	AR	82	VAL
21	AR	84	ASP
23	AU	7	VAL
23	AU	12	LEU
23	AU	14	GLU
23	AU	39	ARG
23	AU	44	LEU
23	AU	61	ARG
23	AU	71	GLU
23	AU	119	ARG
23	AU	130	ASP
24	AV	7	GLU
24	AV	19	ILE
24	AV	23	ILE
24	AV	50	THR
24	AV	56	ILE
24	AV	78	MET
24	AV	88	ILE
25	AW	12	ARG
25	AW	60	ILE
26	AX	12	ILE

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Mol	Chain	Res	Type
26	AX	18	THR
26	AX	32	LEU
26	AX	66	GLU
26	AX	67	ILE
27	AY	9	ILE
27	AY	46	THR
27	AY	48	TRP
28	AZ	22	GLU
28	AZ	159	GLU
28	AZ	175	VAL
28	AZ	192	GLU
28	AZ	193	ILE
29	A0	13	ARG
30	A3	7	VAL
30	A3	23	VAL
30	A3	50	LEU
30	A3	69	LEU
30	A3	102	ILE
31	AT	18	ASN
31	AT	24	LEU
31	AT	26	LYS
31	AT	90	VAL
31	AT	123	THR
31	AT	129	VAL
32	AO	21	LEU
32	AO	31	VAL
32	AO	49	MET
32	AO	72	HIS
32	AO	84	ASP
32	AO	90	ASP
32	AO	91	LEU
32	AO	126	VAL
33	BB	75	GLU
33	BB	96	THR
33	BB	147	GLU
34	BY	78	LYS
35	BO	8	ARG
35	BO	64	THR
35	BO	65	ARG
35	BO	85	LEU
35	BO	90	ILE
35	BO	137	ILE

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Mol	Chain	Res	Type
35	BO	172	LEU
36	BC	56	ASP
36	BC	118	LYS
36	BC	140	ASP
36	BC	199	LYS
36	BC	200	LEU
36	BC	291	LYS
36	BC	293	VAL
37	B5	33	VAL
37	B5	60	ILE
37	B5	61	ASP
37	B5	62	ILE
38	BL	69	VAL
38	BL	115	THR
38	BL	123	VAL
38	BL	146	LEU
39	Bf	47	THR
40	BU	55	MET
41	Bb	84	ILE
41	Bb	108	LYS
42	Be	21	ARG
42	Be	30	VAL
43	BE	29	THR
43	BE	34	VAL
43	BE	82	LEU
43	BE	92	LYS
43	BE	126	VAL
43	BE	144	GLU
43	BE	184	VAL
44	Ba	3	ILE
44	Ba	49	ILE
44	Ba	92	ASP
45	BT	12	ILE
45	BT	17	ILE
46	BW	5	GLU
46	BW	23	LEU
46	BW	27	LYS
47	Bi	51	THR
48	BI	1	MET
48	BI	4	ILE
48	BI	43	GLU
49	BR	77	VAL

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Mol	Chain	Res	Type
37	BK	4	ILE
37	BK	60	ILE
37	BK	75	LEU
50	BQ	40	ASP
50	BQ	71	LYS
50	BQ	122	MET
51	BV	15	GLU
51	BV	54	LYS
52	Bj	33	LEU
52	Bj	63	LYS
52	Bj	65	LEU
30	BG	109	ASP
53	BD	61	ILE
53	BD	92	THR
53	BD	123	ASN
53	BD	147	ASP
53	BD	222	VAL
53	BD	249	ARG
54	BF	15	GLU
54	BF	53	VAL
54	BF	170	ASP
55	BZ	3	LEU
55	BZ	64	GLU
55	BZ	96	LEU
24	B6	22	GLU
24	B6	78	MET
24	B6	90	ASP
56	BP	4	THR
56	BP	94	GLU
56	BP	110	ASN
57	BM	40	GLU
57	BM	102	GLU
58	BS	16	ARG
58	BS	144	THR
59	Bd	29	ARG
60	BN	13	ASP
60	BN	32	THR
60	BN	44	GLU
60	BN	96	GLU
60	BN	107	ARG
60	BN	108	TYR
60	BN	170	ASN

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Mol	Chain	Res	Type
62	Bc	3	ILE
62	Bc	27	LEU
62	Bc	29	VAL
62	Bc	32	ARG
63	BJ	3	LYS
63	BJ	41	ILE
63	BJ	63	VAL
63	BJ	73	MET
63	BJ	136	ILE
64	Bl	13	GLU
64	Bl	59	GLU
30	B4	20	LEU
30	B4	27	ARG
30	B4	43	VAL
30	B4	50	LEU
30	B4	57	VAL
30	B4	69	LEU
30	B4	86	LEU
30	B4	101	ILE
30	B4	113	GLU
30	B4	121	LEU
65	Bk	16	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
4	H	7	GLN
4	H	194	GLN
4	H	237	ASN
4	H	238	ASN
4	H	249	ASN
4	H	277	GLN
4	H	310	ASN
4	H	358	HIS
5	AA	46	ASN
5	AA	70	GLN
5	AA	77	GLN
6	AB	11	GLN
6	AB	18	HIS
6	AB	77	GLN
6	AB	108	ASN
7	AC	34	ASN

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Mol	Chain	Res	Type
8	AD	47	GLN
8	AD	50	ASN
8	AD	65	GLN
8	AD	72	GLN
8	AD	106	GLN
8	AD	123	GLN
8	AD	133	ASN
8	AD	135	GLN
9	AE	67	ASN
9	AE	147	ASN
9	AE	192	ASN
10	AF	58	ASN
10	AF	209	ASN
11	AG	110	ASN
11	AG	118	GLN
11	AG	120	ASN
12	AH	38	ASN
12	AH	90	HIS
12	AH	94	ASN
12	AH	193	ASN
13	AI	9	ASN
13	AI	70	ASN
13	AI	113	HIS
14	AJ	52	ASN
14	AJ	64	ASN
14	AJ	121	ASN
15	AK	131	GLN
16	AL	12	ASN
16	AL	21	ASN
17	AM	24	ASN
17	AM	80	HIS
17	AM	99	GLN
18	AN	66	ASN
20	AQ	104	ASN
20	AQ	123	GLN
21	AR	55	HIS
22	AS	6	GLN
22	AS	18	ASN
23	AU	103	GLN
25	AW	6	ASN
27	AY	3	GLN
28	AZ	77	ASN

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Mol	Chain	Res	Type
28	AZ	101	GLN
32	AO	20	GLN
33	BB	8	GLN
33	BB	50	HIS
33	BB	202	HIS
33	BB	229	HIS
34	BY	14	ASN
34	BY	32	ASN
34	BY	48	GLN
34	BY	77	ASN
34	BY	112	ASN
34	BY	148	ASN
35	BO	42	ASN
35	BO	47	GLN
35	BO	63	HIS
35	BO	130	ASN
35	BO	167	GLN
36	BC	167	GLN
36	BC	194	ASN
36	BC	241	HIS
36	BC	257	HIS
36	BC	270	GLN
36	BC	274	HIS
36	BC	297	ASN
36	BC	309	HIS
37	B5	31	ASN
38	BL	15	HIS
38	BL	57	HIS
39	Bf	20	ASN
39	Bf	38	HIS
40	BU	7	GLN
40	BU	11	GLN
40	BU	96	HIS
40	BU	99	ASN
41	Bb	26	GLN
41	Bb	119	GLN
42	Be	17	HIS
43	BE	112	ASN
43	BE	120	HIS
43	BE	164	HIS
44	Ba	42	HIS
46	BW	40	ASN

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Mol	Chain	Res	Type
47	Bi	55	GLN
48	BI	51	GLN
48	BI	111	GLN
49	BR	33	GLN
49	BR	42	HIS
49	BR	59	HIS
49	BR	89	HIS
49	BR	96	GLN
37	BK	31	ASN
50	BQ	58	GLN
50	BQ	67	HIS
50	BQ	75	HIS
50	BQ	131	GLN
51	BV	46	ASN
30	BG	21	GLN
53	BD	44	GLN
53	BD	123	ASN
53	BD	149	GLN
53	BD	213	ASN
53	BD	214	HIS
53	BD	229	HIS
53	BD	235	HIS
54	BF	22	GLN
54	BF	74	HIS
54	BF	149	GLN
55	BZ	21	ASN
56	BP	10	ASN
56	BP	23	ASN
56	BP	110	ASN
57	BM	87	GLN
57	BM	97	GLN
57	BM	110	ASN
57	BM	154	HIS
57	BM	174	ASN
57	BM	189	ASN
58	BS	70	GLN
58	BS	97	ASN
58	BS	99	GLN
58	BS	104	GLN
59	Bd	25	HIS
59	Bd	35	HIS
59	Bd	70	HIS

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Mol	Chain	Res	Type
60	BN	56	GLN
60	BN	59	GLN
60	BN	60	ASN
60	BN	70	ASN
60	BN	83	HIS
60	BN	97	ASN
60	BN	130	GLN
60	BN	138	ASN
60	BN	170	ASN
62	Bc	17	GLN
62	Bc	18	HIS
62	Bc	28	ASN
63	BJ	47	HIS
63	BJ	102	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3016/3018 (99%)	479 (15%)	22 (0%)
2	2	1495/1512 (98%)	186 (12%)	2 (0%)
3	3	125/128 (97%)	14 (11%)	0
All	All	4636/4658 (99%)	679 (14%)	24 (0%)

All (679) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	5	G
1	1	12	G
1	1	28	A
1	1	39	A
1	1	43	A
1	1	51	A
1	1	52	G
1	1	54	G
1	1	55	U
1	1	56	C
1	1	57	A
1	1	58	A
1	1	59	C
1	1	68	U
1	1	69	U

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Mol	Chain	Res	Type
1	1	75	G
1	1	82	C
1	1	88	G
1	1	94	G
1	1	95	G
1	1	98	C
1	1	99	U
1	1	100	G
1	1	101	U
1	1	102	C
1	1	104	C
1	1	105	C
1	1	107	G
1	1	115	G
1	1	116	G
1	1	118	U
1	1	120	A
1	1	121	G
1	1	122	G
1	1	123	A
1	1	126	C
1	1	127	U
1	1	138	G
1	1	154	G
1	1	160	C
1	1	164	C
1	1	178	A
1	1	184	G
1	1	185	A
1	1	188	A
1	1	189	G
1	1	199	G
1	1	205	G
1	1	231	A
1	1	232	A
1	1	233	U
1	1	238	C
1	1	239	C
1	1	240	U
1	1	241	C
1	1	244	G
1	1	246	G

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Mol	Chain	Res	Type
1	1	247	G
1	1	248	C
1	1	249	U
1	1	250	U
1	1	251	A
1	1	252	U
1	1	253	G
1	1	254	C
1	1	268	A
1	1	269	U
1	1	270	A
1	1	272	G
1	1	273	C
1	1	275	C
1	1	281	G
1	1	285	A
1	1	300	A
1	1	303	A
1	1	319	G
1	1	320	A
1	1	326	A
1	1	332	A
1	1	333	A
1	1	334	G
1	1	352	G
1	1	370	G
1	1	379	G
1	1	392	A
1	1	393	C
1	1	408	G
1	1	413	G
1	1	416	G
1	1	421	G
1	1	422	C
1	1	429	A
1	1	431	G
1	1	433	G
1	1	439	C
1	1	440	G
1	1	447	A
1	1	448	A
1	1	449	G

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Mol	Chain	Res	Type
1	1	456	U
1	1	466	C
1	1	484	G
1	1	485	A
1	1	493	G
1	1	501	A
1	1	507	G
1	1	516	C
1	1	517	G
1	1	522	A
1	1	523	C
1	1	529	G
1	1	544	U
1	1	545	A
1	1	560	G
1	1	565	G
1	1	610	U
1	1	611	A
1	1	621	G
1	1	635	G
1	1	644	G
1	1	657	A
1	1	661	C
1	1	683	A
1	1	684	G
1	1	685	G
1	1	689	C
1	1	696	A
1	1	699	G
1	1	704	G
1	1	731	C
1	1	738	G
1	1	747	G
1	1	769	C
1	1	773	C
1	1	781	A
1	1	785	G
1	1	792	A
1	1	808	G
1	1	809	A
1	1	849	C
1	1	851	U

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Mol	Chain	Res	Type
1	1	852	G
1	1	865	C
1	1	866	C
1	1	867	U
1	1	868	C
1	1	869	G
1	1	870	A
1	1	871	G
1	1	893	A
1	1	925	A
1	1	926	A
1	1	935	U
1	1	951	G
1	1	963	A
1	1	965	C
1	1	975	G
1	1	979	C
1	1	983	C
1	1	993	U
1	1	998	U
1	1	1026	G
1	1	1027	G
1	1	1033	A
1	1	1035	G
1	1	1036	G
1	1	1040	A
1	1	1043	G
1	1	1053	A
1	1	1056	G
1	1	1063	C
1	1	1073	C
1	1	1078	C
1	1	1079	G
1	1	1083	G
1	1	1096	G
1	1	1101	A
1	1	1111	G
1	1	1118	A
1	1	1122	A
1	1	1131	G
1	1	1132	C
1	1	1133	A

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Mol	Chain	Res	Type
1	1	1134	G
1	1	1136	G
1	1	1137	G
1	1	1140	G
1	1	1141	A
1	1	1143	A
1	1	1144	G
1	1	1148	C
1	1	1159	U
1	1	1162	A
1	1	1164	C
1	1	1199	G
1	1	1200	G
1	1	1221	C
1	1	1225	G
1	1	1231	A
1	1	1234	A
1	1	1235	A
1	1	1236	C
1	1	1240	G
1	1	1241	A
1	1	1252	G
1	1	1259	A
1	1	1261	G
1	1	1262	U
1	1	1263	G
1	1	1281	C
1	1	1282	A
1	1	1288	U
1	1	1289	G
1	1	1296	G
1	1	1297	C
1	1	1301	A
1	1	1303	A
1	1	1304	C
1	1	1305	A
1	1	1306	G
1	1	1307	C
1	1	1308	G
1	1	1310	G
1	1	1316	A
1	1	1317	G

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Mol	Chain	Res	Type
1	1	1322	A
1	1	1325	A
1	1	1326	G
1	1	1339	A
1	1	1343	A
1	1	1344	G
1	1	1345	U
1	1	1346	G
1	1	1353	A
1	1	1359	C
1	1	1362	G
1	1	1363	U
1	1	1364	C
1	1	1365	G
1	1	1366	A
1	1	1367	G
1	1	1370	C
1	1	1376	C
1	1	1385	U
1	1	1387	G
1	1	1389	C
1	1	1390	G
1	1	1393	G
1	1	1397	A
1	1	1411	G
1	1	1433	G
1	1	1443	C
1	1	1477	G
1	1	1508	G
1	1	1514	C
1	1	1520	G
1	1	1532	G
1	1	1533	U
1	1	1547	U
1	1	1560	A
1	1	1561	G
1	1	1577	A
1	1	1578	G
1	1	1580	C
1	1	1601	U
1	1	1630	G
1	1	1636	G

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Mol	Chain	Res	Type
1	1	1639	A
1	1	1645	A
1	1	1648	C
1	1	1649	G
1	1	1657	A
1	1	1678	G
1	1	1685	A
1	1	1687	C
1	1	1692	G
1	1	1705	C
1	1	1714	G
1	1	1731	U
1	1	1732	G
1	1	1748	A
1	1	1755	4AC
1	1	1759	G
1	1	1761	G
1	1	1763	G
1	1	1782	G
1	1	1787	A
1	1	1795	A
1	1	1796	U
1	1	1799	C
1	1	1805	C
1	1	1806	G
1	1	1808	U
1	1	1809	A
1	1	1810	G
1	1	1817	U
1	1	1825	U
1	1	1840	A
1	1	1851	G
1	1	1856	U
1	1	1883	A
1	1	1890	C
1	1	1891	A
1	1	1895	G
1	1	1896	C
1	1	1908	A
1	1	1920	U
1	1	1921	G
1	1	1922	U

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Mol	Chain	Res	Type
1	1	1923	C
1	1	1928	G
1	1	1929	A
1	1	1950	G
1	1	1972	G
1	1	1976	A
1	1	1987	G
1	1	1996	U
1	1	1997	A
1	1	2020	G
1	1	2029	A
1	1	2038	U
1	1	2042	A
1	1	2056	C
1	1	2085	A
1	1	2103	U
1	1	2119	A
1	1	2147	OMG
1	1	2154	A
1	1	2155	C
1	1	2157	A
1	1	2170	G
1	1	2171	G
1	1	2177	A
1	1	2178	A
1	1	2179	A
1	1	2181	U
1	1	2196	U
1	1	2205	G
1	1	2208	U
1	1	2211	A
1	1	2212	U
1	1	2213	G
1	1	2232	U
1	1	2233	G
1	1	2234	U
1	1	2253	G
1	1	2267	G
1	1	2271	G
1	1	2272	C
1	1	2273	A
1	1	2276	C

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Mol	Chain	Res	Type
1	1	2295	A
1	1	2299	A
1	1	2300	A
1	1	2301	G
1	1	2302	A
1	1	2303	C
1	1	2309	G
1	1	2310	G
1	1	2333	G
1	1	2340	G
1	1	2341	G
1	1	2342	C
1	1	2345	G
1	1	2347	G
1	1	2348	G
1	1	2350	G
1	1	2351	C
1	1	2352	G
1	1	2353	C
1	1	2354	A
1	1	2355	G
1	1	2356	C
1	1	2357	G
1	1	2363	G
1	1	2366	A
1	1	2368	G
1	1	2372	C
1	1	2373	G
1	1	2376	G
1	1	2386	C
1	1	2388	G
1	1	2397	G
1	1	2398	A
1	1	2401	C
1	1	2403	U
1	1	2405	C
1	1	2410	G
1	1	2411	A
1	1	2413	A
1	1	2418	C
1	1	2420	A
1	1	2430	G

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Mol	Chain	Res	Type
1	1	2431	C
1	1	2432	G
1	1	2438	A
1	1	2446	A
1	1	2449	G
1	1	2455	A
1	1	2456	C
1	1	2465	G
1	1	2468	G
1	1	2469	G
1	1	2488	A
1	1	2497	A
1	1	2498	A
1	1	2499	A
1	1	2510	G
1	1	2514	C
1	1	2518	A
1	1	2519	A
1	1	2536	U
1	1	2539	G
1	1	2543	U
1	1	2550	U
1	1	2551	A
1	1	2553	A
1	1	2556	G
1	1	2566	A
1	1	2574	C
1	1	2576	G
1	1	2588	A
1	1	2592	G
1	1	2617	G
1	1	2618	G
1	1	2619	C
1	1	2625	G
1	1	2626	A
1	1	2636	C
1	1	2659	G
1	1	2664	A
1	1	2665	A
1	1	2666	A
1	1	2673	C
1	1	2677	G

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Mol	Chain	Res	Type
1	1	2680	A
1	1	2706	C
1	1	2707	C
1	1	2710	A
1	1	2716	C
1	1	2723	C
1	1	2726	G
1	1	2730	C
1	1	2733	5MC
1	1	2734	G
1	1	2735	C
1	1	2750	A
1	1	2761	G
1	1	2766	A
1	1	2768	G
1	1	2798	A
1	1	2799	G
1	1	2805	C
1	1	2810	G
1	1	2814	G
1	1	2818	U
1	1	2831	G
1	1	2834	A
1	1	2845	U
1	1	2846	A
1	1	2847	U
1	1	2861	U
1	1	2877	A
1	1	2878	G
1	1	2896	G
1	1	2906	G
1	1	2922	U
1	1	2957	C
1	1	2963	A
1	1	2964	G
1	1	2978	A
1	1	2982	C
1	1	2987	A
1	1	2995	A
1	1	2996	G
1	1	3006	A
1	1	3007	A

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Mol	Chain	Res	Type
1	1	3021	U
1	1	3022	C
2	2	45	U
2	2	52	C
2	2	54	G
2	2	59	A
2	2	72	A
2	2	76	G
2	2	86	U
2	2	87	C
2	2	88	U
2	2	89	G
2	2	115	A
2	2	117	C
2	2	126	A
2	2	128	C
2	2	141	G
2	2	154	G
2	2	189	A
2	2	196	G
2	2	211	A
2	2	212	G
2	2	219	G
2	2	221	A
2	2	222	A
2	2	223	G
2	2	225	C
2	2	229	G
2	2	254	U
2	2	256	G
2	2	260	G
2	2	275	G
2	2	276	C
2	2	290	G
2	2	298	C
2	2	314	G
2	2	315	A
2	2	329	C
2	2	337	C
2	2	338	A
2	2	347	G
2	2	353	A

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Mol	Chain	Res	Type
2	2	354	C
2	2	358	G
2	2	360	G
2	2	361	C
2	2	363	G
2	2	365	A
2	2	371	G
2	2	376	C
2	2	381	C
2	2	406	A
2	2	407	C
2	2	415	G
2	2	424	C
2	2	425	U
2	2	426	G
2	2	430	C
2	2	436	U
2	2	454	U
2	2	460	A
2	2	461	A
2	2	474	A
2	2	476	G
2	2	477	G
2	2	484	G
2	2	487	G
2	2	496	G
2	2	497	U
2	2	513	A
2	2	530	U
2	2	533	G
2	2	539	A
2	2	542	C
2	2	543	G
2	2	562	A
2	2	571	C
2	2	600	G
2	2	609	A
2	2	620	U
2	2	632	A
2	2	642	U
2	2	652	G
2	2	654	A

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Mol	Chain	Res	Type
2	2	660	G
2	2	688	A
2	2	689	G
2	2	690	U
2	2	691	G
2	2	715	G
2	2	722	G
2	2	744	A
2	2	760	U
2	2	761	A
2	2	782	A
2	2	784	G
2	2	786	A
2	2	788	G
2	2	814	A
2	2	861	G
2	2	885	A
2	2	893	G
2	2	905	C
2	2	906	U
2	2	932	U
2	2	934	OMG
2	2	941	A
2	2	943	G
2	2	946	G
2	2	947	G
2	2	949	A
2	2	966	C
2	2	968	G
2	2	975	G
2	2	977	A
2	2	981	C
2	2	984	G
2	2	990	G
2	2	991	G
2	2	996	G
2	2	997	C
2	2	999	G
2	2	1000	G
2	2	1002	C
2	2	1004	C
2	2	1005	G

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Mol	Chain	Res	Type
2	2	1008	G
2	2	1030	U
2	2	1035	U
2	2	1059	G
2	2	1060	U
2	2	1066	A
2	2	1107	U
2	2	1108	C
2	2	1114	G
2	2	1131	A
2	2	1133	U
2	2	1141	A
2	2	1148	G
2	2	1155	G
2	2	1157	G
2	2	1170	A
2	2	1171	G
2	2	1176	G
2	2	1186	A
2	2	1187	A
2	2	1199	A
2	2	1201	A
2	2	1212	A
2	2	1215	G
2	2	1222	A
2	2	1253	A
2	2	1254	A
2	2	1261	A
2	2	1274	G
2	2	1276	U
2	2	1279	G
2	2	1294	C
2	2	1296	C
2	2	1297	G
2	2	1305	G
2	2	1310	U
2	2	1327	G
2	2	1338	U
2	2	1344	G
2	2	1353	G
2	2	1371	C
2	2	1393	G

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Mol	Chain	Res	Type
2	2	1395	G
2	2	1397	G
2	2	1400	C
2	2	1414	A
2	2	1421	U
2	2	1424	G
2	2	1427	G
2	2	1454	G
2	2	1456	G
2	2	1461	A
2	2	1466	G
2	2	1471	A
2	2	1472	A
2	2	1475	U
2	2	1486	G
2	2	1498	5MC
2	2	1499	G
2	2	1503	A
2	2	1504	C
2	2	1505	5MC
3	3	5	C
3	3	9	G
3	3	25	C
3	3	28	C
3	3	30	C
3	3	53	A
3	3	56	U
3	3	57	A
3	3	58	A
3	3	60	C
3	3	79	G
3	3	89	C
3	3	95	G
3	3	115	G

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	68	U
1	1	117	G
1	1	120	A
1	1	122	G

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Mol	Chain	Res	Type
1	1	127	U
1	1	238	C
1	1	250	U
1	1	428	U
1	1	656	A
1	1	866	C
1	1	869	G
1	1	1035	G
1	1	1303	A
1	1	1363	U
1	1	1364	C
1	1	1731	U
1	1	2341	G
1	1	2367	G
1	1	2455	A
1	1	2733	5MC
1	1	2986	U
1	1	3021	U
2	2	406	A
2	2	688	A

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

159 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	5MC	2	535	2	18,22,23	0.93	2 (11%)	26,32,35	1.13	2 (7%)
2	OMU	2	774	2	19,22,23	1.24	3 (15%)	26,31,34	1.73	4 (15%)
1	4AC	1	1068	1	21,24,25	1.04	2 (9%)	29,34,37	1.39	4 (13%)
1	5MC	1	2733	1	18,22,23	0.97	2 (11%)	26,32,35	1.23	3 (11%)
2	4AC	2	394	2	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
2	OMC	2	1376	2	19,22,23	0.81	0	26,31,34	0.77	0
2	4AC	2	839	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	1048	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
2	4AC	2	1239	2	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
2	MA6	2	1488	2	23,26,27	1.47	5 (21%)	34,38,41	2.09	10 (29%)
1	4AC	1	1554	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	OMC	1	615	1	19,22,23	0.81	0	26,31,34	0.82	1 (3%)
2	OMG	2	519	2	23,26,27	1.21	3 (13%)	33,38,41	1.96	5 (15%)
1	4AC	1	2585	1	21,24,25	1.06	2 (9%)	29,34,37	1.81	5 (17%)
1	5MC	1	2203	1	18,22,23	0.93	2 (11%)	26,32,35	1.13	2 (7%)
1	OMG	1	2144	1	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	2642	1	21,24,25	1.01	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	2937	66,1	21,24,25	1.03	2 (9%)	29,34,37	1.55	4 (13%)
2	OMU	2	20	2	19,22,23	1.23	2 (10%)	26,31,34	1.79	5 (19%)
2	4AC	2	17	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
3	4AC	3	32	3	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	2865	1	21,24,25	1.02	2 (9%)	29,34,37	1.28	4 (13%)
2	OMU	2	830	2	19,22,23	1.25	3 (15%)	26,31,34	1.68	4 (15%)
2	4AC	2	479	2	21,24,25	1.02	2 (9%)	29,34,37	1.40	4 (13%)
2	OMG	2	873	2	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
1	5MC	1	2162	1	18,22,23	0.93	2 (11%)	26,32,35	1.18	3 (11%)
2	5MC	2	1374	2	18,22,23	0.92	2 (11%)	26,32,35	1.11	2 (7%)
1	OMG	1	2678	1	23,26,27	1.22	3 (13%)	33,38,41	1.90	6 (18%)
2	4AC	2	718	2	21,24,25	0.99	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	1962	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2908	1	21,24,25	1.01	2 (9%)	29,34,37	1.29	4 (13%)
2	A2M	2	373	2	22,25,26	1.45	4 (18%)	31,36,39	2.08	8 (25%)
1	4AC	1	829	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
2	5MC	2	1505	2	18,22,23	0.97	2 (11%)	26,32,35	1.15	3 (11%)
1	5MC	1	2198	1	18,22,23	0.92	2 (11%)	26,32,35	1.21	3 (11%)
1	4AC	1	60	1	21,24,25	1.02	2 (9%)	29,34,37	1.44	4 (13%)
2	5MC	2	875	2	18,22,23	0.93	2 (11%)	26,32,35	1.20	3 (11%)
1	4AC	1	1878	1	21,24,25	1.01	2 (9%)	29,34,37	1.50	4 (13%)
1	4AC	1	835	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
2	OMC	2	773	2	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
1	4AC	1	22	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	211	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	2495	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
1	5MC	1	2093	1	18,22,23	0.94	2 (11%)	26,32,35	1.13	2 (7%)
2	OMU	2	1177	2	19,22,23	1.23	3 (15%)	26,31,34	1.74	5 (19%)
2	4AC	2	731	2	21,24,25	1.03	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2608	1	21,24,25	1.06	2 (9%)	29,34,37	1.77	6 (20%)
1	4AC	1	341	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	5 (17%)
2	4AC	2	868	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	1184	2	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
2	5MC	2	1025	2	18,22,23	0.95	2 (11%)	26,32,35	1.17	2 (7%)
2	4AC	2	1147	2	21,24,25	1.02	2 (9%)	29,34,37	1.44	4 (13%)
1	4AC	1	1557	1	21,24,25	1.02	2 (9%)	29,34,37	1.26	4 (13%)
1	5MC	1	2163	1	18,22,23	0.93	2 (11%)	26,32,35	1.12	2 (7%)
1	OMC	1	1948	1	19,22,23	0.81	0	26,31,34	0.82	1 (3%)
1	OMG	1	2138	1	23,26,27	1.22	3 (13%)	33,38,41	1.91	6 (18%)
1	4AC	1	1293	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	1695	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2966	1	21,24,25	1.04	2 (9%)	29,34,37	1.36	4 (13%)
2	4AC	2	319	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	1479	2	21,24,25	1.00	2 (9%)	29,34,37	1.30	5 (17%)
1	4AC	1	2136	1	21,24,25	1.02	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	2718	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	UR3	2	1467	2	19,22,23	0.94	0	26,32,35	1.44	2 (7%)
1	4AC	1	1222	66,1	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
1	OMU	1	2784	1	19,22,23	1.23	3 (15%)	26,31,34	1.75	5 (19%)
2	B8H	2	938	2	19,22,23	0.57	0	22,32,35	0.64	0
1	4AC	1	3004	1	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
2	OMG	2	680	2	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	4AC	1	2960	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	828	2	21,24,25	1.00	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	626	2	21,24,25	1.00	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	1662	1	21,24,25	1.00	2 (9%)	29,34,37	1.36	4 (13%)
2	4AC	2	303	2	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	1028	2	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	2027	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	OMG	2	471	2	23,26,27	1.22	3 (13%)	33,38,41	1.92	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	533	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	5 (17%)
2	4AC	2	1233	2	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	OMG	1	923	66,1	23,26,27	1.22	3 (13%)	33,38,41	1.90	6 (18%)
2	4AC	2	848	2	21,24,25	0.99	2 (9%)	29,34,37	1.42	4 (13%)
2	4AC	2	286	2	21,24,25	1.01	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1550	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2925	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1065	1	21,24,25	1.02	2 (9%)	29,34,37	1.42	4 (13%)
2	4AC	2	751	2	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
2	4AC	2	703	2	21,24,25	1.02	1 (4%)	29,34,37	1.44	4 (13%)
1	OMG	1	2147	1	23,26,27	1.20	3 (13%)	33,38,41	1.91	6 (18%)
1	4AC	1	694	1	21,24,25	1.00	2 (9%)	29,34,37	1.30	4 (13%)
2	OMG	2	934	2	23,26,27	1.20	3 (13%)	33,38,41	1.99	6 (18%)
1	4AC	1	1873	1	21,24,25	1.03	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	357	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	2992	1	21,24,25	1.04	2 (9%)	29,34,37	0.90	1 (3%)
1	4AC	1	1885	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	229	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
2	5MC	2	1498	2	18,22,23	0.96	2 (11%)	26,32,35	1.26	3 (11%)
2	OMC	2	129	2	19,22,23	0.80	0	26,31,34	0.83	0
1	4AC	1	1594	66,1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	922	1	21,24,25	1.05	2 (9%)	29,34,37	1.45	4 (13%)
1	4AC	1	1460	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
2	6MZ	2	1469	66,2	22,25,26	1.48	4 (18%)	30,36,39	2.20	9 (30%)
1	4AC	1	451	1	21,24,25	1.01	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	2062	1	21,24,25	1.00	2 (9%)	29,34,37	1.29	4 (13%)
2	4AC	2	546	2	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	2001	1	21,24,25	1.06	2 (9%)	29,34,37	1.51	4 (13%)
1	4AC	1	1667	1	21,24,25	1.00	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2329	1	21,24,25	1.01	2 (9%)	29,34,37	1.41	4 (13%)
1	A2M	1	1055	1	22,25,26	1.44	4 (18%)	31,36,39	2.12	9 (29%)
2	LHH	2	1041	2	22,25,26	0.31	0	29,35,38	0.49	0
1	4AC	1	1934	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	2249	1	21,24,25	1.04	2 (9%)	29,34,37	1.39	4 (13%)
2	OMG	2	913	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	2	1040	2	19,22,23	0.81	0	26,31,34	0.78	0
1	4AC	1	91	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	243	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	A2M	1	2173	1	22,25,26	1.44	4 (18%)	31,36,39	2.05	8 (25%)
2	4AC	2	590	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	314	1	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	1	2083	1	21,24,25	1.04	2 (9%)	29,34,37	1.29	5 (17%)
1	4AC	1	1938	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2570	1	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
2	4AC	2	511	2	21,24,25	1.05	2 (9%)	29,34,37	1.38	4 (13%)
2	MA6	2	1487	2	23,26,27	1.46	5 (21%)	34,38,41	2.11	10 (29%)
1	4AC	1	981	1	21,24,25	1.01	2 (9%)	29,34,37	1.28	4 (13%)
1	OMG	1	328	1	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	1617	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	2545	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	379	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
2	5MC	2	1202	2	18,22,23	0.93	2 (11%)	26,32,35	1.16	3 (11%)
1	OMG	1	789	1	23,26,27	1.23	3 (13%)	33,38,41	1.94	6 (18%)
1	5MC	1	2183	1	18,22,23	0.94	2 (11%)	26,32,35	1.13	2 (7%)
2	OMG	2	467	2	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
2	5MC	2	693	2	18,22,23	0.94	2 (11%)	26,32,35	1.17	3 (11%)
1	4AC	1	1867	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	LHH	1	616	1	22,25,26	0.32	0	29,35,38	0.48	0
2	4AC	2	957	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2548	1	21,24,25	1.00	2 (9%)	29,34,37	1.32	4 (13%)
2	LHH	2	250	2	22,25,26	0.31	0	29,35,38	0.50	0
2	4AC	2	851	2	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
2	5MC	2	1496	2	18,22,23	0.93	2 (11%)	26,32,35	1.18	3 (11%)
2	OMU	2	64	2	19,22,23	1.22	4 (21%)	26,31,34	1.68	4 (15%)
1	4AC	1	136	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1765	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1755	1	21,24,25	1.00	2 (9%)	29,34,37	1.58	4 (13%)
1	4AC	1	1780	1	21,24,25	1.03	2 (9%)	29,34,37	1.55	4 (13%)
1	4AC	1	641	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
2	OMC	2	846	2	19,22,23	0.81	0	26,31,34	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	2	1380	2	19,22,23	1.29	4 (21%)	26,31,34	1.76	4 (15%)
2	OMU	2	787	2	19,22,23	1.21	2 (10%)	26,31,34	1.77	5 (19%)
1	4AC	1	1243	1	21,24,25	1.04	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	802	1	21,24,25	1.01	2 (9%)	29,34,37	1.44	4 (13%)
1	4AC	1	458	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	5 (17%)
2	OMG	2	1069	2	23,26,27	1.21	3 (13%)	33,38,41	1.90	6 (18%)
1	4AC	1	2287	1	21,24,25	1.01	2 (9%)	29,34,37	1.41	4 (13%)
1	4AC	1	161	1	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
2	4AC	2	53	2	21,24,25	1.00	2 (9%)	29,34,37	1.38	4 (13%)
2	4AC	2	636	2	21,24,25	1.02	2 (9%)	29,34,37	1.39	4 (13%)
2	OMG	2	657	2	23,26,27	1.22	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	1621	1	21,24,25	1.02	2 (9%)	29,34,37	1.30	4 (13%)

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
2	5MC	2	535	2	-	0/7/25/26	0/2/2/2
2	OMU	2	774	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1068	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2733	1	-	4/7/25/26	0/2/2/2
2	4AC	2	394	2	-	0/11/29/30	0/2/2/2
2	OMC	2	1376	2	-	0/9/27/28	0/2/2/2
2	4AC	2	839	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1048	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1239	2	-	0/11/29/30	0/2/2/2
2	MA6	2	1488	2	-	2/11/29/30	0/3/3/3
1	4AC	1	1554	1	-	0/11/29/30	0/2/2/2
1	OMC	1	615	1	-	0/9/27/28	0/2/2/2
2	OMG	2	519	2	-	0/9/27/28	0/3/3/3
1	4AC	1	2585	1	-	3/11/29/30	0/2/2/2
1	5MC	1	2203	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2144	1	-	0/9/27/28	0/3/3/3
1	4AC	1	2642	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2937	66,1	-	1/11/29/30	0/2/2/2
2	OMU	2	20	2	-	6/9/27/28	0/2/2/2
2	4AC	2	17	2	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4AC	3	32	3	-	0/11/29/30	0/2/2/2
1	4AC	1	2865	1	-	0/11/29/30	0/2/2/2
2	OMU	2	830	2	-	0/9/27/28	0/2/2/2
2	4AC	2	479	2	-	0/11/29/30	0/2/2/2
2	OMG	2	873	2	-	1/9/27/28	0/3/3/3
1	5MC	1	2162	1	-	0/7/25/26	0/2/2/2
2	5MC	2	1374	2	-	2/7/25/26	0/2/2/2
1	OMG	1	2678	1	-	1/9/27/28	0/3/3/3
2	4AC	2	718	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1962	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2908	1	-	0/11/29/30	0/2/2/2
2	A2M	2	373	2	-	0/9/27/28	0/3/3/3
1	4AC	1	829	1	-	1/11/29/30	0/2/2/2
2	5MC	2	1505	2	-	2/7/25/26	0/2/2/2
1	5MC	1	2198	1	-	0/7/25/26	0/2/2/2
1	4AC	1	60	1	-	0/11/29/30	0/2/2/2
2	5MC	2	875	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1878	1	-	0/11/29/30	0/2/2/2
1	4AC	1	835	1	-	0/11/29/30	0/2/2/2
2	OMC	2	773	2	-	0/9/27/28	0/2/2/2
1	4AC	1	22	1	-	0/11/29/30	0/2/2/2
1	4AC	1	211	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2495	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2093	1	-	0/7/25/26	0/2/2/2
2	OMU	2	1177	2	-	1/9/27/28	0/2/2/2
2	4AC	2	731	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2608	1	-	3/11/29/30	0/2/2/2
1	4AC	1	341	1	-	0/11/29/30	0/2/2/2
2	4AC	2	868	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1184	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1025	2	-	0/7/25/26	0/2/2/2
2	4AC	2	1147	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1557	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2163	1	-	0/7/25/26	0/2/2/2
1	OMC	1	1948	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2138	1	-	0/9/27/28	0/3/3/3
1	4AC	1	1293	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1695	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2966	1	-	0/11/29/30	0/2/2/2
2	4AC	2	319	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1479	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2136	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	2718	1	-	0/11/29/30	0/2/2/2
2	UR3	2	1467	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1222	66,1	-	0/11/29/30	0/2/2/2
1	OMU	1	2784	1	-	0/9/27/28	0/2/2/2
2	B8H	2	938	2	-	1/7/25/26	0/2/2/2
1	4AC	1	3004	1	-	0/11/29/30	0/2/2/2
2	OMG	2	680	2	-	0/9/27/28	0/3/3/3
1	4AC	1	2960	1	-	0/11/29/30	0/2/2/2
2	4AC	2	828	2	-	0/11/29/30	0/2/2/2
2	4AC	2	626	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1662	1	-	0/11/29/30	0/2/2/2
2	4AC	2	303	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1028	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2027	1	-	0/11/29/30	0/2/2/2
2	OMG	2	471	2	-	0/9/27/28	0/3/3/3
1	4AC	1	533	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1233	2	-	0/11/29/30	0/2/2/2
1	OMG	1	923	66,1	-	2/9/27/28	0/3/3/3
2	4AC	2	848	2	-	0/11/29/30	0/2/2/2
2	4AC	2	286	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1550	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2925	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1065	1	-	0/11/29/30	0/2/2/2
2	4AC	2	751	2	-	0/11/29/30	0/2/2/2
2	4AC	2	703	2	-	0/11/29/30	0/2/2/2
1	OMG	1	2147	1	-	3/9/27/28	0/3/3/3
1	4AC	1	694	1	-	0/11/29/30	0/2/2/2
2	OMG	2	934	2	-	2/9/27/28	0/3/3/3
1	4AC	1	1873	1	-	0/11/29/30	0/2/2/2
1	4AC	1	357	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2992	1	-	3/11/29/30	0/2/2/2
1	4AC	1	1885	1	-	0/11/29/30	0/2/2/2
1	4AC	1	229	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1498	2	-	3/7/25/26	0/2/2/2
2	OMC	2	129	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1594	66,1	-	0/11/29/30	0/2/2/2
1	4AC	1	922	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1460	1	-	0/11/29/30	0/2/2/2
2	6MZ	2	1469	66,2	-	0/9/27/28	0/3/3/3
1	4AC	1	451	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2062	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4AC	2	546	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2001	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1667	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2329	1	-	0/11/29/30	0/2/2/2
1	A2M	1	1055	1	-	0/9/27/28	0/3/3/3
2	LHH	2	1041	2	-	0/13/31/32	0/2/2/2
1	4AC	1	1934	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2249	1	-	0/11/29/30	0/2/2/2
2	OMG	2	913	2	-	1/9/27/28	0/3/3/3
2	OMC	2	1040	2	-	0/9/27/28	0/2/2/2
1	4AC	1	91	1	-	0/11/29/30	0/2/2/2
1	4AC	1	243	1	-	0/11/29/30	0/2/2/2
1	A2M	1	2173	1	-	0/9/27/28	0/3/3/3
2	4AC	2	590	2	-	0/11/29/30	0/2/2/2
1	4AC	1	314	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2083	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1938	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2570	1	-	0/11/29/30	0/2/2/2
2	4AC	2	511	2	-	0/11/29/30	0/2/2/2
2	MA6	2	1487	2	-	0/11/29/30	0/3/3/3
1	4AC	1	981	1	-	0/11/29/30	0/2/2/2
1	OMG	1	328	1	-	0/9/27/28	0/3/3/3
1	4AC	1	1617	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2545	1	-	0/11/29/30	0/2/2/2
2	4AC	2	379	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1202	2	-	1/7/25/26	0/2/2/2
1	OMG	1	789	1	-	4/9/27/28	0/3/3/3
1	5MC	1	2183	1	-	0/7/25/26	0/2/2/2
2	OMG	2	467	2	-	0/9/27/28	0/3/3/3
2	5MC	2	693	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1867	1	-	0/11/29/30	0/2/2/2
1	LHH	1	616	1	-	0/13/31/32	0/2/2/2
2	4AC	2	957	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2548	1	-	0/11/29/30	0/2/2/2
2	LHH	2	250	2	-	0/13/31/32	0/2/2/2
2	4AC	2	851	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1496	2	-	0/7/25/26	0/2/2/2
2	OMU	2	64	2	-	0/9/27/28	0/2/2/2
1	4AC	1	136	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1765	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1755	1	-	2/11/29/30	0/2/2/2
1	4AC	1	1780	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	641	1	-	0/11/29/30	0/2/2/2
2	OMC	2	846	2	-	0/9/27/28	0/2/2/2
2	OMU	2	1380	2	-	0/9/27/28	0/2/2/2
2	OMU	2	787	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1243	1	-	0/11/29/30	0/2/2/2
1	4AC	1	802	1	-	0/11/29/30	0/2/2/2
1	4AC	1	458	1	-	0/11/29/30	0/2/2/2
2	OMG	2	1069	2	-	2/9/27/28	0/3/3/3
1	4AC	1	2287	1	-	0/11/29/30	0/2/2/2
1	4AC	1	161	1	-	0/11/29/30	0/2/2/2
2	4AC	2	53	2	-	0/11/29/30	0/2/2/2
2	4AC	2	636	2	-	0/11/29/30	0/2/2/2
2	OMG	2	657	2	-	0/9/27/28	0/3/3/3
1	4AC	1	1621	1	-	0/11/29/30	0/2/2/2

All (331) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1469	6MZ	C5-C4	4.54	1.47	1.39
2	2	1488	MA6	C5-C4	4.42	1.47	1.39
2	2	373	A2M	C5-C4	4.37	1.47	1.39
1	1	1055	A2M	C5-C4	4.36	1.47	1.39
2	2	1487	MA6	C5-C4	4.33	1.47	1.39
1	1	2173	A2M	C5-C4	4.33	1.47	1.39
2	2	657	OMG	C5-C4	3.11	1.47	1.38
1	1	2992	4AC	C5-C4	3.09	1.47	1.40
2	2	680	OMG	C5-C4	3.08	1.47	1.38
2	2	511	4AC	C5-C4	3.01	1.47	1.40
1	1	2147	OMG	C5-C4	3.01	1.47	1.38
2	2	471	OMG	C5-C4	3.01	1.47	1.38
2	2	1069	OMG	C5-C4	3.01	1.47	1.38
2	2	1239	4AC	C5-C4	2.98	1.47	1.40
2	2	873	OMG	C5-C4	2.98	1.47	1.38
1	1	328	OMG	C5-C4	2.97	1.47	1.38
1	1	2138	OMG	C5-C4	2.96	1.47	1.38
1	1	2865	4AC	C5-C4	2.96	1.47	1.40
1	1	2548	4AC	C5-C4	2.96	1.47	1.40
2	2	1028	4AC	C5-C4	2.96	1.47	1.40
1	1	923	OMG	C5-C4	2.96	1.47	1.38
2	2	1147	4AC	C5-C4	2.96	1.47	1.40
1	1	22	4AC	C5-C4	2.96	1.47	1.40
2	2	1233	4AC	C5-C4	2.96	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	467	OMG	C5-C4	2.95	1.47	1.38
1	1	229	4AC	C5-C4	2.95	1.47	1.40
2	2	851	4AC	C5-C4	2.95	1.47	1.40
1	1	922	4AC	C5-C4	2.95	1.47	1.40
1	1	2083	4AC	C5-C4	2.94	1.47	1.40
1	1	641	4AC	C5-C4	2.94	1.47	1.40
2	2	286	4AC	C5-C4	2.94	1.47	1.40
1	1	2495	4AC	C5-C4	2.94	1.47	1.40
1	1	2678	OMG	C5-C4	2.93	1.46	1.38
2	2	626	4AC	C5-C4	2.93	1.47	1.40
1	1	2136	4AC	C5-C4	2.93	1.47	1.40
1	1	2144	OMG	C5-C4	2.92	1.46	1.38
1	1	1867	4AC	C5-C4	2.92	1.47	1.40
1	1	2966	4AC	C5-C4	2.92	1.47	1.40
2	2	751	4AC	C5-C4	2.92	1.47	1.40
1	1	1695	4AC	C5-C4	2.92	1.47	1.40
2	2	957	4AC	C5-C4	2.92	1.47	1.40
2	2	934	OMG	C5-C4	2.92	1.46	1.38
2	2	546	4AC	C5-C4	2.92	1.47	1.40
1	1	2570	4AC	C5-C4	2.92	1.47	1.40
1	1	243	4AC	C5-C4	2.91	1.47	1.40
1	1	1243	4AC	C5-C4	2.91	1.47	1.40
2	2	636	4AC	C5-C4	2.91	1.47	1.40
2	2	731	4AC	C5-C4	2.91	1.47	1.40
2	2	519	OMG	C5-C4	2.91	1.46	1.38
2	2	479	4AC	C5-C4	2.91	1.47	1.40
2	2	913	OMG	C5-C4	2.91	1.46	1.38
1	1	2545	4AC	C5-C4	2.90	1.47	1.40
2	2	1184	4AC	C5-C4	2.90	1.47	1.40
1	1	1048	4AC	C5-C4	2.90	1.47	1.40
1	1	2001	4AC	C5-C4	2.90	1.47	1.40
2	2	868	4AC	C5-C4	2.90	1.47	1.40
2	2	17	4AC	C5-C4	2.90	1.47	1.40
1	1	314	4AC	C5-C4	2.89	1.47	1.40
1	1	458	4AC	C5-C4	2.89	1.47	1.40
2	2	379	4AC	C5-C4	2.89	1.47	1.40
1	1	1667	4AC	C5-C4	2.89	1.47	1.40
2	2	839	4AC	C5-C4	2.89	1.47	1.40
1	1	2937	4AC	C5-C4	2.89	1.47	1.40
1	1	829	4AC	C5-C4	2.88	1.47	1.40
2	2	828	4AC	C5-C4	2.88	1.47	1.40
1	1	1293	4AC	C5-C4	2.88	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	32	4AC	C5-C4	2.88	1.47	1.40
2	2	394	4AC	C5-C4	2.88	1.47	1.40
1	1	835	4AC	C5-C4	2.88	1.47	1.40
1	1	1621	4AC	C5-C4	2.88	1.47	1.40
1	1	60	4AC	C5-C4	2.88	1.47	1.40
1	1	136	4AC	C5-C4	2.88	1.47	1.40
1	1	1873	4AC	C5-C4	2.88	1.47	1.40
2	2	303	4AC	C5-C4	2.87	1.47	1.40
1	1	789	OMG	C5-C4	2.87	1.46	1.38
1	1	1765	4AC	C5-C4	2.87	1.47	1.40
1	1	1222	4AC	C5-C4	2.86	1.47	1.40
1	1	2908	4AC	C5-C4	2.86	1.47	1.40
1	1	451	4AC	C5-C4	2.86	1.47	1.40
1	1	694	4AC	C5-C4	2.86	1.47	1.40
2	2	703	4AC	C5-C4	2.86	1.46	1.40
1	1	341	4AC	C5-C4	2.86	1.46	1.40
1	1	211	4AC	C5-C4	2.86	1.46	1.40
1	1	2642	4AC	C5-C4	2.86	1.46	1.40
1	1	3004	4AC	C5-C4	2.85	1.46	1.40
1	1	1938	4AC	C5-C4	2.85	1.46	1.40
2	2	590	4AC	C5-C4	2.85	1.46	1.40
1	1	2925	4AC	C5-C4	2.84	1.46	1.40
1	1	1617	4AC	C5-C4	2.84	1.46	1.40
1	1	1594	4AC	C5-C4	2.84	1.46	1.40
1	1	2718	4AC	C5-C4	2.83	1.46	1.40
1	1	533	4AC	C5-C4	2.83	1.46	1.40
2	2	53	4AC	C5-C4	2.83	1.46	1.40
1	1	161	4AC	C5-C4	2.83	1.46	1.40
2	2	1488	MA6	C5-C6	2.83	1.49	1.41
1	1	1554	4AC	C5-C4	2.83	1.46	1.40
2	2	319	4AC	C5-C4	2.83	1.46	1.40
1	1	91	4AC	C5-C4	2.82	1.46	1.40
1	1	1962	4AC	C5-C4	2.82	1.46	1.40
1	1	2062	4AC	C5-C4	2.82	1.46	1.40
1	1	2027	4AC	C5-C4	2.82	1.46	1.40
1	1	1068	4AC	C5-C4	2.82	1.46	1.40
1	1	1557	4AC	C5-C4	2.81	1.46	1.40
1	1	2960	4AC	C5-C4	2.81	1.46	1.40
1	1	1550	4AC	C5-C4	2.81	1.46	1.40
1	1	1662	4AC	C5-C4	2.81	1.46	1.40
2	2	718	4AC	C5-C4	2.80	1.46	1.40
2	2	1487	MA6	C5-C6	2.80	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2329	4AC	C5-C4	2.80	1.46	1.40
1	1	1934	4AC	C5-C4	2.79	1.46	1.40
1	1	802	4AC	C5-C4	2.79	1.46	1.40
1	1	1065	4AC	C5-C4	2.79	1.46	1.40
1	1	357	4AC	C5-C4	2.79	1.46	1.40
2	2	1380	OMU	C4-N3	-2.79	1.33	1.38
2	2	1505	5MC	C6-C5	2.79	1.39	1.34
1	1	2249	4AC	C5-C4	2.78	1.46	1.40
2	2	1469	6MZ	C5-C6	2.77	1.49	1.41
1	1	981	4AC	C5-C4	2.77	1.46	1.40
1	1	2138	OMG	C6-N1	-2.77	1.33	1.38
1	1	1460	4AC	C5-C4	2.77	1.46	1.40
1	1	2784	OMU	C4-N3	-2.76	1.33	1.38
1	1	2678	OMG	C6-N1	-2.76	1.33	1.38
2	2	20	OMU	C4-N3	-2.75	1.33	1.38
2	2	848	4AC	C5-C4	2.75	1.46	1.40
2	2	1479	4AC	C5-C4	2.75	1.46	1.40
2	2	471	OMG	C6-N1	-2.74	1.33	1.38
1	1	1885	4AC	C5-C4	2.74	1.46	1.40
1	1	1780	4AC	C5-C4	2.74	1.46	1.40
1	1	2144	OMG	C6-N1	-2.74	1.33	1.38
1	1	2733	5MC	C6-C5	2.73	1.39	1.34
1	1	2287	4AC	C5-C4	2.73	1.46	1.40
1	1	328	OMG	C6-N1	-2.73	1.33	1.38
1	1	923	OMG	C6-N1	-2.73	1.33	1.38
1	1	789	OMG	C6-N1	-2.72	1.33	1.38
1	1	1878	4AC	C5-C4	2.72	1.46	1.40
2	2	873	OMG	C6-N1	-2.71	1.33	1.38
2	2	787	OMU	C4-N3	-2.71	1.33	1.38
2	2	1177	OMU	C4-N3	-2.70	1.33	1.38
1	1	2183	5MC	C6-C5	2.69	1.39	1.34
1	1	1755	4AC	C5-C4	2.69	1.46	1.40
2	2	657	OMG	C6-N1	-2.68	1.33	1.38
1	1	2093	5MC	C6-C5	2.68	1.39	1.34
2	2	913	OMG	C6-N1	-2.67	1.33	1.38
2	2	830	OMU	C4-N3	-2.67	1.33	1.38
1	1	2608	4AC	C5-C4	2.65	1.46	1.40
2	2	934	OMG	C6-N1	-2.65	1.33	1.38
2	2	774	OMU	C4-N3	-2.64	1.33	1.38
2	2	467	OMG	C6-N1	-2.63	1.33	1.38
2	2	680	OMG	C6-N1	-2.63	1.34	1.38
1	1	2173	A2M	C5-C6	2.62	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1025	5MC	C6-C5	2.61	1.38	1.34
2	2	519	OMG	C6-N1	-2.60	1.34	1.38
2	2	373	A2M	C5-C6	2.60	1.48	1.41
2	2	1202	5MC	C6-C5	2.59	1.38	1.34
2	2	1498	5MC	C6-C5	2.58	1.38	1.34
1	1	2585	4AC	C5-C4	2.58	1.46	1.40
1	1	2585	4AC	C4-N3	-2.58	1.28	1.32
2	2	1069	OMG	C6-N1	-2.57	1.34	1.38
1	1	1055	A2M	C5-C6	2.57	1.48	1.41
1	1	2162	5MC	C6-C5	2.55	1.38	1.34
1	1	2163	5MC	C6-C5	2.54	1.38	1.34
1	1	2147	OMG	C6-N1	-2.53	1.34	1.38
2	2	875	5MC	C6-C5	2.53	1.38	1.34
2	2	535	5MC	C6-C5	2.53	1.38	1.34
2	2	1496	5MC	C6-C5	2.53	1.38	1.34
1	1	3004	4AC	C4-N3	-2.52	1.28	1.32
2	2	693	5MC	C6-C5	2.51	1.38	1.34
2	2	1374	5MC	C6-C5	2.50	1.38	1.34
1	1	229	4AC	C4-N3	-2.50	1.28	1.32
1	1	2203	5MC	C6-C5	2.49	1.38	1.34
1	1	2203	5MC	C6-N1	-2.48	1.33	1.38
2	2	64	OMU	C4-N3	-2.48	1.34	1.38
1	1	2784	OMU	C2-N3	-2.48	1.33	1.38
1	1	1885	4AC	C4-N3	-2.48	1.28	1.32
1	1	2001	4AC	C4-N3	-2.48	1.28	1.32
2	2	1498	5MC	C6-N1	-2.48	1.33	1.38
1	1	2608	4AC	C4-N3	-2.47	1.28	1.32
1	1	1938	4AC	C4-N3	-2.46	1.28	1.32
1	1	2198	5MC	C6-N1	-2.45	1.33	1.38
1	1	22	4AC	C4-N3	-2.44	1.28	1.32
2	2	1025	5MC	C6-N1	-2.44	1.33	1.38
1	1	1557	4AC	C4-N3	-2.43	1.28	1.32
2	2	20	OMU	C2-N3	-2.43	1.33	1.38
1	1	2249	4AC	C4-N3	-2.43	1.28	1.32
2	2	535	5MC	C6-N1	-2.42	1.33	1.38
1	1	1873	4AC	C4-N3	-2.41	1.28	1.32
1	1	835	4AC	C4-N3	-2.41	1.28	1.32
2	2	787	OMU	C2-N3	-2.41	1.33	1.38
1	1	789	OMG	C5-N7	-2.41	1.34	1.39
1	1	981	4AC	C4-N3	-2.41	1.28	1.32
2	2	1496	5MC	C6-N1	-2.40	1.33	1.38
2	2	1374	5MC	C6-N1	-2.40	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2083	4AC	C4-N3	-2.40	1.28	1.32
1	1	314	4AC	C4-N3	-2.39	1.28	1.32
2	2	851	4AC	C4-N3	-2.39	1.28	1.32
1	1	2908	4AC	C4-N3	-2.38	1.28	1.32
1	1	341	4AC	C4-N3	-2.38	1.28	1.32
2	2	693	5MC	C6-N1	-2.38	1.34	1.38
1	1	2163	5MC	C6-N1	-2.38	1.34	1.38
1	1	1068	4AC	C4-N3	-2.37	1.28	1.32
1	1	1621	4AC	C4-N3	-2.37	1.28	1.32
2	2	657	OMG	C5-N7	-2.37	1.34	1.39
1	1	2198	5MC	C6-C5	2.37	1.38	1.34
1	1	1222	4AC	C4-N3	-2.36	1.28	1.32
1	1	2173	A2M	C5-N7	-2.36	1.34	1.39
2	2	1380	OMU	C2-N3	-2.36	1.33	1.38
2	2	373	A2M	C5-N7	-2.36	1.34	1.39
2	2	875	5MC	C6-N1	-2.36	1.34	1.38
1	1	2733	5MC	C6-N1	-2.36	1.34	1.38
1	1	641	4AC	C4-N3	-2.36	1.28	1.32
1	1	2162	5MC	C6-N1	-2.36	1.34	1.38
2	2	511	4AC	C4-N3	-2.36	1.28	1.32
2	2	1177	OMU	C2-N3	-2.36	1.33	1.38
1	1	1243	4AC	C4-N3	-2.35	1.28	1.32
1	1	1962	4AC	C4-N3	-2.35	1.28	1.32
1	1	829	4AC	C4-N3	-2.35	1.28	1.32
1	1	2062	4AC	C4-N3	-2.34	1.28	1.32
1	1	328	OMG	C5-N7	-2.33	1.34	1.39
1	1	2865	4AC	C4-N3	-2.33	1.28	1.32
1	1	1055	A2M	C5-N7	-2.33	1.34	1.39
1	1	2678	OMG	C5-N7	-2.33	1.34	1.39
1	1	1765	4AC	C4-N3	-2.33	1.28	1.32
1	1	1065	4AC	C4-N3	-2.33	1.28	1.32
1	1	1460	4AC	C4-N3	-2.32	1.28	1.32
1	1	533	4AC	C4-N3	-2.32	1.28	1.32
2	2	471	OMG	C5-N7	-2.32	1.34	1.39
1	1	2183	5MC	C6-N1	-2.32	1.34	1.38
2	2	830	OMU	C2-N3	-2.32	1.33	1.38
1	1	2495	4AC	C4-N3	-2.32	1.28	1.32
2	2	1202	5MC	C6-N1	-2.32	1.34	1.38
2	2	873	OMG	C5-N7	-2.32	1.34	1.39
1	1	1048	4AC	C4-N3	-2.31	1.28	1.32
1	1	2144	OMG	C5-N7	-2.31	1.34	1.39
1	1	1934	4AC	C4-N3	-2.31	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	923	OMG	C5-N7	-2.31	1.34	1.39
1	1	91	4AC	C4-N3	-2.30	1.28	1.32
1	1	1594	4AC	C4-N3	-2.30	1.28	1.32
1	1	2925	4AC	C4-N3	-2.30	1.28	1.32
1	1	2966	4AC	C4-N3	-2.30	1.28	1.32
1	1	357	4AC	C4-N3	-2.30	1.28	1.32
2	2	1069	OMG	C5-N7	-2.30	1.34	1.39
1	1	2093	5MC	C6-N1	-2.30	1.34	1.38
1	1	2960	4AC	C4-N3	-2.29	1.28	1.32
1	1	922	4AC	C4-N3	-2.28	1.28	1.32
2	2	680	OMG	C5-N7	-2.28	1.34	1.39
1	1	136	4AC	C4-N3	-2.28	1.28	1.32
2	2	17	4AC	C4-N3	-2.28	1.28	1.32
2	2	774	OMU	C2-N3	-2.28	1.33	1.38
1	1	1554	4AC	C4-N3	-2.27	1.28	1.32
1	1	161	4AC	C4-N3	-2.27	1.28	1.32
1	1	2642	4AC	C4-N3	-2.27	1.28	1.32
1	1	2027	4AC	C4-N3	-2.27	1.28	1.32
1	1	694	4AC	C4-N3	-2.26	1.28	1.32
1	1	1878	4AC	C4-N3	-2.26	1.28	1.32
1	1	2992	4AC	C4-N3	-2.26	1.28	1.32
2	2	373	A2M	C8-N7	2.26	1.35	1.31
1	1	2138	OMG	C5-N7	-2.25	1.34	1.39
1	1	451	4AC	C4-N3	-2.25	1.28	1.32
2	2	1488	MA6	C8-N7	2.25	1.35	1.31
1	1	2329	4AC	C4-N3	-2.25	1.28	1.32
1	1	1055	A2M	C8-N7	2.25	1.35	1.31
2	2	53	4AC	C4-N3	-2.25	1.28	1.32
2	2	839	4AC	C4-N3	-2.24	1.28	1.32
1	1	2718	4AC	C4-N3	-2.24	1.28	1.32
2	2	590	4AC	C4-N3	-2.24	1.28	1.32
2	2	913	OMG	C5-N7	-2.24	1.34	1.39
1	1	1667	4AC	C4-N3	-2.24	1.28	1.32
2	2	731	4AC	C4-N3	-2.24	1.28	1.32
2	2	303	4AC	C4-N3	-2.23	1.28	1.32
2	2	751	4AC	C4-N3	-2.23	1.28	1.32
1	1	2570	4AC	C4-N3	-2.23	1.28	1.32
2	2	1505	5MC	C6-N1	-2.23	1.34	1.38
1	1	2937	4AC	C4-N3	-2.23	1.28	1.32
1	1	211	4AC	C4-N3	-2.23	1.28	1.32
2	2	868	4AC	C4-N3	-2.23	1.28	1.32
2	2	1479	4AC	C4-N3	-2.22	1.29	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1550	4AC	C4-N3	-2.21	1.29	1.32
1	1	243	4AC	C4-N3	-2.21	1.29	1.32
2	2	519	OMG	C5-N7	-2.21	1.34	1.39
2	2	286	4AC	C4-N3	-2.20	1.29	1.32
1	1	2545	4AC	C4-N3	-2.20	1.29	1.32
1	1	2287	4AC	C4-N3	-2.20	1.29	1.32
2	2	467	OMG	C5-N7	-2.20	1.34	1.39
1	1	1662	4AC	C4-N3	-2.19	1.29	1.32
1	1	1617	4AC	C4-N3	-2.19	1.29	1.32
1	1	1867	4AC	C4-N3	-2.19	1.29	1.32
2	2	319	4AC	C4-N3	-2.19	1.29	1.32
2	2	64	OMU	C2-N3	-2.19	1.34	1.38
1	1	2147	OMG	C5-N7	-2.19	1.34	1.39
2	2	1487	MA6	C8-N7	2.18	1.35	1.31
2	2	934	OMG	C5-N7	-2.18	1.34	1.39
2	2	1469	6MZ	C5-N7	-2.18	1.34	1.39
2	2	1469	6MZ	C8-N7	2.18	1.35	1.31
1	1	2136	4AC	C4-N3	-2.18	1.29	1.32
2	2	546	4AC	C4-N3	-2.18	1.29	1.32
2	2	1147	4AC	C4-N3	-2.17	1.29	1.32
2	2	1028	4AC	C4-N3	-2.17	1.29	1.32
1	1	2548	4AC	C4-N3	-2.17	1.29	1.32
1	1	1780	4AC	C4-N3	-2.16	1.29	1.32
2	2	957	4AC	C4-N3	-2.16	1.29	1.32
1	1	458	4AC	C4-N3	-2.15	1.29	1.32
2	2	1487	MA6	C5-N7	-2.15	1.35	1.39
2	2	1239	4AC	C4-N3	-2.15	1.29	1.32
2	2	479	4AC	C4-N3	-2.13	1.29	1.32
2	2	828	4AC	C4-N3	-2.13	1.29	1.32
1	1	1293	4AC	C4-N3	-2.13	1.29	1.32
2	2	394	4AC	C4-N3	-2.13	1.29	1.32
2	2	379	4AC	C4-N3	-2.12	1.29	1.32
2	2	848	4AC	C4-N3	-2.12	1.29	1.32
2	2	1380	OMU	C2-N1	2.12	1.41	1.38
2	2	636	4AC	C4-N3	-2.11	1.29	1.32
1	1	802	4AC	C4-N3	-2.11	1.29	1.32
1	1	2173	A2M	C8-N7	2.11	1.35	1.31
3	3	32	4AC	C4-N3	-2.10	1.29	1.32
2	2	1488	MA6	C5-N7	-2.09	1.35	1.39
2	2	1184	4AC	C4-N3	-2.08	1.29	1.32
2	2	718	4AC	C4-N3	-2.08	1.29	1.32
2	2	1380	OMU	C5-C4	-2.08	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1695	4AC	C4-N3	-2.07	1.29	1.32
1	1	1755	4AC	C4-N3	-2.06	1.29	1.32
2	2	1487	MA6	C4-N9	-2.05	1.33	1.37
2	2	1177	OMU	C5-C4	-2.05	1.39	1.43
2	2	64	OMU	C5-C4	-2.04	1.39	1.43
2	2	626	4AC	C4-N3	-2.03	1.29	1.32
2	2	830	OMU	C5-C4	-2.03	1.39	1.43
2	2	1488	MA6	C4-N9	-2.03	1.33	1.37
2	2	1233	4AC	C4-N3	-2.02	1.29	1.32
1	1	2784	OMU	C5-C4	-2.02	1.39	1.43
2	2	774	OMU	C5-C4	-2.01	1.39	1.43
1	1	60	4AC	C4-N3	-2.01	1.29	1.32
2	2	64	OMU	C2-N1	2.01	1.41	1.38

All (639) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1055	A2M	C5-C4-N3	-6.47	118.31	126.75
2	2	373	A2M	C5-C4-N3	-6.37	118.43	126.75
2	2	657	OMG	C5-C4-N3	-6.32	118.21	128.46
2	2	680	OMG	C5-C4-N3	-6.31	118.23	128.46
1	1	2173	A2M	C5-C4-N3	-6.30	118.53	126.75
2	2	471	OMG	C5-C4-N3	-6.14	118.49	128.46
2	2	873	OMG	C5-C4-N3	-6.12	118.53	128.46
1	1	2144	OMG	C5-C4-N3	-6.09	118.58	128.46
1	1	328	OMG	C5-C4-N3	-6.07	118.61	128.46
1	1	789	OMG	C5-C4-N3	-6.07	118.61	128.46
1	1	2138	OMG	C5-C4-N3	-6.06	118.64	128.46
2	2	934	OMG	C5-C4-N3	-6.02	118.70	128.46
2	2	1469	6MZ	C5-C4-N3	-6.00	118.92	126.75
2	2	467	OMG	C5-C4-N3	-5.99	118.75	128.46
2	2	1069	OMG	C5-C4-N3	-5.95	118.81	128.46
1	1	923	OMG	C5-C4-N3	-5.92	118.86	128.46
2	2	913	OMG	C5-C4-N3	-5.91	118.87	128.46
2	2	519	OMG	C5-C4-N3	-5.89	118.91	128.46
1	1	2678	OMG	C5-C4-N3	-5.88	118.92	128.46
1	1	2147	OMG	C5-C4-N3	-5.84	118.98	128.46
2	2	1488	MA6	C5-C4-N3	-5.74	119.27	126.75
2	2	1487	MA6	C5-C4-N3	-5.61	119.43	126.75
2	2	1467	UR3	C4-N3-C2	-5.60	119.29	124.56
1	1	2001	4AC	O7-C7-N4	5.17	130.19	121.82
1	1	1780	4AC	O7-C7-N4	5.03	129.96	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1878	4AC	O7-C7-N4	5.02	129.95	121.82
1	1	1755	4AC	O7-C7-N4	4.99	129.89	121.82
1	1	1055	A2M	N3-C4-N9	4.98	135.28	127.08
2	2	467	OMG	C2-N3-C4	4.92	121.06	112.30
2	2	680	OMG	C2-N3-C4	4.90	121.04	112.30
2	2	934	OMG	C2-N3-C4	4.90	121.03	112.30
1	1	2585	4AC	N4-C4-N3	4.89	122.06	113.85
1	1	789	OMG	C2-N3-C4	4.89	121.01	112.30
2	2	373	A2M	N3-C4-N9	4.88	135.13	127.08
2	2	519	OMG	C2-N3-C4	4.88	120.99	112.30
2	2	787	OMU	C4-N3-C2	-4.85	120.18	126.58
2	2	913	OMG	C2-N3-C4	4.82	120.89	112.30
2	2	873	OMG	C2-N3-C4	4.81	120.87	112.30
1	1	2147	OMG	C2-N3-C4	4.81	120.87	112.30
1	1	2608	4AC	N4-C4-N3	4.81	121.92	113.85
1	1	2173	A2M	N3-C4-N9	4.80	135.00	127.08
2	2	20	OMU	C4-N3-C2	-4.80	120.25	126.58
2	2	471	OMG	C2-N3-C4	4.79	120.84	112.30
1	1	2144	OMG	C2-N3-C4	4.79	120.84	112.30
1	1	923	OMG	C2-N3-C4	4.79	120.84	112.30
1	1	2138	OMG	C2-N3-C4	4.79	120.83	112.30
1	1	2608	4AC	C5-C4-N4	-4.79	114.61	122.92
2	2	657	OMG	C2-N3-C4	4.79	120.83	112.30
2	2	1069	OMG	C2-N3-C4	4.78	120.81	112.30
1	1	2678	OMG	C2-N3-C4	4.77	120.81	112.30
2	2	657	OMG	N9-C4-N3	4.77	135.52	125.94
2	2	680	OMG	N9-C4-N3	4.75	135.47	125.94
1	1	2784	OMU	C4-N3-C2	-4.72	120.36	126.58
1	1	328	OMG	N9-C4-N3	4.71	135.40	125.94
1	1	1065	4AC	O7-C7-N4	4.70	129.43	121.82
1	1	328	OMG	C2-N3-C4	4.68	120.64	112.30
2	2	873	OMG	N9-C4-N3	4.67	135.32	125.94
1	1	2937	4AC	C5-C4-N4	-4.66	114.83	122.92
3	3	32	4AC	O7-C7-N4	4.62	129.30	121.82
2	2	1177	OMU	C4-N3-C2	-4.62	120.49	126.58
2	2	471	OMG	N9-C4-N3	4.61	135.21	125.94
2	2	848	4AC	O7-C7-N4	4.61	129.28	121.82
1	1	2287	4AC	O7-C7-N4	4.61	129.28	121.82
2	2	1487	MA6	C2-N1-C6	4.61	122.63	111.75
1	1	789	OMG	N9-C4-N3	4.59	135.16	125.94
1	1	1873	4AC	O7-C7-N4	4.59	129.25	121.82
1	1	2937	4AC	N4-C4-N3	4.59	121.55	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1934	4AC	O7-C7-N4	4.58	129.24	121.82
1	1	1068	4AC	O7-C7-N4	4.58	129.23	121.82
1	1	2585	4AC	C5-C4-N4	-4.57	114.98	122.92
2	2	53	4AC	O7-C7-N4	4.57	129.21	121.82
1	1	2136	4AC	O7-C7-N4	4.56	129.20	121.82
1	1	2138	OMG	N9-C4-N3	4.56	135.09	125.94
1	1	2144	OMG	N9-C4-N3	4.56	135.09	125.94
1	1	802	4AC	O7-C7-N4	4.55	129.19	121.82
2	2	1028	4AC	O7-C7-N4	4.55	129.19	121.82
1	1	2249	4AC	O7-C7-N4	4.55	129.19	121.82
2	2	636	4AC	O7-C7-N4	4.55	129.18	121.82
1	1	1667	4AC	O7-C7-N4	4.55	129.18	121.82
1	1	1554	4AC	O7-C7-N4	4.54	129.17	121.82
1	1	1460	4AC	O7-C7-N4	4.54	129.17	121.82
2	2	934	OMG	N9-C4-N3	4.54	135.05	125.94
2	2	718	4AC	O7-C7-N4	4.54	129.16	121.82
1	1	922	4AC	O7-C7-N4	4.54	129.16	121.82
2	2	774	OMU	C4-N3-C2	-4.54	120.60	126.58
2	2	1184	4AC	O7-C7-N4	4.54	129.16	121.82
2	2	626	4AC	O7-C7-N4	4.52	129.14	121.82
2	2	546	4AC	O7-C7-N4	4.52	129.14	121.82
2	2	1147	4AC	O7-C7-N4	4.52	129.13	121.82
1	1	641	4AC	O7-C7-N4	4.52	129.13	121.82
1	1	1243	4AC	O7-C7-N4	4.52	129.13	121.82
1	1	243	4AC	O7-C7-N4	4.51	129.12	121.82
1	1	2329	4AC	O7-C7-N4	4.51	129.12	121.82
2	2	303	4AC	O7-C7-N4	4.51	129.12	121.82
2	2	479	4AC	O7-C7-N4	4.51	129.12	121.82
1	1	2966	4AC	O7-C7-N4	4.51	129.12	121.82
1	1	1617	4AC	O7-C7-N4	4.50	129.11	121.82
1	1	1962	4AC	O7-C7-N4	4.50	129.11	121.82
1	1	829	4AC	O7-C7-N4	4.50	129.11	121.82
1	1	1662	4AC	O7-C7-N4	4.50	129.10	121.82
2	2	319	4AC	O7-C7-N4	4.50	129.10	121.82
2	2	17	4AC	O7-C7-N4	4.50	129.09	121.82
2	2	1380	OMU	C4-N3-C2	-4.49	120.65	126.58
2	2	731	4AC	O7-C7-N4	4.49	129.09	121.82
1	1	91	4AC	O7-C7-N4	4.49	129.08	121.82
2	2	957	4AC	O7-C7-N4	4.48	129.07	121.82
2	2	1233	4AC	O7-C7-N4	4.48	129.07	121.82
1	1	1867	4AC	O7-C7-N4	4.48	129.07	121.82
2	2	1069	OMG	N9-C4-N3	4.48	134.93	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1695	4AC	O7-C7-N4	4.48	129.06	121.82
1	1	161	4AC	O7-C7-N4	4.47	129.06	121.82
1	1	1550	4AC	O7-C7-N4	4.47	129.05	121.82
1	1	60	4AC	O7-C7-N4	4.47	129.05	121.82
1	1	1048	4AC	O7-C7-N4	4.47	129.04	121.82
1	1	1293	4AC	O7-C7-N4	4.46	129.04	121.82
1	1	357	4AC	O7-C7-N4	4.46	129.04	121.82
1	1	2570	4AC	O7-C7-N4	4.46	129.03	121.82
1	1	2718	4AC	O7-C7-N4	4.46	129.03	121.82
2	2	839	4AC	O7-C7-N4	4.46	129.03	121.82
1	1	923	OMG	N9-C4-N3	4.45	134.87	125.94
1	1	2548	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	1488	MA6	C2-N1-C6	4.44	122.25	111.75
1	1	1938	4AC	O7-C7-N4	4.44	129.01	121.82
1	1	2545	4AC	O7-C7-N4	4.44	129.01	121.82
2	2	511	4AC	O7-C7-N4	4.44	129.00	121.82
1	1	1885	4AC	O7-C7-N4	4.43	128.99	121.82
2	2	394	4AC	O7-C7-N4	4.43	128.98	121.82
1	1	1621	4AC	O7-C7-N4	4.42	128.97	121.82
1	1	1594	4AC	O7-C7-N4	4.42	128.97	121.82
2	2	379	4AC	O7-C7-N4	4.41	128.96	121.82
2	2	830	OMU	C4-N3-C2	-4.41	120.76	126.58
1	1	451	4AC	O7-C7-N4	4.41	128.96	121.82
1	1	835	4AC	O7-C7-N4	4.41	128.95	121.82
1	1	2960	4AC	O7-C7-N4	4.40	128.95	121.82
2	2	868	4AC	O7-C7-N4	4.40	128.94	121.82
2	2	1469	6MZ	C6-C5-N7	4.40	137.15	132.39
1	1	2925	4AC	O7-C7-N4	4.39	128.93	121.82
1	1	1765	4AC	O7-C7-N4	4.39	128.93	121.82
1	1	314	4AC	O7-C7-N4	4.39	128.93	121.82
2	2	64	OMU	C4-N3-C2	-4.39	120.79	126.58
1	1	136	4AC	O7-C7-N4	4.39	128.92	121.82
2	2	590	4AC	O7-C7-N4	4.38	128.91	121.82
2	2	20	OMU	N3-C2-N1	4.38	120.70	114.89
2	2	467	OMG	N9-C4-N3	4.38	134.73	125.94
2	2	751	4AC	O7-C7-N4	4.37	128.90	121.82
1	1	2784	OMU	N3-C2-N1	4.37	120.70	114.89
2	2	828	4AC	O7-C7-N4	4.37	128.90	121.82
1	1	211	4AC	O7-C7-N4	4.37	128.89	121.82
1	1	3004	4AC	O7-C7-N4	4.37	128.89	121.82
1	1	2027	4AC	O7-C7-N4	4.37	128.89	121.82
1	1	229	4AC	O7-C7-N4	4.37	128.89	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	703	4AC	O7-C7-N4	4.37	128.89	121.82
1	1	1222	4AC	O7-C7-N4	4.36	128.88	121.82
1	1	2908	4AC	O7-C7-N4	4.35	128.86	121.82
1	1	2147	OMG	N9-C4-N3	4.35	134.68	125.94
1	1	2678	OMG	N9-C4-N3	4.35	134.67	125.94
2	2	1469	6MZ	N3-C4-N9	4.35	134.25	127.08
2	2	913	OMG	N9-C4-N3	4.34	134.66	125.94
1	1	694	4AC	O7-C7-N4	4.33	128.83	121.82
1	1	981	4AC	O7-C7-N4	4.33	128.83	121.82
1	1	2062	4AC	O7-C7-N4	4.33	128.82	121.82
2	2	1380	OMU	N3-C2-N1	4.32	120.62	114.89
1	1	22	4AC	O7-C7-N4	4.30	128.78	121.82
1	1	2495	4AC	O7-C7-N4	4.29	128.76	121.82
1	1	533	4AC	O7-C7-N4	4.28	128.74	121.82
1	1	2865	4AC	O7-C7-N4	4.27	128.73	121.82
2	2	286	4AC	O7-C7-N4	4.26	128.71	121.82
2	2	519	OMG	N9-C4-N3	4.25	134.48	125.94
2	2	1177	OMU	N3-C2-N1	4.25	120.53	114.89
2	2	1239	4AC	O7-C7-N4	4.24	128.68	121.82
1	1	1557	4AC	O7-C7-N4	4.23	128.66	121.82
1	1	2083	4AC	O7-C7-N4	4.23	128.66	121.82
1	1	458	4AC	O7-C7-N4	4.23	128.66	121.82
2	2	1487	MA6	N3-C4-N9	4.21	134.01	127.08
2	2	787	OMU	N3-C2-N1	4.20	120.46	114.89
1	1	341	4AC	O7-C7-N4	4.19	128.61	121.82
1	1	2642	4AC	O7-C7-N4	4.19	128.59	121.82
2	2	774	OMU	N3-C2-N1	4.16	120.41	114.89
2	2	1479	4AC	O7-C7-N4	4.15	128.54	121.82
2	2	1488	MA6	N3-C4-N9	4.14	133.91	127.08
2	2	851	4AC	O7-C7-N4	4.14	128.51	121.82
2	2	830	OMU	N3-C2-N1	4.13	120.38	114.89
2	2	64	OMU	N3-C2-N1	3.99	120.19	114.89
2	2	1488	MA6	C4-C5-N7	-3.97	105.78	110.62
1	1	1055	A2M	C2-N3-C4	3.97	121.12	111.75
2	2	373	A2M	C2-N3-C4	3.95	121.08	111.75
2	2	1469	6MZ	C2-N3-C4	3.94	121.06	111.75
1	1	2173	A2M	C2-N3-C4	3.91	121.00	111.75
2	2	1469	6MZ	C4-C5-N7	-3.91	105.86	110.62
2	2	1487	MA6	C2-N3-C4	3.86	120.87	111.75
2	2	1025	5MC	C5-C6-N1	-3.84	119.38	123.34
2	2	1487	MA6	C4-C5-N7	-3.84	105.95	110.62
2	2	787	OMU	C5-C4-N3	3.81	120.55	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1488	MA6	C2-N3-C4	3.79	120.70	111.75
1	1	2784	OMU	C5-C4-N3	3.71	120.39	114.84
1	1	1755	4AC	N4-C4-N3	3.68	120.03	113.85
2	2	1374	5MC	C5-C6-N1	-3.66	119.57	123.34
2	2	20	OMU	C5-C4-N3	3.66	120.31	114.84
2	2	1177	OMU	C5-C4-N3	3.63	120.27	114.84
1	1	2733	5MC	C5-C6-N1	-3.62	119.62	123.34
1	1	2937	4AC	O7-C7-N4	3.61	127.66	121.82
2	2	774	OMU	C5-C4-N3	3.61	120.23	114.84
1	1	1755	4AC	C5-C4-N4	-3.60	116.66	122.92
2	2	1380	OMU	C5-C4-N3	3.59	120.21	114.84
2	2	830	OMU	C5-C4-N3	3.58	120.20	114.84
2	2	1202	5MC	C5-C6-N1	-3.58	119.66	123.34
2	2	535	5MC	C5-C6-N1	-3.57	119.66	123.34
1	1	2093	5MC	C5-C6-N1	-3.57	119.67	123.34
2	2	703	4AC	N4-C4-N3	3.57	119.84	113.85
1	1	1780	4AC	N4-C4-N3	3.56	119.83	113.85
2	2	64	OMU	C5-C4-N3	3.55	120.14	114.84
1	1	2198	5MC	C5-C6-N1	-3.52	119.72	123.34
1	1	2183	5MC	C5-C6-N1	-3.51	119.73	123.34
1	1	1780	4AC	C5-C4-N4	-3.51	116.83	122.92
2	2	519	OMG	C6-C5-N7	3.49	136.75	130.25
2	2	1487	MA6	N1-C2-N3	-3.49	123.14	128.60
1	1	2163	5MC	C5-C6-N1	-3.49	119.75	123.34
2	2	875	5MC	C5-C6-N1	-3.47	119.77	123.34
1	1	60	4AC	N4-C4-N3	3.46	119.67	113.85
1	1	2585	4AC	O7-C7-N4	3.46	127.42	121.82
1	1	2203	5MC	C5-C6-N1	-3.46	119.78	123.34
1	1	2608	4AC	O7-C7-N4	3.44	127.38	121.82
1	1	2162	5MC	C5-C6-N1	-3.43	119.81	123.34
2	2	1496	5MC	C5-C6-N1	-3.42	119.82	123.34
2	2	1469	6MZ	N1-C2-N3	-3.41	123.28	128.60
2	2	467	OMG	C6-C5-N7	3.40	136.57	130.25
2	2	913	OMG	C6-C5-N7	3.40	136.57	130.25
1	1	2147	OMG	C6-C5-N7	3.38	136.53	130.25
2	2	1505	5MC	C5-C6-N1	-3.36	119.89	123.34
2	2	693	5MC	C5-C6-N1	-3.33	119.91	123.34
1	1	2678	OMG	C6-C5-N7	3.32	136.42	130.25
1	1	2173	A2M	C4-C5-N7	-3.31	106.59	110.62
2	2	934	OMG	C6-C5-N7	3.30	136.39	130.25
2	2	1498	5MC	C5-C6-N1	-3.29	119.95	123.34
1	1	1878	4AC	CM7-C7-N4	-3.28	109.61	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	373	A2M	C4-C5-N7	-3.27	106.64	110.62
1	1	2001	4AC	N4-C4-N3	3.26	119.33	113.85
1	1	2585	4AC	O2-C2-N3	-3.25	117.04	122.33
1	1	923	OMG	C6-C5-N7	3.24	136.28	130.25
2	2	703	4AC	C5-C4-N4	-3.23	117.31	122.92
1	1	1878	4AC	C5-C4-N4	-3.23	117.31	122.92
1	1	2966	4AC	CM7-C7-N4	-3.22	109.73	115.29
1	1	2138	OMG	C6-C5-N7	3.21	136.21	130.25
1	1	922	4AC	N4-C4-N3	3.20	119.22	113.85
1	1	1055	A2M	C4-C5-N7	-3.19	106.73	110.62
1	1	2329	4AC	N4-C4-N3	3.19	119.20	113.85
2	2	1488	MA6	N1-C2-N3	-3.19	123.62	128.60
2	2	1069	OMG	C6-C5-N7	3.18	136.17	130.25
1	1	1873	4AC	CM7-C7-N4	-3.18	109.79	115.29
1	1	1065	4AC	N4-C4-N3	3.18	119.20	113.85
2	2	626	4AC	N4-C4-N3	3.17	119.17	113.85
1	1	2144	OMG	C6-C5-N7	3.16	136.13	130.25
1	1	789	OMG	C6-C5-N7	3.16	136.12	130.25
1	1	802	4AC	N4-C4-N3	3.15	119.15	113.85
2	2	373	A2M	N3-C2-N1	-3.14	123.69	128.60
1	1	2287	4AC	N4-C4-N3	3.13	119.11	113.85
1	1	641	4AC	CM7-C7-N4	-3.13	109.88	115.29
2	2	848	4AC	CM7-C7-N4	-3.13	109.88	115.29
2	2	873	OMG	C6-C5-N7	3.12	136.05	130.25
1	1	2173	A2M	N3-C2-N1	-3.12	123.72	128.60
1	1	1055	A2M	N3-C2-N1	-3.11	123.73	128.60
1	1	1243	4AC	CM7-C7-N4	-3.10	109.93	115.29
2	2	1487	MA6	C5-N7-C8	3.10	107.91	103.51
1	1	229	4AC	CM7-C7-N4	-3.09	109.94	115.29
2	2	1488	MA6	C5-N7-C8	3.08	107.89	103.51
1	1	1878	4AC	N4-C4-N3	3.07	119.01	113.85
1	1	1885	4AC	CM7-C7-N4	-3.07	109.98	115.29
2	2	394	4AC	N4-C4-N3	3.07	119.00	113.85
2	2	471	OMG	C6-C5-N7	3.07	135.95	130.25
2	2	1233	4AC	N4-C4-N3	3.06	119.00	113.85
1	1	829	4AC	CM7-C7-N4	-3.06	110.00	115.29
1	1	60	4AC	C5-C4-N4	-3.06	117.60	122.92
2	2	1239	4AC	N4-C4-N3	3.06	118.99	113.85
2	2	319	4AC	N4-C4-N3	3.06	118.99	113.85
1	1	3004	4AC	CM7-C7-N4	-3.06	110.01	115.29
2	2	1469	6MZ	C5-N7-C8	3.05	107.85	103.51
1	1	1962	4AC	CM7-C7-N4	-3.05	110.01	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	802	4AC	C5-C4-N4	-3.05	117.62	122.92
2	2	848	4AC	C5-C4-N4	-3.05	117.63	122.92
2	2	379	4AC	N4-C4-N3	3.04	118.96	113.85
1	1	2249	4AC	CM7-C7-N4	-3.04	110.03	115.29
1	1	2287	4AC	C5-C4-N4	-3.04	117.64	122.92
2	2	53	4AC	CM7-C7-N4	-3.04	110.04	115.29
1	1	2136	4AC	N4-C4-N3	3.03	118.93	113.85
1	1	1293	4AC	N4-C4-N3	3.02	118.93	113.85
1	1	1867	4AC	CM7-C7-N4	-3.02	110.07	115.29
1	1	1065	4AC	C5-C4-N4	-3.02	117.67	122.92
2	2	319	4AC	C5-C4-N4	-3.02	117.67	122.92
2	2	1028	4AC	CM7-C7-N4	-3.02	110.07	115.29
2	2	1184	4AC	N4-C4-N3	3.01	118.91	113.85
3	3	32	4AC	CM7-C7-N4	-3.01	110.09	115.29
1	1	357	4AC	CM7-C7-N4	-3.00	110.10	115.29
1	1	1068	4AC	CM7-C7-N4	-3.00	110.10	115.29
2	2	546	4AC	N4-C4-N3	3.00	118.88	113.85
2	2	828	4AC	CM7-C7-N4	-3.00	110.11	115.29
1	1	2001	4AC	C5-C4-N4	-2.99	117.72	122.92
2	2	479	4AC	N4-C4-N3	2.99	118.88	113.85
1	1	1293	4AC	C5-C4-N4	-2.99	117.73	122.92
1	1	1550	4AC	N4-C4-N3	2.99	118.86	113.85
2	2	718	4AC	N4-C4-N3	2.99	118.86	113.85
1	1	22	4AC	CM7-C7-N4	-2.98	110.13	115.29
2	2	848	4AC	N4-C4-N3	2.98	118.86	113.85
1	1	328	OMG	C6-C5-N7	2.98	135.79	130.25
1	1	211	4AC	CM7-C7-N4	-2.98	110.14	115.29
2	2	1147	4AC	CM7-C7-N4	-2.98	110.15	115.29
1	1	1662	4AC	CM7-C7-N4	-2.97	110.15	115.29
1	1	835	4AC	CM7-C7-N4	-2.97	110.16	115.29
2	2	64	OMU	O4-C4-C5	-2.97	119.94	125.16
2	2	626	4AC	C5-C4-N4	-2.97	117.76	122.92
2	2	680	OMG	C6-C5-N7	2.97	135.77	130.25
2	2	1177	OMU	O4-C4-C5	-2.96	119.95	125.16
2	2	53	4AC	N4-C4-N3	2.96	118.83	113.85
1	1	981	4AC	CM7-C7-N4	-2.96	110.17	115.29
2	2	731	4AC	N4-C4-N3	2.96	118.83	113.85
1	1	2329	4AC	C5-C4-N4	-2.96	117.77	122.92
2	2	17	4AC	CM7-C7-N4	-2.96	110.17	115.29
2	2	479	4AC	CM7-C7-N4	-2.96	110.17	115.29
2	2	636	4AC	N4-C4-N3	2.96	118.82	113.85
3	3	32	4AC	N4-C4-N3	2.96	118.81	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2570	4AC	N4-C4-N3	2.96	118.81	113.85
1	1	1934	4AC	N4-C4-N3	2.95	118.81	113.85
1	1	2608	4AC	O2-C2-N3	-2.95	117.53	122.33
2	2	787	OMU	O4-C4-C5	-2.95	119.97	125.16
1	1	1667	4AC	CM7-C7-N4	-2.95	110.19	115.29
1	1	357	4AC	N4-C4-N3	2.95	118.80	113.85
1	1	1621	4AC	CM7-C7-N4	-2.94	110.20	115.29
1	1	1780	4AC	CM7-C7-N4	-2.94	110.20	115.29
1	1	2083	4AC	CM7-C7-N4	-2.94	110.20	115.29
2	2	957	4AC	N4-C4-N3	2.94	118.79	113.85
1	1	458	4AC	N4-C4-N3	2.94	118.78	113.85
1	1	2718	4AC	N4-C4-N3	2.93	118.78	113.85
1	1	1662	4AC	C5-C4-N4	-2.93	117.83	122.92
1	1	1554	4AC	CM7-C7-N4	-2.93	110.23	115.29
2	2	511	4AC	CM7-C7-N4	-2.93	110.23	115.29
1	1	2548	4AC	CM7-C7-N4	-2.92	110.24	115.29
1	1	91	4AC	N4-C4-N3	2.92	118.76	113.85
1	1	922	4AC	C5-C4-N4	-2.92	117.85	122.92
1	1	1695	4AC	CM7-C7-N4	-2.92	110.25	115.29
1	1	1934	4AC	C5-C4-N4	-2.92	117.85	122.92
1	1	1460	4AC	N4-C4-N3	2.92	118.75	113.85
1	1	2136	4AC	C5-C4-N4	-2.92	117.85	122.92
1	1	136	4AC	CM7-C7-N4	-2.91	110.25	115.29
1	1	1048	4AC	CM7-C7-N4	-2.91	110.25	115.29
1	1	2545	4AC	CM7-C7-N4	-2.91	110.26	115.29
2	2	1233	4AC	C5-C4-N4	-2.91	117.86	122.92
2	2	774	OMU	O4-C4-C5	-2.91	120.05	125.16
1	1	802	4AC	CM7-C7-N4	-2.91	110.26	115.29
2	2	636	4AC	CM7-C7-N4	-2.91	110.26	115.29
2	2	839	4AC	N4-C4-N3	2.91	118.73	113.85
2	2	731	4AC	CM7-C7-N4	-2.90	110.27	115.29
1	1	161	4AC	CM7-C7-N4	-2.90	110.27	115.29
1	1	1293	4AC	CM7-C7-N4	-2.90	110.28	115.29
2	2	1184	4AC	C5-C4-N4	-2.90	117.88	122.92
3	3	32	4AC	C5-C4-N4	-2.90	117.88	122.92
2	2	303	4AC	CM7-C7-N4	-2.90	110.28	115.29
2	2	718	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	1	1695	4AC	C5-C4-N4	-2.89	117.89	122.92
1	1	2062	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	1	2585	4AC	C1'-N1-C2	2.89	124.87	118.42
2	2	957	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	1	1662	4AC	N4-C4-N3	2.89	118.70	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	479	4AC	C5-C4-N4	-2.88	117.91	122.92
2	2	1487	MA6	C4-N9-C8	2.88	108.85	105.73
2	2	1147	4AC	N4-C4-N3	2.88	118.69	113.85
1	1	314	4AC	CM7-C7-N4	-2.88	110.31	115.29
1	1	2570	4AC	C5-C4-N4	-2.88	117.92	122.92
1	1	1765	4AC	CM7-C7-N4	-2.88	110.31	115.29
2	2	590	4AC	CM7-C7-N4	-2.88	110.31	115.29
2	2	718	4AC	C5-C4-N4	-2.88	117.92	122.92
1	1	2027	4AC	N4-C4-N3	2.87	118.68	113.85
1	1	1934	4AC	CM7-C7-N4	-2.87	110.33	115.29
1	1	1550	4AC	C5-C4-N4	-2.87	117.94	122.92
1	1	2784	OMU	O4-C4-C5	-2.86	120.12	125.16
2	2	957	4AC	C5-C4-N4	-2.86	117.94	122.92
1	1	1460	4AC	CM7-C7-N4	-2.86	110.34	115.29
2	2	20	OMU	O4-C4-C5	-2.86	120.13	125.16
2	2	1380	OMU	O4-C4-C5	-2.86	120.13	125.16
1	1	2545	4AC	N4-C4-N3	2.86	118.65	113.85
1	1	243	4AC	N4-C4-N3	2.86	118.65	113.85
2	2	636	4AC	C5-C4-N4	-2.85	117.96	122.92
2	2	379	4AC	C5-C4-N4	-2.85	117.96	122.92
1	1	1695	4AC	N4-C4-N3	2.85	118.64	113.85
2	2	839	4AC	CM7-C7-N4	-2.85	110.36	115.29
1	1	1938	4AC	CM7-C7-N4	-2.85	110.36	115.29
1	1	1617	4AC	N4-C4-N3	2.85	118.64	113.85
1	1	2287	4AC	CM7-C7-N4	-2.84	110.37	115.29
1	1	91	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	1	694	4AC	CM7-C7-N4	-2.84	110.39	115.29
2	2	868	4AC	N4-C4-N3	2.83	118.61	113.85
1	1	1068	4AC	N4-C4-N3	2.83	118.61	113.85
1	1	2925	4AC	C5-C4-N4	-2.83	118.00	122.92
2	2	394	4AC	CM7-C7-N4	-2.83	110.40	115.29
2	2	519	OMG	C4-C5-N7	-2.83	106.24	110.72
2	2	751	4AC	CM7-C7-N4	-2.83	110.40	115.29
2	2	394	4AC	C5-C4-N4	-2.83	118.01	122.92
1	1	1667	4AC	N4-C4-N3	2.83	118.60	113.85
1	1	243	4AC	CM7-C7-N4	-2.83	110.41	115.29
2	2	1479	4AC	N4-C4-N3	2.82	118.58	113.85
1	1	1867	4AC	N4-C4-N3	2.82	118.58	113.85
1	1	2027	4AC	CM7-C7-N4	-2.82	110.42	115.29
2	2	751	4AC	N4-C4-N3	2.81	118.58	113.85
2	2	830	OMU	O4-C4-C5	-2.81	120.21	125.16
2	2	657	OMG	C6-C5-N7	2.81	135.48	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1554	4AC	N4-C4-N3	2.81	118.57	113.85
1	1	161	4AC	N4-C4-N3	2.81	118.57	113.85
2	2	1184	4AC	CM7-C7-N4	-2.81	110.43	115.29
2	2	590	4AC	N4-C4-N3	2.81	118.57	113.85
2	2	731	4AC	C5-C4-N4	-2.81	118.04	122.92
1	1	2865	4AC	CM7-C7-N4	-2.81	110.44	115.29
1	1	1460	4AC	C5-C4-N4	-2.81	118.05	122.92
1	1	2718	4AC	C5-C4-N4	-2.80	118.05	122.92
1	1	1867	4AC	C5-C4-N4	-2.80	118.05	122.92
1	1	2570	4AC	CM7-C7-N4	-2.80	110.45	115.29
1	1	1550	4AC	CM7-C7-N4	-2.80	110.45	115.29
1	1	2642	4AC	N4-C4-N3	2.80	118.55	113.85
2	2	1147	4AC	C5-C4-N4	-2.80	118.06	122.92
2	2	1239	4AC	C5-C4-N4	-2.80	118.06	122.92
2	2	546	4AC	C5-C4-N4	-2.80	118.06	122.92
1	1	1594	4AC	CM7-C7-N4	-2.80	110.46	115.29
1	1	1222	4AC	N4-C4-N3	2.79	118.54	113.85
2	2	1233	4AC	CM7-C7-N4	-2.79	110.47	115.29
1	1	451	4AC	N4-C4-N3	2.78	118.53	113.85
1	1	2136	4AC	CM7-C7-N4	-2.78	110.48	115.29
2	2	303	4AC	N4-C4-N3	2.78	118.51	113.85
1	1	243	4AC	C5-C4-N4	-2.78	118.10	122.92
2	2	626	4AC	CM7-C7-N4	-2.77	110.50	115.29
1	1	1065	4AC	CM7-C7-N4	-2.77	110.50	115.29
1	1	1617	4AC	CM7-C7-N4	-2.77	110.50	115.29
2	2	546	4AC	CM7-C7-N4	-2.77	110.51	115.29
1	1	2495	4AC	CM7-C7-N4	-2.76	110.52	115.29
1	1	1755	4AC	CM7-C7-N4	-2.76	110.52	115.29
1	1	533	4AC	N4-C4-N3	2.75	118.48	113.85
2	2	53	4AC	C5-C4-N4	-2.75	118.14	122.92
1	1	2718	4AC	CM7-C7-N4	-2.75	110.54	115.29
1	1	2960	4AC	CM7-C7-N4	-2.75	110.55	115.29
1	1	451	4AC	CM7-C7-N4	-2.74	110.55	115.29
1	1	2925	4AC	CM7-C7-N4	-2.74	110.55	115.29
1	1	1667	4AC	C5-C4-N4	-2.74	118.16	122.92
1	1	2960	4AC	N4-C4-N3	2.74	118.45	113.85
2	2	17	4AC	C5-C4-N4	-2.73	118.18	122.92
2	2	1028	4AC	N4-C4-N3	2.73	118.43	113.85
1	1	1594	4AC	N4-C4-N3	2.73	118.43	113.85
1	1	1068	4AC	C5-C4-N4	-2.73	118.18	122.92
1	1	91	4AC	C5-C4-N4	-2.72	118.19	122.92
2	2	319	4AC	CM7-C7-N4	-2.72	110.58	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1554	4AC	C5-C4-N4	-2.72	118.19	122.92
1	1	2027	4AC	C5-C4-N4	-2.72	118.19	122.92
2	2	828	4AC	N4-C4-N3	2.72	118.42	113.85
1	1	1765	4AC	C5-C4-N4	-2.72	118.19	122.92
1	1	694	4AC	N4-C4-N3	2.72	118.42	113.85
2	2	693	5MC	C5-C4-N3	-2.72	118.74	121.67
1	1	1055	A2M	C2'-C1'-N9	-2.72	108.96	113.53
1	1	1765	4AC	N4-C4-N3	2.72	118.41	113.85
2	2	286	4AC	N4-C4-N3	2.71	118.41	113.85
1	1	2545	4AC	C5-C4-N4	-2.71	118.21	122.92
2	2	868	4AC	C5-C4-N4	-2.71	118.21	122.92
2	2	467	OMG	C4-C5-N7	-2.71	106.43	110.72
2	2	379	4AC	CM7-C7-N4	-2.71	110.61	115.29
2	2	303	4AC	C5-C4-N4	-2.71	118.21	122.92
2	2	839	4AC	C5-C4-N4	-2.71	118.21	122.92
2	2	868	4AC	CM7-C7-N4	-2.71	110.61	115.29
2	2	913	OMG	C4-C5-N7	-2.71	106.44	110.72
1	1	211	4AC	N4-C4-N3	2.71	118.39	113.85
1	1	2908	4AC	CM7-C7-N4	-2.70	110.62	115.29
1	1	161	4AC	C5-C4-N4	-2.70	118.22	122.92
1	1	341	4AC	N4-C4-N3	2.70	118.39	113.85
1	1	2733	5MC	C5-C4-N3	-2.70	118.76	121.67
2	2	286	4AC	CM7-C7-N4	-2.70	110.62	115.29
1	1	2925	4AC	N4-C4-N3	2.70	118.38	113.85
2	2	828	4AC	C5-C4-N4	-2.70	118.23	122.92
1	1	2548	4AC	N4-C4-N3	2.70	118.38	113.85
2	2	17	4AC	N4-C4-N3	2.69	118.37	113.85
1	1	357	4AC	C5-C4-N4	-2.69	118.25	122.92
1	1	2960	4AC	C5-C4-N4	-2.69	118.25	122.92
1	1	1048	4AC	N4-C4-N3	2.69	118.36	113.85
2	2	373	A2M	C5-N7-C8	2.69	107.33	103.51
1	1	2173	A2M	C5-N7-C8	2.68	107.31	103.51
1	1	1617	4AC	C5-C4-N4	-2.68	118.27	122.92
1	1	2001	4AC	CM7-C7-N4	-2.67	110.67	115.29
1	1	2966	4AC	C5-C4-N4	-2.67	118.28	122.92
1	1	2147	OMG	C4-C5-N7	-2.66	106.52	110.72
2	2	851	4AC	CM7-C7-N4	-2.65	110.70	115.29
1	1	2062	4AC	N4-C4-N3	2.65	118.31	113.85
1	1	60	4AC	CM7-C7-N4	-2.65	110.71	115.29
1	1	694	4AC	C5-C4-N4	-2.65	118.32	122.92
1	1	2144	OMG	C4-C5-N7	-2.65	106.53	110.72
1	1	1048	4AC	C5-C4-N4	-2.65	118.32	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2162	5MC	C5-C4-N3	-2.65	118.82	121.67
1	1	2203	5MC	C5-C4-N3	-2.64	118.82	121.67
2	2	934	OMG	C4-C5-N7	-2.64	106.54	110.72
1	1	1962	4AC	N4-C4-N3	2.64	118.29	113.85
1	1	2329	4AC	CM7-C7-N4	-2.64	110.72	115.29
2	2	1028	4AC	C5-C4-N4	-2.64	118.33	122.92
2	2	511	4AC	N4-C4-N3	2.64	118.28	113.85
1	1	1594	4AC	C5-C4-N4	-2.64	118.33	122.92
2	2	703	4AC	CM7-C7-N4	-2.64	110.73	115.29
1	1	2093	5MC	C5-C4-N3	-2.64	118.83	121.67
2	2	1498	5MC	O2-C2-N3	-2.64	118.04	122.33
1	1	341	4AC	CM7-C7-N4	-2.63	110.74	115.29
1	1	1222	4AC	C5-C4-N4	-2.63	118.35	122.92
2	2	1488	MA6	C4-N9-C8	2.63	108.58	105.73
1	1	829	4AC	C5-C4-N4	-2.63	118.35	122.92
2	2	1202	5MC	C5-C4-N3	-2.63	118.84	121.67
2	2	751	4AC	C5-C4-N4	-2.62	118.36	122.92
2	2	1498	5MC	C5-C4-N3	-2.62	118.84	121.67
1	1	1873	4AC	C5-C4-N4	-2.62	118.36	122.92
1	1	1938	4AC	N4-C4-N3	2.62	118.25	113.85
1	1	2249	4AC	N4-C4-N3	2.62	118.25	113.85
2	2	875	5MC	C5-C4-N3	-2.62	118.85	121.67
1	1	922	4AC	CM7-C7-N4	-2.61	110.77	115.29
1	1	2678	OMG	C4-C5-N7	-2.61	106.59	110.72
1	1	1055	A2M	C5-N7-C8	2.61	107.21	103.51
1	1	2198	5MC	C5-C4-N3	-2.61	118.86	121.67
1	1	1557	4AC	N4-C4-N3	2.60	118.22	113.85
1	1	2138	OMG	C4-C5-N7	-2.60	106.60	110.72
1	1	829	4AC	N4-C4-N3	2.60	118.22	113.85
2	2	20	OMU	O2-C2-N1	-2.60	119.33	122.79
1	1	1962	4AC	C5-C4-N4	-2.60	118.41	122.92
1	1	2608	4AC	C1'-N1-C2	2.60	124.21	118.42
2	2	1069	OMG	C4-C5-N7	-2.59	106.62	110.72
1	1	2249	4AC	C5-C4-N4	-2.59	118.42	122.92
1	1	2548	4AC	C5-C4-N4	-2.59	118.43	122.92
2	2	1496	5MC	C5-C4-N3	-2.58	118.89	121.67
1	1	1222	4AC	CM7-C7-N4	-2.57	110.85	115.29
2	2	680	OMG	C4-C5-N7	-2.57	106.66	110.72
2	2	1505	5MC	C5-C4-N3	-2.57	118.91	121.67
2	2	471	OMG	C4-C5-N7	-2.56	106.66	110.72
1	1	458	4AC	CM7-C7-N4	-2.56	110.86	115.29
2	2	873	OMG	C4-C5-N7	-2.55	106.68	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	835	4AC	N4-C4-N3	2.55	118.14	113.85
2	2	1479	4AC	C5-C4-N4	-2.54	118.50	122.92
1	1	1873	4AC	N4-C4-N3	2.54	118.12	113.85
1	1	136	4AC	N4-C4-N3	2.54	118.11	113.85
1	1	2495	4AC	N4-C4-N3	2.54	118.11	113.85
1	1	458	4AC	C5-C4-N4	-2.53	118.52	122.92
1	1	2908	4AC	N4-C4-N3	2.53	118.11	113.85
1	1	2966	4AC	N4-C4-N3	2.53	118.10	113.85
1	1	835	4AC	C5-C4-N4	-2.53	118.52	122.92
1	1	533	4AC	CM7-C7-N4	-2.53	110.92	115.29
1	1	641	4AC	C5-C4-N4	-2.53	118.52	122.92
1	1	2865	4AC	N4-C4-N3	2.53	118.10	113.85
1	1	641	4AC	N4-C4-N3	2.53	118.09	113.85
1	1	2062	4AC	C5-C4-N4	-2.52	118.53	122.92
1	1	328	OMG	C4-C5-N7	-2.52	106.73	110.72
1	1	923	OMG	C4-C5-N7	-2.52	106.73	110.72
1	1	789	OMG	C4-C5-N7	-2.52	106.74	110.72
1	1	211	4AC	C5-C4-N4	-2.51	118.55	122.92
1	1	451	4AC	C5-C4-N4	-2.51	118.55	122.92
1	1	2642	4AC	C5-C4-N4	-2.51	118.56	122.92
2	2	657	OMG	C4-C5-N7	-2.50	106.76	110.72
1	1	1885	4AC	N4-C4-N3	2.50	118.05	113.85
1	1	2642	4AC	CM7-C7-N4	-2.50	110.97	115.29
2	2	511	4AC	C5-C4-N4	-2.50	118.57	122.92
2	2	286	4AC	C5-C4-N4	-2.50	118.58	122.92
1	1	1243	4AC	C5-C4-N4	-2.49	118.60	122.92
1	1	2163	5MC	C5-C4-N3	-2.48	119.00	121.67
1	1	1938	4AC	C5-C4-N4	-2.47	118.62	122.92
1	1	1243	4AC	N4-C4-N3	2.47	118.00	113.85
1	1	1885	4AC	C5-C4-N4	-2.47	118.62	122.92
2	2	590	4AC	C5-C4-N4	-2.46	118.64	122.92
2	2	1488	MA6	C6-C5-N7	2.46	137.42	133.28
1	1	1621	4AC	N4-C4-N3	2.46	117.98	113.85
1	1	22	4AC	N4-C4-N3	2.46	117.98	113.85
1	1	2183	5MC	C5-C4-N3	-2.46	119.02	121.67
2	2	1487	MA6	C6-C5-N7	2.46	137.41	133.28
1	1	2865	4AC	C5-C4-N4	-2.44	118.67	122.92
2	2	1025	5MC	C5-C4-N3	-2.44	119.04	121.67
1	1	533	4AC	C5-C4-N4	-2.43	118.70	122.92
2	2	1239	4AC	CM7-C7-N4	-2.43	111.10	115.29
1	1	981	4AC	N4-C4-N3	2.42	117.91	113.85
1	1	981	4AC	C5-C4-N4	-2.41	118.72	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2992	4AC	CM7-C7-N4	2.41	119.47	115.29
1	1	2495	4AC	C5-C4-N4	-2.41	118.73	122.92
2	2	535	5MC	C5-C4-N3	-2.39	119.09	121.67
1	1	1557	4AC	CM7-C7-N4	-2.38	111.17	115.29
2	2	787	OMU	O2-C2-N1	-2.38	119.62	122.79
1	1	1557	4AC	C5-C4-N4	-2.38	118.79	122.92
1	1	1621	4AC	C5-C4-N4	-2.37	118.80	122.92
2	2	1374	5MC	C5-C4-N3	-2.37	119.11	121.67
2	2	1479	4AC	CM7-C7-N4	-2.37	111.19	115.29
1	1	136	4AC	C5-C4-N4	-2.37	118.81	122.92
1	1	314	4AC	N4-C4-N3	2.36	117.82	113.85
1	1	2908	4AC	C5-C4-N4	-2.36	118.82	122.92
1	1	314	4AC	C5-C4-N4	-2.33	118.87	122.92
2	2	875	5MC	O2-C2-N3	-2.33	118.55	122.33
2	2	1487	MA6	N9-C8-N7	-2.33	110.73	113.91
1	1	2162	5MC	O2-C2-N3	-2.32	118.55	122.33
1	1	2733	5MC	O2-C2-N3	-2.31	118.57	122.33
1	1	341	4AC	C5-C4-N4	-2.30	118.93	122.92
1	1	22	4AC	C5-C4-N4	-2.29	118.94	122.92
2	2	851	4AC	N4-C4-N3	2.29	117.70	113.85
2	2	1505	5MC	O2-C2-N3	-2.28	118.62	122.33
1	1	2198	5MC	O2-C2-N3	-2.28	118.63	122.33
1	1	3004	4AC	C5-C4-N4	-2.26	118.99	122.92
2	2	373	A2M	C4-N9-C8	2.25	108.17	105.73
1	1	2784	OMU	O2-C2-N1	-2.24	119.81	122.79
2	2	1469	6MZ	C4-N9-C8	2.23	108.14	105.73
1	1	1055	A2M	C4-N9-C8	2.23	108.14	105.73
1	1	2173	A2M	C6-C5-N7	2.22	136.16	132.02
1	1	229	4AC	C5-C4-N4	-2.22	119.06	122.92
2	2	1467	UR3	C1'-N1-C2	2.22	120.73	116.99
2	2	1469	6MZ	C2-N1-C6	2.21	122.69	115.25
2	2	1202	5MC	O2-C2-N3	-2.21	118.74	122.33
2	2	1488	MA6	N9-C8-N7	-2.19	110.91	113.91
1	1	2173	A2M	C4-N9-C8	2.19	108.10	105.73
1	1	229	4AC	N4-C4-N3	2.19	117.52	113.85
2	2	773	OMC	O2-C2-N3	-2.18	118.78	122.33
1	1	2083	4AC	N4-C4-N3	2.18	117.50	113.85
1	1	2083	4AC	O2-C2-N3	-2.14	118.84	122.33
2	2	693	5MC	O2-C2-N3	-2.14	118.85	122.33
1	1	2608	4AC	CM7-C7-N4	-2.14	111.60	115.29
2	2	373	A2M	C6-C5-N7	2.12	135.97	132.02
2	2	873	OMG	O6-C6-C5	-2.11	121.00	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2937	4AC	CM7-C7-N4	-2.10	111.66	115.29
1	1	2678	OMG	O6-C6-C5	-2.10	121.04	126.60
2	2	934	OMG	O6-C6-C5	-2.09	121.05	126.60
2	2	680	OMG	O6-C6-C5	-2.09	121.05	126.60
2	2	851	4AC	C5-C4-N4	-2.08	119.30	122.92
2	2	471	OMG	O6-C6-C5	-2.08	121.08	126.60
1	1	615	OMC	O2-C2-N3	-2.08	118.95	122.33
2	2	1496	5MC	O2-C2-N3	-2.08	118.95	122.33
1	1	3004	4AC	N4-C4-N3	2.07	117.33	113.85
2	2	467	OMG	O6-C6-C5	-2.06	121.14	126.60
2	2	657	OMG	O6-C6-C5	-2.06	121.14	126.60
1	1	789	OMG	O6-C6-C5	-2.05	121.16	126.60
1	1	328	OMG	O6-C6-C5	-2.04	121.19	126.60
1	1	923	OMG	O6-C6-C5	-2.04	121.19	126.60
1	1	2147	OMG	O6-C6-C5	-2.03	121.21	126.60
1	1	2083	4AC	C5-C4-N4	-2.03	119.39	122.92
1	1	1055	A2M	C6-C5-N7	2.03	135.79	132.02
1	1	2144	OMG	O6-C6-C5	-2.02	121.23	126.60
1	1	458	4AC	O2-C2-N3	-2.02	119.05	122.33
2	2	1177	OMU	O2-C2-N1	-2.02	120.11	122.79
1	1	1948	OMC	O2-C2-N3	-2.02	119.05	122.33
1	1	341	4AC	O2-C2-N3	-2.01	119.06	122.33
2	2	1479	4AC	O2-C2-N3	-2.01	119.07	122.33
1	1	2138	OMG	O6-C6-C5	-2.01	121.28	126.60
1	1	533	4AC	O2-C2-N3	-2.01	119.07	122.33
2	2	1069	OMG	O6-C6-C5	-2.00	121.29	126.60

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2147	OMG	C3'-C4'-C5'-O5'
1	1	2585	4AC	O4'-C1'-N1-C2
1	1	2585	4AC	O4'-C1'-N1-C6
1	1	2608	4AC	O4'-C1'-N1-C2
1	1	2608	4AC	O4'-C1'-N1-C6
1	1	2733	5MC	C2'-C1'-N1-C6
2	2	934	OMG	O4'-C4'-C5'-O5'
2	2	1505	5MC	O4'-C4'-C5'-O5'
1	1	789	OMG	C3'-C4'-C5'-O5'
1	1	2147	OMG	O4'-C4'-C5'-O5'
2	2	934	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	2	1505	5MC	C3'-C4'-C5'-O5'
1	1	789	OMG	O4'-C4'-C5'-O5'
2	2	1488	MA6	O4'-C4'-C5'-O5'
1	1	2733	5MC	C2'-C1'-N1-C2
2	2	20	OMU	C2'-C1'-N1-C6
1	1	1755	4AC	O4'-C4'-C5'-O5'
1	1	1755	4AC	C3'-C4'-C5'-O5'
2	2	20	OMU	O4'-C4'-C5'-O5'
1	1	2992	4AC	O7-C7-N4-C4
1	1	2992	4AC	CM7-C7-N4-C4
1	1	789	OMG	C1'-C2'-O2'-CM2
1	1	923	OMG	C1'-C2'-O2'-CM2
2	2	1498	5MC	O4'-C1'-N1-C6
2	2	1498	5MC	O4'-C1'-N1-C2
2	2	20	OMU	O4'-C1'-N1-C6
1	1	2678	OMG	C3'-C2'-O2'-CM2
1	1	2585	4AC	N3-C4-N4-C7
1	1	2608	4AC	N3-C4-N4-C7
1	1	2937	4AC	N3-C4-N4-C7
2	2	1488	MA6	C3'-C4'-C5'-O5'
1	1	2733	5MC	O4'-C1'-N1-C2
1	1	829	4AC	O4'-C4'-C5'-O5'
1	1	2992	4AC	O4'-C4'-C5'-O5'
2	2	20	OMU	C3'-C4'-C5'-O5'
2	2	1202	5MC	O4'-C4'-C5'-O5'
2	2	1374	5MC	O4'-C4'-C5'-O5'
1	1	2733	5MC	O4'-C1'-N1-C6
1	1	923	OMG	C3'-C2'-O2'-CM2
2	2	1177	OMU	C3'-C2'-O2'-CM2
2	2	20	OMU	C2'-C1'-N1-C2
2	2	20	OMU	O4'-C1'-N1-C2
2	2	938	B8H	O4'-C1'-C5-C4
1	1	789	OMG	C3'-C2'-O2'-CM2
2	2	913	OMG	C3'-C2'-O2'-CM2
2	2	1069	OMG	C1'-C2'-O2'-CM2
2	2	1374	5MC	C3'-C4'-C5'-O5'
2	2	873	OMG	C4'-C5'-O5'-P
1	1	2147	OMG	C3'-C2'-O2'-CM2
2	2	1069	OMG	C3'-C2'-O2'-CM2
2	2	1498	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

84 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	774	OMU	2	0
2	2	394	4AC	2	0
2	2	1376	OMC	1	0
2	2	839	4AC	1	0
2	2	1239	4AC	1	0
2	2	1488	MA6	3	0
2	2	519	OMG	1	0
1	1	2585	4AC	3	0
3	3	32	4AC	2	0
2	2	830	OMU	1	0
2	2	479	4AC	1	0
1	1	2678	OMG	1	0
1	1	2908	4AC	1	0
2	2	373	A2M	2	0
1	1	829	4AC	2	0
2	2	1505	5MC	1	0
1	1	2198	5MC	1	0
1	1	60	4AC	1	0
1	1	1878	4AC	2	0
1	1	211	4AC	1	0
2	2	1177	OMU	1	0
2	2	731	4AC	2	0
1	1	2608	4AC	2	0
1	1	341	4AC	1	0
2	2	1184	4AC	2	0
2	2	1025	5MC	1	0
1	1	1293	4AC	1	0
1	1	1695	4AC	1	0
2	2	319	4AC	1	0
2	2	1479	4AC	1	0
1	1	2136	4AC	1	0
1	1	2718	4AC	2	0
1	1	3004	4AC	1	0
2	2	680	OMG	1	0
1	1	2960	4AC	1	0
2	2	828	4AC	1	0
2	2	626	4AC	3	0
1	1	1662	4AC	1	0
1	1	2027	4AC	1	0
1	1	533	4AC	1	0
2	2	848	4AC	1	0
1	1	1550	4AC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2925	4AC	1	0
1	1	1065	4AC	3	0
2	2	703	4AC	3	0
2	2	934	OMG	1	0
1	1	357	4AC	1	0
1	1	2992	4AC	1	0
1	1	229	4AC	1	0
1	1	1594	4AC	1	0
1	1	922	4AC	1	0
1	1	451	4AC	1	0
2	2	546	4AC	1	0
1	1	2001	4AC	2	0
1	1	1667	4AC	2	0
1	1	2329	4AC	1	0
1	1	1055	A2M	2	0
1	1	1934	4AC	2	0
1	1	91	4AC	1	0
2	2	590	4AC	1	0
1	1	314	4AC	1	0
1	1	2570	4AC	1	0
2	2	511	4AC	2	0
2	2	1487	MA6	2	0
1	1	1617	4AC	2	0
2	2	379	4AC	2	0
1	1	789	OMG	2	0
1	1	2183	5MC	1	0
2	2	467	OMG	1	0
1	1	1867	4AC	1	0
2	2	957	4AC	1	0
2	2	851	4AC	1	0
2	2	1496	5MC	1	0
2	2	64	OMU	1	0
1	1	1765	4AC	1	0
1	1	1755	4AC	2	0
1	1	1780	4AC	3	0
2	2	1380	OMU	2	0
1	1	802	4AC	2	0
1	1	458	4AC	1	0
2	2	1069	OMG	1	0
1	1	2287	4AC	2	0
2	2	636	4AC	2	0
2	2	657	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 257 ligands modelled in this entry, 257 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	107:G	O3'	112:A	P	11.57

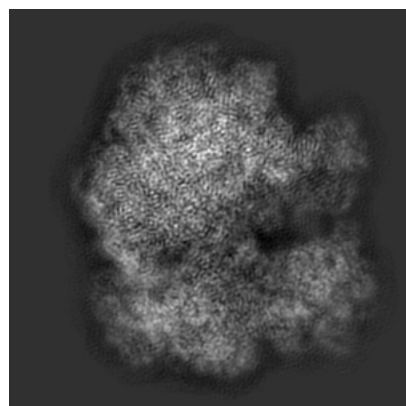
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55137. These allow visual inspection of the internal detail of the map and identification of artifacts.

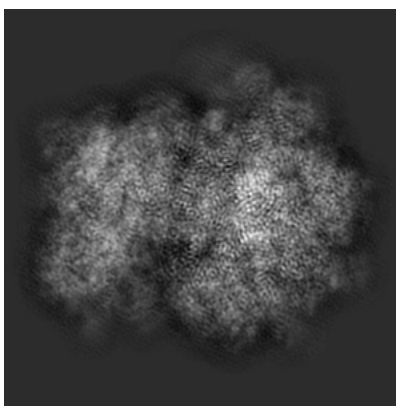
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

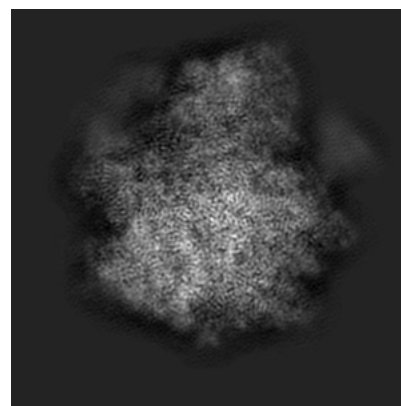
6.1.1 Primary map



X

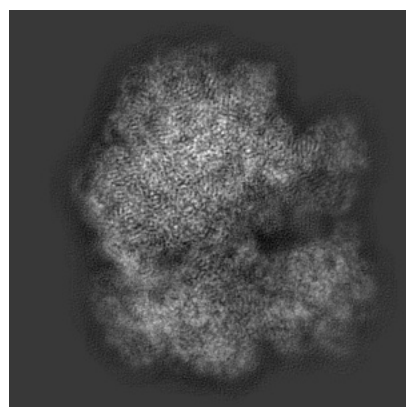


Y

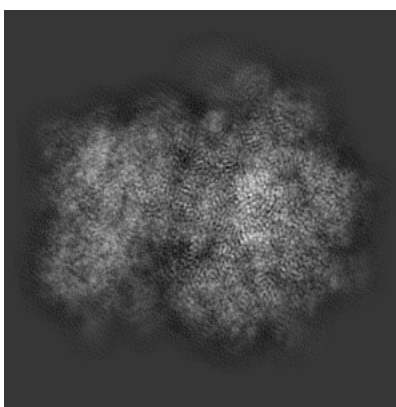


Z

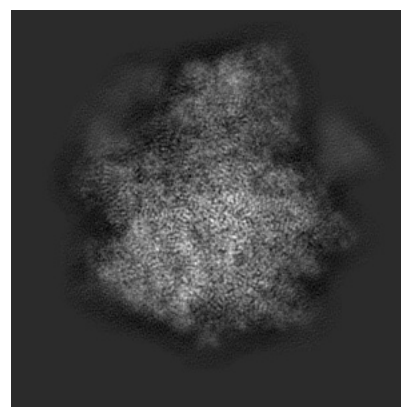
6.1.2 Raw map



X



Y

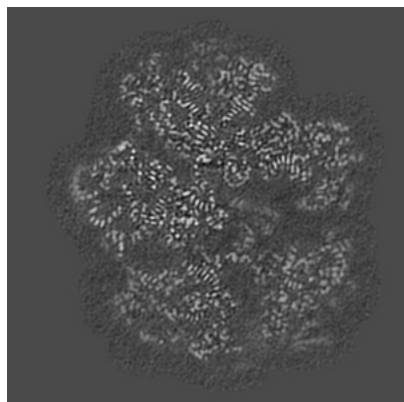


Z

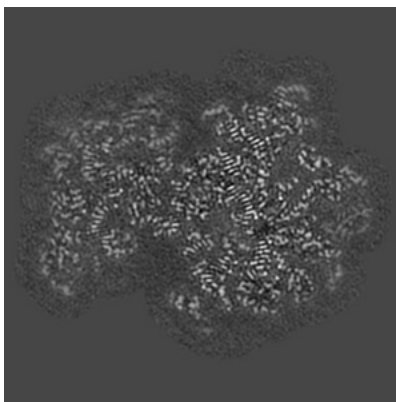
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

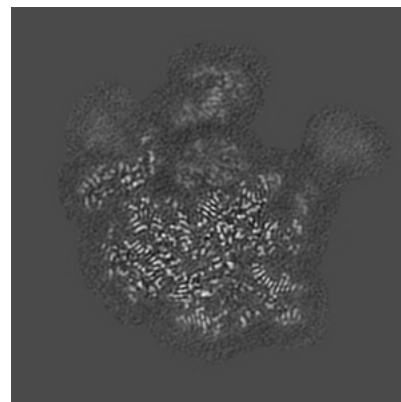
6.2.1 Primary map



X Index: 180

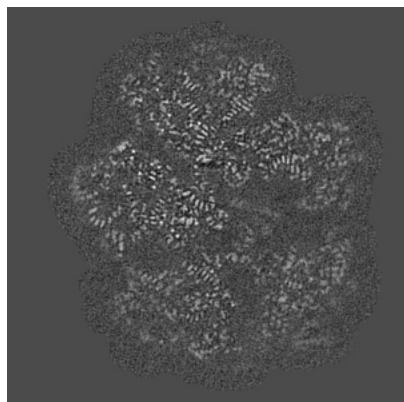


Y Index: 180

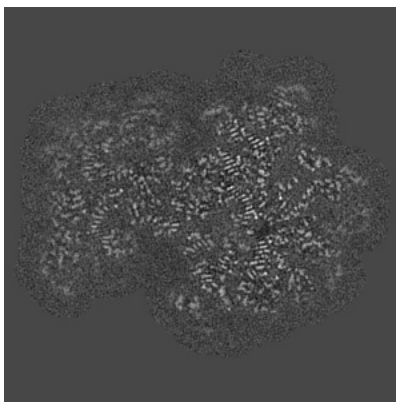


Z Index: 180

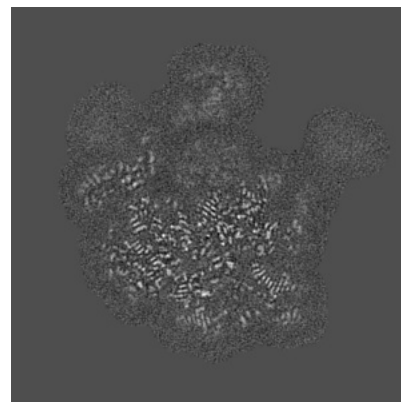
6.2.2 Raw map



X Index: 180



Y Index: 180

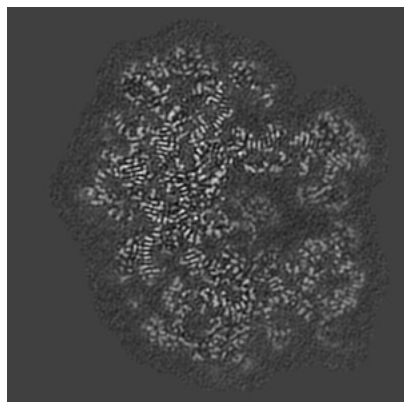


Z Index: 180

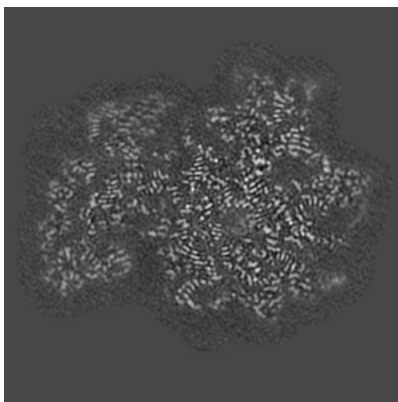
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

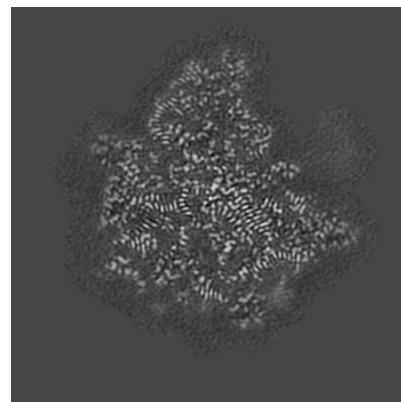
6.3.1 Primary map



X Index: 195

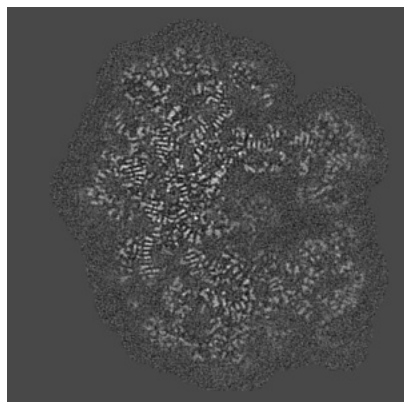


Y Index: 170

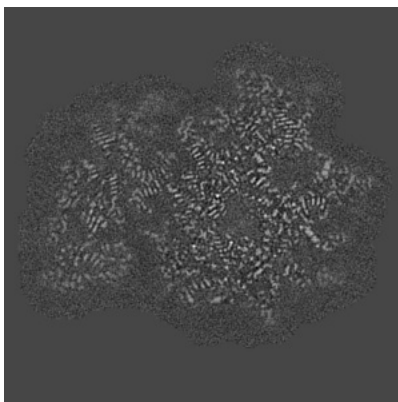


Z Index: 232

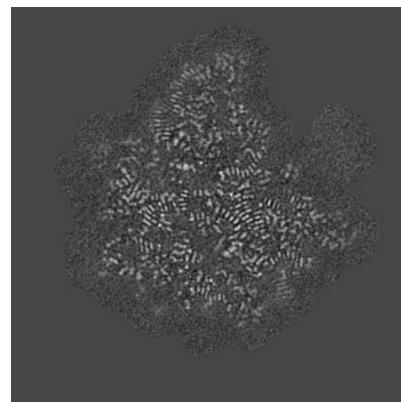
6.3.2 Raw map



X Index: 195



Y Index: 166

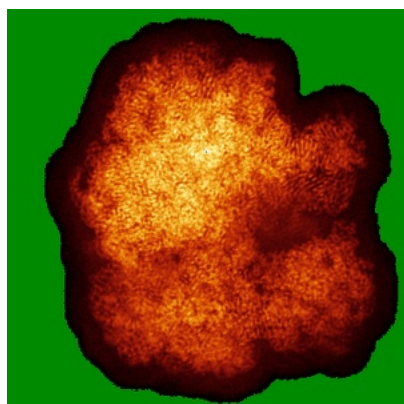


Z Index: 229

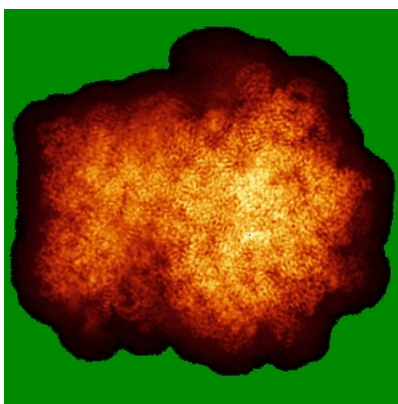
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

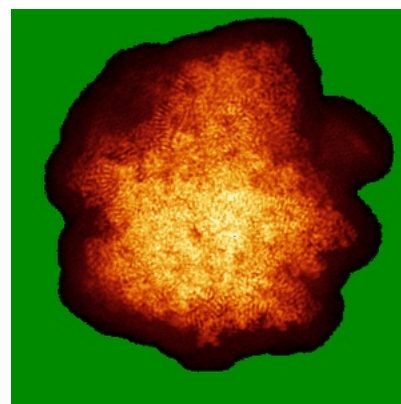
6.4.1 Primary map



X

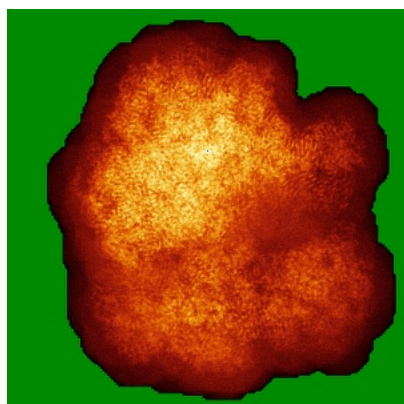


Y

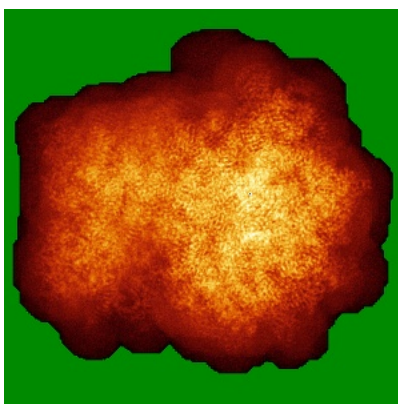


Z

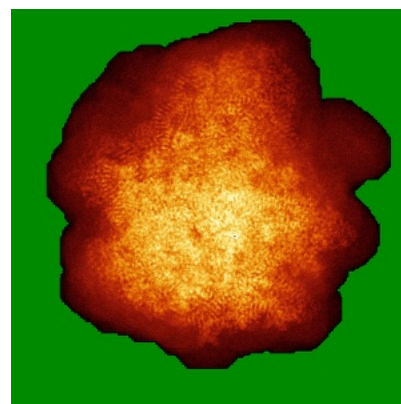
6.4.2 Raw map



X



Y

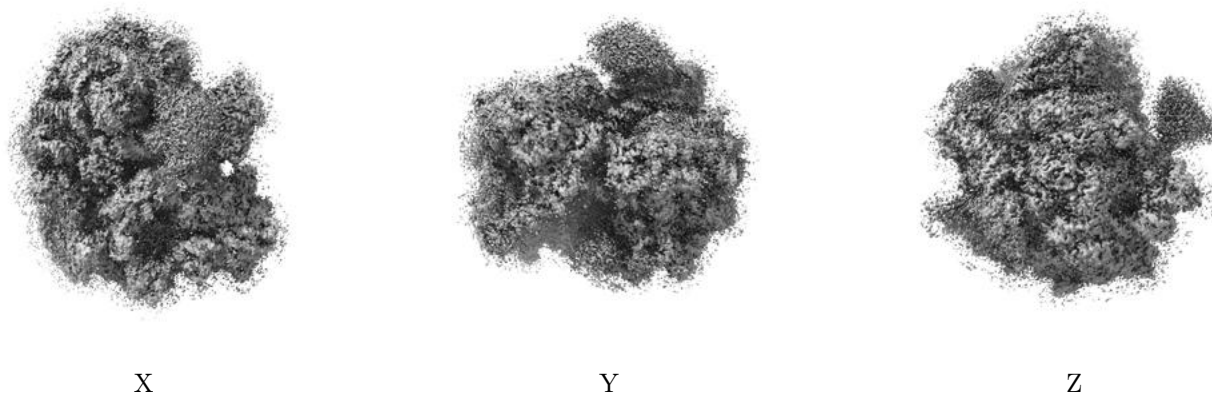


Z

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.

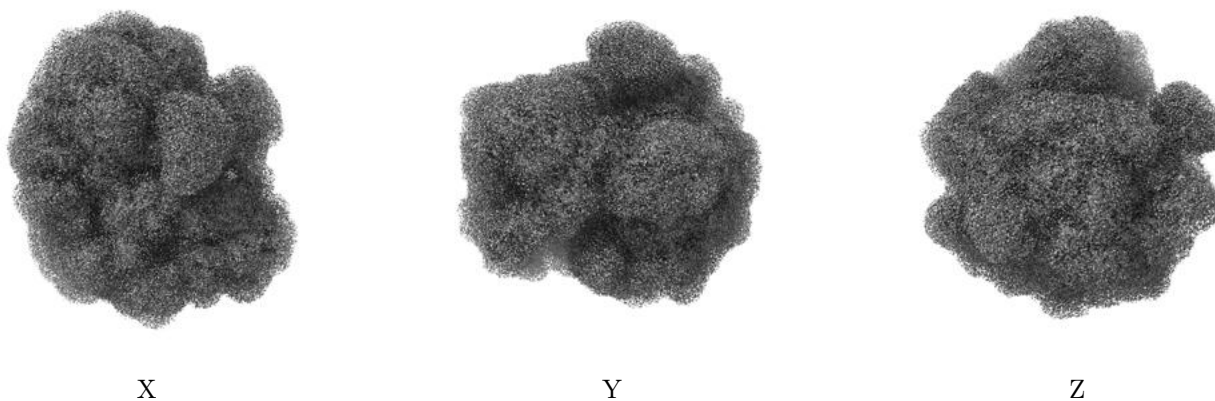
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

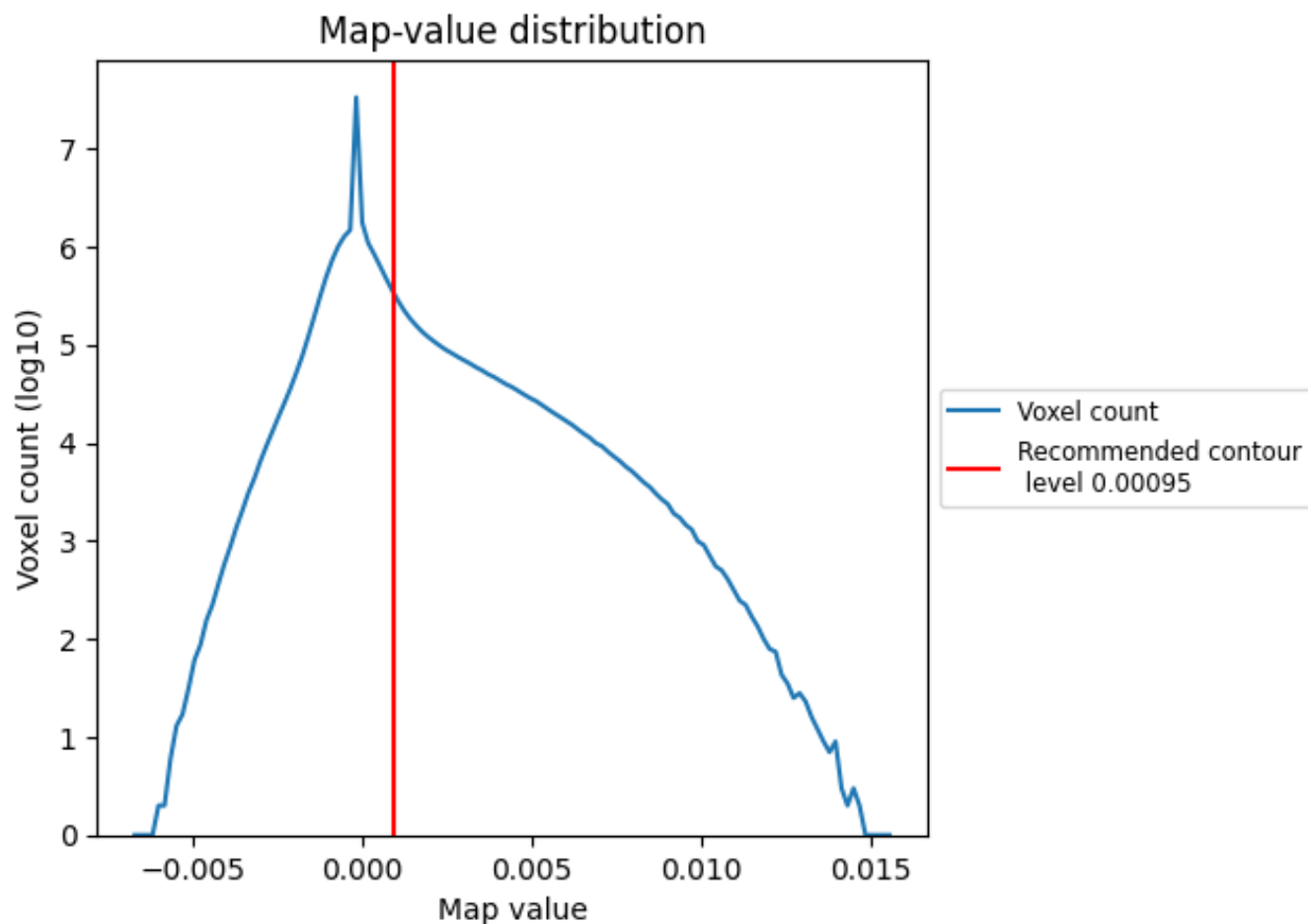
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

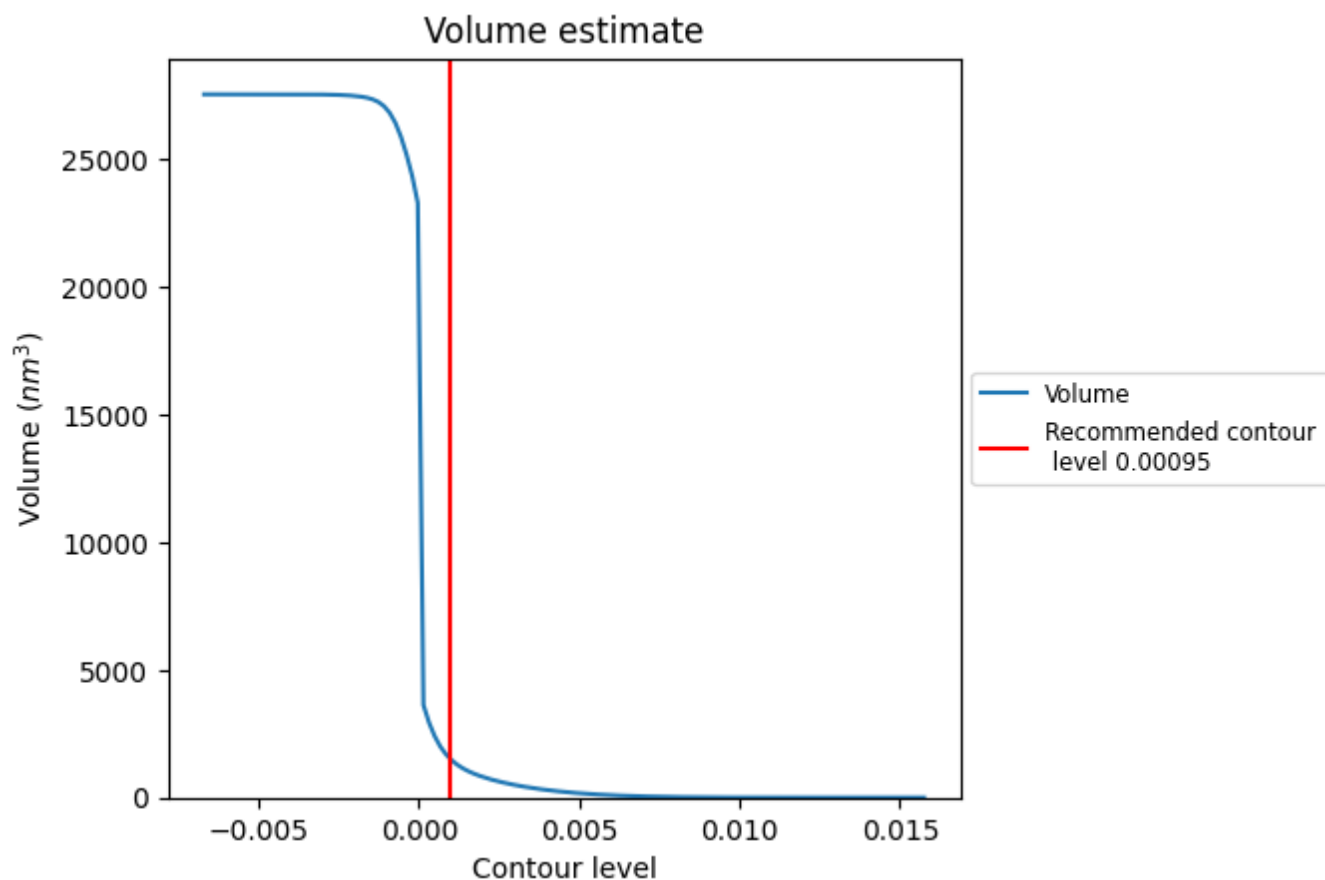
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

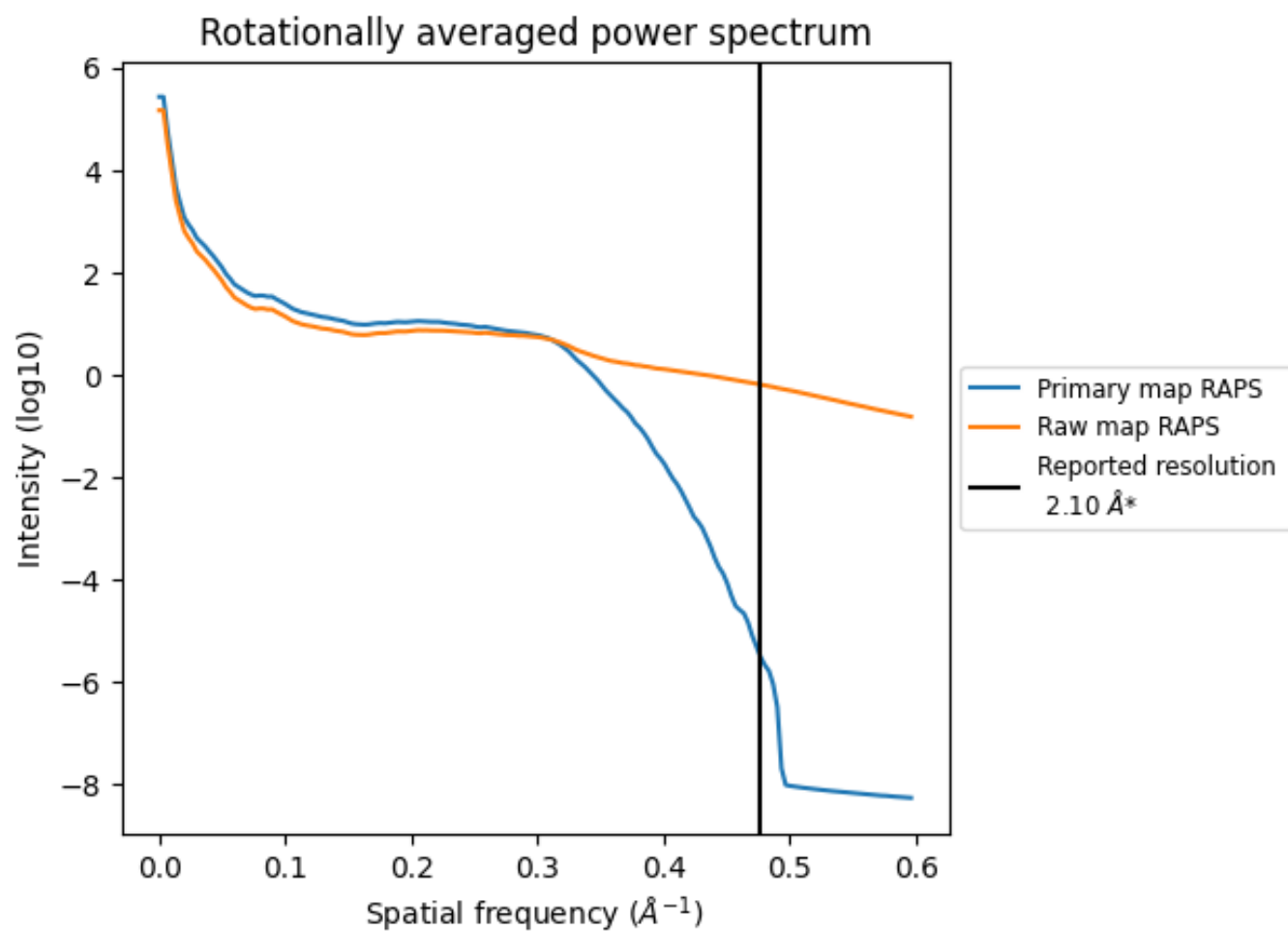
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1560 nm^3 ; this corresponds to an approximate mass of 1409 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 ⓘ

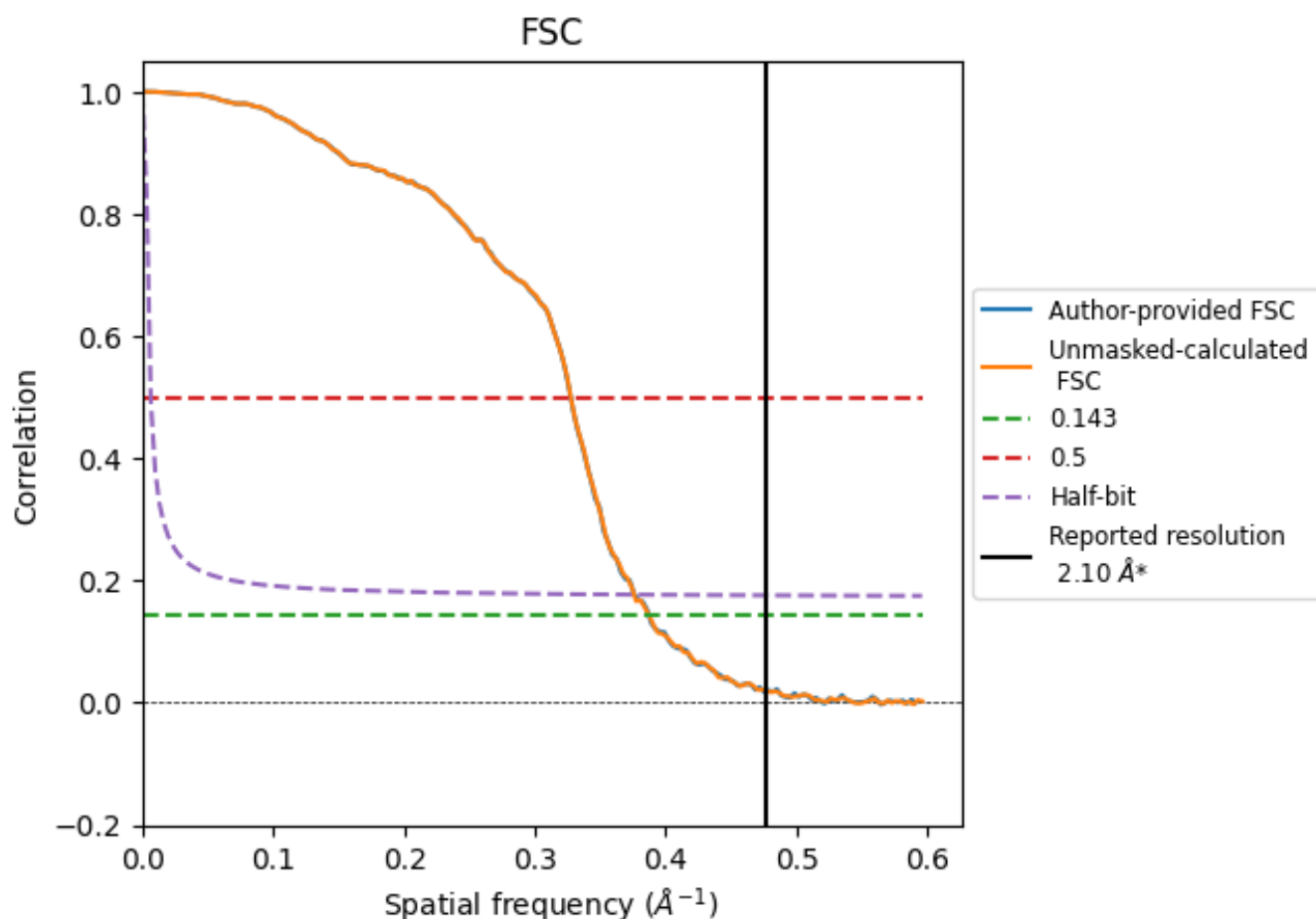


*Reported resolution corresponds to spatial frequency of $0.476 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.58	3.05	2.66
Unmasked-calculated*	2.58	3.05	2.66

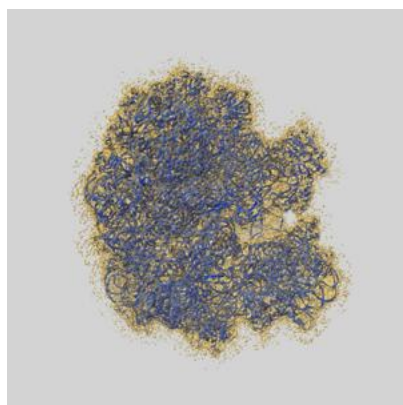
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.58 differs from the reported value 2.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.58 differs from the reported value 2.1 by more than 10 %

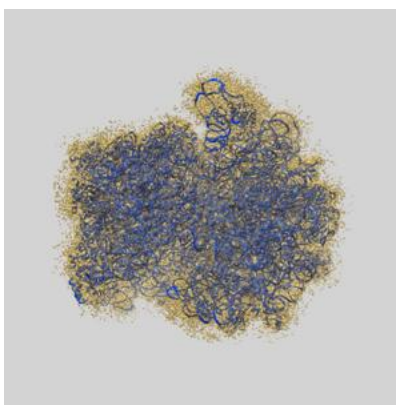
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55137 and PDB model 9SRC. Per-residue inclusion information can be found in section [3](#) on page [17](#).

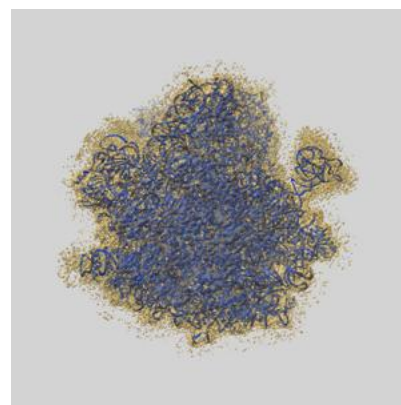
9.1 Map-model overlay [i](#)



X



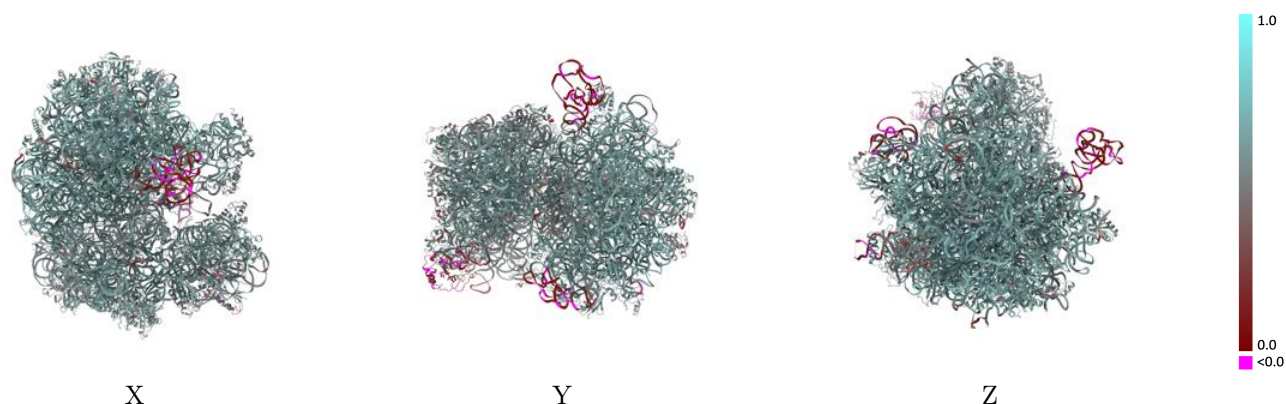
Y



Z

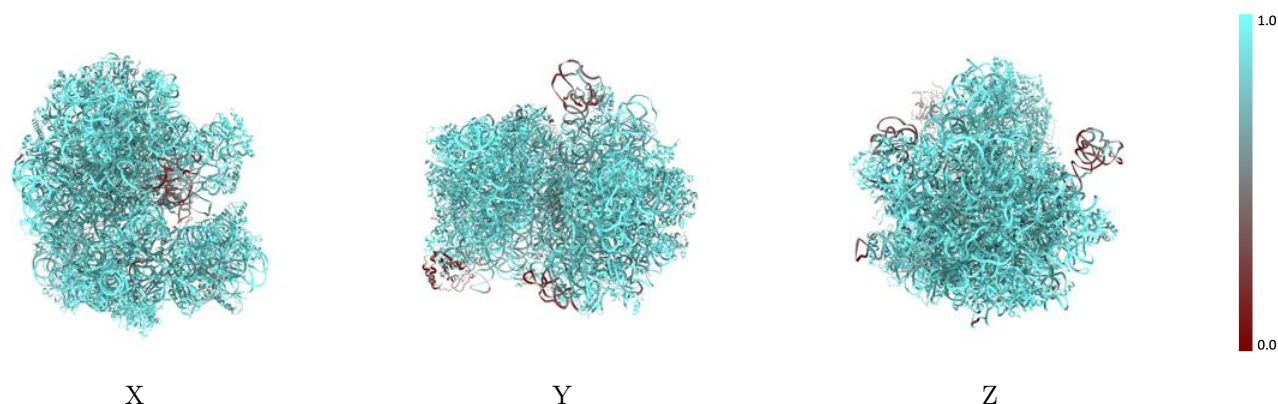
The images above show the 3D surface view of the map at the recommended contour level 0.00095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



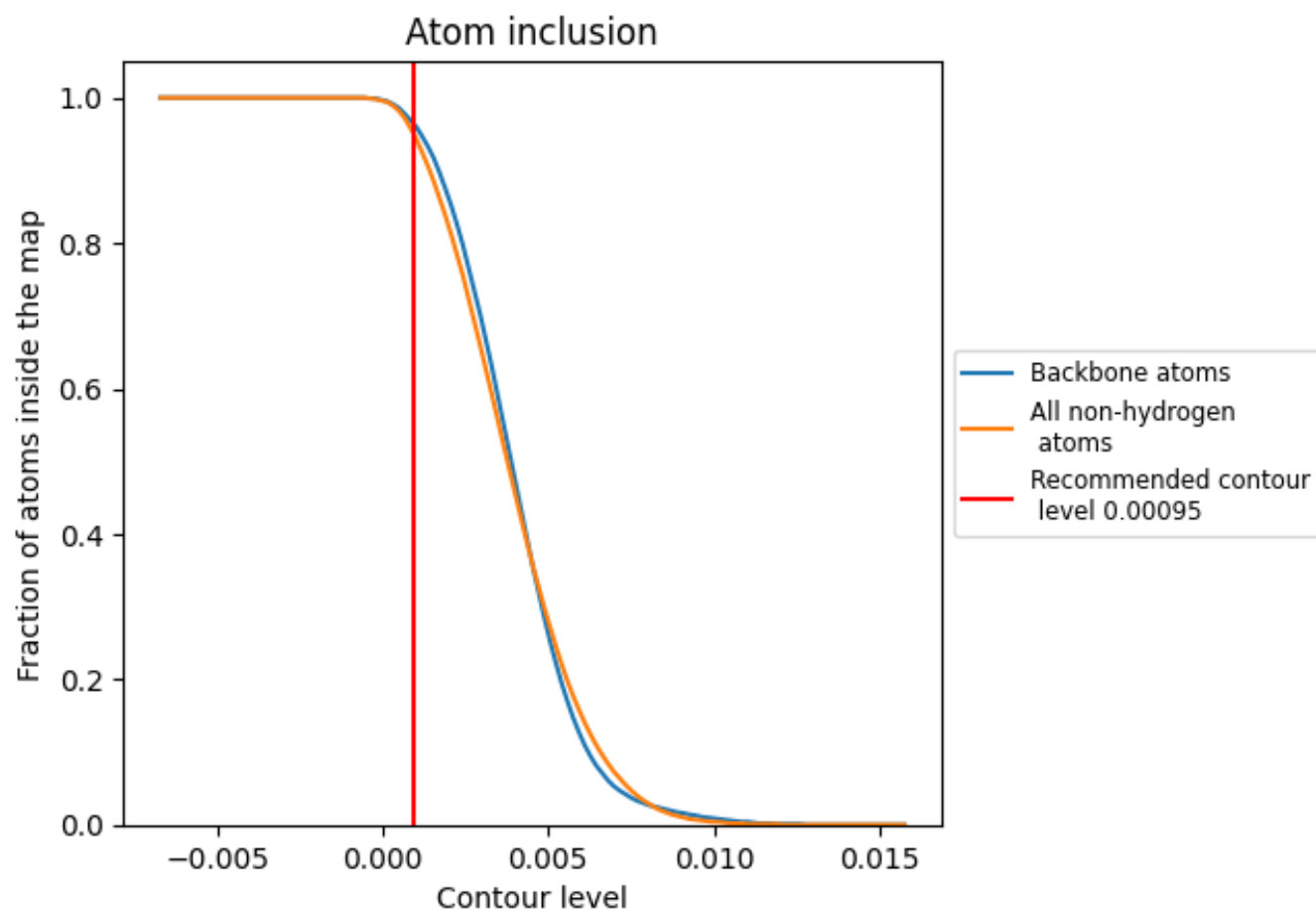
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.00095).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.00095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.5870
1	 0.9580	 0.5980
2	 0.9790	 0.5850
3	 0.9940	 0.5990
A0	 0.9750	 0.6480
A3	 0.3140	 0.1390
AA	 0.8690	 0.5040
AB	 0.9580	 0.5550
AC	 0.9640	 0.5770
AD	 0.9630	 0.5960
AE	 0.9590	 0.5610
AF	 0.9740	 0.6070
AG	 0.8960	 0.4970
AH	 0.9450	 0.5670
AI	 0.9710	 0.6070
AJ	 0.9490	 0.5800
AK	 0.9640	 0.5690
AL	 0.8580	 0.4930
AM	 0.9250	 0.5500
AN	 0.9460	 0.6000
AO	 0.9220	 0.5370
AP	 0.9170	 0.5590
AQ	 0.9300	 0.5570
AR	 0.9490	 0.5900
AS	 0.9370	 0.5400
AT	 0.8830	 0.5220
AU	 0.9590	 0.5680
AV	 0.9200	 0.5220
AW	 0.9060	 0.4980
AX	 0.9130	 0.5300
AY	 0.1810	 0.1380
AZ	 0.8780	 0.5100
B4	 0.7540	 0.4060
B5	 0.9700	 0.5870
B6	 0.7810	 0.5550



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Chain	Atom inclusion	Q-score
BB	 0.9780	 0.6470
BC	 0.9760	 0.6390
BD	 0.9830	 0.6350
BE	 0.9270	 0.5470
BF	 0.9410	 0.6010
BG	 0.9540	 0.5930
BI	 0.9740	 0.6360
BJ	 0.9780	 0.6390
BK	 0.9490	 0.5650
BL	 0.9660	 0.6090
BM	 0.9920	 0.6520
BN	 0.9510	 0.6160
BO	 0.9690	 0.5910
BP	 0.9900	 0.6320
BQ	 0.9700	 0.6270
BR	 0.9820	 0.6440
BS	 0.9780	 0.6380
BT	 0.9800	 0.6190
BU	 0.9660	 0.6150
BV	 0.9760	 0.6320
BW	 0.8950	 0.5720
BY	 0.9810	 0.6350
BZ	 0.9200	 0.5660
Ba	 0.9590	 0.6060
Bb	 0.9820	 0.6420
Bc	 0.9810	 0.6390
Bd	 0.9700	 0.6260
Be	 0.9980	 0.6470
Bf	 0.9980	 0.6410
Bg	 0.9730	 0.6230
Bi	 0.9560	 0.6400
Bj	 0.9720	 0.6320
Bk	 0.9610	 0.6050
Bl	 0.9280	 0.5970
H	 0.7590	 0.5310