



Full wwPDB EM Validation Report ⓘ

Jul 13, 2026 – 12:25 pm BST

PDB ID : 9SRE / pdb_00009sre
EMDB ID : EMD-55139
Title : Cryo-EM structure of P. abyssi 70S ribosome in complex with hibernation factor HibA (PTC conformation with E-site tRNA)
Authors : Madru, C.M.; Bourgeois, G.B.; Mechulam, Y.M.; Schmitt, E.S.
Deposited on : 2025-09-24
Resolution : 2.11 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

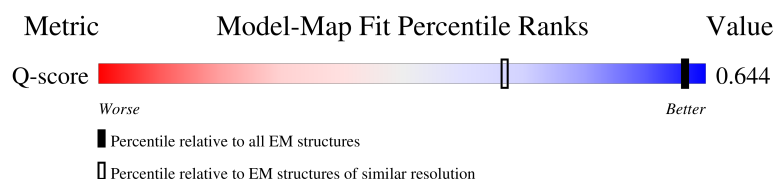
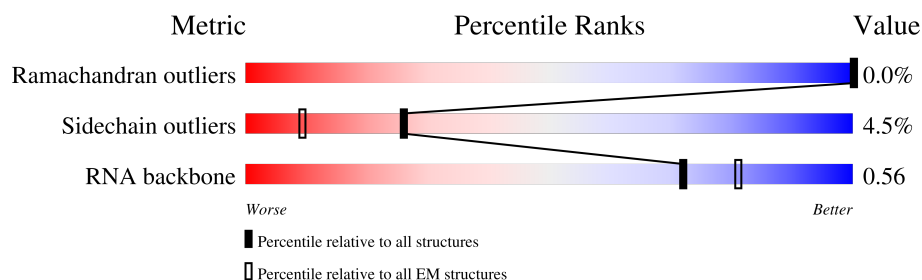
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.11 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.



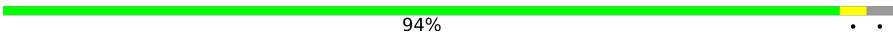
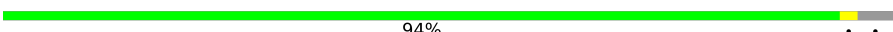
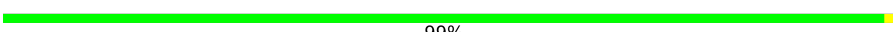
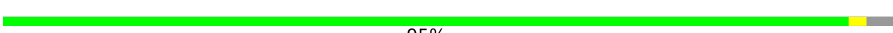
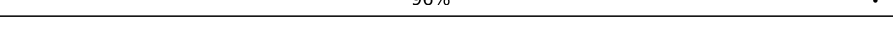
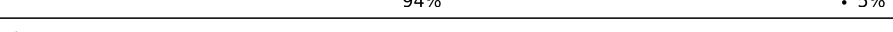
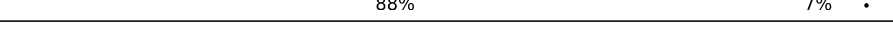
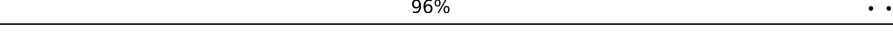
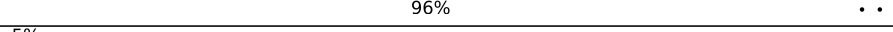
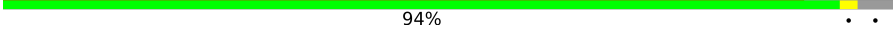
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2361 (1.64 - 2.61)

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	3	128	
2	4	77	
3	H	392	
4	AA	199	

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Mol	Chain	Length	Quality of chain
5	AB	202	
6	AC	63	
7	AD	180	
8	AE	243	
9	AF	236	
10	AG	125	
11	AH	215	
12	AI	130	
13	AJ	127	
14	AK	135	
15	AL	102	
16	AM	137	
17	AN	147	
18	AP	56	
19	AQ	158	
20	AR	113	
21	AS	67	
22	AU	150	
23	AV	99	
23	B6	99	
24	AW	65	
25	AX	71	
26	AY	51	
27	AZ	210	
28	A0	37	

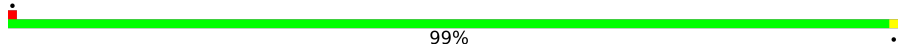
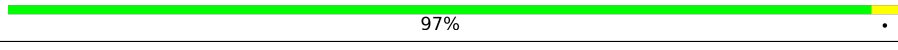
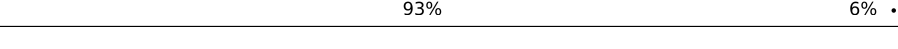
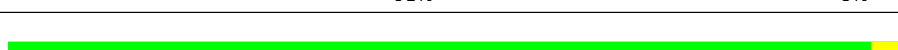
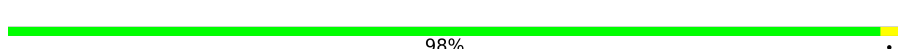
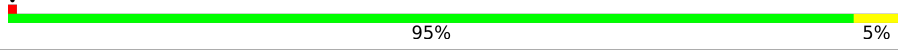
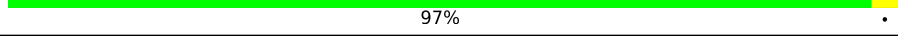
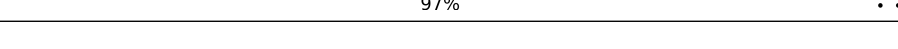
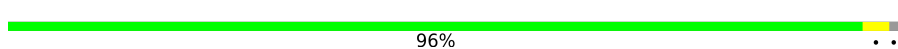
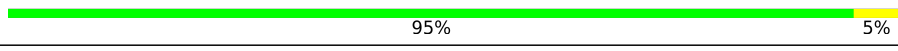
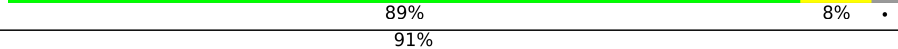
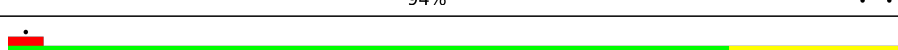
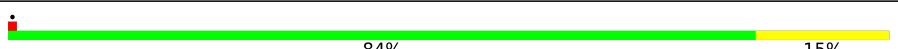
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Mol	Chain	Length	Quality of chain
29	A3	123	97%
29	B4	123	25% 94% 5%
29	BG	123	91% 8%
30	AT	132	5% 94% 5%
31	AO	148	91% 7%
32	BB	239	96%
33	BY	155	97%
34	BO	203	91% 7%
35	BC	361	98%
36	B5	82	94% 5%
36	BK	82	91% 6%
37	BL	147	93% 7%
38	Bf	51	94%
39	BU	121	96%
40	Bb	130	98%
41	Be	62	97%
42	BE	188	87% 12%
43	Ba	94	98%
44	BT	86	99%
45	BW	68	97%
46	Bi	83	95%
47	BI	142	99%
48	BR	97	97%
49	BQ	151	98%
50	BV	67	91% 6%

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Mol	Chain	Length	Quality of chain
51	Bj	94	 99%
52	BD	255	 97%
53	BF	184	 93% 6%
54	BZ	99	 91% 8%
55	BP	120	 97%
56	BM	194	 98%
57	BS	155	 95% 5%
58	Bd	91	 97%
59	BN	181	 97%
60	Bg	51	 94% 6%
61	Bc	87	 98%
62	BJ	141	 96%
63	Bl	77	 95% 5%
64	Bk	65	 89% 8%
65	BA	219	 91% 9%
66	1	3018	 81% 19%
67	2	1496	 84% 15%

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 198152 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 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	126	Total	C	N	O	P	0	0
			2703	1203	498	876	126		

- Molecule 2 is a RNA chain called tRNAMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	4	77	Total	C	N	O	P	S	0	0
			1644	734	296	536	77	1		

- Molecule 3 is a protein called Dehydrogenase.

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

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

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

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called Zn-ribbon RNA-binding protein involved in translation.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S4e.

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

- Molecule 9 is a protein called 30S ribosomal protein S5.

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

- Molecule 10 is a protein called 30S ribosomal protein S6e.

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

- Molecule 11 is a protein called 30S ribosomal protein S7.

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

- Molecule 12 is a protein called 30S ribosomal protein S8.

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

- Molecule 13 is a protein called 30S ribosomal protein S8e.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

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

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 19 is a protein called 30S ribosomal protein S15.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S17e.

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

- Molecule 22 is a protein called 30S ribosomal protein S19e.

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

- Molecule 23 is a protein called 30S ribosomal protein S24e.

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

- Molecule 24 is a protein called 30S ribosomal protein S27e.

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

- Molecule 25 is a protein called 30S ribosomal protein S28e.

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

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

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

- Molecule 27 is a protein called 30S ribosomal protein S3.

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

- Molecule 28 is a protein called Small ribosomal subunit protein eS32.

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

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S13.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 36 is a protein called Large ribosomal subunit protein eL14.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 38 is a protein called Large ribosomal subunit protein eL39.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL32.

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL31.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 46 is a protein called Large ribosomal subunit protein eL43.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 48 is a protein called Large ribosomal subunit protein eL21.

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

- Molecule 49 is a protein called Large ribosomal subunit protein eL19.

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

- Molecule 50 is a protein called Large ribosomal subunit protein eL24.

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

- Molecule 51 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 54 is a protein called Large ribosomal subunit protein eL30.

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

- Molecule 55 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 56 is a protein called Large ribosomal subunit protein eL15.

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

- Molecule 57 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 58 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 59 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 60 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 61 is a protein called Large ribosomal subunit protein eL33.

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

- Molecule 62 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 63 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 64 is a protein called C2H2-type domain-containing protein.

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

- Molecule 65 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BA	215	Total	C	N	O	S	0	0
			1675	1065	301	304	5		

- Molecule 66 is a RNA chain called rRNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	1	3018	Total	C	N	O	P	0	0
			65181	29055	12094	21014	3018		

- Molecule 67 is a RNA chain called rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	2	1496	Total	C	N	O	P	0	0
			32291	14408	5957	10430	1496		

- Molecule 68 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
68	3	1	Total	Mg	0
			1	1	
68	AK	1	Total	Mg	0
			1	1	
68	AN	1	Total	Mg	0
			1	1	
68	BB	2	Total	Mg	0
			2	2	
68	Bb	1	Total	Mg	0
			1	1	
68	BD	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
68	BM	1	Total 1	Mg 1	0
68	BS	1	Total 1	Mg 1	0
68	1	166	Total 166	Mg 166	0
68	2	69	Total 69	Mg 69	0

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 70 is water.

Mol	Chain	Residues	Atoms		AltConf
70	3	424	Total 424	O 424	0

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Mol	Chain	Residues	Atoms		AltConf
70	4	4	Total 4	O 4	0
70	H	474	Total 474	O 474	0
70	AA	288	Total 288	O 288	0
70	AB	295	Total 295	O 295	0
70	AC	61	Total 61	O 61	0
70	AD	190	Total 190	O 190	0
70	AE	207	Total 207	O 207	0
70	AF	194	Total 194	O 194	0
70	AG	227	Total 227	O 227	0
70	AH	249	Total 249	O 249	0
70	AI	109	Total 109	O 109	0
70	AJ	125	Total 125	O 125	0
70	AK	113	Total 113	O 113	0
70	AL	136	Total 136	O 136	0
70	AM	88	Total 88	O 88	0
70	AN	142	Total 142	O 142	0
70	AP	61	Total 61	O 61	0
70	AQ	162	Total 162	O 162	0
70	AR	67	Total 67	O 67	0
70	AU	172	Total 172	O 172	0
70	AV	165	Total 165	O 165	0

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Mol	Chain	Residues	Atoms		AltConf
70	AW	85	Total 85	O 85	0
70	AX	82	Total 82	O 82	0
70	AZ	4	Total 4	O 4	0
70	A0	42	Total 42	O 42	0
70	AT	230	Total 230	O 230	0
70	AO	1	Total 1	O 1	0
70	BB	170	Total 170	O 170	0
70	BY	115	Total 115	O 115	0
70	BO	204	Total 204	O 204	0
70	BC	238	Total 238	O 238	0
70	B5	77	Total 77	O 77	0
70	BL	101	Total 101	O 101	0
70	Bf	36	Total 36	O 36	0
70	BU	95	Total 95	O 95	0
70	Bb	120	Total 120	O 120	0
70	Be	56	Total 56	O 56	0
70	BE	6	Total 6	O 6	0
70	Ba	77	Total 77	O 77	0
70	BT	67	Total 67	O 67	0
70	BW	67	Total 67	O 67	0
70	Bi	62	Total 62	O 62	0

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Mol	Chain	Residues	Atoms		AltConf
70	BI	93	Total 93	O 93	0
70	BR	78	Total 78	O 78	0
70	BK	121	Total 121	O 121	0
70	BQ	119	Total 119	O 119	0
70	BV	47	Total 47	O 47	0
70	Bj	85	Total 85	O 85	0
70	BG	231	Total 231	O 231	0
70	BD	197	Total 197	O 197	0
70	BF	224	Total 224	O 224	0
70	BZ	102	Total 102	O 102	0
70	B6	214	Total 214	O 214	0
70	BP	99	Total 99	O 99	0
70	BM	138	Total 138	O 138	0
70	BS	119	Total 119	O 119	0
70	Bd	69	Total 69	O 69	0
70	BN	133	Total 133	O 133	0
70	Bg	44	Total 44	O 44	0
70	Bc	61	Total 61	O 61	0
70	BJ	84	Total 84	O 84	0
70	Bl	107	Total 107	O 107	0
70	B4	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
70	Bk	47	Total 47	O 47	0
70	1	10842	Total 10842	O 10842	0
70	2	5225	Total 5225	O 5225	0

3 Residue-property plots [i](#)

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

- Molecule 1: rRNA 5S

Chain 3: 

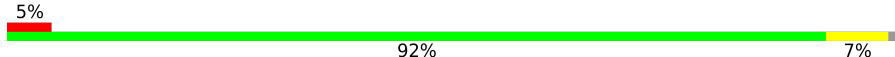


- Molecule 2: tRNA^{Met}

Chain 4: 



- Molecule 3: Dehydrogenase

Chain H: 

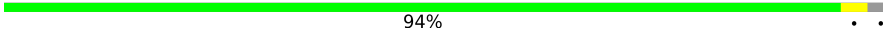


- Molecule 4: 30S ribosomal protein S3Ae

Chain AA: 

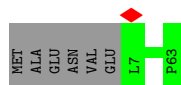


- Molecule 5: 30S ribosomal protein S2

Chain AB: 



- Molecule 6: Zn-ribbon RNA-binding protein involved in translation



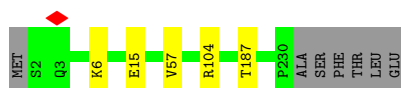
- Molecule 7: 30S ribosomal protein S4



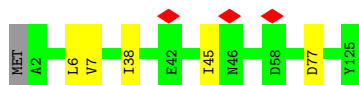
- Molecule 8: 30S ribosomal protein S4e



- Molecule 9: 30S ribosomal protein S5



- Molecule 10: 30S ribosomal protein S6e



- Molecule 11: 30S ribosomal protein S7



- Molecule 12: 30S ribosomal protein S8





- Molecule 13: 30S ribosomal protein S8e

Chain AJ: 95%



- Molecule 14: 30S ribosomal protein S9

Chain AK: 95%



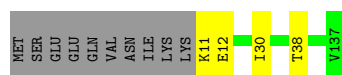
- Molecule 15: 30S ribosomal protein S10

Chain AL: 24% 90% 8%



- Molecule 16: 30S ribosomal protein S11

Chain AM: 90% 7%



- Molecule 17: 30S ribosomal protein S12

Chain AN: 97%



- Molecule 18: 30S ribosomal protein S14 type Z

Chain AP: 89% 9%



- Molecule 19: 30S ribosomal protein S15

Chain AQ: 96%



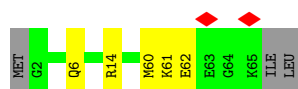
- Molecule 20: 30S ribosomal protein S17

Chain AR: 94% 5%



- Molecule 21: 30S ribosomal protein S17e

Chain AS: 88% 7% 5%



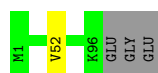
- Molecule 22: 30S ribosomal protein S19e

Chain AU: 96% 4%



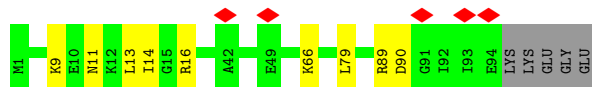
- Molecule 23: 30S ribosomal protein S24e

Chain AV: 96% 4%



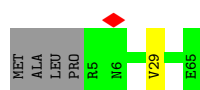
- Molecule 23: 30S ribosomal protein S24e

Chain B6: 5% 86% 9% 5%



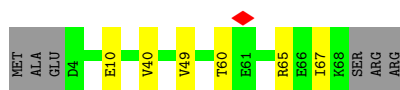
- Molecule 24: 30S ribosomal protein S27e

Chain AW: 92% 6% 2%

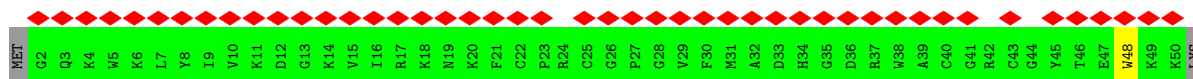


- Molecule 25: 30S ribosomal protein S28e

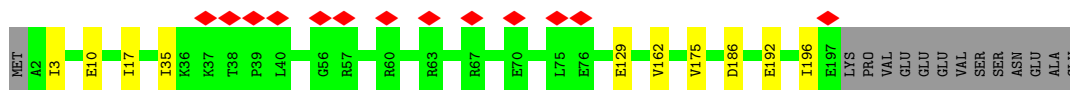
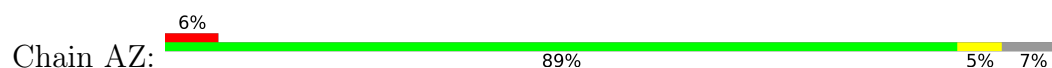
Chain AX: 83% 8% 8%



- Molecule 26: 30S ribosomal protein S27ae



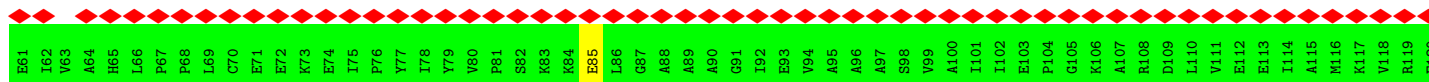
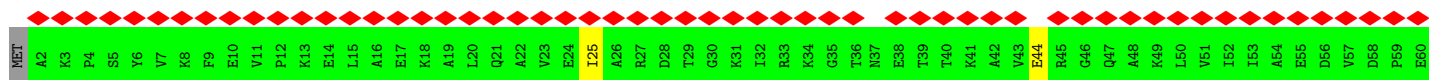
- Molecule 27: 30S ribosomal protein S3



- Molecule 28: Small ribosomal subunit protein eS32



- Molecule 29: 50S ribosomal protein L7Ae

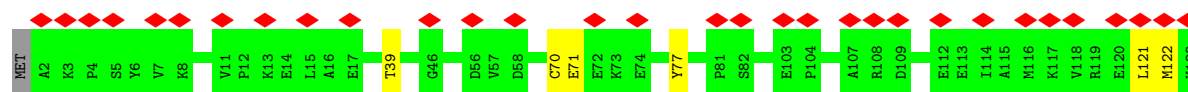


- Molecule 29: 50S ribosomal protein L7Ae



- Molecule 29: 50S ribosomal protein L7Ae





- Molecule 30: 30S ribosomal protein S19



- Molecule 31: 30S ribosomal protein S13



- Molecule 32: Large ribosomal subunit protein uL2



- Molecule 33: Large ribosomal subunit protein uL30



- Molecule 34: Large ribosomal subunit protein uL18



- Molecule 35: Large ribosomal subunit protein uL3



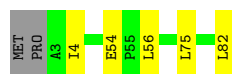
- Molecule 36: Large ribosomal subunit protein eL14

Chain B5:  94% 5%



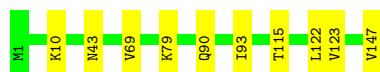
- Molecule 36: Large ribosomal subunit protein eL14

Chain BK:  91% 6%



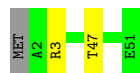
- Molecule 37: Large ribosomal subunit protein uL15

Chain BL:  93% 7%

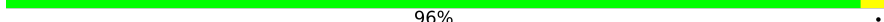


- Molecule 38: Large ribosomal subunit protein eL39

Chain Bf:  94%

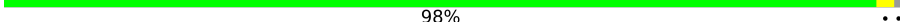


- Molecule 39: Large ribosomal subunit protein uL24

Chain BU:  96%

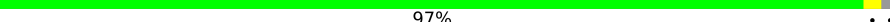


- Molecule 40: Large ribosomal subunit protein eL32

Chain Bb:  98%



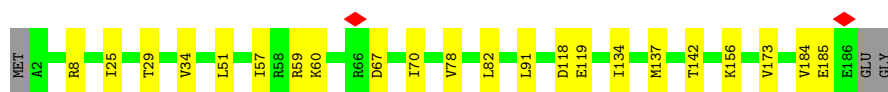
- Molecule 41: Large ribosomal subunit protein eL37

Chain Be:  97%

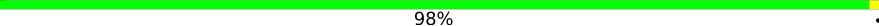


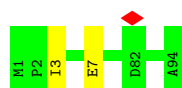
- Molecule 42: Large ribosomal subunit protein uL5

Chain BE:  87% 12%

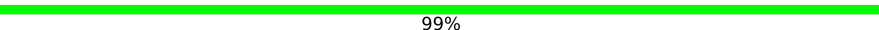


- Molecule 43: Large ribosomal subunit protein eL31

Chain Ba:  98%

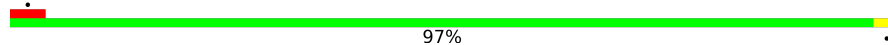


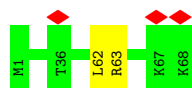
- Molecule 44: Large ribosomal subunit protein uL23

Chain BT:  99%

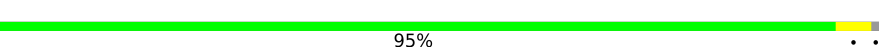


- Molecule 45: Large ribosomal subunit protein uL29

Chain BW:  97%

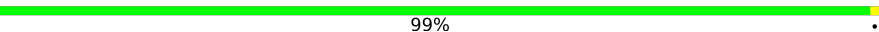


- Molecule 46: Large ribosomal subunit protein eL43

Chain Bi:  95%

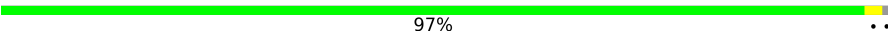


- Molecule 47: Large ribosomal subunit protein uL13

Chain BI:  99%

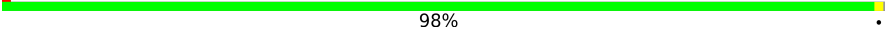


- Molecule 48: Large ribosomal subunit protein eL21

Chain BR:  97%



- Molecule 49: Large ribosomal subunit protein eL19

Chain BQ:  98% ..



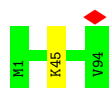
- Molecule 50: Large ribosomal subunit protein eL24

Chain BV:  91% • 6%

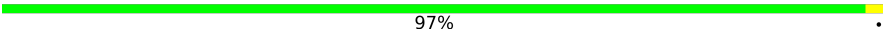


- Molecule 51: Large ribosomal subunit protein eL42

Chain Bj:  99% .

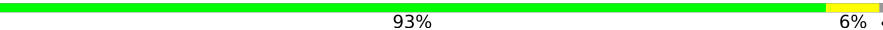


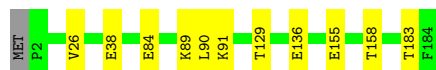
- Molecule 52: Large ribosomal subunit protein uL4

Chain BD:  97% .



- Molecule 53: Large ribosomal subunit protein uL6

Chain BF:  93% • 6% .

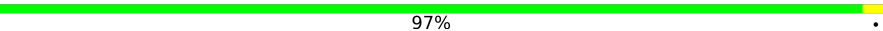


- Molecule 54: Large ribosomal subunit protein eL30

Chain BZ:  91% • 8% .

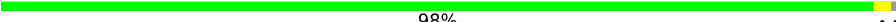


- Molecule 55: Large ribosomal subunit protein eL18

Chain BP:  97% .



- Molecule 56: Large ribosomal subunit protein eL15

Chain BM:  98% ..

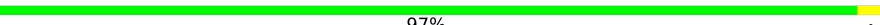


- Molecule 57: Large ribosomal subunit protein uL22

Chain BS:  95% 5% .

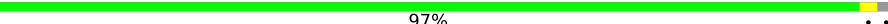


- Molecule 58: Large ribosomal subunit protein eL34

Chain Bd:  97% .



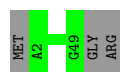
- Molecule 59: Large ribosomal subunit protein uL16

Chain BN:  97% ..

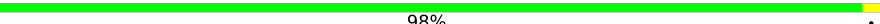


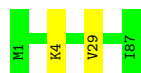
- Molecule 60: Large ribosomal subunit protein eL40

Chain Bg:  94% 6%



- Molecule 61: Large ribosomal subunit protein eL33

Chain Bc:  98% .

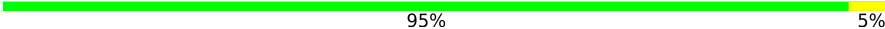


- Molecule 62: Large ribosomal subunit protein uL14

Chain BJ:  96% ..



- Molecule 63: Large ribosomal subunit protein eL20

Chain Bl:  95% 5%



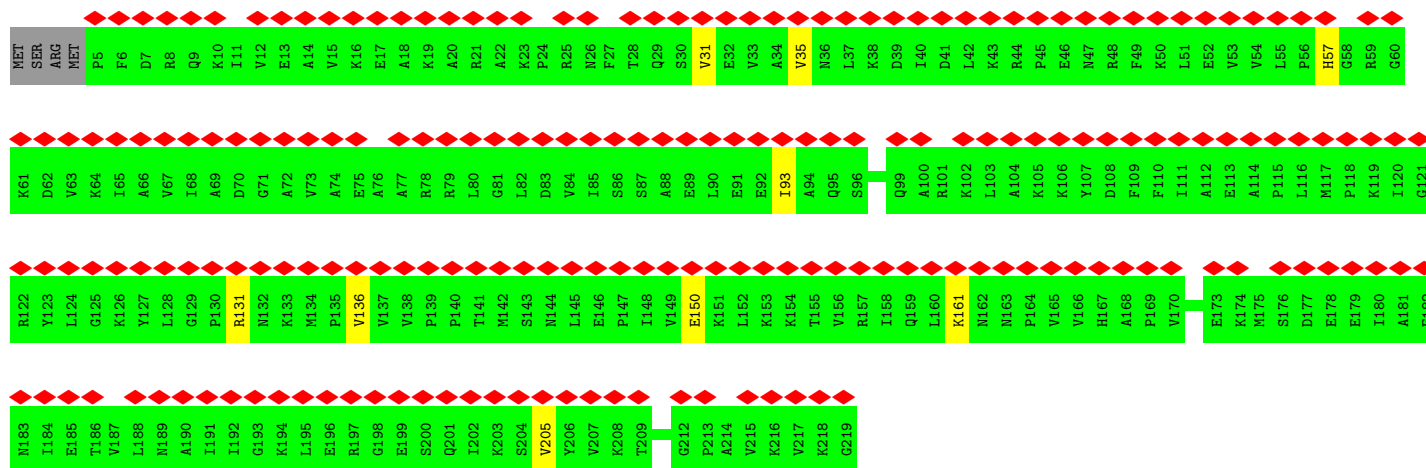
- Molecule 64: C2H2-type domain-containing protein

Chain Bk:  89% 8%



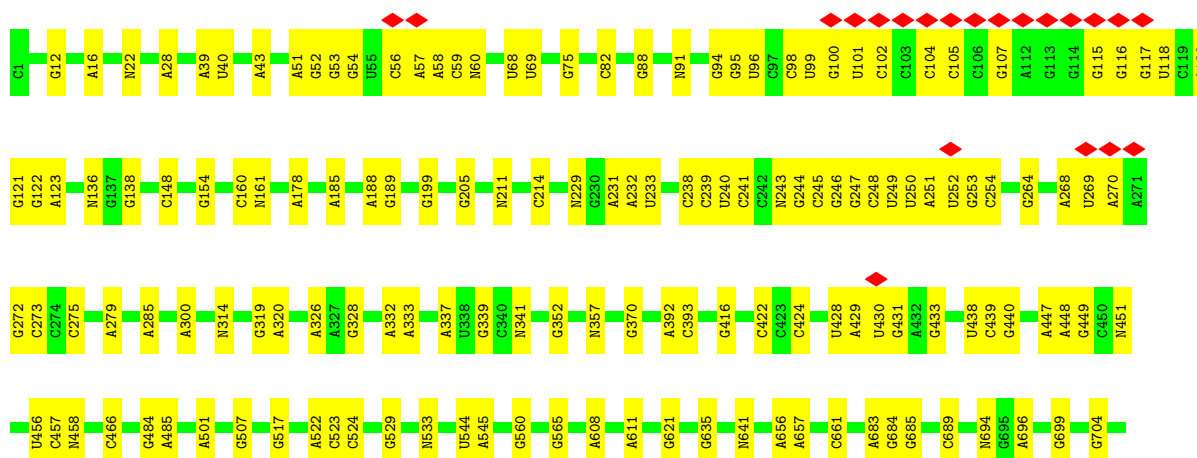
- Molecule 65: Large ribosomal subunit protein uL1

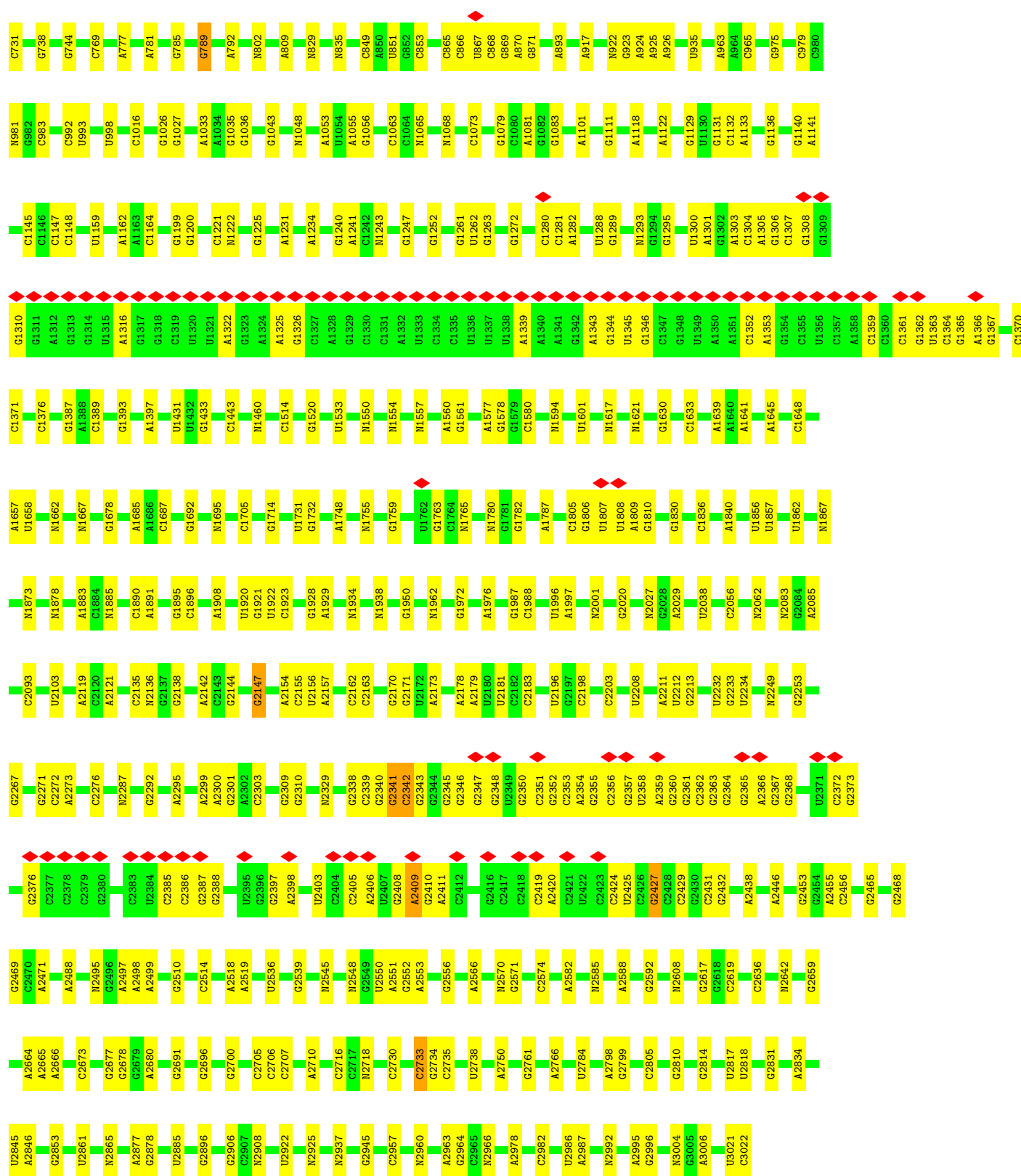
Chain BA:  91% 94%

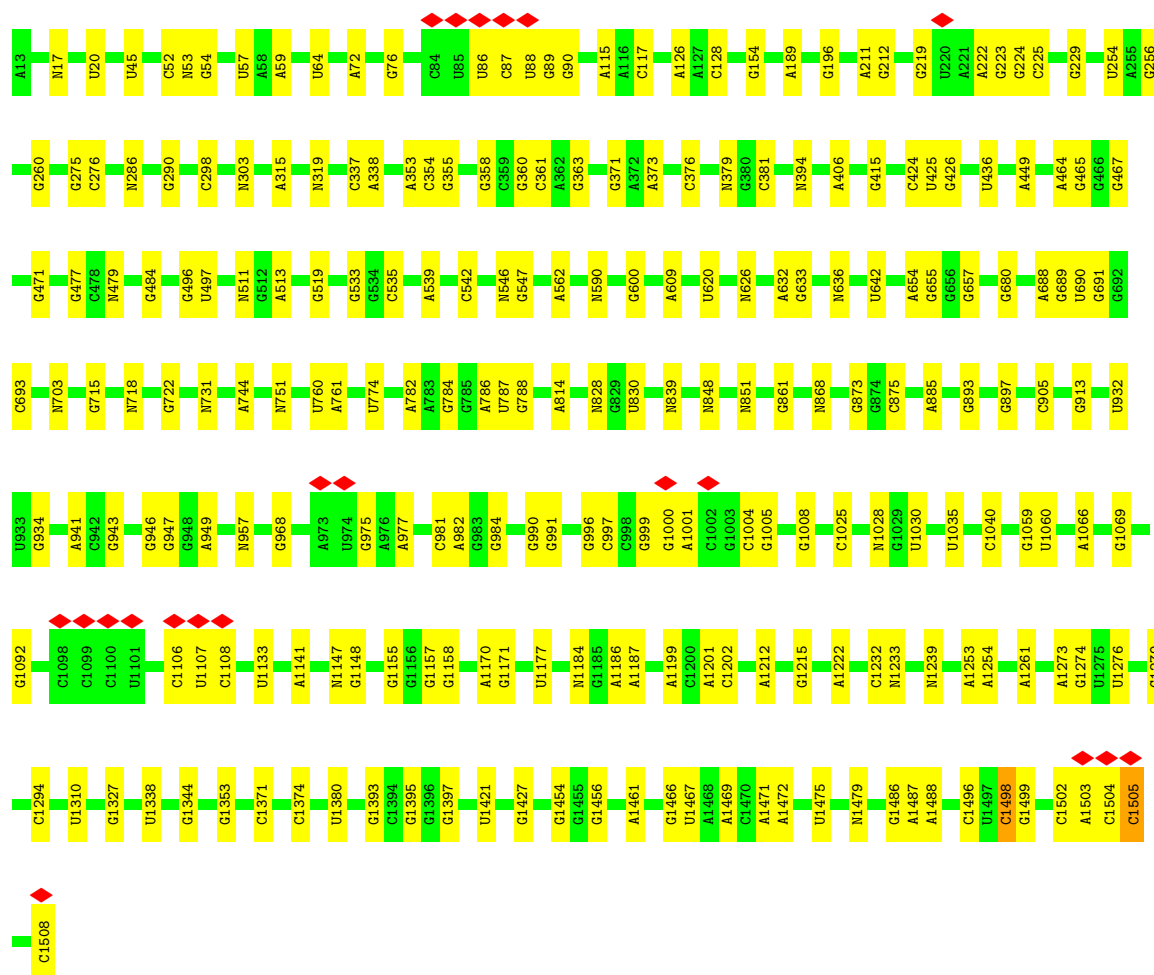


- Molecule 66: rRNA 23S

Chain 1:  81% 19%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182000	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	0.042	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	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: MA6, LHH, 5MU, UR3, PSU, OMG, 4AC, 4SU, H2U, MG, OMC, OMU, 6MZ, ZN, 5MC, A2M, 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	3	0.20	0/2995	0.32	0/4669
2	4	0.21	1/1724 (0.1%)	0.42	0/2687
3	H	0.17	0/3120	0.33	0/4209
4	AA	0.15	0/1557	0.29	0/2087
5	AB	0.14	0/1602	0.29	0/2165
6	AC	0.14	0/463	0.30	0/628
7	AD	0.13	0/1476	0.25	0/1980
8	AE	0.15	0/2032	0.31	0/2742
9	AF	0.15	0/1838	0.30	0/2478
10	AG	0.16	0/993	0.33	0/1329
11	AH	0.13	0/1762	0.29	0/2366
12	AI	0.16	0/1055	0.29	0/1415
13	AJ	0.16	0/995	0.27	0/1327
14	AK	0.14	0/1089	0.29	0/1459
15	AL	0.14	0/817	0.31	0/1097
16	AM	0.16	0/973	0.34	0/1311
17	AN	0.15	0/1165	0.30	0/1547
18	AP	0.15	0/465	0.34	0/613
19	AQ	0.14	0/1333	0.29	0/1791
20	AR	0.16	0/907	0.31	0/1225
21	AS	0.13	0/548	0.29	0/725
22	AU	0.14	0/1253	0.29	0/1689
23	AV	0.13	0/826	0.26	0/1108
23	B6	0.16	0/808	0.36	0/1086
24	AW	0.14	0/476	0.31	0/641
25	AX	0.10	0/518	0.25	0/694
26	AY	0.09	0/412	0.25	0/549
27	AZ	0.12	0/1563	0.26	0/2099
28	A0	0.20	0/349	0.40	0/451
29	A3	0.11	0/945	0.32	0/1274
29	B4	0.15	0/945	0.35	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	BG	0.19	0/944	0.34	0/1274
30	AT	0.15	0/1077	0.30	0/1439
31	AO	0.12	0/1135	0.29	0/1526
32	BB	0.21	0/1882	0.37	0/2538
33	BY	0.19	0/1254	0.33	0/1677
34	BO	0.18	0/1645	0.34	0/2209
35	BC	0.18	0/2933	0.36	0/3943
36	B5	0.17	0/619	0.35	0/830
36	BK	0.15	0/611	0.35	0/819
37	BL	0.19	0/1167	0.38	0/1552
38	Bf	0.21	0/443	0.35	0/589
39	BU	0.34	0/1027	0.44	0/1368
40	Bb	0.18	0/1120	0.32	0/1494
41	Be	0.20	0/514	0.35	0/676
42	BE	0.20	0/1509	0.39	0/2022
43	Ba	0.17	0/793	0.33	0/1064
44	BT	0.17	0/705	0.33	0/945
45	BW	0.17	0/566	0.31	0/747
46	Bi	0.15	0/630	0.35	0/839
47	BI	0.17	0/1166	0.32	0/1559
48	BR	0.18	0/819	0.33	0/1098
49	BQ	0.17	0/1281	0.32	0/1689
50	BV	0.17	0/547	0.33	0/729
51	Bj	0.18	0/807	0.32	0/1070
52	BD	0.20	0/2069	0.37	0/2787
53	BF	0.18	0/1485	0.31	0/2003
54	BZ	0.17	0/759	0.36	0/1023
55	BP	0.16	0/984	0.30	0/1314
56	BM	0.21	0/1627	0.35	0/2170
57	BS	0.28	0/1275	0.49	2/1715 (0.1%)
58	Bd	0.18	0/778	0.31	0/1036
59	BN	0.17	0/1483	0.32	0/1992
60	Bg	0.18	0/396	0.30	0/526
61	Bc	0.17	0/693	0.35	0/926
62	BJ	0.20	0/1080	0.34	0/1456
63	Bl	0.18	0/669	0.32	0/886
64	Bk	0.21	0/538	0.33	0/709
65	BA	0.15	0/1700	0.38	0/2288
66	1	0.26	1/70601 (0.0%)	0.38	5/110066 (0.0%)
67	2	0.21	0/34413	0.31	0/53647
All	All	0.22	2/182748 (0.0%)	0.35	7/268955 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	1	96	U	C1'-N1	5.75	1.57	1.48
2	4	8	4SU	O3'-P	5.01	1.61	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	2341	G	C2'-C3'-O3'	9.21	127.52	113.70
57	BS	79	GLY	N-CA-C	-8.59	94.82	112.34
66	1	2409	A	C2'-C3'-O3'	7.07	124.30	113.70
66	1	2427	G	C4'-C3'-O3'	6.09	122.14	113.00
57	BS	78	PHE	N-CA-C	5.85	118.06	108.52
66	1	2341	G	C3'-C2'-O2'	5.75	119.32	110.70
66	1	2342	C	C4'-C3'-O3'	-5.07	105.40	113.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
3	H	384/392 (98%)	382 (100%)	2 (0%)	0	100	100
4	AA	186/199 (94%)	181 (97%)	5 (3%)	0	100	100
5	AB	194/202 (96%)	192 (99%)	2 (1%)	0	100	100
6	AC	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
7	AD	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
8	AE	240/243 (99%)	238 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AF	227/236 (96%)	221 (97%)	6 (3%)	0	100	100
10	AG	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
11	AH	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
12	AI	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
13	AJ	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
14	AK	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
15	AL	98/102 (96%)	96 (98%)	2 (2%)	0	100	100
16	AM	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
17	AN	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
18	AP	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
19	AQ	155/158 (98%)	151 (97%)	4 (3%)	0	100	100
20	AR	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
21	AS	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
22	AU	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
23	AV	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
23	B6	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
24	AW	59/65 (91%)	56 (95%)	3 (5%)	0	100	100
25	AX	63/71 (89%)	63 (100%)	0	0	100	100
26	AY	47/51 (92%)	42 (89%)	5 (11%)	0	100	100
27	AZ	194/210 (92%)	182 (94%)	12 (6%)	0	100	100
28	A0	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
29	A3	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
29	B4	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
29	BG	120/123 (98%)	120 (100%)	0	0	100	100
30	AT	128/132 (97%)	127 (99%)	1 (1%)	0	100	100
31	AO	136/148 (92%)	129 (95%)	7 (5%)	0	100	100
32	BB	236/239 (99%)	229 (97%)	6 (2%)	1 (0%)	30	28
33	BY	152/155 (98%)	150 (99%)	2 (1%)	0	100	100
34	BO	196/203 (97%)	195 (100%)	1 (0%)	0	100	100
35	BC	358/361 (99%)	348 (97%)	10 (3%)	0	100	100
36	B5	79/82 (96%)	78 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BK	78/82 (95%)	75 (96%)	3 (4%)	0	100	100
37	BL	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
38	Bf	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
39	BU	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
40	Bb	127/130 (98%)	127 (100%)	0	0	100	100
41	Be	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
42	BE	183/188 (97%)	183 (100%)	0	0	100	100
43	Ba	92/94 (98%)	92 (100%)	0	0	100	100
44	BT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
45	BW	66/68 (97%)	66 (100%)	0	0	100	100
46	Bi	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
47	BI	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
48	BR	94/97 (97%)	94 (100%)	0	0	100	100
49	BQ	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
50	BV	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
51	Bj	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
52	BD	253/255 (99%)	250 (99%)	3 (1%)	0	100	100
53	BF	181/184 (98%)	181 (100%)	0	0	100	100
54	BZ	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
55	BP	118/120 (98%)	118 (100%)	0	0	100	100
56	BM	191/194 (98%)	189 (99%)	2 (1%)	0	100	100
57	BS	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
58	Bd	89/91 (98%)	89 (100%)	0	0	100	100
59	BN	176/181 (97%)	171 (97%)	5 (3%)	0	100	100
60	Bg	46/51 (90%)	46 (100%)	0	0	100	100
61	Bc	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
62	BJ	138/141 (98%)	138 (100%)	0	0	100	100
63	Bl	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
64	Bk	61/65 (94%)	61 (100%)	0	0	100	100
65	BA	213/219 (97%)	206 (97%)	7 (3%)	0	100	100
All	All	8781/9080 (97%)	8612 (98%)	168 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	BB	122	VAL

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	
3	H	332/338 (98%)	305 (92%)	27 (8%)	11	8
4	AA	160/167 (96%)	151 (94%)	9 (6%)	19	17
5	AB	168/173 (97%)	162 (96%)	6 (4%)	31	33
6	AC	50/55 (91%)	50 (100%)	0	100	100
7	AD	156/160 (98%)	153 (98%)	3 (2%)	50	57
8	AE	213/214 (100%)	211 (99%)	2 (1%)	70	78
9	AF	192/198 (97%)	187 (97%)	5 (3%)	40	45
10	AG	107/108 (99%)	102 (95%)	5 (5%)	23	23
11	AH	183/184 (100%)	175 (96%)	8 (4%)	25	25
12	AI	106/107 (99%)	104 (98%)	2 (2%)	50	57
13	AJ	101/103 (98%)	97 (96%)	4 (4%)	28	28
14	AK	111/111 (100%)	104 (94%)	7 (6%)	16	13
15	AL	89/91 (98%)	81 (91%)	8 (9%)	9	6
16	AM	94/104 (90%)	90 (96%)	4 (4%)	26	26
17	AN	120/121 (99%)	117 (98%)	3 (2%)	42	47
18	AP	45/46 (98%)	40 (89%)	5 (11%)	6	3
19	AQ	142/143 (99%)	136 (96%)	6 (4%)	26	27
20	AR	96/102 (94%)	95 (99%)	1 (1%)	68	76
21	AS	58/61 (95%)	53 (91%)	5 (9%)	10	7
22	AU	126/127 (99%)	121 (96%)	5 (4%)	28	28
23	AV	88/90 (98%)	87 (99%)	1 (1%)	65	74
23	B6	86/90 (96%)	77 (90%)	9 (10%)	6	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AW	53/56 (95%)	52 (98%)	1 (2%)	50	57
25	AX	55/60 (92%)	49 (89%)	6 (11%)	6	3
26	AY	40/42 (95%)	39 (98%)	1 (2%)	42	47
27	AZ	155/168 (92%)	145 (94%)	10 (6%)	15	13
28	A0	34/35 (97%)	33 (97%)	1 (3%)	37	41
29	A3	98/99 (99%)	95 (97%)	3 (3%)	35	38
29	B4	98/99 (99%)	92 (94%)	6 (6%)	17	14
29	BG	98/99 (99%)	88 (90%)	10 (10%)	7	4
30	AT	113/114 (99%)	107 (95%)	6 (5%)	20	18
31	AO	115/123 (94%)	111 (96%)	4 (4%)	32	34
32	BB	188/189 (100%)	181 (96%)	7 (4%)	30	31
33	BY	132/133 (99%)	128 (97%)	4 (3%)	36	40
34	BO	167/170 (98%)	153 (92%)	14 (8%)	10	7
35	BC	306/307 (100%)	299 (98%)	7 (2%)	44	50
36	B5	65/66 (98%)	61 (94%)	4 (6%)	16	14
36	BK	64/66 (97%)	59 (92%)	5 (8%)	11	9
37	BL	118/118 (100%)	108 (92%)	10 (8%)	10	7
38	Bf	46/47 (98%)	44 (96%)	2 (4%)	26	26
39	BU	109/109 (100%)	104 (95%)	5 (5%)	24	24
40	Bb	117/118 (99%)	115 (98%)	2 (2%)	53	61
41	Be	52/53 (98%)	51 (98%)	1 (2%)	50	57
42	BE	158/160 (99%)	136 (86%)	22 (14%)	3	1
43	Ba	84/84 (100%)	82 (98%)	2 (2%)	43	48
44	BT	77/77 (100%)	76 (99%)	1 (1%)	61	69
45	BW	63/63 (100%)	61 (97%)	2 (3%)	34	37
46	Bi	61/62 (98%)	58 (95%)	3 (5%)	22	21
47	BI	122/122 (100%)	120 (98%)	2 (2%)	55	63
48	BR	86/87 (99%)	84 (98%)	2 (2%)	44	50
49	BQ	132/133 (99%)	130 (98%)	2 (2%)	57	65
50	BV	54/58 (93%)	52 (96%)	2 (4%)	30	31
51	Bj	83/84 (99%)	82 (99%)	1 (1%)	63	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	BD	212/212 (100%)	205 (97%)	7 (3%)	33	36
53	BF	156/157 (99%)	145 (93%)	11 (7%)	13	10
54	BZ	79/80 (99%)	71 (90%)	8 (10%)	7	4
55	BP	102/102 (100%)	98 (96%)	4 (4%)	28	29
56	BM	160/161 (99%)	157 (98%)	3 (2%)	50	57
57	BS	130/131 (99%)	125 (96%)	5 (4%)	29	30
58	Bd	82/82 (100%)	79 (96%)	3 (4%)	30	31
59	BN	149/151 (99%)	146 (98%)	3 (2%)	48	55
60	Bg	37/39 (95%)	37 (100%)	0	100	100
61	Bc	74/74 (100%)	72 (97%)	2 (3%)	39	44
62	BJ	108/109 (99%)	104 (96%)	4 (4%)	30	31
63	Bl	72/72 (100%)	68 (94%)	4 (6%)	19	17
64	Bk	55/57 (96%)	50 (91%)	5 (9%)	9	6
65	BA	182/186 (98%)	173 (95%)	9 (5%)	22	21
All	All	7564/7707 (98%)	7223 (96%)	341 (4%)	26	24

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	12	ASP
3	H	23	LEU
3	H	27	ILE
3	H	37	LEU
3	H	51	THR
3	H	61	LYS
3	H	68	LYS
3	H	85	LEU
3	H	93	LEU
3	H	98	ARG
3	H	99	SER
3	H	108	GLU
3	H	110	LEU
3	H	112	VAL
3	H	123	VAL
3	H	129	LYS
3	H	132	VAL
3	H	218	VAL

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Mol	Chain	Res	Type
3	H	221	ILE
3	H	268	VAL
3	H	269	GLU
3	H	277	GLN
3	H	350	THR
3	H	373	GLU
3	H	378	ILE
3	H	379	ARG
3	H	385	ILE
4	AA	18	GLN
4	AA	26	ASP
4	AA	31	VAL
4	AA	57	THR
4	AA	97	VAL
4	AA	153	LEU
4	AA	160	LEU
4	AA	161	GLU
4	AA	185	GLU
5	AB	4	GLU
5	AB	9	LEU
5	AB	32	ILE
5	AB	74	LEU
5	AB	170	ILE
5	AB	193	GLU
7	AD	20	LYS
7	AD	102	GLU
7	AD	119	ARG
8	AE	122	ILE
8	AE	191	LYS
9	AF	6	LYS
9	AF	15	GLU
9	AF	57	VAL
9	AF	104	ARG
9	AF	187	THR
10	AG	6	LEU
10	AG	7	VAL
10	AG	38	ILE
10	AG	45	ILE
10	AG	77	ASP
11	AH	67	LEU
11	AH	74	SER
11	AH	128	GLU

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Mol	Chain	Res	Type
11	AH	140	MET
11	AH	145	ARG
11	AH	146	TYR
11	AH	190	LEU
11	AH	209	ARG
12	AI	55	ASP
12	AI	117	ARG
13	AJ	18	VAL
13	AJ	42	LYS
13	AJ	91	ARG
13	AJ	96	THR
14	AK	20	ARG
14	AK	23	LYS
14	AK	39	GLU
14	AK	56	ILE
14	AK	82	ILE
14	AK	88	GLU
14	AK	114	THR
15	AL	6	ILE
15	AL	73	ILE
15	AL	75	ILE
15	AL	76	GLU
15	AL	89	ARG
15	AL	96	ILE
15	AL	97	GLU
15	AL	101	ILE
16	AM	11	LYS
16	AM	12	GLU
16	AM	30	ILE
16	AM	38	THR
17	AN	18	LEU
17	AN	64	GLN
17	AN	143	GLU
18	AP	9	ARG
18	AP	10	LYS
18	AP	20	ARG
18	AP	46	VAL
18	AP	49	LYS
19	AQ	24	ILE
19	AQ	30	VAL
19	AQ	60	ILE
19	AQ	77	THR

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Mol	Chain	Res	Type
19	AQ	87	LEU
19	AQ	111	GLN
20	AR	38	VAL
21	AS	6	GLN
21	AS	14	ARG
21	AS	60	MET
21	AS	61	LYS
21	AS	62	GLU
22	AU	18	GLN
22	AU	22	GLU
22	AU	25	GLU
22	AU	68	VAL
22	AU	121	ILE
23	AV	52	VAL
24	AW	29	VAL
25	AX	10	GLU
25	AX	40	VAL
25	AX	49	VAL
25	AX	60	THR
25	AX	65	ARG
25	AX	67	ILE
26	AY	48	TRP
27	AZ	3	ILE
27	AZ	10	GLU
27	AZ	17	ILE
27	AZ	35	ILE
27	AZ	129	GLU
27	AZ	162	VAL
27	AZ	175	VAL
27	AZ	186	ASP
27	AZ	192	GLU
27	AZ	196	ILE
28	A0	36	LEU
29	A3	25	ILE
29	A3	44	GLU
29	A3	85	GLU
30	AT	36	LEU
30	AT	47	LEU
30	AT	49	ARG
30	AT	53	LEU
30	AT	93	GLU
30	AT	112	ARG

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Mol	Chain	Res	Type
31	AO	21	LEU
31	AO	31	VAL
31	AO	122	LEU
31	AO	126	VAL
32	BB	62	ARG
32	BB	83	ILE
32	BB	96	THR
32	BB	127	THR
32	BB	201	ASN
32	BB	225	ARG
32	BB	239	LYS
33	BY	17	ARG
33	BY	55	THR
33	BY	82	ASP
33	BY	105	MET
34	BO	23	LYS
34	BO	36	VAL
34	BO	37	VAL
34	BO	39	LYS
34	BO	48	ILE
34	BO	54	LYS
34	BO	59	LEU
34	BO	67	LEU
34	BO	100	GLU
34	BO	112	VAL
34	BO	137	ILE
34	BO	162	GLU
34	BO	172	LEU
34	BO	176	LEU
35	BC	3	LYS
35	BC	56	ASP
35	BC	105	GLU
35	BC	154	GLU
35	BC	170	VAL
35	BC	171	ILE
35	BC	191	GLU
36	B5	29	ASP
36	B5	33	VAL
36	B5	60	ILE
36	B5	77	LYS
37	BL	10	LYS
37	BL	43	ASN

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Mol	Chain	Res	Type
37	BL	69	VAL
37	BL	79	LYS
37	BL	90	GLN
37	BL	93	ILE
37	BL	115	THR
37	BL	122	LEU
37	BL	123	VAL
37	BL	147	VAL
38	Bf	3	ARG
38	Bf	47	THR
39	BU	1	MET
39	BU	27	MET
39	BU	68	GLU
39	BU	83	LEU
39	BU	118	ARG
40	Bb	80	GLU
40	Bb	113	GLU
41	Be	21	ARG
42	BE	8	ARG
42	BE	25	ILE
42	BE	29	THR
42	BE	34	VAL
42	BE	51	LEU
42	BE	57	ILE
42	BE	59	ARG
42	BE	60	LYS
42	BE	67	ASP
42	BE	70	ILE
42	BE	78	VAL
42	BE	82	LEU
42	BE	91	LEU
42	BE	118	ASP
42	BE	119	GLU
42	BE	134	ILE
42	BE	137	MET
42	BE	142	THR
42	BE	156	LYS
42	BE	173	VAL
42	BE	184	VAL
42	BE	185	GLU
43	Ba	3	ILE
43	Ba	7	GLU

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Mol	Chain	Res	Type
44	BT	41	ARG
45	BW	62	LEU
45	BW	63	ARG
46	Bi	2	SER
46	Bi	34	GLN
46	Bi	43	ARG
47	BI	1	MET
47	BI	27	GLU
48	BR	36	GLU
48	BR	66	VAL
36	BK	4	ILE
36	BK	54	GLU
36	BK	56	LEU
36	BK	75	LEU
36	BK	82	LEU
49	BQ	111	GLU
49	BQ	115	ILE
50	BV	15	GLU
50	BV	58	GLU
51	Bj	45	LYS
29	BG	3	LYS
29	BG	13	LYS
29	BG	28	ASP
29	BG	34	LYS
29	BG	72	GLU
29	BG	73	LYS
29	BG	74	GLU
29	BG	103	GLU
29	BG	106	LYS
29	BG	109	ASP
52	BD	61	ILE
52	BD	75	THR
52	BD	92	THR
52	BD	150	LYS
52	BD	162	LYS
52	BD	222	VAL
52	BD	243	THR
53	BF	26	VAL
53	BF	38	GLU
53	BF	84	GLU
53	BF	89	LYS
53	BF	90	LEU

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Mol	Chain	Res	Type
53	BF	91	LYS
53	BF	129	THR
53	BF	136	GLU
53	BF	155	GLU
53	BF	158	THR
53	BF	183	THR
54	BZ	3	LEU
54	BZ	6	GLU
54	BZ	11	LEU
54	BZ	55	LEU
54	BZ	79	VAL
54	BZ	94	LEU
54	BZ	96	LEU
54	BZ	99	ARG
23	B6	9	LYS
23	B6	11	ASN
23	B6	13	LEU
23	B6	14	ILE
23	B6	16	ARG
23	B6	66	LYS
23	B6	79	LEU
23	B6	89	ARG
23	B6	90	ASP
55	BP	4	THR
55	BP	16	ARG
55	BP	99	GLU
55	BP	104	GLU
56	BM	3	MET
56	BM	5	LYS
56	BM	76	TRP
57	BS	65	ARG
57	BS	103	LYS
57	BS	126	ARG
57	BS	144	THR
57	BS	155	ARG
58	Bd	80	MET
58	Bd	82	GLU
58	Bd	83	GLN
59	BN	108	TYR
59	BN	167	LYS
59	BN	174	THR
61	Bc	4	LYS

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Mol	Chain	Res	Type
61	Bc	29	VAL
62	BJ	41	ILE
62	BJ	63	VAL
62	BJ	112	VAL
62	BJ	117	GLU
63	Bl	7	ARG
63	Bl	13	GLU
63	Bl	17	ARG
63	Bl	20	LYS
29	B4	39	THR
29	B4	70	CYS
29	B4	71	GLU
29	B4	77	TYR
29	B4	121	LEU
29	B4	122	MET
64	Bk	16	GLU
64	Bk	23	CYS
64	Bk	39	LYS
64	Bk	44	LEU
64	Bk	49	LYS
65	BA	31	VAL
65	BA	35	VAL
65	BA	57	HIS
65	BA	93	ILE
65	BA	131	ARG
65	BA	136	VAL
65	BA	150	GLU
65	BA	161	LYS
65	BA	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	52	GLN
3	H	87	HIS
3	H	194	GLN
3	H	237	ASN
3	H	238	ASN
3	H	277	GLN
4	AA	77	GLN
4	AA	109	ASN
4	AA	164	ASN

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Mol	Chain	Res	Type
5	AB	11	GLN
5	AB	108	ASN
5	AB	124	HIS
5	AB	145	ASN
7	AD	47	GLN
7	AD	50	ASN
7	AD	65	GLN
7	AD	72	GLN
7	AD	123	GLN
7	AD	162	ASN
7	AD	164	GLN
8	AE	38	ASN
8	AE	143	HIS
9	AF	58	ASN
9	AF	115	ASN
9	AF	120	ASN
9	AF	186	GLN
9	AF	209	ASN
10	AG	18	GLN
10	AG	110	ASN
10	AG	118	GLN
10	AG	120	ASN
11	AH	55	HIS
11	AH	90	HIS
11	AH	94	ASN
11	AH	147	HIS
11	AH	164	ASN
11	AH	193	ASN
12	AI	9	ASN
12	AI	16	ASN
12	AI	64	GLN
12	AI	70	ASN
12	AI	108	GLN
13	AJ	34	ASN
13	AJ	40	GLN
13	AJ	52	ASN
13	AJ	64	ASN
13	AJ	83	ASN
13	AJ	121	ASN
14	AK	5	GLN
14	AK	67	GLN
15	AL	22	GLN

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Mol	Chain	Res	Type
15	AL	84	GLN
16	AM	99	GLN
17	AN	64	GLN
17	AN	66	ASN
17	AN	76	GLN
18	AP	26	GLN
19	AQ	71	ASN
19	AQ	111	GLN
19	AQ	123	GLN
20	AR	55	HIS
20	AR	74	ASN
21	AS	18	ASN
22	AU	18	GLN
22	AU	47	GLN
25	AX	26	GLN
27	AZ	77	ASN
27	AZ	95	GLN
29	A3	37	ASN
29	A3	47	GLN
29	A3	65	HIS
30	AT	15	GLN
30	AT	114	GLN
31	AO	20	GLN
31	AO	67	GLN
32	BB	8	GLN
32	BB	34	ASN
32	BB	50	HIS
32	BB	201	ASN
32	BB	202	HIS
32	BB	210	HIS
32	BB	229	HIS
33	BY	48	GLN
33	BY	148	ASN
34	BO	42	ASN
34	BO	44	HIS
34	BO	47	GLN
34	BO	63	HIS
34	BO	76	HIS
34	BO	109	HIS
35	BC	62	ASN
35	BC	123	GLN
35	BC	143	GLN

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Mol	Chain	Res	Type
35	BC	167	GLN
35	BC	257	HIS
35	BC	270	GLN
35	BC	274	HIS
35	BC	309	HIS
36	B5	31	ASN
37	BL	15	HIS
37	BL	43	ASN
37	BL	57	HIS
37	BL	84	ASN
37	BL	90	GLN
38	Bf	19	GLN
38	Bf	20	ASN
38	Bf	38	HIS
39	BU	7	GLN
39	BU	96	HIS
39	BU	106	ASN
40	Bb	104	HIS
41	Be	17	HIS
42	BE	120	HIS
42	BE	164	HIS
43	Ba	42	HIS
43	Ba	46	GLN
44	BT	37	GLN
45	BW	40	ASN
47	BI	41	ASN
47	BI	51	GLN
47	BI	111	GLN
47	BI	119	HIS
48	BR	6	HIS
48	BR	19	HIS
48	BR	33	GLN
48	BR	42	HIS
48	BR	59	HIS
48	BR	89	HIS
36	BK	31	ASN
49	BQ	58	GLN
49	BQ	75	HIS
49	BQ	131	GLN
49	BQ	136	HIS
51	Bj	37	GLN
52	BD	44	GLN

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Mol	Chain	Res	Type
52	BD	123	ASN
52	BD	213	ASN
52	BD	214	HIS
52	BD	229	HIS
52	BD	235	HIS
53	BF	74	HIS
53	BF	149	GLN
54	BZ	21	ASN
23	B6	11	ASN
55	BP	10	ASN
55	BP	23	ASN
55	BP	110	ASN
56	BM	87	GLN
56	BM	97	GLN
56	BM	110	ASN
56	BM	154	HIS
56	BM	174	ASN
56	BM	189	ASN
57	BS	10	GLN
57	BS	70	GLN
57	BS	97	ASN
57	BS	116	HIS
58	Bd	35	HIS
59	BN	38	ASN
59	BN	56	GLN
59	BN	59	GLN
59	BN	70	ASN
59	BN	76	ASN
59	BN	81	ASN
59	BN	83	HIS
59	BN	97	ASN
59	BN	130	GLN
59	BN	170	ASN
61	Bc	17	GLN
61	Bc	18	HIS
61	Bc	28	ASN
61	Bc	30	ASN
62	BJ	47	HIS
62	BJ	102	ASN
29	B4	65	HIS
64	Bk	38	ASN
65	BA	36	ASN

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Mol	Chain	Res	Type
65	BA	163	ASN
65	BA	167	HIS
65	BA	201	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	125/128 (97%)	17 (13%)	0
2	4	76/77 (98%)	29 (38%)	1 (1%)
66	1	3016/3018 (99%)	491 (16%)	33 (1%)
67	2	1495/1496 (99%)	170 (11%)	4 (0%)
All	All	4712/4719 (99%)	707 (15%)	38 (0%)

All (707) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	5	C
1	3	24	G
1	3	25	C
1	3	26	C
1	3	30	C
1	3	44	G
1	3	53	A
1	3	56	U
1	3	57	A
1	3	58	A
1	3	60	C
1	3	67	G
1	3	79	G
1	3	89	C
1	3	95	G
1	3	115	G
1	3	125	A
2	4	3	C
2	4	6	G
2	4	7	G
2	4	8	4SU
2	4	14	A
2	4	16	C
2	4	17	C
2	4	17(A)	U

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Mol	Chain	Res	Type
2	4	18	G
2	4	19	G
2	4	20	H2U
2	4	22	G
2	4	23	C
2	4	35	A
2	4	36	U
2	4	42	G
2	4	47	U
2	4	48	C
2	4	55	PSU
2	4	56	C
2	4	57	A
2	4	58	A
2	4	59	A
2	4	60	U
2	4	61	C
2	4	67	C
2	4	69	C
2	4	72	U
2	4	76	A
66	1	12	G
66	1	16	A
66	1	28	A
66	1	39	A
66	1	40	U
66	1	43	A
66	1	51	A
66	1	52	G
66	1	53	G
66	1	54	G
66	1	56	C
66	1	57	A
66	1	58	A
66	1	59	C
66	1	69	U
66	1	75	G
66	1	82	C
66	1	88	G
66	1	94	G
66	1	95	G
66	1	98	C

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Mol	Chain	Res	Type
66	1	99	U
66	1	100	G
66	1	101	U
66	1	102	C
66	1	104	C
66	1	105	C
66	1	107	G
66	1	115	G
66	1	116	G
66	1	118	U
66	1	120	A
66	1	121	G
66	1	122	G
66	1	123	A
66	1	138	G
66	1	148	C
66	1	154	G
66	1	160	C
66	1	178	A
66	1	185	A
66	1	188	A
66	1	189	G
66	1	199	G
66	1	205	G
66	1	214	C
66	1	231	A
66	1	232	A
66	1	233	U
66	1	238	C
66	1	239	C
66	1	240	U
66	1	241	C
66	1	244	G
66	1	245	C
66	1	246	G
66	1	247	G
66	1	248	C
66	1	249	U
66	1	250	U
66	1	251	A
66	1	252	U
66	1	253	G

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Mol	Chain	Res	Type
66	1	254	C
66	1	264	G
66	1	268	A
66	1	269	U
66	1	270	A
66	1	272	G
66	1	273	C
66	1	275	C
66	1	279	A
66	1	285	A
66	1	300	A
66	1	319	G
66	1	320	A
66	1	326	A
66	1	332	A
66	1	333	A
66	1	337	A
66	1	339	G
66	1	352	G
66	1	370	G
66	1	392	A
66	1	393	C
66	1	416	G
66	1	422	C
66	1	424	C
66	1	428	U
66	1	429	A
66	1	430	U
66	1	431	G
66	1	433	G
66	1	438	U
66	1	439	C
66	1	440	G
66	1	447	A
66	1	448	A
66	1	449	G
66	1	456	U
66	1	457	C
66	1	466	C
66	1	484	G
66	1	485	A
66	1	501	A

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Mol	Chain	Res	Type
66	1	507	G
66	1	517	G
66	1	522	A
66	1	523	C
66	1	524	C
66	1	529	G
66	1	544	U
66	1	545	A
66	1	560	G
66	1	565	G
66	1	608	A
66	1	611	A
66	1	621	G
66	1	635	G
66	1	657	A
66	1	661	C
66	1	683	A
66	1	684	G
66	1	685	G
66	1	689	C
66	1	696	A
66	1	699	G
66	1	704	G
66	1	731	C
66	1	738	G
66	1	744	G
66	1	769	C
66	1	777	A
66	1	781	A
66	1	785	G
66	1	789	OMG
66	1	792	A
66	1	809	A
66	1	849	C
66	1	851	U
66	1	853	C
66	1	865	C
66	1	866	C
66	1	867	U
66	1	868	C
66	1	869	G
66	1	870	A

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Mol	Chain	Res	Type
66	1	871	G
66	1	893	A
66	1	917	A
66	1	924	A
66	1	925	A
66	1	926	A
66	1	935	U
66	1	963	A
66	1	965	C
66	1	975	G
66	1	979	C
66	1	983	C
66	1	993	U
66	1	998	U
66	1	1016	C
66	1	1026	G
66	1	1027	G
66	1	1033	A
66	1	1035	G
66	1	1036	G
66	1	1043	G
66	1	1053	A
66	1	1056	G
66	1	1063	C
66	1	1073	C
66	1	1079	G
66	1	1081	A
66	1	1083	G
66	1	1101	A
66	1	1111	G
66	1	1118	A
66	1	1122	A
66	1	1129	G
66	1	1131	G
66	1	1132	C
66	1	1133	A
66	1	1136	G
66	1	1140	G
66	1	1141	A
66	1	1145	C
66	1	1147	C
66	1	1148	C

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Mol	Chain	Res	Type
66	1	1159	U
66	1	1162	A
66	1	1164	C
66	1	1199	G
66	1	1200	G
66	1	1221	C
66	1	1225	G
66	1	1231	A
66	1	1234	A
66	1	1240	G
66	1	1241	A
66	1	1247	G
66	1	1252	G
66	1	1261	G
66	1	1262	U
66	1	1263	G
66	1	1272	G
66	1	1280	C
66	1	1281	C
66	1	1282	A
66	1	1288	U
66	1	1289	G
66	1	1295	G
66	1	1300	U
66	1	1301	A
66	1	1303	A
66	1	1304	C
66	1	1305	A
66	1	1306	G
66	1	1307	C
66	1	1308	G
66	1	1310	G
66	1	1316	A
66	1	1322	A
66	1	1325	A
66	1	1326	G
66	1	1339	A
66	1	1343	A
66	1	1344	G
66	1	1345	U
66	1	1346	G
66	1	1352	C

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Mol	Chain	Res	Type
66	1	1353	A
66	1	1359	C
66	1	1361	C
66	1	1362	G
66	1	1363	U
66	1	1364	C
66	1	1365	G
66	1	1366	A
66	1	1367	G
66	1	1370	C
66	1	1371	C
66	1	1376	C
66	1	1387	G
66	1	1389	C
66	1	1393	G
66	1	1397	A
66	1	1431	U
66	1	1433	G
66	1	1443	C
66	1	1514	C
66	1	1520	G
66	1	1533	U
66	1	1560	A
66	1	1561	G
66	1	1577	A
66	1	1578	G
66	1	1580	C
66	1	1601	U
66	1	1630	G
66	1	1633	C
66	1	1639	A
66	1	1641	A
66	1	1645	A
66	1	1648	C
66	1	1657	A
66	1	1658	U
66	1	1678	G
66	1	1685	A
66	1	1687	C
66	1	1692	G
66	1	1705	C
66	1	1714	G

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Mol	Chain	Res	Type
66	1	1731	U
66	1	1732	G
66	1	1748	A
66	1	1759	G
66	1	1763	G
66	1	1782	G
66	1	1787	A
66	1	1805	C
66	1	1806	G
66	1	1807	U
66	1	1808	U
66	1	1809	A
66	1	1810	G
66	1	1830	G
66	1	1836	C
66	1	1840	A
66	1	1856	U
66	1	1857	U
66	1	1862	U
66	1	1883	A
66	1	1890	C
66	1	1891	A
66	1	1895	G
66	1	1896	C
66	1	1908	A
66	1	1920	U
66	1	1921	G
66	1	1922	U
66	1	1923	C
66	1	1928	G
66	1	1929	A
66	1	1950	G
66	1	1972	G
66	1	1976	A
66	1	1987	G
66	1	1988	C
66	1	1996	U
66	1	1997	A
66	1	2020	G
66	1	2029	A
66	1	2038	U
66	1	2056	C

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Mol	Chain	Res	Type
66	1	2085	A
66	1	2103	U
66	1	2119	A
66	1	2121	A
66	1	2135	C
66	1	2142	A
66	1	2147	OMG
66	1	2154	A
66	1	2155	C
66	1	2156	U
66	1	2157	A
66	1	2170	G
66	1	2171	G
66	1	2178	A
66	1	2179	A
66	1	2181	U
66	1	2196	U
66	1	2208	U
66	1	2211	A
66	1	2212	U
66	1	2213	G
66	1	2232	U
66	1	2233	G
66	1	2234	U
66	1	2253	G
66	1	2267	G
66	1	2271	G
66	1	2272	C
66	1	2273	A
66	1	2276	C
66	1	2292	G
66	1	2295	A
66	1	2299	A
66	1	2300	A
66	1	2301	G
66	1	2303	C
66	1	2309	G
66	1	2310	G
66	1	2338	G
66	1	2339	C
66	1	2340	G
66	1	2341	G

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Mol	Chain	Res	Type
66	1	2342	C
66	1	2343	G
66	1	2345	G
66	1	2346	G
66	1	2347	G
66	1	2348	G
66	1	2350	G
66	1	2351	C
66	1	2352	G
66	1	2353	C
66	1	2354	A
66	1	2355	G
66	1	2356	C
66	1	2357	G
66	1	2358	U
66	1	2359	A
66	1	2360	G
66	1	2361	G
66	1	2362	C
66	1	2363	G
66	1	2364	G
66	1	2365	G
66	1	2366	A
66	1	2368	G
66	1	2372	C
66	1	2373	G
66	1	2376	G
66	1	2385	C
66	1	2386	C
66	1	2387	G
66	1	2388	G
66	1	2397	G
66	1	2398	A
66	1	2403	U
66	1	2405	C
66	1	2406	A
66	1	2408	G
66	1	2410	G
66	1	2411	A
66	1	2419	C
66	1	2420	A
66	1	2424	C

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Mol	Chain	Res	Type
66	1	2425	U
66	1	2427	G
66	1	2429	C
66	1	2431	C
66	1	2432	G
66	1	2438	A
66	1	2446	A
66	1	2453	G
66	1	2455	A
66	1	2456	C
66	1	2465	G
66	1	2468	G
66	1	2469	G
66	1	2471	A
66	1	2488	A
66	1	2497	A
66	1	2498	A
66	1	2499	A
66	1	2510	G
66	1	2514	C
66	1	2518	A
66	1	2519	A
66	1	2536	U
66	1	2539	G
66	1	2550	U
66	1	2551	A
66	1	2552	G
66	1	2553	A
66	1	2556	G
66	1	2566	A
66	1	2571	G
66	1	2574	C
66	1	2582	A
66	1	2588	A
66	1	2592	G
66	1	2617	G
66	1	2619	C
66	1	2636	C
66	1	2659	G
66	1	2664	A
66	1	2665	A
66	1	2666	A

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Mol	Chain	Res	Type
66	1	2673	C
66	1	2677	G
66	1	2680	A
66	1	2691	G
66	1	2696	G
66	1	2700	G
66	1	2705	C
66	1	2706	C
66	1	2707	C
66	1	2710	A
66	1	2716	C
66	1	2730	C
66	1	2733	5MC
66	1	2734	G
66	1	2735	C
66	1	2738	U
66	1	2750	A
66	1	2761	G
66	1	2766	A
66	1	2798	A
66	1	2799	G
66	1	2805	C
66	1	2810	G
66	1	2814	G
66	1	2817	U
66	1	2818	U
66	1	2831	G
66	1	2834	A
66	1	2845	U
66	1	2846	A
66	1	2853	G
66	1	2861	U
66	1	2877	A
66	1	2878	G
66	1	2885	U
66	1	2896	G
66	1	2906	G
66	1	2922	U
66	1	2945	G
66	1	2957	C
66	1	2963	A
66	1	2964	G

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Mol	Chain	Res	Type
66	1	2978	A
66	1	2982	C
66	1	2987	A
66	1	2995	A
66	1	2996	G
66	1	3006	A
66	1	3021	U
66	1	3022	C
67	2	45	U
67	2	52	C
67	2	54	G
67	2	57	U
67	2	59	A
67	2	72	A
67	2	76	G
67	2	86	U
67	2	87	C
67	2	88	U
67	2	89	G
67	2	90	G
67	2	115	A
67	2	117	C
67	2	126	A
67	2	128	C
67	2	154	G
67	2	189	A
67	2	196	G
67	2	211	A
67	2	212	G
67	2	219	G
67	2	222	A
67	2	223	G
67	2	224	G
67	2	225	C
67	2	229	G
67	2	254	U
67	2	256	G
67	2	260	G
67	2	275	G
67	2	276	C
67	2	290	G
67	2	298	C

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Mol	Chain	Res	Type
67	2	315	A
67	2	337	C
67	2	338	A
67	2	353	A
67	2	354	C
67	2	355	G
67	2	358	G
67	2	360	G
67	2	361	C
67	2	363	G
67	2	371	G
67	2	376	C
67	2	381	C
67	2	406	A
67	2	415	G
67	2	424	C
67	2	425	U
67	2	426	G
67	2	436	U
67	2	449	A
67	2	465	G
67	2	477	G
67	2	484	G
67	2	496	G
67	2	497	U
67	2	513	A
67	2	533	G
67	2	539	A
67	2	542	C
67	2	547	G
67	2	562	A
67	2	600	G
67	2	609	A
67	2	620	U
67	2	632	A
67	2	633	G
67	2	642	U
67	2	654	A
67	2	655	G
67	2	689	G
67	2	690	U
67	2	691	G

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Mol	Chain	Res	Type
67	2	715	G
67	2	722	G
67	2	744	A
67	2	760	U
67	2	761	A
67	2	782	A
67	2	784	G
67	2	786	A
67	2	788	G
67	2	814	A
67	2	861	G
67	2	885	A
67	2	893	G
67	2	897	G
67	2	905	C
67	2	932	U
67	2	941	A
67	2	943	G
67	2	946	G
67	2	947	G
67	2	949	A
67	2	968	G
67	2	975	G
67	2	977	A
67	2	981	C
67	2	982	A
67	2	984	G
67	2	990	G
67	2	991	G
67	2	996	G
67	2	997	C
67	2	999	G
67	2	1000	G
67	2	1001	A
67	2	1004	C
67	2	1005	G
67	2	1008	G
67	2	1030	U
67	2	1035	U
67	2	1059	G
67	2	1060	U
67	2	1066	A

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Mol	Chain	Res	Type
67	2	1092	G
67	2	1107	U
67	2	1108	C
67	2	1133	U
67	2	1141	A
67	2	1148	G
67	2	1155	G
67	2	1157	G
67	2	1158	G
67	2	1170	A
67	2	1171	G
67	2	1186	A
67	2	1187	A
67	2	1199	A
67	2	1201	A
67	2	1212	A
67	2	1215	G
67	2	1222	A
67	2	1232	C
67	2	1253	A
67	2	1254	A
67	2	1261	A
67	2	1273	A
67	2	1274	G
67	2	1276	U
67	2	1279	G
67	2	1294	C
67	2	1310	U
67	2	1327	G
67	2	1338	U
67	2	1344	G
67	2	1353	G
67	2	1371	C
67	2	1393	G
67	2	1395	G
67	2	1397	G
67	2	1421	U
67	2	1427	G
67	2	1454	G
67	2	1456	G
67	2	1461	A
67	2	1466	G

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Mol	Chain	Res	Type
67	2	1471	A
67	2	1472	A
67	2	1475	U
67	2	1486	G
67	2	1498	5MC
67	2	1499	G
67	2	1503	A
67	2	1504	C
67	2	1505	5MC
67	2	1508	C

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	4	68	C
66	1	68	U
66	1	117	G
66	1	120	A
66	1	122	G
66	1	238	C
66	1	250	U
66	1	428	U
66	1	656	A
66	1	866	C
66	1	867	U
66	1	869	G
66	1	870	A
66	1	992	C
66	1	1035	G
66	1	1288	U
66	1	1303	A
66	1	1363	U
66	1	1364	C
66	1	1657	A
66	1	1731	U
66	1	2341	G
66	1	2352	G
66	1	2359	A
66	1	2362	C
66	1	2364	G
66	1	2367	G
66	1	2409	A

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Mol	Chain	Res	Type
66	1	2455	A
66	1	2551	A
66	1	2664	A
66	1	2733	5MC
66	1	2986	U
66	1	3021	U
67	2	464	A
67	2	688	A
67	2	1106	C
67	2	1502	C

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

165 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	$\# Z > 2$
66	4AC	1	1557	66	21,24,25	1.01	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	1048	66	21,24,25	1.09	2 (9%)	29,34,37	1.34	3 (10%)
66	4AC	1	451	66	21,24,25	1.06	2 (9%)	29,34,37	1.37	4 (13%)
67	4AC	2	636	67	21,24,25	1.02	2 (9%)	29,34,37	1.54	4 (13%)
66	4AC	1	314	66	21,24,25	1.07	2 (9%)	29,34,37	1.25	4 (13%)
66	4AC	1	1550	66	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
67	OMU	2	787	67	19,22,23	1.22	2 (10%)	26,31,34	1.86	6 (23%)
1	4AC	3	32	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
66	4AC	1	2287	66	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
67	OMG	2	467	67	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
67	4AC	2	1233	67	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
67	OMU	2	20	67	19,22,23	1.26	3 (15%)	26,31,34	1.77	5 (19%)
66	4AC	1	161	66	21,24,25	1.05	2 (9%)	29,34,37	1.31	4 (13%)
67	OMG	2	913	67	23,26,27	1.21	3 (13%)	33,38,41	1.96	6 (18%)
66	4AC	1	2027	66	21,24,25	1.05	2 (9%)	29,34,37	1.24	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	4AC	2	1184	67	21,24,25	1.05	2 (9%)	29,34,37	1.45	4 (13%)
66	4AC	1	2718	66	21,24,25	1.04	2 (9%)	29,34,37	1.28	4 (13%)
67	5MC	2	1374	67	18,22,23	0.91	2 (11%)	26,32,35	1.12	2 (7%)
67	4AC	2	851	67	21,24,25	1.05	2 (9%)	29,34,37	1.32	4 (13%)
66	4AC	1	1068	66	21,24,25	1.09	2 (9%)	29,34,37	1.36	5 (17%)
66	4AC	1	694	66	21,24,25	1.03	2 (9%)	29,34,37	1.27	4 (13%)
66	5MC	1	2203	66	18,22,23	0.92	2 (11%)	26,32,35	1.18	2 (7%)
67	OMG	2	471	67	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
67	OMU	2	830	67	19,22,23	1.26	4 (21%)	26,31,34	1.69	5 (19%)
2	OMC	4	32	2	19,22,23	0.82	0	26,31,34	0.73	0
66	OMG	1	2678	66	23,26,27	1.22	4 (17%)	33,38,41	1.92	6 (18%)
66	4AC	1	2992	66	21,24,25	1.04	2 (9%)	29,34,37	0.88	1 (3%)
67	4AC	2	319	67	21,24,25	1.05	2 (9%)	29,34,37	1.29	4 (13%)
66	4AC	1	1878	66	21,24,25	1.06	2 (9%)	29,34,37	1.53	4 (13%)
66	4AC	1	60	66	21,24,25	1.01	2 (9%)	29,34,37	1.40	5 (17%)
67	B8H	2	938	67	19,22,23	0.57	0	22,32,35	0.62	0
67	LHH	2	250	67	22,25,26	0.33	0	29,35,38	0.48	0
67	OMG	2	680	67	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
66	OMG	1	789	66	23,26,27	1.27	3 (13%)	33,38,41	2.00	6 (18%)
67	5MC	2	535	67	18,22,23	0.93	2 (11%)	26,32,35	1.15	3 (11%)
67	5MC	2	1498	67	18,22,23	0.93	2 (11%)	26,32,35	1.30	4 (15%)
67	OMG	2	657	67	23,26,27	1.23	3 (13%)	33,38,41	1.97	6 (18%)
66	4AC	1	3004	66	21,24,25	1.06	2 (9%)	29,34,37	1.23	4 (13%)
66	4AC	1	1621	66	21,24,25	1.08	2 (9%)	29,34,37	1.32	4 (13%)
66	4AC	1	22	66	21,24,25	1.05	2 (9%)	29,34,37	1.39	4 (13%)
66	4AC	1	1667	66	21,24,25	1.06	2 (9%)	29,34,37	1.30	4 (13%)
67	4AC	2	303	67	21,24,25	1.04	2 (9%)	29,34,37	1.31	4 (13%)
66	4AC	1	243	66	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
66	OMC	1	1948	66	19,22,23	0.76	0	26,31,34	0.76	0
67	4AC	2	626	67	21,24,25	1.02	2 (9%)	29,34,37	1.40	4 (13%)
66	4AC	1	1460	66	21,24,25	1.04	2 (9%)	29,34,37	1.29	4 (13%)
66	4AC	1	1662	66	21,24,25	1.00	2 (9%)	29,34,37	1.32	4 (13%)
66	4AC	1	1938	66	21,24,25	1.11	2 (9%)	29,34,37	1.32	5 (17%)
66	OMG	1	2144	66	23,26,27	1.21	3 (13%)	33,38,41	1.99	6 (18%)
66	OMU	1	2784	66	19,22,23	1.20	2 (10%)	26,31,34	1.74	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	A2M	2	373	67	22,25,26	1.44	4 (18%)	31,36,39	2.06	8 (25%)
67	4AC	2	957	67	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
67	4AC	2	718	67	21,24,25	1.02	2 (9%)	29,34,37	1.26	4 (13%)
66	4AC	1	2570	66	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
66	OMG	1	2147	66	23,26,27	1.21	3 (13%)	33,38,41	1.88	6 (18%)
66	4AC	1	1554	66	21,24,25	1.07	2 (9%)	29,34,37	1.24	4 (13%)
67	4AC	2	868	67	21,24,25	1.03	2 (9%)	29,34,37	1.29	4 (13%)
66	4AC	1	2865	66	21,24,25	1.04	2 (9%)	29,34,37	1.28	4 (13%)
66	4AC	1	2908	66	21,24,25	1.06	2 (9%)	29,34,37	1.28	4 (13%)
67	OMC	2	1040	67	19,22,23	0.81	0	26,31,34	0.89	1 (3%)
66	4AC	1	1934	66	21,24,25	1.06	2 (9%)	29,34,37	1.30	4 (13%)
67	4AC	2	1239	67	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
66	4AC	1	2495	66	21,24,25	1.09	2 (9%)	29,34,37	1.35	5 (17%)
66	A2M	1	1055	66	22,25,26	1.44	4 (18%)	31,36,39	2.10	8 (25%)
67	OMG	2	519	67	23,26,27	1.17	3 (13%)	33,38,41	2.01	7 (21%)
66	4AC	1	2585	66	21,24,25	1.07	2 (9%)	29,34,37	1.79	5 (17%)
66	4AC	1	2960	66	21,24,25	1.05	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	802	66	21,24,25	1.05	2 (9%)	29,34,37	1.28	4 (13%)
66	4AC	1	829	66	21,24,25	1.04	2 (9%)	29,34,37	1.31	4 (13%)
67	4AC	2	828	67	21,24,25	1.03	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	211	66	21,24,25	1.08	2 (9%)	29,34,37	1.30	4 (13%)
67	OMG	2	1069	67	23,26,27	1.18	3 (13%)	33,38,41	1.95	6 (18%)
66	4AC	1	1695	66	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
2	5MU	4	54	2	19,22,23	1.43	6 (31%)	28,32,35	2.04	5 (17%)
2	PSU	4	55	2	18,21,22	1.38	3 (16%)	22,30,33	2.31	7 (31%)
66	4AC	1	922	66	21,24,25	1.07	2 (9%)	29,34,37	1.40	4 (13%)
66	4AC	1	2249	66	21,24,25	1.10	2 (9%)	29,34,37	1.38	4 (13%)
67	MA6	2	1488	67	23,26,27	1.45	5 (21%)	34,38,41	2.11	10 (29%)
67	OMG	2	873	67	23,26,27	1.20	3 (13%)	33,38,41	1.98	6 (18%)
66	5MC	1	2093	66	18,22,23	0.96	2 (11%)	26,32,35	1.12	2 (7%)
66	4AC	1	91	66	21,24,25	1.04	2 (9%)	29,34,37	1.45	4 (13%)
67	UR3	2	1467	67	19,22,23	0.92	0	26,32,35	1.41	3 (11%)
66	4AC	1	136	66	21,24,25	1.06	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	2136	66	21,24,25	1.06	2 (9%)	29,34,37	1.44	5 (17%)
66	4AC	1	2937	68,66	21,24,25	1.05	2 (9%)	29,34,37	1.47	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	LHH	2	1041	67	21,24,26	0.33	0	29,34,38	0.35	0
67	4AC	2	751	67	21,24,25	1.04	2 (9%)	29,34,37	1.31	4 (13%)
66	5MC	1	2163	66	18,22,23	0.95	2 (11%)	26,32,35	1.17	3 (11%)
67	4AC	2	731	67	21,24,25	1.05	2 (9%)	29,34,37	1.33	4 (13%)
67	6MZ	2	1469	68,67	22,25,26	1.48	4 (18%)	30,36,39	2.18	9 (30%)
66	4AC	1	357	66	21,24,25	1.08	2 (9%)	29,34,37	1.25	4 (13%)
67	4AC	2	590	67	21,24,25	1.02	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	981	66	21,24,25	1.03	2 (9%)	29,34,37	1.19	4 (13%)
66	5MC	1	2733	66	18,22,23	0.96	2 (11%)	26,32,35	1.30	3 (11%)
67	5MC	2	1496	67	18,22,23	0.94	2 (11%)	26,32,35	1.16	3 (11%)
66	4AC	1	2966	66	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
66	4AC	1	1873	66	21,24,25	1.08	2 (9%)	29,34,37	1.29	4 (13%)
66	OMG	1	923	68,66	23,26,27	1.20	3 (13%)	33,38,41	1.98	8 (24%)
66	4AC	1	1867	66	21,24,25	1.03	2 (9%)	29,34,37	1.29	4 (13%)
67	4AC	2	17	67	21,24,25	1.04	2 (9%)	29,34,37	1.35	4 (13%)
66	4AC	1	2545	66	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
66	4AC	1	2062	66	21,24,25	1.05	2 (9%)	29,34,37	1.27	4 (13%)
2	H2U	4	20	2	18,21,22	0.98	2 (11%)	21,30,33	2.01	5 (23%)
66	4AC	1	2329	66	21,24,25	1.05	2 (9%)	29,34,37	1.36	4 (13%)
67	4AC	2	703	67	21,24,25	1.03	2 (9%)	29,34,37	1.46	4 (13%)
66	4AC	1	1617	66	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
66	4AC	1	533	66	21,24,25	1.07	2 (9%)	29,34,37	1.37	4 (13%)
66	4AC	1	1222	68,66	21,24,25	1.06	2 (9%)	29,34,37	1.21	4 (13%)
66	4AC	1	341	66	21,24,25	1.06	2 (9%)	29,34,37	1.30	4 (13%)
66	4AC	1	2608	66	21,24,25	1.08	2 (9%)	29,34,37	1.77	5 (17%)
66	4AC	1	2925	66	21,24,25	1.07	2 (9%)	29,34,37	1.32	4 (13%)
67	4AC	2	379	67	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
66	4AC	1	2642	66	21,24,25	1.05	2 (9%)	29,34,37	1.29	4 (13%)
67	OMU	2	774	67	19,22,23	1.23	3 (15%)	26,31,34	1.70	4 (15%)
67	OMU	2	64	67	19,22,23	1.25	4 (21%)	26,31,34	1.68	5 (19%)
67	OMU	2	1177	67	19,22,23	1.25	3 (15%)	26,31,34	1.72	4 (15%)
66	4AC	1	1065	66	21,24,25	1.05	2 (9%)	29,34,37	1.33	4 (13%)
66	4AC	1	1293	66	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
67	4AC	2	839	67	21,24,25	1.04	2 (9%)	29,34,37	1.38	4 (13%)
67	4AC	2	1479	67	21,24,25	0.99	2 (9%)	29,34,37	1.27	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	5MC	2	875	67	18,22,23	0.91	2 (11%)	26,32,35	1.13	3 (11%)
67	OMC	2	1036	67	19,22,23	0.80	0	26,31,34	0.79	0
66	4AC	1	1765	66	21,24,25	1.06	2 (9%)	29,34,37	1.28	4 (13%)
66	4AC	1	1962	66	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
67	4AC	2	1147	67	21,24,25	1.05	2 (9%)	29,34,37	1.56	5 (17%)
67	OMC	2	773	67	19,22,23	0.81	0	26,31,34	0.81	0
66	OMG	1	2138	66	23,26,27	1.20	3 (13%)	33,38,41	1.90	6 (18%)
66	4AC	1	835	66	21,24,25	1.08	2 (9%)	29,34,37	1.28	5 (17%)
66	5MC	1	2198	66	18,22,23	0.88	2 (11%)	26,32,35	1.10	2 (7%)
67	4AC	2	511	67	21,24,25	1.04	2 (9%)	29,34,37	1.40	4 (13%)
67	OMU	2	1380	67	19,22,23	1.33	3 (15%)	26,31,34	1.75	4 (15%)
66	4AC	1	458	66	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
67	4AC	2	286	67	21,24,25	1.04	2 (9%)	29,34,37	1.36	4 (13%)
2	4SU	4	8	2	18,21,22	1.80	5 (27%)	26,30,33	2.25	5 (19%)
66	4AC	1	1780	66	21,24,25	1.07	2 (9%)	29,34,37	1.80	5 (17%)
66	4AC	1	2083	66	21,24,25	1.12	2 (9%)	29,34,37	1.24	2 (6%)
66	OMG	1	328	66	23,26,27	1.22	3 (13%)	33,38,41	1.97	6 (18%)
66	5MC	1	2183	66	18,22,23	0.93	2 (11%)	26,32,35	1.09	2 (7%)
67	MA6	2	1487	67	23,26,27	1.48	5 (21%)	34,38,41	2.12	11 (32%)
67	OMC	2	129	67	19,22,23	0.81	0	26,31,34	0.81	0
67	5MC	2	1505	67	18,22,23	0.97	2 (11%)	26,32,35	1.38	4 (15%)
67	4AC	2	394	67	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
67	5MC	2	693	67	18,22,23	0.93	2 (11%)	26,32,35	1.17	3 (11%)
66	4AC	1	1755	66	21,24,25	1.07	2 (9%)	29,34,37	1.76	4 (13%)
67	4AC	2	546	67	21,24,25	1.03	2 (9%)	29,34,37	1.27	4 (13%)
66	OMC	1	615	66	19,22,23	0.77	0	26,31,34	0.73	0
67	OMC	2	846	67	19,22,23	0.81	0	26,31,34	0.79	0
66	5MC	1	2162	66	18,22,23	0.95	2 (11%)	26,32,35	1.28	4 (15%)
67	OMG	2	934	67	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
67	4AC	2	848	67	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
66	4AC	1	641	66	21,24,25	1.07	2 (9%)	29,34,37	1.34	4 (13%)
66	LHH	1	616	66	22,25,26	0.33	0	29,35,38	0.41	0
67	4AC	2	1028	67	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
67	5MC	2	1202	67	18,22,23	0.97	2 (11%)	26,32,35	1.14	3 (11%)
66	A2M	1	2173	66	22,25,26	1.46	4 (18%)	31,36,39	2.02	8 (25%)
67	4AC	2	479	67	21,24,25	1.02	2 (9%)	29,34,37	1.40	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	4AC	2	53	67	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
66	4AC	1	2548	66	21,24,25	1.03	2 (9%)	29,34,37	1.39	4 (13%)
66	4AC	1	229	66	21,24,25	1.10	2 (9%)	29,34,37	1.32	3 (10%)
66	4AC	1	1885	66	21,24,25	1.04	2 (9%)	29,34,37	1.22	4 (13%)
66	4AC	1	1594	68,66	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
67	5MC	2	1025	67	18,22,23	0.93	2 (11%)	26,32,35	1.08	2 (7%)
66	4AC	1	2001	66	21,24,25	1.07	2 (9%)	29,34,37	1.31	4 (13%)
66	4AC	1	1243	66	21,24,25	1.06	2 (9%)	29,34,37	1.35	4 (13%)
67	OMC	2	1376	67	19,22,23	0.79	0	26,31,34	0.76	0

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
66	4AC	1	1557	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1048	66	-	0/11/29/30	0/2/2/2
66	4AC	1	451	66	-	0/11/29/30	0/2/2/2
67	4AC	2	636	67	-	0/11/29/30	0/2/2/2
66	4AC	1	314	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1550	66	-	0/11/29/30	0/2/2/2
67	OMU	2	787	67	-	4/9/27/28	0/2/2/2
1	4AC	3	32	1	-	2/11/29/30	0/2/2/2
66	4AC	1	2287	66	-	0/11/29/30	0/2/2/2
67	OMG	2	467	67	-	0/9/27/28	0/3/3/3
67	4AC	2	1233	67	-	0/11/29/30	0/2/2/2
67	OMU	2	20	67	-	5/9/27/28	0/2/2/2
66	4AC	1	161	66	-	0/11/29/30	0/2/2/2
67	OMG	2	913	67	-	0/9/27/28	0/3/3/3
66	4AC	1	2027	66	-	0/11/29/30	0/2/2/2
67	4AC	2	1184	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2718	66	-	0/11/29/30	0/2/2/2
67	5MC	2	1374	67	-	0/7/25/26	0/2/2/2
67	4AC	2	851	67	-	0/11/29/30	0/2/2/2
66	4AC	1	1068	66	-	0/11/29/30	0/2/2/2
66	4AC	1	694	66	-	0/11/29/30	0/2/2/2
66	5MC	1	2203	66	-	0/7/25/26	0/2/2/2
67	OMG	2	471	67	-	0/9/27/28	0/3/3/3
67	OMU	2	830	67	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	4	32	2	-	0/9/27/28	0/2/2/2
66	OMG	1	2678	66	-	0/9/27/28	0/3/3/3
66	4AC	1	2992	66	-	2/11/29/30	0/2/2/2
67	4AC	2	319	67	-	0/11/29/30	0/2/2/2
66	4AC	1	1878	66	-	0/11/29/30	0/2/2/2
66	4AC	1	60	66	-	0/11/29/30	0/2/2/2
67	B8H	2	938	67	-	0/7/25/26	0/2/2/2
67	LHH	2	250	67	-	0/13/31/32	0/2/2/2
67	OMG	2	680	67	-	0/9/27/28	0/3/3/3
66	OMG	1	789	66	-	2/9/27/28	0/3/3/3
67	5MC	2	535	67	-	0/7/25/26	0/2/2/2
67	5MC	2	1498	67	-	4/7/25/26	0/2/2/2
67	OMG	2	657	67	-	0/9/27/28	0/3/3/3
66	4AC	1	3004	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1621	66	-	0/11/29/30	0/2/2/2
66	4AC	1	22	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1667	66	-	0/11/29/30	0/2/2/2
67	4AC	2	303	67	-	0/11/29/30	0/2/2/2
66	4AC	1	243	66	-	0/11/29/30	0/2/2/2
66	OMC	1	1948	66	-	0/9/27/28	0/2/2/2
67	4AC	2	626	67	-	0/11/29/30	0/2/2/2
66	4AC	1	1460	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1662	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1938	66	-	0/11/29/30	0/2/2/2
66	OMG	1	2144	66	-	0/9/27/28	0/3/3/3
66	OMU	1	2784	66	-	0/9/27/28	0/2/2/2
67	A2M	2	373	67	-	0/9/27/28	0/3/3/3
67	4AC	2	957	67	-	0/11/29/30	0/2/2/2
67	4AC	2	718	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2570	66	-	0/11/29/30	0/2/2/2
66	OMG	1	2147	66	-	2/9/27/28	0/3/3/3
66	4AC	1	1554	66	-	0/11/29/30	0/2/2/2
67	4AC	2	868	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2865	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2908	66	-	0/11/29/30	0/2/2/2
67	OMC	2	1040	67	-	0/9/27/28	0/2/2/2
66	4AC	1	1934	66	-	0/11/29/30	0/2/2/2
67	4AC	2	1239	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2495	66	-	0/11/29/30	0/2/2/2
66	A2M	1	1055	66	-	0/9/27/28	0/3/3/3
67	OMG	2	519	67	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	4AC	1	2585	66	-	3/11/29/30	0/2/2/2
66	4AC	1	2960	66	-	0/11/29/30	0/2/2/2
66	4AC	1	802	66	-	0/11/29/30	0/2/2/2
66	4AC	1	829	66	-	0/11/29/30	0/2/2/2
67	4AC	2	828	67	-	0/11/29/30	0/2/2/2
66	4AC	1	211	66	-	0/11/29/30	0/2/2/2
67	OMG	2	1069	67	-	1/9/27/28	0/3/3/3
66	4AC	1	1695	66	-	0/11/29/30	0/2/2/2
2	5MU	4	54	2	-	0/7/25/26	0/2/2/2
2	PSU	4	55	2	-	2/7/25/26	0/2/2/2
66	4AC	1	922	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2249	66	-	0/11/29/30	0/2/2/2
67	MA6	2	1488	67	-	2/11/29/30	0/3/3/3
67	OMG	2	873	67	-	1/9/27/28	0/3/3/3
66	5MC	1	2093	66	-	0/7/25/26	0/2/2/2
66	4AC	1	91	66	-	0/11/29/30	0/2/2/2
67	UR3	2	1467	67	-	0/7/25/26	0/2/2/2
66	4AC	1	136	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2136	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2937	68,66	-	1/11/29/30	0/2/2/2
67	LHH	2	1041	67	-	0/11/29/32	0/2/2/2
67	4AC	2	751	67	-	0/11/29/30	0/2/2/2
66	5MC	1	2163	66	-	0/7/25/26	0/2/2/2
67	4AC	2	731	67	-	0/11/29/30	0/2/2/2
67	6MZ	2	1469	68,67	-	0/9/27/28	0/3/3/3
66	4AC	1	357	66	-	0/11/29/30	0/2/2/2
67	4AC	2	590	67	-	0/11/29/30	0/2/2/2
66	4AC	1	981	66	-	0/11/29/30	0/2/2/2
66	5MC	1	2733	66	-	5/7/25/26	0/2/2/2
67	5MC	2	1496	67	-	0/7/25/26	0/2/2/2
66	4AC	1	2966	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1873	66	-	0/11/29/30	0/2/2/2
66	OMG	1	923	68,66	-	0/9/27/28	0/3/3/3
66	4AC	1	1867	66	-	0/11/29/30	0/2/2/2
67	4AC	2	17	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2545	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2062	66	-	0/11/29/30	0/2/2/2
2	H2U	4	20	2	-	3/7/38/39	0/2/2/2
66	4AC	1	2329	66	-	0/11/29/30	0/2/2/2
67	4AC	2	703	67	-	0/11/29/30	0/2/2/2
66	4AC	1	1617	66	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	4AC	1	533	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1222	68,66	-	0/11/29/30	0/2/2/2
66	4AC	1	341	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2608	66	-	3/11/29/30	0/2/2/2
66	4AC	1	2925	66	-	0/11/29/30	0/2/2/2
67	4AC	2	379	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2642	66	-	0/11/29/30	0/2/2/2
67	OMU	2	774	67	-	0/9/27/28	0/2/2/2
67	OMU	2	64	67	-	0/9/27/28	0/2/2/2
67	OMU	2	1177	67	-	0/9/27/28	0/2/2/2
66	4AC	1	1065	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1293	66	-	0/11/29/30	0/2/2/2
67	4AC	2	839	67	-	0/11/29/30	0/2/2/2
67	4AC	2	1479	67	-	0/11/29/30	0/2/2/2
67	5MC	2	875	67	-	0/7/25/26	0/2/2/2
67	OMC	2	1036	67	-	0/9/27/28	0/2/2/2
66	4AC	1	1765	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1962	66	-	0/11/29/30	0/2/2/2
67	4AC	2	1147	67	-	1/11/29/30	0/2/2/2
67	OMC	2	773	67	-	0/9/27/28	0/2/2/2
66	OMG	1	2138	66	-	0/9/27/28	0/3/3/3
66	4AC	1	835	66	-	0/11/29/30	0/2/2/2
66	5MC	1	2198	66	-	0/7/25/26	0/2/2/2
67	4AC	2	511	67	-	0/11/29/30	0/2/2/2
67	OMU	2	1380	67	-	0/9/27/28	0/2/2/2
66	4AC	1	458	66	-	0/11/29/30	0/2/2/2
67	4AC	2	286	67	-	0/11/29/30	0/2/2/2
2	4SU	4	8	2	-	2/7/25/26	0/2/2/2
66	4AC	1	1780	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2083	66	-	0/11/29/30	0/2/2/2
66	OMG	1	328	66	-	0/9/27/28	0/3/3/3
66	5MC	1	2183	66	-	0/7/25/26	0/2/2/2
67	MA6	2	1487	67	-	0/11/29/30	0/3/3/3
67	OMC	2	129	67	-	0/9/27/28	0/2/2/2
67	5MC	2	1505	67	-	2/7/25/26	0/2/2/2
67	4AC	2	394	67	-	0/11/29/30	0/2/2/2
67	5MC	2	693	67	-	0/7/25/26	0/2/2/2
66	4AC	1	1755	66	-	0/11/29/30	0/2/2/2
67	4AC	2	546	67	-	0/11/29/30	0/2/2/2
66	OMC	1	615	66	-	0/9/27/28	0/2/2/2
67	OMC	2	846	67	-	0/9/27/28	0/2/2/2
66	5MC	1	2162	66	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	OMG	2	934	67	-	0/9/27/28	0/3/3/3
67	4AC	2	848	67	-	0/11/29/30	0/2/2/2
66	4AC	1	641	66	-	0/11/29/30	0/2/2/2
66	LHH	1	616	66	-	0/13/31/32	0/2/2/2
67	4AC	2	1028	67	-	0/11/29/30	0/2/2/2
67	5MC	2	1202	67	-	1/7/25/26	0/2/2/2
66	A2M	1	2173	66	-	0/9/27/28	0/3/3/3
67	4AC	2	479	67	-	0/11/29/30	0/2/2/2
67	4AC	2	53	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2548	66	-	0/11/29/30	0/2/2/2
66	4AC	1	229	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1885	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1594	68,66	-	0/11/29/30	0/2/2/2
67	5MC	2	1025	67	-	0/7/25/26	0/2/2/2
66	4AC	1	2001	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1243	66	-	0/11/29/30	0/2/2/2
67	OMC	2	1376	67	-	0/9/27/28	0/2/2/2

All (349) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	8	4SU	C4-S4	-4.63	1.59	1.68
67	2	1469	6MZ	C5-C4	4.58	1.47	1.39
66	1	1055	A2M	C5-C4	4.33	1.47	1.39
67	2	1487	MA6	C5-C4	4.31	1.47	1.39
67	2	373	A2M	C5-C4	4.27	1.47	1.39
66	1	2173	A2M	C5-C4	4.26	1.47	1.39
67	2	1488	MA6	C5-C4	4.19	1.46	1.39
2	4	8	4SU	C4-N3	-3.37	1.34	1.37
66	1	2083	4AC	C5-C4	3.20	1.47	1.40
66	1	314	4AC	C5-C4	3.13	1.47	1.40
66	1	229	4AC	C5-C4	3.13	1.47	1.40
66	1	1048	4AC	C5-C4	3.13	1.47	1.40
66	1	1621	4AC	C5-C4	3.13	1.47	1.40
66	1	1765	4AC	C5-C4	3.11	1.47	1.40
66	1	1222	4AC	C5-C4	3.10	1.47	1.40
66	1	357	4AC	C5-C4	3.10	1.47	1.40
66	1	1873	4AC	C5-C4	3.10	1.47	1.40
66	1	341	4AC	C5-C4	3.09	1.47	1.40
67	2	1380	OMU	C4-N3	-3.09	1.33	1.38
66	1	2908	4AC	C5-C4	3.09	1.47	1.40
67	2	657	OMG	C5-C4	3.09	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	1	1938	4AC	C5-C4	3.08	1.47	1.40
66	1	835	4AC	C5-C4	3.08	1.47	1.40
66	1	1934	4AC	C5-C4	3.08	1.47	1.40
66	1	2001	4AC	C5-C4	3.07	1.47	1.40
66	1	211	4AC	C5-C4	3.07	1.47	1.40
66	1	2960	4AC	C5-C4	3.07	1.47	1.40
67	2	1239	4AC	C5-C4	3.06	1.47	1.40
66	1	533	4AC	C5-C4	3.05	1.47	1.40
66	1	136	4AC	C5-C4	3.05	1.47	1.40
66	1	2992	4AC	C5-C4	3.05	1.47	1.40
66	1	2495	4AC	C5-C4	3.04	1.47	1.40
67	2	590	4AC	C5-C4	3.04	1.47	1.40
67	2	828	4AC	C5-C4	3.04	1.47	1.40
66	1	2249	4AC	C5-C4	3.04	1.47	1.40
67	2	17	4AC	C5-C4	3.04	1.47	1.40
66	1	1065	4AC	C5-C4	3.03	1.47	1.40
66	1	3004	4AC	C5-C4	3.02	1.47	1.40
66	1	1867	4AC	C5-C4	3.02	1.47	1.40
66	1	1554	4AC	C5-C4	3.01	1.47	1.40
66	1	641	4AC	C5-C4	3.01	1.47	1.40
66	1	243	4AC	C5-C4	3.01	1.47	1.40
66	1	451	4AC	C5-C4	3.01	1.47	1.40
67	2	751	4AC	C5-C4	3.00	1.47	1.40
66	1	1695	4AC	C5-C4	3.00	1.47	1.40
66	1	2718	4AC	C5-C4	3.00	1.47	1.40
66	1	2062	4AC	C5-C4	2.99	1.47	1.40
67	2	1233	4AC	C5-C4	2.99	1.47	1.40
66	1	328	OMG	C5-C4	2.99	1.47	1.38
66	1	829	4AC	C5-C4	2.99	1.47	1.40
2	4	55	PSU	C6-C5	2.99	1.38	1.35
66	1	1667	4AC	C5-C4	2.99	1.47	1.40
67	2	471	OMG	C5-C4	2.98	1.47	1.38
67	2	303	4AC	C5-C4	2.98	1.47	1.40
66	1	2329	4AC	C5-C4	2.98	1.47	1.40
66	1	802	4AC	C5-C4	2.98	1.47	1.40
67	2	546	4AC	C5-C4	2.98	1.47	1.40
67	2	511	4AC	C5-C4	2.97	1.47	1.40
67	2	934	OMG	C5-C4	2.97	1.47	1.38
67	2	851	4AC	C5-C4	2.97	1.47	1.40
66	1	2642	4AC	C5-C4	2.97	1.47	1.40
67	2	1028	4AC	C5-C4	2.96	1.47	1.40
67	2	286	4AC	C5-C4	2.96	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	1	1878	4AC	C5-C4	2.96	1.47	1.40
66	1	1594	4AC	C5-C4	2.95	1.47	1.40
67	2	379	4AC	C5-C4	2.95	1.47	1.40
66	1	1068	4AC	C5-C4	2.95	1.47	1.40
67	2	680	OMG	C5-C4	2.95	1.47	1.38
66	1	1550	4AC	C5-C4	2.95	1.47	1.40
67	2	731	4AC	C5-C4	2.95	1.47	1.40
66	1	2570	4AC	C5-C4	2.95	1.47	1.40
66	1	2138	OMG	C5-C4	2.95	1.47	1.38
66	1	161	4AC	C5-C4	2.95	1.47	1.40
67	2	913	OMG	C5-C4	2.95	1.46	1.38
66	1	2027	4AC	C5-C4	2.94	1.47	1.40
67	2	868	4AC	C5-C4	2.94	1.47	1.40
66	1	1243	4AC	C5-C4	2.94	1.47	1.40
67	2	957	4AC	C5-C4	2.94	1.47	1.40
66	1	1293	4AC	C5-C4	2.94	1.47	1.40
67	2	319	4AC	C5-C4	2.94	1.47	1.40
66	1	2136	4AC	C5-C4	2.93	1.47	1.40
66	1	2925	4AC	C5-C4	2.93	1.47	1.40
66	1	981	4AC	C5-C4	2.92	1.47	1.40
66	1	22	4AC	C5-C4	2.92	1.47	1.40
66	1	458	4AC	C5-C4	2.92	1.47	1.40
67	2	479	4AC	C5-C4	2.92	1.47	1.40
66	1	694	4AC	C5-C4	2.92	1.47	1.40
67	2	394	4AC	C5-C4	2.91	1.47	1.40
66	1	1460	4AC	C5-C4	2.91	1.47	1.40
66	1	1962	4AC	C5-C4	2.91	1.47	1.40
66	1	2966	4AC	C5-C4	2.90	1.47	1.40
66	1	2548	4AC	C5-C4	2.90	1.47	1.40
66	1	2144	OMG	C5-C4	2.90	1.46	1.38
66	1	2287	4AC	C5-C4	2.89	1.47	1.40
67	2	636	4AC	C5-C4	2.89	1.47	1.40
67	2	53	4AC	C5-C4	2.89	1.47	1.40
67	2	467	OMG	C5-C4	2.89	1.46	1.38
66	1	2865	4AC	C5-C4	2.89	1.47	1.40
66	1	1885	4AC	C5-C4	2.89	1.47	1.40
66	1	2147	OMG	C5-C4	2.89	1.46	1.38
66	1	60	4AC	C5-C4	2.88	1.47	1.40
67	2	1184	4AC	C5-C4	2.88	1.47	1.40
67	2	1069	OMG	C5-C4	2.87	1.46	1.38
67	2	703	4AC	C5-C4	2.87	1.47	1.40
66	1	2733	5MC	C6-C5	2.86	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	1	1617	4AC	C5-C4	2.86	1.47	1.40
67	2	626	4AC	C5-C4	2.86	1.47	1.40
67	2	873	OMG	C5-C4	2.86	1.46	1.38
66	1	922	4AC	C5-C4	2.86	1.46	1.40
66	1	2545	4AC	C5-C4	2.86	1.46	1.40
67	2	1202	5MC	C6-C5	2.85	1.39	1.34
67	2	471	OMG	C6-N1	-2.85	1.33	1.38
66	1	923	OMG	C5-C4	2.85	1.46	1.38
66	1	1557	4AC	C5-C4	2.84	1.46	1.40
67	2	848	4AC	C5-C4	2.84	1.46	1.40
67	2	787	OMU	C4-N3	-2.84	1.33	1.38
67	2	718	4AC	C5-C4	2.83	1.46	1.40
67	2	20	OMU	C4-N3	-2.82	1.33	1.38
66	1	2937	4AC	C5-C4	2.81	1.46	1.40
1	3	32	4AC	C5-C4	2.81	1.46	1.40
66	1	2678	OMG	C6-N1	-2.81	1.33	1.38
66	1	789	OMG	C5-C4	2.81	1.46	1.38
67	2	1469	6MZ	C5-C6	2.80	1.49	1.41
67	2	1487	MA6	C5-C6	2.80	1.48	1.41
67	2	519	OMG	C5-C4	2.80	1.46	1.38
66	1	1662	4AC	C5-C4	2.78	1.46	1.40
66	1	2093	5MC	C6-C5	2.78	1.39	1.34
67	2	1479	4AC	C5-C4	2.78	1.46	1.40
67	2	1147	4AC	C5-C4	2.77	1.46	1.40
67	2	467	OMG	C6-N1	-2.75	1.33	1.38
67	2	1488	MA6	C5-C6	2.75	1.48	1.41
66	1	2083	4AC	C4-N3	-2.75	1.28	1.32
66	1	2144	OMG	C6-N1	-2.75	1.33	1.38
67	2	839	4AC	C5-C4	2.75	1.46	1.40
67	2	873	OMG	C6-N1	-2.75	1.33	1.38
66	1	2678	OMG	C5-C4	2.75	1.46	1.38
67	2	1505	5MC	C6-C5	2.74	1.39	1.34
66	1	2608	4AC	C4-N3	-2.74	1.28	1.32
66	1	91	4AC	C5-C4	2.74	1.46	1.40
66	1	2784	OMU	C4-N3	-2.74	1.33	1.38
66	1	2585	4AC	C4-N3	-2.74	1.28	1.32
67	2	657	OMG	C6-N1	-2.74	1.33	1.38
66	1	2138	OMG	C6-N1	-2.73	1.33	1.38
66	1	328	OMG	C6-N1	-2.73	1.33	1.38
66	1	2183	5MC	C6-C5	2.72	1.39	1.34
2	4	8	4SU	C5-C4	-2.72	1.39	1.42
67	2	774	OMU	C4-N3	-2.72	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	2	913	OMG	C6-N1	-2.72	1.33	1.38
66	1	923	OMG	C6-N1	-2.71	1.33	1.38
67	2	1177	OMU	C4-N3	-2.70	1.33	1.38
67	2	64	OMU	C4-N3	-2.70	1.33	1.38
66	1	1055	A2M	C5-C6	2.70	1.48	1.41
66	1	789	OMG	C6-N1	-2.69	1.33	1.38
2	4	54	5MU	C6-C5	2.69	1.39	1.34
66	1	229	4AC	C4-N3	-2.69	1.28	1.32
67	2	1496	5MC	C6-C5	2.67	1.39	1.34
67	2	830	OMU	C4-N3	-2.67	1.33	1.38
66	1	1755	4AC	C5-C4	2.66	1.46	1.40
67	2	1380	OMU	C2-N3	-2.66	1.33	1.38
67	2	20	OMU	C2-N3	-2.65	1.33	1.38
67	2	1374	5MC	C6-C5	2.65	1.39	1.34
2	4	54	5MU	C4-N3	-2.64	1.33	1.38
67	2	1025	5MC	C6-C5	2.62	1.38	1.34
66	1	2147	OMG	C6-N1	-2.61	1.34	1.38
66	1	2163	5MC	C6-C5	2.60	1.38	1.34
67	2	1069	OMG	C6-N1	-2.59	1.34	1.38
66	1	2249	4AC	C4-N3	-2.59	1.28	1.32
66	1	2173	A2M	C5-C6	2.59	1.48	1.41
66	1	2162	5MC	C6-C5	2.59	1.38	1.34
67	2	934	OMG	C6-N1	-2.59	1.34	1.38
66	1	1873	4AC	C4-N3	-2.58	1.28	1.32
67	2	680	OMG	C6-N1	-2.57	1.34	1.38
66	1	2203	5MC	C6-C5	2.57	1.38	1.34
66	1	1621	4AC	C4-N3	-2.57	1.28	1.32
66	1	1780	4AC	C5-C4	2.57	1.46	1.40
66	1	922	4AC	C4-N3	-2.57	1.28	1.32
67	2	657	OMG	C5-N7	-2.57	1.34	1.39
2	4	55	PSU	C4-N3	-2.57	1.34	1.38
67	2	373	A2M	C5-C6	2.57	1.48	1.41
67	2	693	5MC	C6-C5	2.56	1.38	1.34
66	1	1554	4AC	C4-N3	-2.56	1.28	1.32
67	2	787	OMU	C2-N3	-2.55	1.33	1.38
67	2	875	5MC	C6-C5	2.54	1.38	1.34
2	4	20	H2U	C4-N3	-2.54	1.33	1.37
66	1	3004	4AC	C4-N3	-2.54	1.28	1.32
67	2	519	OMG	C6-N1	-2.53	1.34	1.38
66	1	2495	4AC	C4-N3	-2.53	1.28	1.32
67	2	535	5MC	C6-C5	2.52	1.38	1.34
66	1	1885	4AC	C4-N3	-2.52	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	1	1068	4AC	C4-N3	-2.51	1.28	1.32
66	1	1938	4AC	C4-N3	-2.51	1.28	1.32
66	1	22	4AC	C4-N3	-2.51	1.28	1.32
66	1	211	4AC	C4-N3	-2.51	1.28	1.32
66	1	835	4AC	C4-N3	-2.50	1.28	1.32
66	1	1048	4AC	C4-N3	-2.50	1.28	1.32
66	1	2163	5MC	C6-N1	-2.50	1.33	1.38
67	2	1498	5MC	C6-N1	-2.50	1.33	1.38
66	1	2173	A2M	C5-N7	-2.50	1.34	1.39
66	1	2062	4AC	C4-N3	-2.49	1.28	1.32
66	1	1765	4AC	C4-N3	-2.48	1.28	1.32
66	1	2001	4AC	C4-N3	-2.48	1.28	1.32
66	1	2608	4AC	C5-C4	2.48	1.46	1.40
67	2	1505	5MC	C6-N1	-2.48	1.33	1.38
67	2	851	4AC	C4-N3	-2.48	1.28	1.32
66	1	2678	OMG	C5-N7	-2.47	1.34	1.39
66	1	2198	5MC	C6-C5	2.47	1.38	1.34
66	1	923	OMG	C5-N7	-2.47	1.34	1.39
67	2	319	4AC	C4-N3	-2.47	1.28	1.32
66	1	1243	4AC	C4-N3	-2.47	1.28	1.32
66	1	2784	OMU	C2-N3	-2.46	1.33	1.38
66	1	981	4AC	C4-N3	-2.46	1.28	1.32
67	2	1498	5MC	C6-C5	2.46	1.38	1.34
66	1	2162	5MC	C6-N1	-2.46	1.33	1.38
67	2	373	A2M	C5-N7	-2.45	1.34	1.39
66	1	2027	4AC	C4-N3	-2.45	1.28	1.32
66	1	1667	4AC	C4-N3	-2.45	1.28	1.32
66	1	641	4AC	C4-N3	-2.44	1.28	1.32
66	1	2585	4AC	C5-C4	2.44	1.46	1.40
2	4	20	H2U	C2-N3	-2.44	1.33	1.38
66	1	357	4AC	C4-N3	-2.44	1.28	1.32
67	2	535	5MC	C6-N1	-2.44	1.33	1.38
67	2	718	4AC	C4-N3	-2.43	1.28	1.32
66	1	2925	4AC	C4-N3	-2.43	1.28	1.32
67	2	848	4AC	C4-N3	-2.43	1.28	1.32
66	1	1934	4AC	C4-N3	-2.43	1.28	1.32
66	1	2908	4AC	C4-N3	-2.43	1.28	1.32
66	1	91	4AC	C4-N3	-2.41	1.28	1.32
66	1	314	4AC	C4-N3	-2.41	1.28	1.32
66	1	694	4AC	C4-N3	-2.41	1.28	1.32
66	1	136	4AC	C4-N3	-2.40	1.28	1.32
66	1	2548	4AC	C4-N3	-2.40	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	1	1594	4AC	C4-N3	-2.40	1.28	1.32
66	1	789	OMG	C5-N7	-2.39	1.34	1.39
67	2	286	4AC	C4-N3	-2.39	1.28	1.32
67	2	511	4AC	C4-N3	-2.39	1.28	1.32
2	4	54	5MU	C2-N1	2.39	1.42	1.38
67	2	839	4AC	C4-N3	-2.39	1.28	1.32
66	1	2203	5MC	C6-N1	-2.39	1.34	1.38
67	2	868	4AC	C4-N3	-2.38	1.28	1.32
67	2	731	4AC	C4-N3	-2.37	1.28	1.32
66	1	2144	OMG	C5-N7	-2.37	1.34	1.39
66	1	2093	5MC	C6-N1	-2.36	1.34	1.38
67	2	1177	OMU	C2-N3	-2.36	1.33	1.38
67	2	1496	5MC	C6-N1	-2.36	1.34	1.38
66	1	2642	4AC	C4-N3	-2.36	1.28	1.32
66	1	2147	OMG	C5-N7	-2.36	1.34	1.39
66	1	1460	4AC	C4-N3	-2.35	1.28	1.32
2	4	54	5MU	C4-C5	2.35	1.48	1.44
66	1	829	4AC	C4-N3	-2.35	1.28	1.32
66	1	2865	4AC	C4-N3	-2.35	1.28	1.32
67	2	17	4AC	C4-N3	-2.34	1.28	1.32
66	1	2136	4AC	C4-N3	-2.34	1.28	1.32
66	1	1557	4AC	C4-N3	-2.34	1.28	1.32
66	1	2992	4AC	C4-N3	-2.34	1.28	1.32
2	4	8	4SU	C2-N1	2.34	1.42	1.38
67	2	546	4AC	C4-N3	-2.34	1.28	1.32
66	1	2718	4AC	C4-N3	-2.33	1.28	1.32
67	2	471	OMG	C5-N7	-2.33	1.34	1.39
67	2	873	OMG	C5-N7	-2.32	1.34	1.39
66	1	2329	4AC	C4-N3	-2.32	1.28	1.32
66	1	451	4AC	C4-N3	-2.32	1.28	1.32
66	1	243	4AC	C4-N3	-2.31	1.28	1.32
66	1	1962	4AC	C4-N3	-2.31	1.28	1.32
66	1	802	4AC	C4-N3	-2.31	1.28	1.32
67	2	1488	MA6	C8-N7	2.31	1.36	1.31
66	1	1055	A2M	C5-N7	-2.31	1.34	1.39
66	1	1617	4AC	C4-N3	-2.31	1.28	1.32
66	1	161	4AC	C4-N3	-2.31	1.28	1.32
67	2	828	4AC	C4-N3	-2.30	1.28	1.32
67	2	467	OMG	C5-N7	-2.30	1.34	1.39
66	1	2183	5MC	C6-N1	-2.30	1.34	1.38
67	2	64	OMU	C2-N3	-2.29	1.33	1.38
66	1	2937	4AC	C4-N3	-2.29	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	1	2138	OMG	C5-N7	-2.29	1.34	1.39
67	2	875	5MC	C6-N1	-2.29	1.34	1.38
67	2	774	OMU	C2-N3	-2.29	1.33	1.38
66	1	341	4AC	C4-N3	-2.29	1.28	1.32
66	1	1867	4AC	C4-N3	-2.29	1.28	1.32
66	1	328	OMG	C5-N7	-2.28	1.34	1.39
67	2	1469	6MZ	C5-N7	-2.28	1.34	1.39
67	2	303	4AC	C4-N3	-2.28	1.28	1.32
66	1	2966	4AC	C4-N3	-2.28	1.28	1.32
67	2	693	5MC	C6-N1	-2.27	1.34	1.38
2	4	55	PSU	C2'-C1'	-2.27	1.50	1.53
66	1	2960	4AC	C4-N3	-2.27	1.28	1.32
67	2	1488	MA6	C5-N7	-2.27	1.34	1.39
67	2	751	4AC	C4-N3	-2.27	1.28	1.32
66	1	533	4AC	C4-N3	-2.27	1.28	1.32
67	2	1487	MA6	C8-N7	2.27	1.35	1.31
66	1	1065	4AC	C4-N3	-2.26	1.28	1.32
66	1	1878	4AC	C4-N3	-2.26	1.28	1.32
66	1	1222	4AC	C4-N3	-2.26	1.28	1.32
66	1	60	4AC	C4-N3	-2.26	1.28	1.32
66	1	2173	A2M	C8-N7	2.26	1.35	1.31
66	1	1662	4AC	C4-N3	-2.26	1.28	1.32
67	2	1374	5MC	C6-N1	-2.25	1.34	1.38
66	1	2545	4AC	C4-N3	-2.25	1.28	1.32
67	2	53	4AC	C4-N3	-2.25	1.28	1.32
67	2	680	OMG	C5-N7	-2.24	1.34	1.39
66	1	1293	4AC	C4-N3	-2.23	1.28	1.32
66	1	2198	5MC	C6-N1	-2.23	1.34	1.38
67	2	1025	5MC	C6-N1	-2.23	1.34	1.38
66	1	1550	4AC	C4-N3	-2.23	1.28	1.32
67	2	934	OMG	C5-N7	-2.22	1.34	1.39
67	2	830	OMU	C2-N3	-2.22	1.34	1.38
67	2	1487	MA6	C5-N7	-2.22	1.34	1.39
66	1	2678	OMG	C4-N9	-2.22	1.32	1.38
67	2	703	4AC	C4-N3	-2.22	1.29	1.32
67	2	957	4AC	C4-N3	-2.21	1.29	1.32
66	1	2570	4AC	C4-N3	-2.20	1.29	1.32
67	2	1479	4AC	C4-N3	-2.20	1.29	1.32
67	2	379	4AC	C4-N3	-2.20	1.29	1.32
66	1	1055	A2M	C8-N7	2.20	1.35	1.31
66	1	1695	4AC	C4-N3	-2.19	1.29	1.32
66	1	1755	4AC	C4-N3	-2.19	1.29	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	2	394	4AC	C4-N3	-2.19	1.29	1.32
67	2	1184	4AC	C4-N3	-2.19	1.29	1.32
67	2	590	4AC	C4-N3	-2.18	1.29	1.32
67	2	636	4AC	C4-N3	-2.18	1.29	1.32
2	4	54	5MU	C6-N1	-2.18	1.34	1.38
67	2	1069	OMG	C5-N7	-2.17	1.34	1.39
66	1	2733	5MC	C6-N1	-2.17	1.34	1.38
67	2	1233	4AC	C4-N3	-2.16	1.29	1.32
67	2	1239	4AC	C4-N3	-2.15	1.29	1.32
67	2	830	OMU	C2-N1	2.15	1.41	1.38
66	1	2287	4AC	C4-N3	-2.14	1.29	1.32
67	2	626	4AC	C4-N3	-2.14	1.29	1.32
67	2	1202	5MC	C6-N1	-2.14	1.34	1.38
67	2	913	OMG	C5-N7	-2.13	1.34	1.39
67	2	830	OMU	C5-C4	-2.13	1.38	1.43
67	2	1177	OMU	C5-C4	-2.13	1.38	1.43
67	2	1487	MA6	C4-N9	-2.12	1.33	1.37
67	2	1028	4AC	C4-N3	-2.11	1.29	1.32
2	4	8	4SU	C2-N3	-2.11	1.34	1.38
67	2	479	4AC	C4-N3	-2.11	1.29	1.32
67	2	20	OMU	C5-C4	-2.10	1.39	1.43
67	2	1469	6MZ	C8-N7	2.09	1.35	1.31
67	2	1147	4AC	C4-N3	-2.08	1.29	1.32
66	1	1780	4AC	C4-N3	-2.08	1.29	1.32
1	3	32	4AC	C4-N3	-2.08	1.29	1.32
67	2	64	OMU	C5-C4	-2.08	1.39	1.43
67	2	373	A2M	C8-N7	2.06	1.35	1.31
67	2	1488	MA6	C4-N9	-2.06	1.33	1.37
67	2	519	OMG	C5-N7	-2.06	1.35	1.39
2	4	54	5MU	C2-N3	-2.04	1.34	1.38
67	2	1380	OMU	C2-N1	2.03	1.41	1.38
66	1	458	4AC	C4-N3	-2.03	1.29	1.32
67	2	774	OMU	C5-C4	-2.00	1.39	1.43
67	2	64	OMU	C2-N1	2.00	1.41	1.38

All (668) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	20	H2U	C4-N3-C2	-7.53	119.55	125.79
67	2	657	OMG	C5-C4-N3	-6.50	117.92	128.46
2	4	8	4SU	C4-N3-C2	-6.46	121.07	127.34
66	1	1055	A2M	C5-C4-N3	-6.31	118.52	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	2	471	OMG	C5-C4-N3	-6.28	118.28	128.46
67	2	373	A2M	C5-C4-N3	-6.17	118.70	126.75
66	1	789	OMG	C5-C4-N3	-6.17	118.46	128.46
66	1	2144	OMG	C5-C4-N3	-6.16	118.47	128.46
66	1	328	OMG	C5-C4-N3	-6.14	118.50	128.46
67	2	467	OMG	C5-C4-N3	-6.11	118.55	128.46
66	1	2173	A2M	C5-C4-N3	-6.07	118.83	126.75
67	2	1469	6MZ	C5-C4-N3	-6.03	118.88	126.75
2	4	55	PSU	N1-C2-N3	6.02	121.95	115.13
67	2	913	OMG	C5-C4-N3	-6.01	118.72	128.46
67	2	680	OMG	C5-C4-N3	-5.94	118.82	128.46
67	2	1069	OMG	C5-C4-N3	-5.89	118.90	128.46
67	2	873	OMG	C5-C4-N3	-5.89	118.90	128.46
2	4	8	4SU	C5-C4-N3	5.89	120.15	114.69
66	1	2138	OMG	C5-C4-N3	-5.89	118.91	128.46
66	1	1755	4AC	O7-C7-N4	5.87	131.32	121.82
67	2	519	OMG	C5-C4-N3	-5.87	118.94	128.46
67	2	934	OMG	C5-C4-N3	-5.86	118.95	128.46
66	1	1780	4AC	O7-C7-N4	5.78	131.18	121.82
66	1	2147	OMG	C5-C4-N3	-5.77	119.11	128.46
66	1	2678	OMG	C5-C4-N3	-5.75	119.13	128.46
66	1	923	OMG	C5-C4-N3	-5.66	119.28	128.46
67	2	1467	UR3	C4-N3-C2	-5.48	119.40	124.56
67	2	1487	MA6	C5-C4-N3	-5.46	119.62	126.75
66	1	1878	4AC	O7-C7-N4	5.42	130.59	121.82
67	2	1488	MA6	C5-C4-N3	-5.39	119.72	126.75
66	1	2144	OMG	C2-N3-C4	5.12	121.43	112.30
2	4	54	5MU	C4-N3-C2	-5.05	120.81	127.35
67	2	787	OMU	C4-N3-C2	-4.99	119.99	126.58
67	2	519	OMG	C2-N3-C4	4.99	121.19	112.30
66	1	789	OMG	C2-N3-C4	4.97	121.15	112.30
67	2	680	OMG	C2-N3-C4	4.96	121.13	112.30
67	2	873	OMG	C2-N3-C4	4.94	121.10	112.30
67	2	467	OMG	C2-N3-C4	4.94	121.09	112.30
67	2	657	OMG	C2-N3-C4	4.93	121.08	112.30
67	2	703	4AC	O7-C7-N4	4.93	129.79	121.82
67	2	657	OMG	N9-C4-N3	4.92	135.82	125.94
67	2	913	OMG	C2-N3-C4	4.90	121.04	112.30
67	2	1069	OMG	C2-N3-C4	4.90	121.03	112.30
67	2	471	OMG	C2-N3-C4	4.90	121.03	112.30
66	1	91	4AC	O7-C7-N4	4.88	129.71	121.82
67	2	1184	4AC	O7-C7-N4	4.87	129.70	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	923	OMG	C2-N3-C4	4.87	120.97	112.30
66	1	2678	OMG	C2-N3-C4	4.83	120.90	112.30
2	4	54	5MU	N3-C2-N1	4.83	121.30	114.89
66	1	1055	A2M	N3-C4-N9	4.80	134.99	127.08
67	2	373	A2M	N3-C4-N9	4.80	134.99	127.08
67	2	471	OMG	N9-C4-N3	4.80	135.57	125.94
66	1	2138	OMG	C2-N3-C4	4.77	120.81	112.30
66	1	328	OMG	N9-C4-N3	4.76	135.50	125.94
66	1	2608	4AC	N4-C4-N3	4.75	121.83	113.85
67	2	636	4AC	O7-C7-N4	4.74	129.49	121.82
66	1	451	4AC	O7-C7-N4	4.72	129.46	121.82
67	2	839	4AC	O7-C7-N4	4.72	129.46	121.82
66	1	328	OMG	C2-N3-C4	4.71	120.70	112.30
66	1	2585	4AC	N4-C4-N3	4.70	121.75	113.85
66	1	2548	4AC	O7-C7-N4	4.70	129.43	121.82
66	1	2144	OMG	N9-C4-N3	4.69	135.37	125.94
67	2	20	OMU	C4-N3-C2	-4.67	120.42	126.58
1	3	32	4AC	O7-C7-N4	4.67	129.38	121.82
67	2	934	OMG	C2-N3-C4	4.67	120.61	112.30
67	2	1487	MA6	C2-N1-C6	4.66	122.77	111.75
66	1	2147	OMG	C2-N3-C4	4.65	120.58	112.30
66	1	2173	A2M	N3-C4-N9	4.65	134.74	127.08
67	2	1380	OMU	C4-N3-C2	-4.62	120.49	126.58
67	2	626	4AC	O7-C7-N4	4.61	129.28	121.82
66	1	533	4AC	O7-C7-N4	4.58	129.24	121.82
66	1	2249	4AC	O7-C7-N4	4.57	129.22	121.82
67	2	467	OMG	N9-C4-N3	4.57	135.12	125.94
66	1	458	4AC	O7-C7-N4	4.56	129.19	121.82
66	1	1243	4AC	O7-C7-N4	4.54	129.16	121.82
67	2	1380	OMU	N3-C2-N1	4.53	120.90	114.89
66	1	2147	OMG	N9-C4-N3	4.53	135.03	125.94
67	2	1488	MA6	C2-N1-C6	4.52	122.44	111.75
67	2	53	4AC	O7-C7-N4	4.52	129.14	121.82
66	1	2784	OMU	C4-N3-C2	-4.52	120.62	126.58
66	1	923	OMG	N9-C4-N3	4.50	134.98	125.94
66	1	2966	4AC	O7-C7-N4	4.50	129.11	121.82
67	2	286	4AC	O7-C7-N4	4.50	129.10	121.82
66	1	2608	4AC	C5-C4-N4	-4.50	115.11	122.92
66	1	2545	4AC	O7-C7-N4	4.49	129.09	121.82
67	2	479	4AC	O7-C7-N4	4.49	129.09	121.82
66	1	60	4AC	O7-C7-N4	4.48	129.07	121.82
67	2	774	OMU	C4-N3-C2	-4.48	120.67	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	789	OMG	N9-C4-N3	4.48	134.93	125.94
66	1	1068	4AC	O7-C7-N4	4.47	129.06	121.82
67	2	718	4AC	O7-C7-N4	4.47	129.06	121.82
67	2	1177	OMU	C4-N3-C2	-4.47	120.68	126.58
66	1	1617	4AC	O7-C7-N4	4.47	129.05	121.82
66	1	922	4AC	O7-C7-N4	4.46	129.04	121.82
67	2	787	OMU	N3-C2-N1	4.46	120.81	114.89
66	1	1293	4AC	O7-C7-N4	4.45	129.03	121.82
67	2	873	OMG	N9-C4-N3	4.45	134.88	125.94
66	1	1048	4AC	O7-C7-N4	4.44	129.00	121.82
67	2	379	4AC	O7-C7-N4	4.44	129.00	121.82
66	1	1065	4AC	O7-C7-N4	4.44	129.00	121.82
67	2	511	4AC	O7-C7-N4	4.43	128.99	121.82
67	2	934	OMG	N9-C4-N3	4.43	134.84	125.94
66	1	1780	4AC	N4-C4-N3	4.43	121.29	113.85
66	1	2138	OMG	N9-C4-N3	4.43	134.83	125.94
67	2	957	4AC	O7-C7-N4	4.42	128.98	121.82
67	2	303	4AC	O7-C7-N4	4.41	128.96	121.82
67	2	848	4AC	O7-C7-N4	4.40	128.95	121.82
67	2	913	OMG	N9-C4-N3	4.40	134.78	125.94
66	1	1934	4AC	O7-C7-N4	4.40	128.94	121.82
67	2	1069	OMG	N9-C4-N3	4.40	134.77	125.94
67	2	1469	6MZ	N3-C4-N9	4.40	134.33	127.08
67	2	1147	4AC	O7-C7-N4	4.40	128.93	121.82
66	1	2329	4AC	O7-C7-N4	4.39	128.93	121.82
67	2	1028	4AC	O7-C7-N4	4.39	128.92	121.82
66	1	1873	4AC	O7-C7-N4	4.38	128.91	121.82
66	1	1662	4AC	O7-C7-N4	4.37	128.90	121.82
66	1	641	4AC	O7-C7-N4	4.37	128.89	121.82
66	1	229	4AC	O7-C7-N4	4.37	128.89	121.82
66	1	1460	4AC	O7-C7-N4	4.36	128.88	121.82
67	2	731	4AC	O7-C7-N4	4.36	128.88	121.82
67	2	17	4AC	O7-C7-N4	4.36	128.88	121.82
66	1	2570	4AC	O7-C7-N4	4.36	128.88	121.82
2	4	54	5MU	C5-C4-N3	4.36	119.03	115.31
66	1	2784	OMU	N3-C2-N1	4.36	120.68	114.89
66	1	2062	4AC	O7-C7-N4	4.35	128.86	121.82
66	1	1557	4AC	O7-C7-N4	4.35	128.86	121.82
66	1	1667	4AC	O7-C7-N4	4.35	128.86	121.82
67	2	751	4AC	O7-C7-N4	4.35	128.86	121.82
67	2	680	OMG	N9-C4-N3	4.35	134.67	125.94
67	2	1233	4AC	O7-C7-N4	4.35	128.85	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	341	4AC	O7-C7-N4	4.34	128.85	121.82
66	1	1962	4AC	O7-C7-N4	4.34	128.85	121.82
66	1	1594	4AC	O7-C7-N4	4.34	128.84	121.82
66	1	1780	4AC	C5-C4-N4	-4.33	115.39	122.92
66	1	2495	4AC	O7-C7-N4	4.33	128.83	121.82
66	1	1695	4AC	O7-C7-N4	4.33	128.83	121.82
66	1	2937	4AC	C5-C4-N4	-4.33	115.41	122.92
66	1	2136	4AC	O7-C7-N4	4.32	128.81	121.82
67	2	851	4AC	O7-C7-N4	4.32	128.81	121.82
66	1	2001	4AC	O7-C7-N4	4.32	128.81	121.82
66	1	2925	4AC	O7-C7-N4	4.32	128.81	121.82
66	1	211	4AC	O7-C7-N4	4.31	128.80	121.82
66	1	1621	4AC	O7-C7-N4	4.31	128.79	121.82
67	2	1505	5MC	C5-C6-N1	-4.31	118.91	123.34
67	2	20	OMU	N3-C2-N1	4.31	120.61	114.89
66	1	22	4AC	O7-C7-N4	4.31	128.79	121.82
67	2	519	OMG	N9-C4-N3	4.31	134.59	125.94
66	1	243	4AC	O7-C7-N4	4.30	128.78	121.82
67	2	64	OMU	C4-N3-C2	-4.30	120.90	126.58
67	2	546	4AC	O7-C7-N4	4.29	128.77	121.82
67	2	868	4AC	O7-C7-N4	4.29	128.76	121.82
66	1	2718	4AC	O7-C7-N4	4.28	128.74	121.82
67	2	1239	4AC	O7-C7-N4	4.27	128.72	121.82
67	2	1469	6MZ	C6-C5-N7	4.26	137.00	132.39
66	1	2937	4AC	N4-C4-N3	4.26	121.00	113.85
66	1	694	4AC	O7-C7-N4	4.26	128.71	121.82
66	1	2585	4AC	C5-C4-N4	-4.25	115.53	122.92
66	1	2287	4AC	O7-C7-N4	4.25	128.69	121.82
67	2	394	4AC	O7-C7-N4	4.25	128.69	121.82
66	1	2642	4AC	O7-C7-N4	4.24	128.67	121.82
66	1	2908	4AC	O7-C7-N4	4.24	128.67	121.82
66	1	1938	4AC	O7-C7-N4	4.23	128.67	121.82
67	2	319	4AC	O7-C7-N4	4.22	128.65	121.82
67	2	774	OMU	N3-C2-N1	4.21	120.48	114.89
66	1	1867	4AC	O7-C7-N4	4.21	128.63	121.82
67	2	828	4AC	O7-C7-N4	4.21	128.63	121.82
66	1	1554	4AC	O7-C7-N4	4.21	128.63	121.82
66	1	2865	4AC	O7-C7-N4	4.21	128.62	121.82
66	1	1550	4AC	O7-C7-N4	4.20	128.62	121.82
66	1	161	4AC	O7-C7-N4	4.20	128.62	121.82
67	2	830	OMU	C4-N3-C2	-4.20	121.05	126.58
2	4	55	PSU	O2'-C2'-C1'	-4.19	101.24	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	2960	4AC	O7-C7-N4	4.18	128.58	121.82
66	1	829	4AC	O7-C7-N4	4.17	128.57	121.82
66	1	802	4AC	O7-C7-N4	4.17	128.57	121.82
66	1	2083	4AC	O7-C7-N4	4.16	128.54	121.82
67	2	590	4AC	O7-C7-N4	4.15	128.53	121.82
66	1	357	4AC	O7-C7-N4	4.15	128.53	121.82
66	1	1755	4AC	C5-C4-N4	-4.14	115.73	122.92
66	1	2678	OMG	N9-C4-N3	4.13	134.23	125.94
67	2	1479	4AC	O7-C7-N4	4.12	128.49	121.82
66	1	835	4AC	O7-C7-N4	4.11	128.47	121.82
66	1	3004	4AC	O7-C7-N4	4.10	128.46	121.82
66	1	314	4AC	O7-C7-N4	4.08	128.42	121.82
66	1	1765	4AC	O7-C7-N4	4.06	128.39	121.82
2	4	55	PSU	C4-N3-C2	-4.06	120.49	126.34
66	1	136	4AC	O7-C7-N4	4.05	128.37	121.82
67	2	830	OMU	N3-C2-N1	4.05	120.26	114.89
67	2	1487	MA6	N3-C4-N9	4.04	133.74	127.08
2	4	8	4SU	N3-C2-N1	4.03	120.24	114.89
67	2	1177	OMU	N3-C2-N1	4.02	120.22	114.89
66	1	981	4AC	O7-C7-N4	4.02	128.32	121.82
66	1	2027	4AC	O7-C7-N4	4.01	128.31	121.82
66	1	1055	A2M	C2-N3-C4	4.01	121.22	111.75
67	2	1488	MA6	N3-C4-N9	3.98	133.65	127.08
66	1	2203	5MC	C5-C6-N1	-3.98	119.24	123.34
66	1	1755	4AC	N4-C4-N3	3.98	120.53	113.85
67	2	64	OMU	N3-C2-N1	3.96	120.15	114.89
66	1	1885	4AC	O7-C7-N4	3.96	128.22	121.82
67	2	373	A2M	C2-N3-C4	3.94	121.06	111.75
66	1	2173	A2M	C2-N3-C4	3.91	120.98	111.75
67	2	1487	MA6	C2-N3-C4	3.89	120.93	111.75
67	2	1469	6MZ	C2-N3-C4	3.88	120.91	111.75
67	2	1488	MA6	C2-N3-C4	3.87	120.90	111.75
66	1	2162	5MC	C5-C6-N1	-3.87	119.35	123.34
66	1	1222	4AC	O7-C7-N4	3.86	128.07	121.82
66	1	1878	4AC	CM7-C7-N4	-3.86	108.62	115.29
67	2	1469	6MZ	C4-C5-N7	-3.84	105.94	110.62
67	2	787	OMU	C5-C4-N3	3.83	120.58	114.84
67	2	1488	MA6	C4-C5-N7	-3.83	105.96	110.62
67	2	1487	MA6	C4-C5-N7	-3.78	106.01	110.62
2	4	54	5MU	O4-C4-C5	-3.77	120.53	124.90
2	4	54	5MU	C5-C6-N1	-3.75	119.48	123.34
66	1	2093	5MC	C5-C6-N1	-3.74	119.49	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	2	20	OMU	C5-C4-N3	3.72	120.40	114.84
67	2	1177	OMU	C5-C4-N3	3.68	120.35	114.84
67	2	535	5MC	C5-C6-N1	-3.68	119.55	123.34
67	2	1380	OMU	C5-C4-N3	3.66	120.31	114.84
67	2	1374	5MC	C5-C6-N1	-3.65	119.58	123.34
67	2	1147	4AC	N4-C4-N3	3.65	119.98	113.85
66	1	2198	5MC	C5-C6-N1	-3.65	119.59	123.34
67	2	875	5MC	C5-C6-N1	-3.64	119.59	123.34
66	1	2784	OMU	C5-C4-N3	3.62	120.26	114.84
67	2	64	OMU	C5-C4-N3	3.62	120.26	114.84
66	1	2163	5MC	C5-C6-N1	-3.59	119.64	123.34
67	2	1487	MA6	N1-C2-N3	-3.58	123.00	128.60
67	2	519	OMG	C6-C5-N7	3.53	136.82	130.25
66	1	2937	4AC	O7-C7-N4	3.52	127.52	121.82
67	2	774	OMU	C5-C4-N3	3.51	120.10	114.84
2	4	8	4SU	C1'-N1-C2	3.51	123.92	117.57
66	1	2678	OMG	C6-C5-N7	3.50	136.76	130.25
67	2	636	4AC	C5-C4-N4	-3.48	116.88	122.92
66	1	2183	5MC	C5-C6-N1	-3.47	119.77	123.34
66	1	2585	4AC	O2-C2-N3	-3.47	116.69	122.33
67	2	1488	MA6	N1-C2-N3	-3.46	123.19	128.60
67	2	636	4AC	N4-C4-N3	3.46	119.66	113.85
67	2	830	OMU	C5-C4-N3	3.43	119.97	114.84
67	2	680	OMG	C6-C5-N7	3.43	136.63	130.25
2	4	8	4SU	C5-C4-S4	-3.42	120.05	124.47
67	2	913	OMG	C6-C5-N7	3.42	136.61	130.25
66	1	923	OMG	C6-C5-N7	3.42	136.60	130.25
67	2	1069	OMG	C6-C5-N7	3.41	136.59	130.25
2	4	55	PSU	O2-C2-N1	-3.40	119.04	122.79
66	1	2733	5MC	C5-C6-N1	-3.39	119.85	123.34
66	1	2249	4AC	CM7-C7-N4	-3.38	109.44	115.29
66	1	1055	A2M	C4-C5-N7	-3.37	106.52	110.62
67	2	873	OMG	C6-C5-N7	3.36	136.49	130.25
66	1	2585	4AC	O7-C7-N4	3.33	127.21	121.82
67	2	636	4AC	CM7-C7-N4	-3.33	109.54	115.29
66	1	2608	4AC	O2-C2-N3	-3.33	116.92	122.33
66	1	2608	4AC	O7-C7-N4	3.32	127.19	121.82
66	1	789	OMG	C6-C5-N7	3.31	136.41	130.25
67	2	1496	5MC	C5-C6-N1	-3.31	119.94	123.34
67	2	1147	4AC	C5-C4-N4	-3.30	117.18	122.92
66	1	2062	4AC	CM7-C7-N4	-3.30	109.58	115.29
67	2	373	A2M	N3-C2-N1	-3.30	123.44	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	2	693	5MC	C5-C6-N1	-3.30	119.95	123.34
66	1	1055	A2M	N3-C2-N1	-3.28	123.47	128.60
66	1	2173	A2M	N3-C2-N1	-3.28	123.47	128.60
66	1	2144	OMG	C6-C5-N7	3.27	136.32	130.25
66	1	2138	OMG	C6-C5-N7	3.26	136.31	130.25
67	2	1025	5MC	C5-C6-N1	-3.26	119.99	123.34
67	2	467	OMG	C6-C5-N7	3.25	136.30	130.25
67	2	1469	6MZ	N1-C2-N3	-3.24	123.53	128.60
66	1	2083	4AC	CM7-C7-N4	-3.23	109.71	115.29
67	2	934	OMG	C6-C5-N7	3.23	136.25	130.25
67	2	373	A2M	C4-C5-N7	-3.20	106.72	110.62
66	1	2495	4AC	CM7-C7-N4	-3.20	109.76	115.29
66	1	2173	A2M	C4-C5-N7	-3.19	106.73	110.62
66	1	2548	4AC	CM7-C7-N4	-3.16	109.83	115.29
67	2	626	4AC	N4-C4-N3	3.15	119.14	113.85
67	2	703	4AC	CM7-C7-N4	-3.14	109.86	115.29
67	2	703	4AC	C5-C4-N4	-3.12	117.50	122.92
67	2	703	4AC	N4-C4-N3	3.12	119.08	113.85
67	2	1488	MA6	C5-N7-C8	3.11	107.93	103.51
67	2	1469	6MZ	C5-N7-C8	3.10	107.91	103.51
67	2	839	4AC	CM7-C7-N4	-3.09	109.96	115.29
67	2	1184	4AC	N4-C4-N3	3.09	119.03	113.85
1	3	32	4AC	N4-C4-N3	3.08	119.03	113.85
66	1	458	4AC	N4-C4-N3	3.06	119.00	113.85
66	1	2287	4AC	N4-C4-N3	3.06	118.99	113.85
66	1	229	4AC	CM7-C7-N4	-3.06	110.00	115.29
67	2	479	4AC	N4-C4-N3	3.05	118.97	113.85
67	2	64	OMU	O4-C4-C5	-3.04	119.81	125.16
67	2	286	4AC	CM7-C7-N4	-3.04	110.03	115.29
67	2	511	4AC	CM7-C7-N4	-3.04	110.04	115.29
67	2	479	4AC	C5-C4-N4	-3.03	117.66	122.92
66	1	91	4AC	N4-C4-N3	3.02	118.92	113.85
66	1	1695	4AC	CM7-C7-N4	-3.02	110.07	115.29
66	1	328	OMG	C6-C5-N7	3.01	135.84	130.25
66	1	1550	4AC	N4-C4-N3	3.00	118.89	113.85
67	2	1184	4AC	C5-C4-N4	-3.00	117.71	122.92
66	1	211	4AC	CM7-C7-N4	-2.99	110.12	115.29
67	2	1177	OMU	O4-C4-C5	-2.99	119.90	125.16
67	2	1479	4AC	N4-C4-N3	2.99	118.87	113.85
66	1	2147	OMG	C6-C5-N7	2.98	135.80	130.25
66	1	533	4AC	N4-C4-N3	2.98	118.86	113.85
66	1	1878	4AC	C5-C4-N4	-2.98	117.74	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	243	4AC	N4-C4-N3	2.98	118.85	113.85
67	2	1028	4AC	N4-C4-N3	2.98	118.85	113.85
66	1	2136	4AC	N4-C4-N3	2.97	118.84	113.85
66	1	1065	4AC	N4-C4-N3	2.97	118.84	113.85
66	1	1068	4AC	CM7-C7-N4	-2.97	110.16	115.29
67	2	1184	4AC	CM7-C7-N4	-2.97	110.16	115.29
66	1	2545	4AC	CM7-C7-N4	-2.96	110.17	115.29
66	1	2865	4AC	CM7-C7-N4	-2.96	110.17	115.29
66	1	1755	4AC	CM7-C7-N4	-2.96	110.17	115.29
67	2	53	4AC	CM7-C7-N4	-2.96	110.17	115.29
67	2	1487	MA6	C5-N7-C8	2.96	107.72	103.51
66	1	60	4AC	N4-C4-N3	2.96	118.81	113.85
66	1	1867	4AC	CM7-C7-N4	-2.96	110.18	115.29
66	1	60	4AC	CM7-C7-N4	-2.95	110.19	115.29
66	1	1048	4AC	CM7-C7-N4	-2.95	110.19	115.29
67	2	718	4AC	CM7-C7-N4	-2.95	110.19	115.29
66	1	2642	4AC	CM7-C7-N4	-2.94	110.20	115.29
67	2	1233	4AC	N4-C4-N3	2.94	118.79	113.85
66	1	91	4AC	C5-C4-N4	-2.94	117.81	122.92
67	2	1239	4AC	N4-C4-N3	2.94	118.78	113.85
67	2	848	4AC	CM7-C7-N4	-2.94	110.22	115.29
66	1	22	4AC	CM7-C7-N4	-2.93	110.22	115.29
67	2	1496	5MC	C5-C4-N3	-2.93	118.51	121.67
67	2	731	4AC	CM7-C7-N4	-2.93	110.23	115.29
66	1	1293	4AC	CM7-C7-N4	-2.93	110.23	115.29
67	2	17	4AC	CM7-C7-N4	-2.92	110.24	115.29
67	2	479	4AC	CM7-C7-N4	-2.92	110.24	115.29
67	2	1498	5MC	C5-C6-N1	-2.92	120.33	123.34
66	1	2733	5MC	C5-C4-N3	-2.92	118.52	121.67
66	1	2162	5MC	C5-C4-N3	-2.92	118.53	121.67
66	1	451	4AC	CM7-C7-N4	-2.91	110.25	115.29
66	1	1621	4AC	CM7-C7-N4	-2.91	110.26	115.29
67	2	379	4AC	CM7-C7-N4	-2.91	110.26	115.29
66	1	1557	4AC	CM7-C7-N4	-2.91	110.26	115.29
66	1	2966	4AC	CM7-C7-N4	-2.90	110.28	115.29
66	1	1938	4AC	CM7-C7-N4	-2.90	110.28	115.29
66	1	2329	4AC	CM7-C7-N4	-2.90	110.28	115.29
67	2	471	OMG	C6-C5-N7	2.90	135.63	130.25
66	1	1962	4AC	N4-C4-N3	2.90	118.71	113.85
66	1	2784	OMU	O4-C4-C5	-2.90	120.07	125.16
67	2	1488	MA6	C4-N9-C8	2.89	108.86	105.73
66	1	1243	4AC	CM7-C7-N4	-2.88	110.31	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	2	957	4AC	N4-C4-N3	2.87	118.68	113.85
67	2	626	4AC	C5-C4-N4	-2.87	117.93	122.92
66	1	1460	4AC	CM7-C7-N4	-2.87	110.33	115.29
67	2	1233	4AC	C5-C4-N4	-2.87	117.94	122.92
67	2	830	OMU	O4-C4-C5	-2.86	120.12	125.16
66	1	2585	4AC	C1'-N1-C2	2.86	124.80	118.42
66	1	2329	4AC	C5-C4-N4	-2.86	117.95	122.92
66	1	1055	A2M	C5-N7-C8	2.85	107.56	103.51
66	1	2960	4AC	N4-C4-N3	2.85	118.64	113.85
66	1	1550	4AC	C5-C4-N4	-2.85	117.97	122.92
66	1	2287	4AC	C5-C4-N4	-2.84	117.98	122.92
67	2	1028	4AC	CM7-C7-N4	-2.84	110.37	115.29
67	2	1505	5MC	C5-C4-N3	-2.84	118.61	121.67
66	1	2570	4AC	CM7-C7-N4	-2.84	110.39	115.29
66	1	1293	4AC	N4-C4-N3	2.83	118.61	113.85
67	2	394	4AC	N4-C4-N3	2.83	118.61	113.85
66	1	2718	4AC	CM7-C7-N4	-2.83	110.39	115.29
66	1	243	4AC	C5-C4-N4	-2.83	118.01	122.92
66	1	1962	4AC	CM7-C7-N4	-2.82	110.41	115.29
66	1	789	OMG	C4-C5-N7	-2.82	106.26	110.72
66	1	458	4AC	C5-C4-N4	-2.82	118.02	122.92
67	2	828	4AC	CM7-C7-N4	-2.82	110.42	115.29
66	1	91	4AC	CM7-C7-N4	-2.81	110.43	115.29
67	2	53	4AC	N4-C4-N3	2.81	118.57	113.85
66	1	533	4AC	CM7-C7-N4	-2.81	110.43	115.29
67	2	379	4AC	N4-C4-N3	2.81	118.57	113.85
66	1	1662	4AC	N4-C4-N3	2.81	118.57	113.85
66	1	314	4AC	CM7-C7-N4	-2.81	110.44	115.29
66	1	2925	4AC	CM7-C7-N4	-2.80	110.44	115.29
66	1	1662	4AC	C5-C4-N4	-2.80	118.05	122.92
66	1	1962	4AC	C5-C4-N4	-2.80	118.05	122.92
67	2	957	4AC	C5-C4-N4	-2.80	118.06	122.92
66	1	2608	4AC	C1'-N1-C2	2.80	124.67	118.42
67	2	303	4AC	CM7-C7-N4	-2.80	110.45	115.29
1	3	32	4AC	C5-C4-N4	-2.80	118.06	122.92
66	1	1873	4AC	CM7-C7-N4	-2.80	110.46	115.29
66	1	1934	4AC	N4-C4-N3	2.79	118.54	113.85
67	2	1487	MA6	C4-N9-C8	2.79	108.75	105.73
67	2	1488	MA6	C6-C5-N7	2.79	137.96	133.28
67	2	657	OMG	C6-C5-N7	2.78	135.43	130.25
66	1	641	4AC	CM7-C7-N4	-2.78	110.48	115.29
67	2	1028	4AC	C5-C4-N4	-2.78	118.08	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	22	4AC	N4-C4-N3	2.78	118.52	113.85
66	1	161	4AC	N4-C4-N3	2.78	118.52	113.85
67	2	751	4AC	CM7-C7-N4	-2.78	110.49	115.29
67	2	1202	5MC	C5-C6-N1	-2.78	120.48	123.34
66	1	533	4AC	C5-C4-N4	-2.77	118.10	122.92
67	2	848	4AC	N4-C4-N3	2.77	118.51	113.85
67	2	1498	5MC	C5-C4-N3	-2.77	118.69	121.67
67	2	53	4AC	C5-C4-N4	-2.77	118.11	122.92
67	2	1239	4AC	C5-C4-N4	-2.77	118.11	122.92
66	1	2908	4AC	CM7-C7-N4	-2.76	110.52	115.29
66	1	922	4AC	N4-C4-N3	2.76	118.49	113.85
66	1	1222	4AC	N4-C4-N3	2.76	118.49	113.85
66	1	802	4AC	N4-C4-N3	2.76	118.48	113.85
66	1	2570	4AC	N4-C4-N3	2.76	118.48	113.85
66	1	2136	4AC	O2-C2-N3	-2.76	117.85	122.33
66	1	2329	4AC	N4-C4-N3	2.76	118.48	113.85
67	2	774	OMU	O4-C4-C5	-2.75	120.32	125.16
67	2	848	4AC	C5-C4-N4	-2.75	118.14	122.92
66	1	2545	4AC	N4-C4-N3	2.75	118.47	113.85
67	2	751	4AC	N4-C4-N3	2.75	118.47	113.85
66	1	835	4AC	CM7-C7-N4	-2.75	110.54	115.29
67	2	731	4AC	N4-C4-N3	2.75	118.46	113.85
67	2	546	4AC	N4-C4-N3	2.75	118.46	113.85
66	1	341	4AC	N4-C4-N3	2.74	118.46	113.85
67	2	519	OMG	C4-C5-N7	-2.74	106.38	110.72
67	2	851	4AC	CM7-C7-N4	-2.74	110.56	115.29
66	1	22	4AC	C5-C4-N4	-2.73	118.17	122.92
66	1	451	4AC	C5-C4-N4	-2.73	118.17	122.92
67	2	680	OMG	C4-C5-N7	-2.73	106.40	110.72
66	1	458	4AC	CM7-C7-N4	-2.73	110.57	115.29
67	2	1233	4AC	CM7-C7-N4	-2.73	110.57	115.29
1	3	32	4AC	CM7-C7-N4	-2.73	110.58	115.29
66	1	451	4AC	N4-C4-N3	2.73	118.43	113.85
66	1	2545	4AC	C5-C4-N4	-2.73	118.18	122.92
66	1	161	4AC	CM7-C7-N4	-2.73	110.58	115.29
66	1	1667	4AC	CM7-C7-N4	-2.73	110.58	115.29
67	2	1202	5MC	C5-C4-N3	-2.73	118.73	121.67
67	2	303	4AC	N4-C4-N3	2.72	118.43	113.85
66	1	1617	4AC	CM7-C7-N4	-2.72	110.58	115.29
67	2	913	OMG	C4-C5-N7	-2.72	106.41	110.72
67	2	379	4AC	C5-C4-N4	-2.72	118.19	122.92
67	2	626	4AC	CM7-C7-N4	-2.72	110.58	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	1293	4AC	C5-C4-N4	-2.72	118.19	122.92
67	2	957	4AC	CM7-C7-N4	-2.72	110.59	115.29
67	2	319	4AC	N4-C4-N3	2.72	118.42	113.85
67	2	373	A2M	C5-N7-C8	2.72	107.37	103.51
67	2	20	OMU	O4-C4-C5	-2.72	120.38	125.16
67	2	17	4AC	C5-C4-N4	-2.71	118.20	122.92
66	1	981	4AC	CM7-C7-N4	-2.71	110.61	115.29
67	2	1479	4AC	C5-C4-N4	-2.71	118.22	122.92
66	1	2570	4AC	C5-C4-N4	-2.71	118.22	122.92
66	1	1617	4AC	N4-C4-N3	2.70	118.39	113.85
66	1	1662	4AC	CM7-C7-N4	-2.70	110.62	115.29
66	1	2001	4AC	CM7-C7-N4	-2.70	110.63	115.29
66	1	2966	4AC	C5-C4-N4	-2.70	118.24	122.92
67	2	17	4AC	N4-C4-N3	2.69	118.37	113.85
66	1	1617	4AC	C5-C4-N4	-2.69	118.25	122.92
66	1	1594	4AC	CM7-C7-N4	-2.69	110.64	115.29
66	1	694	4AC	N4-C4-N3	2.69	118.36	113.85
66	1	161	4AC	C5-C4-N4	-2.68	118.26	122.92
67	2	787	OMU	O4-C4-C5	-2.67	120.46	125.16
66	1	2678	OMG	C4-C5-N7	-2.67	106.50	110.72
66	1	641	4AC	C5-C4-N4	-2.67	118.29	122.92
66	1	829	4AC	CM7-C7-N4	-2.67	110.68	115.29
66	1	641	4AC	N4-C4-N3	2.67	118.33	113.85
66	1	1765	4AC	N4-C4-N3	2.66	118.32	113.85
67	2	394	4AC	CM7-C7-N4	-2.66	110.69	115.29
66	1	2784	OMU	O2-C2-N1	-2.66	119.25	122.79
66	1	1594	4AC	N4-C4-N3	2.65	118.30	113.85
66	1	357	4AC	CM7-C7-N4	-2.65	110.71	115.29
66	1	694	4AC	CM7-C7-N4	-2.65	110.71	115.29
66	1	829	4AC	C5-C4-N4	-2.65	118.32	122.92
66	1	2173	A2M	C5-N7-C8	2.65	107.27	103.51
66	1	2001	4AC	N4-C4-N3	2.65	118.30	113.85
66	1	802	4AC	CM7-C7-N4	-2.64	110.72	115.29
67	2	731	4AC	C5-C4-N4	-2.64	118.33	122.92
66	1	60	4AC	C5-C4-N4	-2.64	118.33	122.92
67	2	286	4AC	N4-C4-N3	2.64	118.29	113.85
66	1	2925	4AC	N4-C4-N3	2.64	118.28	113.85
66	1	136	4AC	N4-C4-N3	2.63	118.27	113.85
66	1	2027	4AC	CM7-C7-N4	-2.63	110.74	115.29
67	2	1069	OMG	C4-C5-N7	-2.63	106.55	110.72
67	2	693	5MC	C5-C4-N3	-2.63	118.83	121.67
66	1	829	4AC	N4-C4-N3	2.63	118.27	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	2136	4AC	C5-C4-N4	-2.63	118.35	122.92
67	2	546	4AC	CM7-C7-N4	-2.63	110.75	115.29
66	1	2548	4AC	C5-C4-N4	-2.63	118.36	122.92
67	2	394	4AC	C5-C4-N4	-2.63	118.36	122.92
67	2	934	OMG	C4-C5-N7	-2.63	106.56	110.72
66	1	1667	4AC	C5-C4-N4	-2.62	118.37	122.92
67	2	1239	4AC	CM7-C7-N4	-2.62	110.77	115.29
66	1	2966	4AC	N4-C4-N3	2.62	118.25	113.85
66	1	1065	4AC	C5-C4-N4	-2.61	118.38	122.92
66	1	2548	4AC	N4-C4-N3	2.61	118.24	113.85
66	1	1885	4AC	CM7-C7-N4	-2.61	110.78	115.29
67	2	868	4AC	CM7-C7-N4	-2.61	110.78	115.29
67	2	286	4AC	C5-C4-N4	-2.61	118.39	122.92
66	1	1554	4AC	CM7-C7-N4	-2.61	110.78	115.29
67	2	1498	5MC	O2-C2-N3	-2.61	118.09	122.33
66	1	2718	4AC	N4-C4-N3	2.60	118.21	113.85
66	1	1667	4AC	N4-C4-N3	2.60	118.21	113.85
67	2	1487	MA6	N1-C6-N6	2.59	119.92	117.08
67	2	839	4AC	C5-C4-N4	-2.59	118.42	122.92
66	1	2287	4AC	CM7-C7-N4	-2.59	110.82	115.29
67	2	467	OMG	C4-C5-N7	-2.59	106.63	110.72
66	1	1780	4AC	CM7-C7-N4	-2.58	110.83	115.29
66	1	1765	4AC	CM7-C7-N4	-2.58	110.83	115.29
67	2	873	OMG	C4-C5-N7	-2.58	106.64	110.72
67	2	511	4AC	C5-C4-N4	-2.58	118.44	122.92
67	2	303	4AC	C5-C4-N4	-2.58	118.44	122.92
66	1	2183	5MC	C5-C4-N3	-2.57	118.90	121.67
67	2	590	4AC	CM7-C7-N4	-2.57	110.84	115.29
66	1	2203	5MC	C5-C4-N3	-2.57	118.90	121.67
66	1	1550	4AC	CM7-C7-N4	-2.57	110.84	115.29
67	2	590	4AC	N4-C4-N3	2.57	118.17	113.85
67	2	868	4AC	N4-C4-N3	2.57	118.16	113.85
66	1	2733	5MC	O2-C2-N3	-2.57	118.16	122.33
66	1	1065	4AC	CM7-C7-N4	-2.57	110.86	115.29
67	2	830	OMU	C1'-N1-C2	2.56	122.21	117.57
67	2	1202	5MC	O2-C2-N3	-2.56	118.16	122.33
67	2	511	4AC	N4-C4-N3	2.56	118.15	113.85
66	1	2865	4AC	N4-C4-N3	2.56	118.15	113.85
66	1	2144	OMG	C4-C5-N7	-2.56	106.67	110.72
67	2	546	4AC	C5-C4-N4	-2.56	118.47	122.92
66	1	3004	4AC	CM7-C7-N4	-2.55	110.88	115.29
67	2	828	4AC	N4-C4-N3	2.55	118.13	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	2138	OMG	C4-C5-N7	-2.54	106.69	110.72
66	1	1243	4AC	C5-C4-N4	-2.54	118.50	122.92
67	2	319	4AC	C5-C4-N4	-2.54	118.50	122.92
66	1	2865	4AC	C5-C4-N4	-2.54	118.51	122.92
67	2	787	OMU	O2-C2-N1	-2.54	119.41	122.79
66	1	1934	4AC	CM7-C7-N4	-2.54	110.91	115.29
66	1	243	4AC	CM7-C7-N4	-2.53	110.91	115.29
66	1	2198	5MC	C5-C4-N3	-2.53	118.94	121.67
66	1	1222	4AC	C5-C4-N4	-2.53	118.52	122.92
67	2	319	4AC	CM7-C7-N4	-2.53	110.92	115.29
66	1	2925	4AC	C5-C4-N4	-2.53	118.53	122.92
66	1	2093	5MC	C5-C4-N3	-2.52	118.95	121.67
66	1	694	4AC	C5-C4-N4	-2.51	118.56	122.92
66	1	1621	4AC	N4-C4-N3	2.51	118.07	113.85
66	1	136	4AC	CM7-C7-N4	-2.51	110.95	115.29
66	1	1695	4AC	N4-C4-N3	2.51	118.06	113.85
66	1	1068	4AC	N4-C4-N3	2.50	118.06	113.85
67	2	657	OMG	C4-C5-N7	-2.50	106.76	110.72
2	4	20	H2U	C3'-C2'-C1'	2.50	106.18	101.43
66	1	2163	5MC	C5-C4-N3	-2.49	118.98	121.67
67	2	1025	5MC	C5-C4-N3	-2.49	118.98	121.67
67	2	828	4AC	C5-C4-N4	-2.49	118.59	122.92
66	1	328	OMG	C4-C5-N7	-2.49	106.78	110.72
66	1	1594	4AC	C5-C4-N4	-2.49	118.59	122.92
67	2	839	4AC	N4-C4-N3	2.49	118.03	113.85
66	1	2136	4AC	CM7-C7-N4	-2.48	111.01	115.29
66	1	1934	4AC	C5-C4-N4	-2.48	118.62	122.92
67	2	1498	5MC	C1'-N1-C6	-2.47	117.00	121.12
66	1	1695	4AC	C5-C4-N4	-2.47	118.62	122.92
66	1	2960	4AC	CM7-C7-N4	-2.47	111.03	115.29
2	4	55	PSU	C2'-C3'-C4'	-2.47	97.85	102.64
66	1	2960	4AC	C5-C4-N4	-2.46	118.64	122.92
67	2	751	4AC	C5-C4-N4	-2.46	118.64	122.92
66	1	922	4AC	CM7-C7-N4	-2.45	111.05	115.29
67	2	1487	MA6	C6-C5-N7	2.44	137.39	133.28
2	4	55	PSU	O4'-C1'-C2'	-2.44	101.70	105.14
66	1	341	4AC	CM7-C7-N4	-2.43	111.08	115.29
67	2	875	5MC	C5-C4-N3	-2.43	119.05	121.67
66	1	1867	4AC	C5-C4-N4	-2.43	118.70	122.92
66	1	1867	4AC	N4-C4-N3	2.43	117.93	113.85
66	1	2992	4AC	CM7-C7-N4	2.43	119.49	115.29
66	1	2718	4AC	C5-C4-N4	-2.43	118.70	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	2	1479	4AC	CM7-C7-N4	-2.42	111.11	115.29
67	2	1488	MA6	N9-C8-N7	-2.42	110.61	113.91
66	1	1938	4AC	N4-C4-N3	2.41	117.90	113.85
66	1	2027	4AC	N4-C4-N3	2.41	117.90	113.85
66	1	802	4AC	C5-C4-N4	-2.41	118.73	122.92
66	1	922	4AC	C5-C4-N4	-2.41	118.74	122.92
66	1	1243	4AC	N4-C4-N3	2.40	117.89	113.85
67	2	471	OMG	C4-C5-N7	-2.40	106.92	110.72
66	1	1878	4AC	N4-C4-N3	2.40	117.88	113.85
66	1	1557	4AC	N4-C4-N3	2.40	117.88	113.85
66	1	2642	4AC	N4-C4-N3	2.39	117.87	113.85
67	2	851	4AC	N4-C4-N3	2.39	117.86	113.85
66	1	211	4AC	C5-C4-N4	-2.38	118.79	122.92
66	1	1765	4AC	C5-C4-N4	-2.38	118.79	122.92
67	2	535	5MC	C5-C4-N3	-2.38	119.11	121.67
67	2	1147	4AC	CM7-C7-N4	-2.38	111.18	115.29
66	1	2001	4AC	C5-C4-N4	-2.38	118.79	122.92
66	1	923	OMG	O6-C6-C5	-2.37	120.31	126.60
66	1	1885	4AC	N4-C4-N3	2.37	117.83	113.85
66	1	923	OMG	C4-C5-N7	-2.37	106.97	110.72
67	2	693	5MC	O2-C2-N3	-2.36	118.49	122.33
67	2	1380	OMU	O4-C4-C5	-2.36	121.02	125.16
66	1	2173	A2M	C4-N9-C8	2.34	108.27	105.73
66	1	2249	4AC	C5-C4-N4	-2.34	118.85	122.92
66	1	1460	4AC	N4-C4-N3	2.34	117.78	113.85
66	1	2678	OMG	O6-C6-C5	-2.34	120.40	126.60
66	1	1068	4AC	C5-C4-N4	-2.34	118.86	122.92
67	2	373	A2M	C4-N9-C8	2.34	108.26	105.73
66	1	211	4AC	N4-C4-N3	2.34	117.78	113.85
66	1	60	4AC	O2-C2-N3	-2.34	118.53	122.33
67	2	851	4AC	C5-C4-N4	-2.32	118.88	122.92
66	1	341	4AC	C5-C4-N4	-2.32	118.89	122.92
66	1	314	4AC	N4-C4-N3	2.31	117.73	113.85
66	1	1621	4AC	C5-C4-N4	-2.31	118.91	122.92
66	1	1055	A2M	C6-C5-N7	2.31	136.32	132.02
66	1	1885	4AC	C5-C4-N4	-2.31	118.91	122.92
67	2	1374	5MC	C5-C4-N3	-2.30	119.19	121.67
66	1	357	4AC	N4-C4-N3	2.30	117.72	113.85
66	1	1554	4AC	N4-C4-N3	2.30	117.71	113.85
66	1	1460	4AC	C5-C4-N4	-2.30	118.93	122.92
67	2	873	OMG	O6-C6-C5	-2.30	120.51	126.60
67	2	20	OMU	O2-C2-N1	-2.29	119.74	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	2642	4AC	C5-C4-N4	-2.28	118.95	122.92
2	4	55	PSU	C3'-C2'-C1'	-2.28	98.98	101.64
66	1	2173	A2M	C6-C5-N7	2.27	136.25	132.02
67	2	718	4AC	C5-C4-N4	-2.27	118.98	122.92
66	1	1554	4AC	C5-C4-N4	-2.26	118.98	122.92
66	1	328	OMG	O6-C6-C5	-2.26	120.60	126.60
66	1	2147	OMG	C4-C5-N7	-2.26	107.14	110.72
67	2	1505	5MC	O2-C2-N3	-2.26	118.66	122.33
66	1	2147	OMG	O6-C6-C5	-2.26	120.62	126.60
66	1	1055	A2M	C4-N9-C8	2.25	108.17	105.73
67	2	1147	4AC	O3'-C3'-C2'	2.25	119.09	111.82
67	2	868	4AC	C5-C4-N4	-2.24	119.03	122.92
67	2	590	4AC	C5-C4-N4	-2.23	119.05	122.92
66	1	981	4AC	N4-C4-N3	2.23	117.59	113.85
66	1	1557	4AC	C5-C4-N4	-2.22	119.06	122.92
67	2	519	OMG	O6-C6-C5	-2.22	120.71	126.60
66	1	2908	4AC	N4-C4-N3	2.22	117.58	113.85
67	2	1487	MA6	N9-C8-N7	-2.22	110.88	113.91
66	1	136	4AC	C5-C4-N4	-2.21	119.08	122.92
66	1	835	4AC	N4-C4-N3	2.21	117.56	113.85
67	2	1496	5MC	O2-C2-N3	-2.21	118.74	122.33
66	1	2144	OMG	O6-C6-C5	-2.20	120.75	126.60
66	1	2162	5MC	O2-C2-N3	-2.20	118.75	122.33
66	1	2249	4AC	N4-C4-N3	2.20	117.55	113.85
67	2	718	4AC	N4-C4-N3	2.19	117.53	113.85
66	1	1780	4AC	O7-C7-CM7	-2.19	118.00	122.06
67	2	373	A2M	C6-C5-N7	2.18	136.09	132.02
66	1	2062	4AC	C5-C4-N4	-2.18	119.13	122.92
67	2	1469	6MZ	C4-N9-C8	2.17	108.08	105.73
66	1	1222	4AC	CM7-C7-N4	-2.16	111.55	115.29
66	1	2027	4AC	C5-C4-N4	-2.16	119.16	122.92
66	1	2908	4AC	C5-C4-N4	-2.16	119.17	122.92
66	1	835	4AC	O2-C2-N3	-2.16	118.82	122.33
2	4	20	H2U	O2-C2-N1	-2.16	120.40	123.11
66	1	1873	4AC	N4-C4-N3	2.16	117.47	113.85
66	1	314	4AC	C5-C4-N4	-2.15	119.19	122.92
67	2	680	OMG	O6-C6-C5	-2.15	120.91	126.60
67	2	467	OMG	O6-C6-C5	-2.14	120.92	126.60
66	1	789	OMG	C2'-C1'-N9	-2.14	110.06	114.22
67	2	1469	6MZ	C2-N1-C6	2.14	122.44	115.25
66	1	2062	4AC	N4-C4-N3	2.14	117.45	113.85
67	2	535	5MC	O2-C2-N3	-2.14	118.85	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	2495	4AC	O2-C2-N3	-2.13	118.86	122.33
2	4	20	H2U	N3-C2-N1	2.13	118.91	116.65
66	1	357	4AC	O2-C2-N3	-2.13	118.87	122.33
67	2	875	5MC	O2-C2-N3	-2.13	118.87	122.33
66	1	2138	OMG	O6-C6-C5	-2.12	120.97	126.60
67	2	471	OMG	O6-C6-C5	-2.12	120.98	126.60
66	1	1873	4AC	C5-C4-N4	-2.11	119.25	122.92
66	1	1938	4AC	C5-C4-N4	-2.11	119.25	122.92
66	1	2495	4AC	C5-C4-N4	-2.11	119.25	122.92
67	2	1040	OMC	O2-C2-N3	-2.11	118.90	122.33
67	2	787	OMU	C5-C6-N1	-2.10	118.29	121.81
66	1	2163	5MC	O2-C2-N3	-2.10	118.92	122.33
66	1	1068	4AC	O2-C2-N3	-2.10	118.92	122.33
66	1	923	OMG	C2'-C1'-N9	-2.10	110.15	114.22
66	1	1048	4AC	C5-C4-N4	-2.10	119.28	122.92
66	1	229	4AC	O2-C2-N3	-2.10	118.92	122.33
66	1	923	OMG	C5-C6-N1	2.09	118.49	113.19
67	2	1069	OMG	O6-C6-C5	-2.08	121.07	126.60
66	1	2495	4AC	N4-C4-N3	2.08	117.34	113.85
67	2	657	OMG	O6-C6-C5	-2.08	121.09	126.60
67	2	1505	5MC	C1'-N1-C6	-2.08	117.67	121.12
66	1	1938	4AC	O2-C2-N3	-2.07	118.96	122.33
66	1	3004	4AC	N4-C4-N3	2.07	117.33	113.85
2	4	20	H2U	O4-C4-N3	2.07	123.56	120.28
66	1	2162	5MC	CM5-C5-C6	-2.05	120.11	122.85
67	2	64	OMU	C1'-N1-C2	2.04	121.27	117.57
67	2	934	OMG	O6-C6-C5	-2.04	121.20	126.60
66	1	3004	4AC	C5-C4-N4	-2.03	119.38	122.92
66	1	835	4AC	C5-C4-N4	-2.03	119.39	122.92
67	2	1467	UR3	C6-N1-C2	-2.02	119.98	121.79
67	2	1467	UR3	C1'-N1-C2	2.02	120.40	116.99
67	2	913	OMG	O6-C6-C5	-2.02	121.25	126.60
66	1	981	4AC	C5-C4-N4	-2.02	119.42	122.92
67	2	519	OMG	C5-C6-N1	2.00	118.28	113.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	4	20	H2U	O4'-C1'-N1-C6
66	1	789	OMG	O4'-C4'-C5'-O5'
66	1	789	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
66	1	2147	OMG	C3'-C4'-C5'-O5'
66	1	2585	4AC	O4'-C1'-N1-C2
66	1	2585	4AC	O4'-C1'-N1-C6
66	1	2608	4AC	O4'-C1'-N1-C2
66	1	2608	4AC	O4'-C1'-N1-C6
67	2	1505	5MC	O4'-C4'-C5'-O5'
2	4	8	4SU	O4'-C1'-N1-C2
67	2	1488	MA6	O4'-C4'-C5'-O5'
67	2	1505	5MC	C3'-C4'-C5'-O5'
2	4	20	H2U	O4'-C1'-N1-C2
66	1	2147	OMG	O4'-C4'-C5'-O5'
66	1	2733	5MC	O4'-C4'-C5'-O5'
67	2	1488	MA6	C3'-C4'-C5'-O5'
2	4	8	4SU	O4'-C1'-N1-C6
66	1	2733	5MC	C3'-C4'-C5'-O5'
67	2	20	OMU	C2'-C1'-N1-C6
2	4	55	PSU	O4'-C4'-C5'-O5'
2	4	55	PSU	C3'-C4'-C5'-O5'
66	1	2992	4AC	O7-C7-N4-C4
66	1	2992	4AC	CM7-C7-N4-C4
67	2	20	OMU	O4'-C1'-N1-C6
67	2	1498	5MC	O4'-C1'-N1-C6
2	4	20	H2U	C4'-C5'-O5'-P
67	2	1069	OMG	C3'-C2'-O2'-CM2
66	1	2585	4AC	N3-C4-N4-C7
66	1	2608	4AC	N3-C4-N4-C7
66	1	2937	4AC	N3-C4-N4-C7
1	3	32	4AC	O4'-C4'-C5'-O5'
1	3	32	4AC	C3'-C4'-C5'-O5'
67	2	1498	5MC	O4'-C1'-N1-C2
67	2	787	OMU	C2'-C1'-N1-C6
67	2	20	OMU	O4'-C1'-N1-C2
67	2	20	OMU	C2'-C1'-N1-C2
66	1	2733	5MC	C2'-C1'-N1-C6
67	2	787	OMU	O4'-C1'-N1-C2
66	1	2733	5MC	O4'-C1'-N1-C6
67	2	787	OMU	O4'-C1'-N1-C6
67	2	1202	5MC	O4'-C4'-C5'-O5'
67	2	20	OMU	O4'-C4'-C5'-O5'
67	2	1147	4AC	C3'-C4'-C5'-O5'
67	2	787	OMU	C2'-C1'-N1-C2
67	2	1498	5MC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
67	2	1498	5MC	O4'-C4'-C5'-O5'
66	1	2733	5MC	O4'-C1'-N1-C2
67	2	873	OMG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

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
66	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

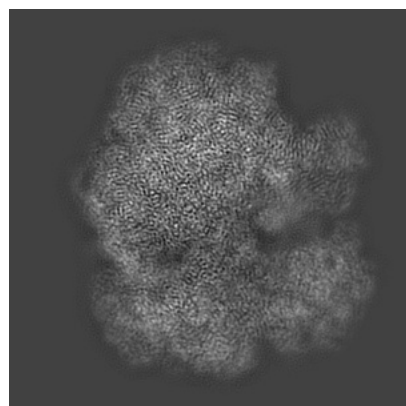
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55139. These allow visual inspection of the internal detail of the map and identification of artifacts.

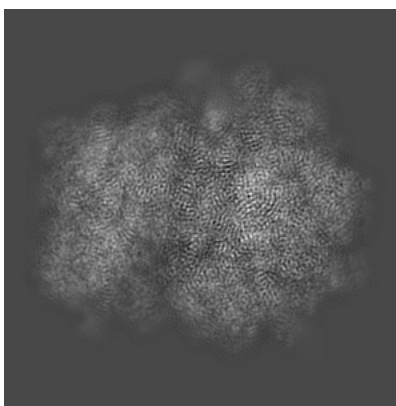
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

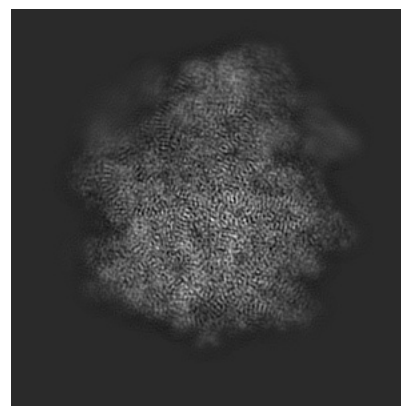
6.1.1 Primary map



X

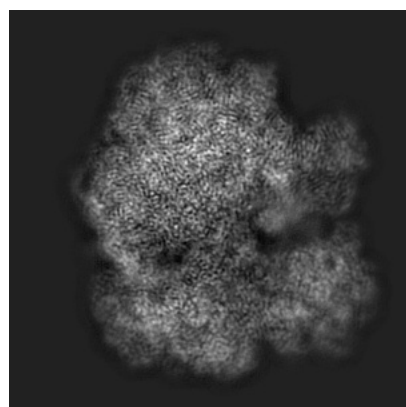


Y

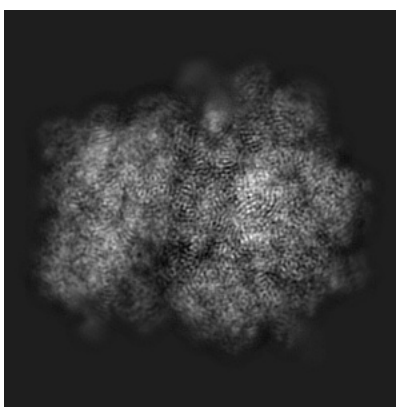


Z

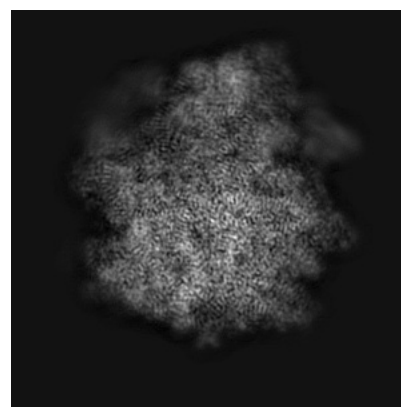
6.1.2 Raw map



X



Y

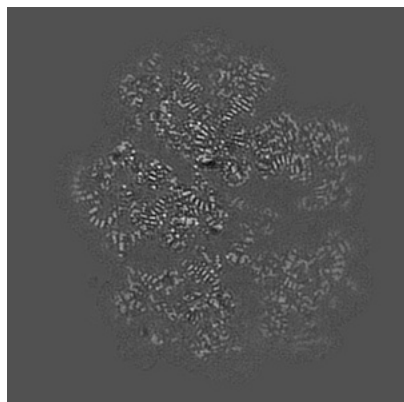


Z

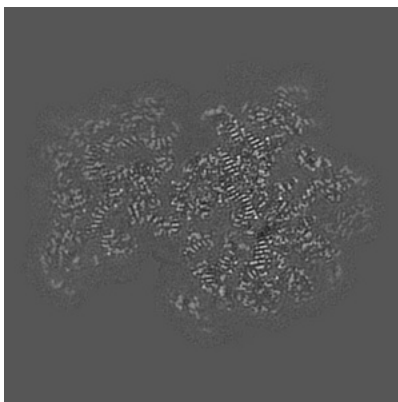
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

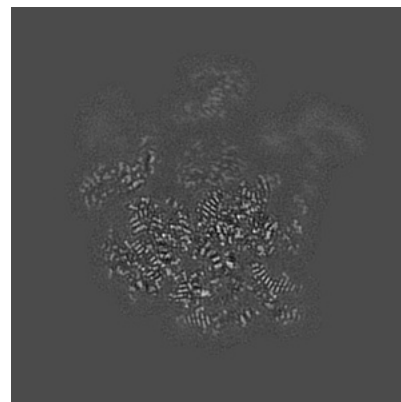
6.2.1 Primary map



X Index: 180

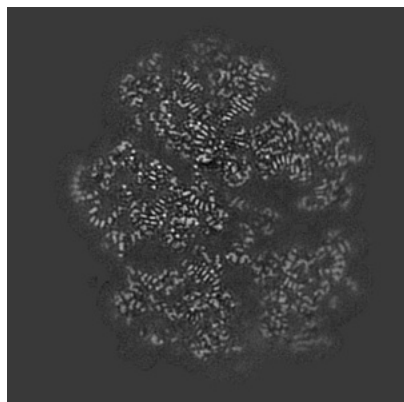


Y Index: 180

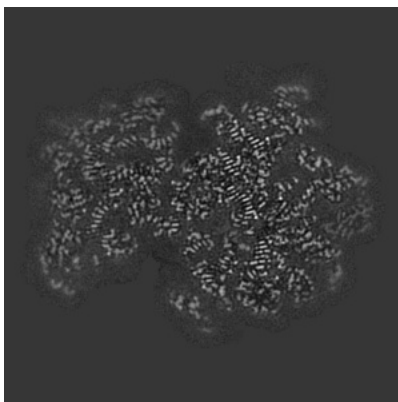


Z Index: 180

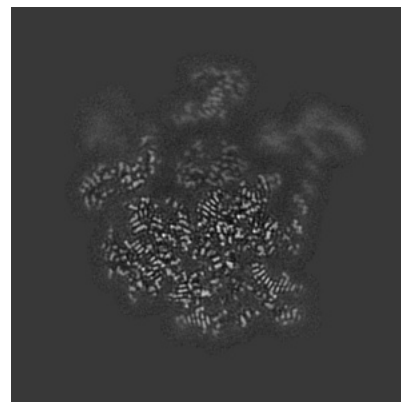
6.2.2 Raw map



X Index: 180



Y Index: 180

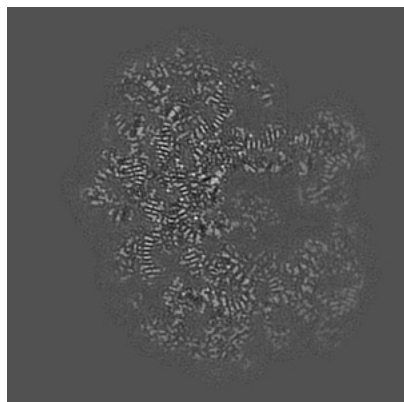


Z Index: 180

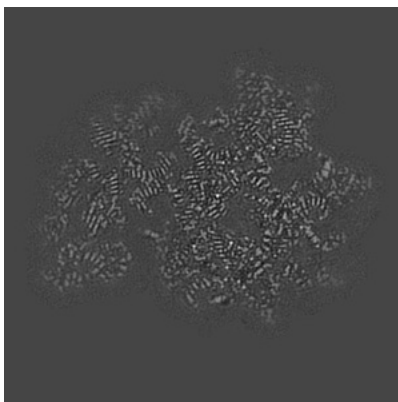
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

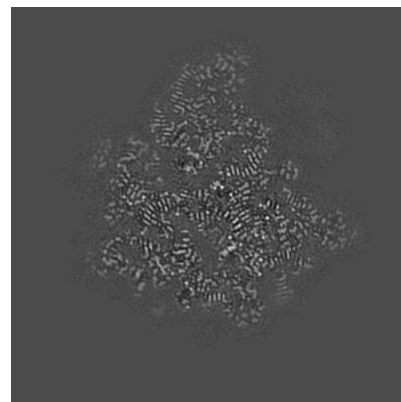
6.3.1 Primary map



X Index: 195

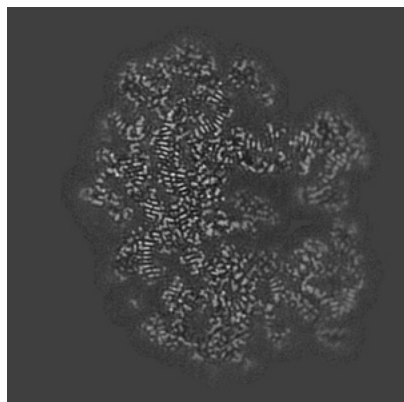


Y Index: 166

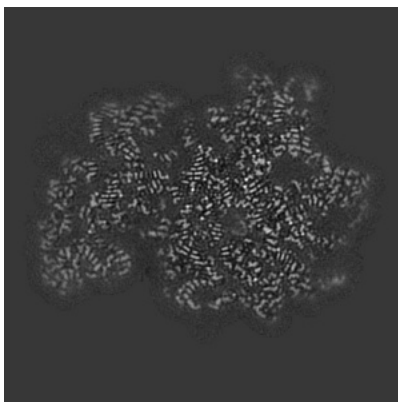


Z Index: 228

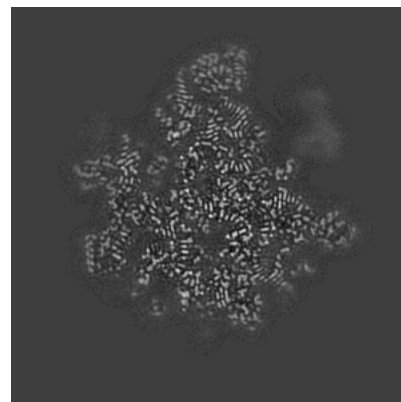
6.3.2 Raw map



X Index: 196



Y Index: 170

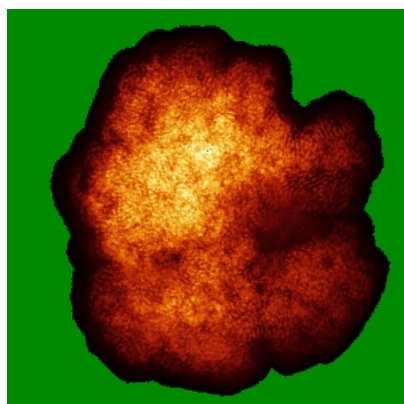


Z Index: 222

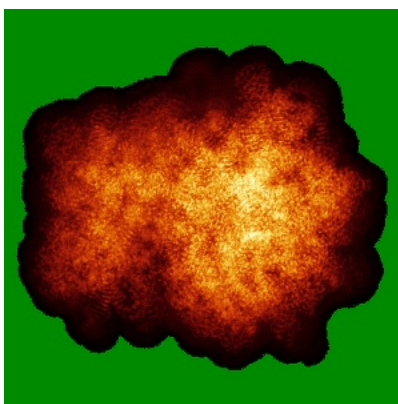
The images above show the largest variance slices of the map in three orthogonal directions.

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

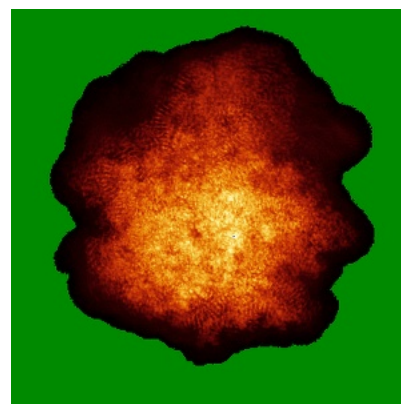
6.4.1 Primary map



X

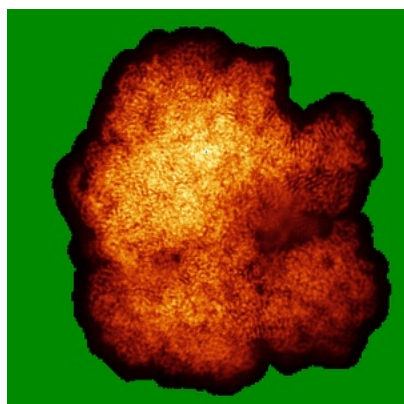


Y

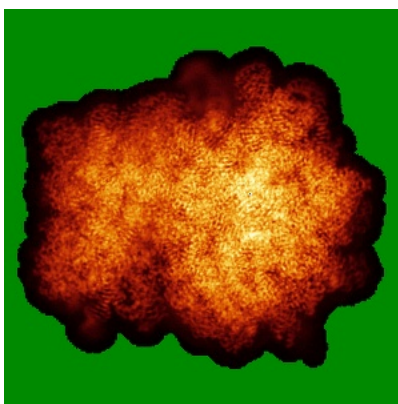


Z

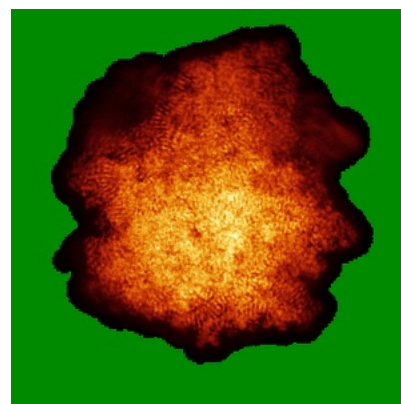
6.4.2 Raw map



X



Y

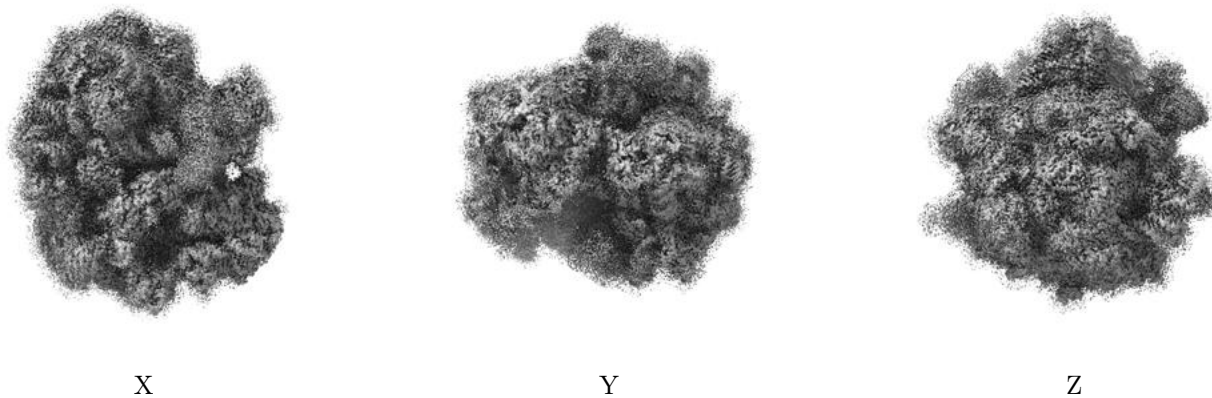


Z

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.

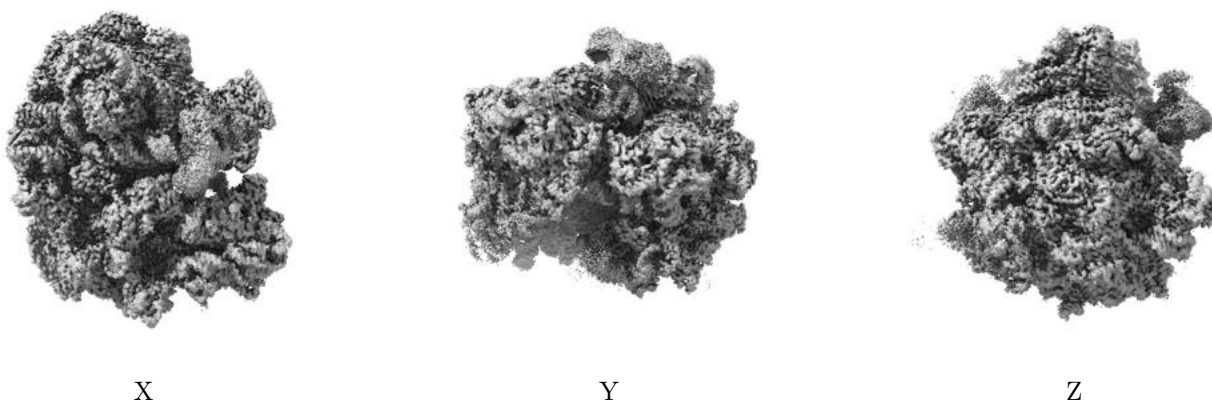
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0015. 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.

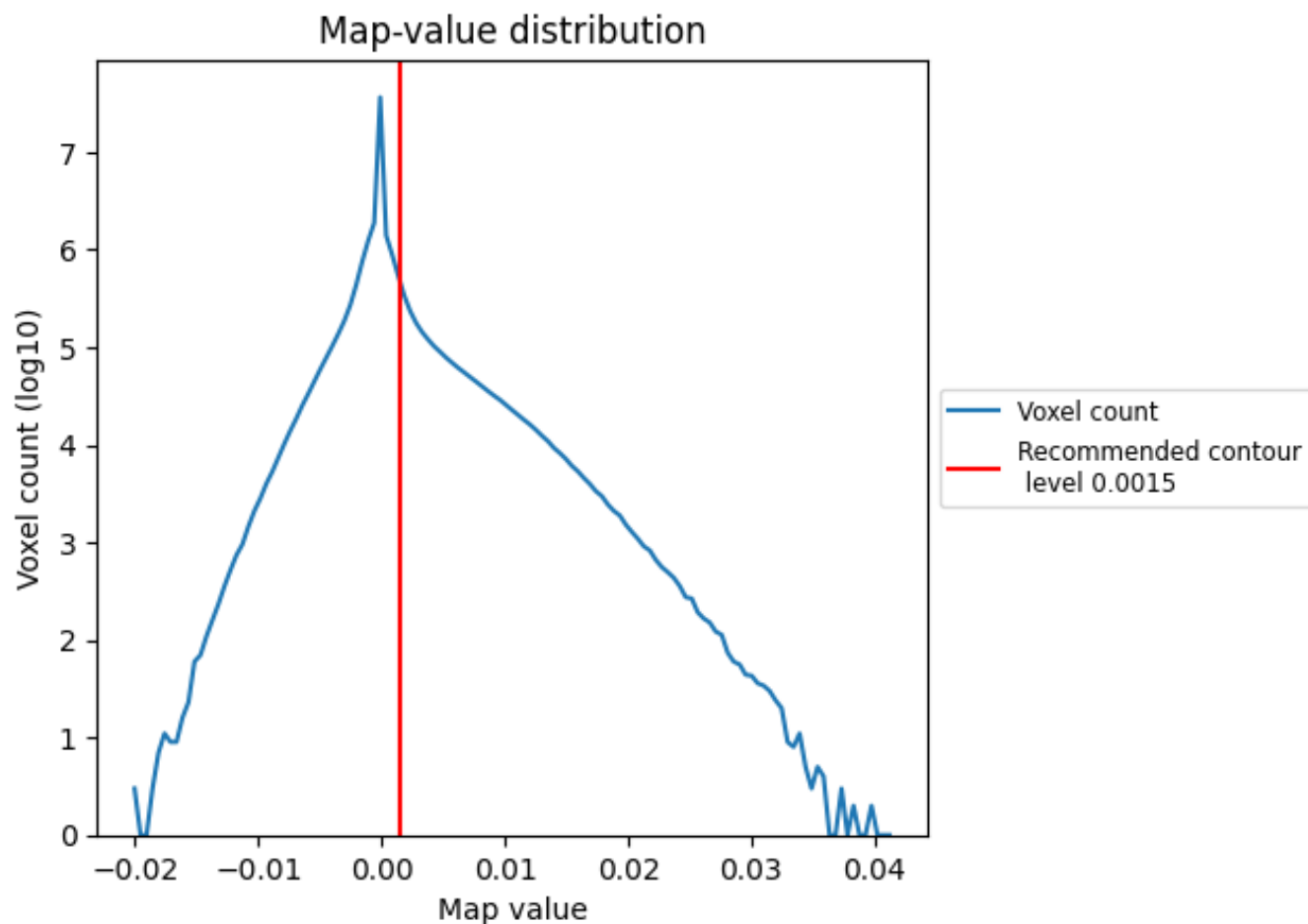
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

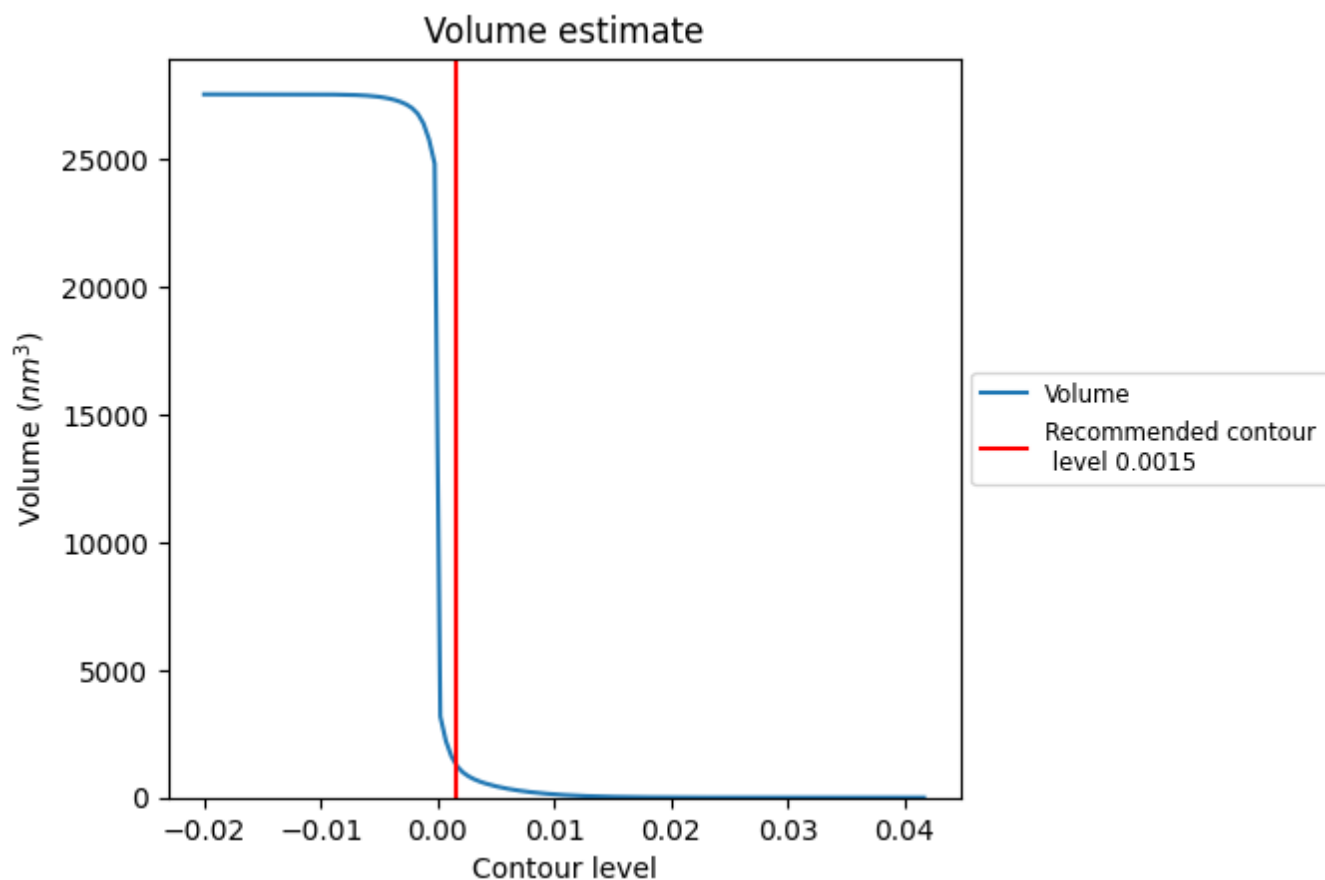
This section contains the results of statistical analysis of the map.

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.

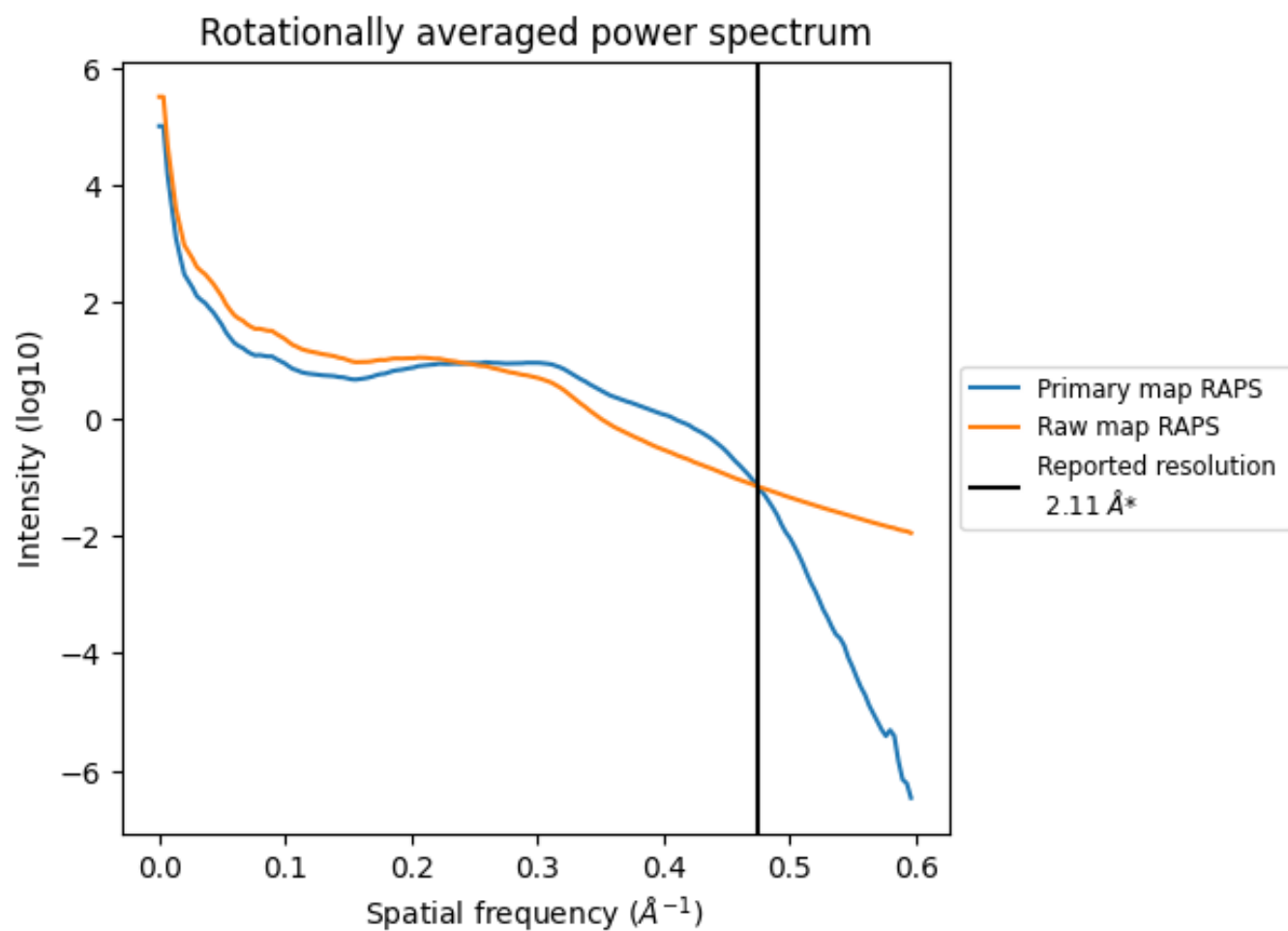
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1353 nm^3 ; this corresponds to an approximate mass of 1222 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 ⓘ

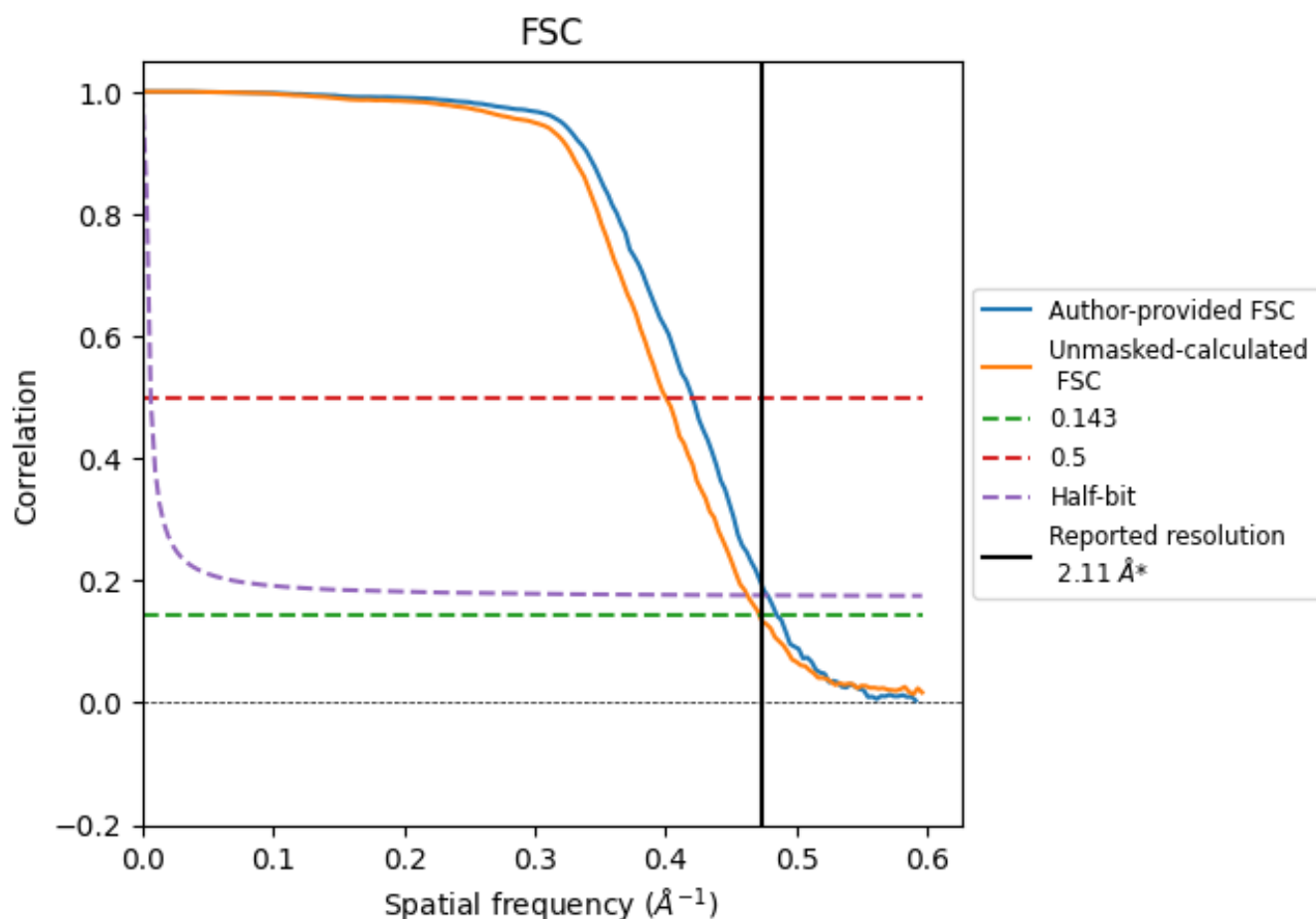


*Reported resolution corresponds to spatial frequency of $0.474 \text{ \AA}^{-1}$

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 0.474 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

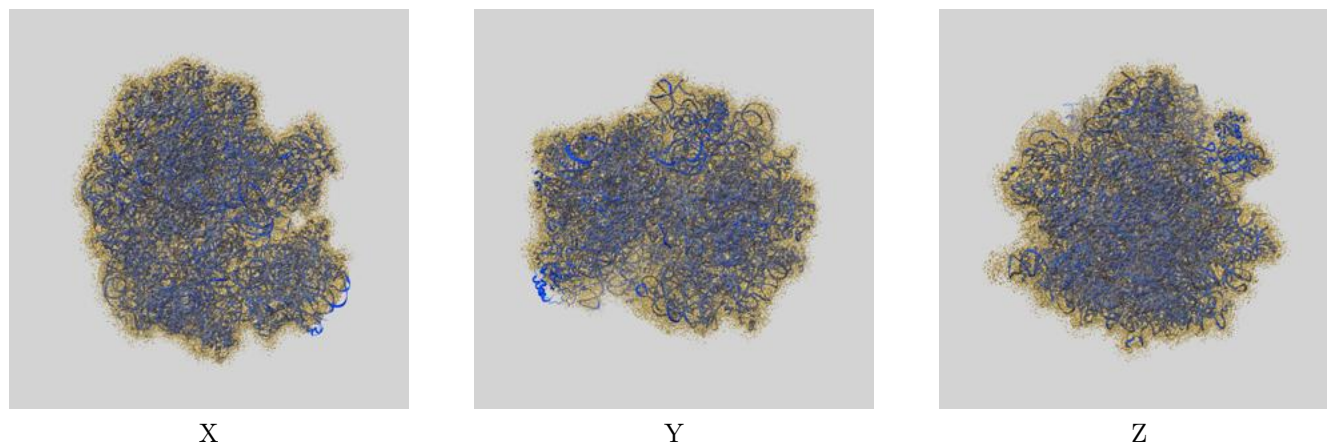
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.11	-	-
Author-provided FSC curve	2.06	2.38	2.09
Unmasked-calculated*	2.12	2.50	2.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

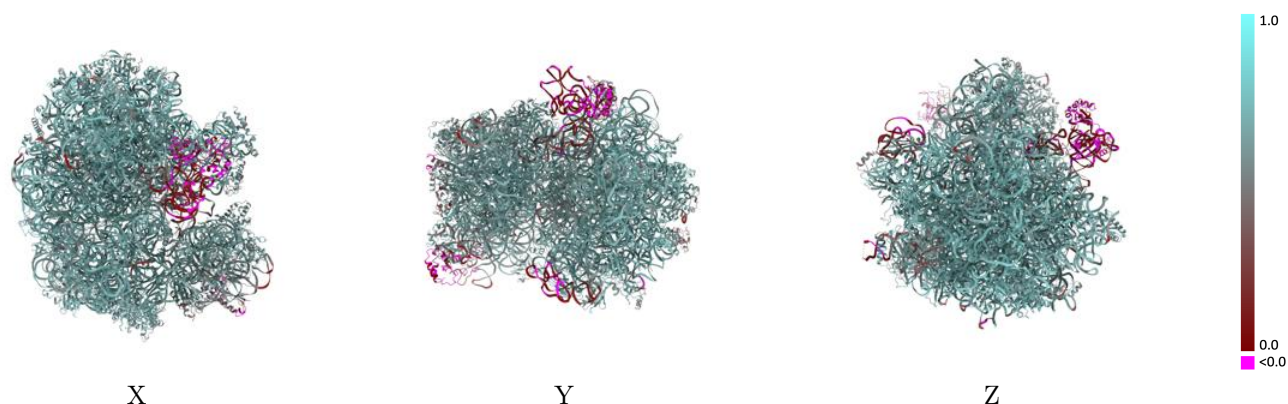
This section contains information regarding the fit between EMDB map EMD-55139 and PDB model 9SRE. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



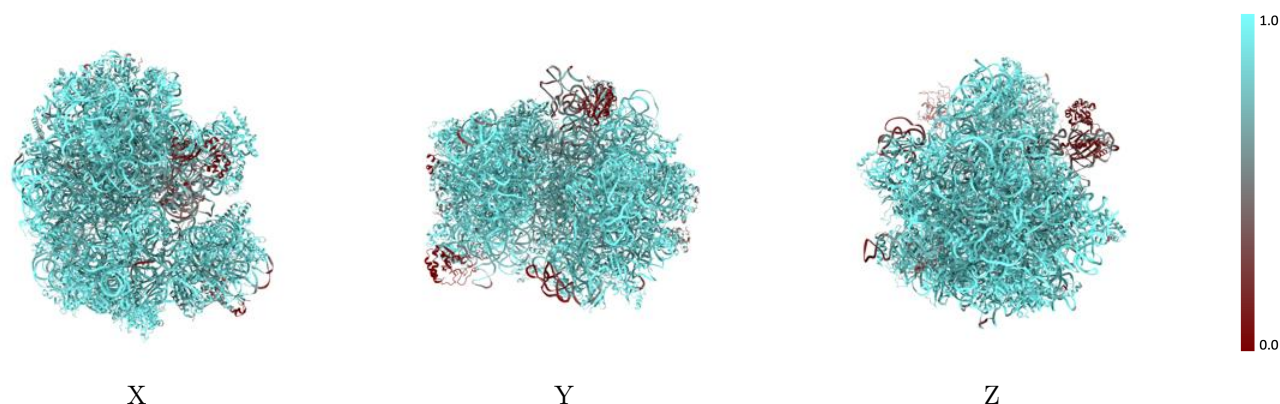
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



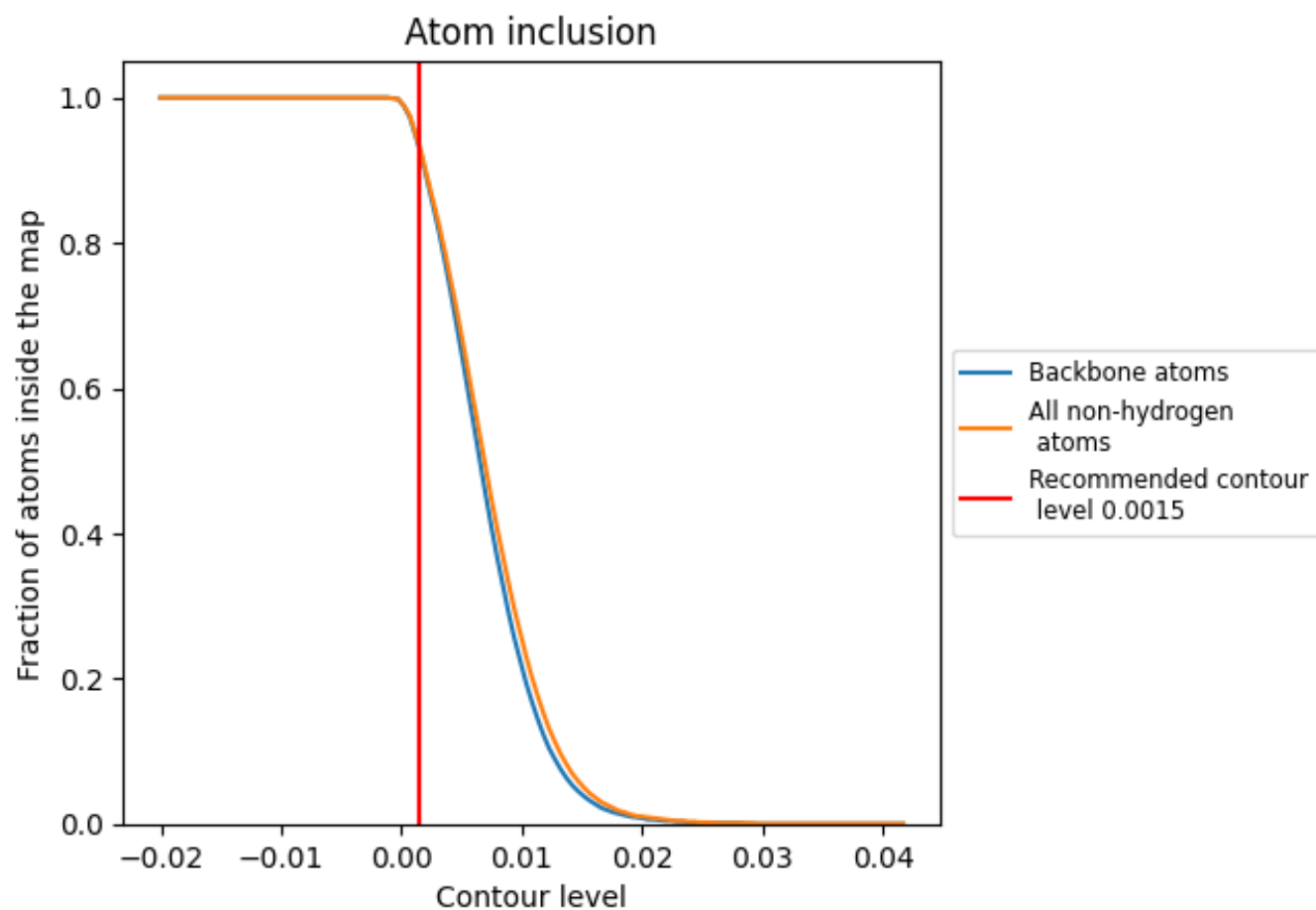
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.6440
1	 0.9510	 0.6610
2	 0.9710	 0.6530
3	 0.9890	 0.6570
4	 0.5780	 0.2760
A0	 0.9780	 0.7200
A3	 0.0620	 0.0830
AA	 0.9100	 0.6190
AB	 0.9490	 0.6240
AC	 0.9430	 0.6470
AD	 0.9710	 0.6700
AE	 0.9740	 0.6750
AF	 0.9610	 0.6670
AG	 0.8860	 0.5720
AH	 0.9440	 0.6180
AI	 0.9830	 0.6910
AJ	 0.9680	 0.6870
AK	 0.9420	 0.6100
AL	 0.6820	 0.4510
AM	 0.9570	 0.6600
AN	 0.9750	 0.6940
AO	 0.9220	 0.6070
AP	 0.9260	 0.6170
AQ	 0.9520	 0.6600
AR	 0.9750	 0.6930
AS	 0.8800	 0.5390
AT	 0.8820	 0.5770
AU	 0.9400	 0.6040
AV	 0.9500	 0.6330
AW	 0.9190	 0.5930
AX	 0.8990	 0.5940
AY	 0.1010	 0.1260
AZ	 0.8440	 0.5420
B4	 0.5960	 0.4050
B5	 0.9680	 0.6580



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Chain	Atom inclusion	Q-score
B6	 0.8060	 0.6150
BA	 0.1380	 0.0390
BB	 0.9800	 0.7290
BC	 0.9800	 0.7170
BD	 0.9820	 0.7090
BE	 0.9130	 0.5960
BF	 0.9480	 0.6600
BG	 0.9490	 0.6640
BI	 0.9790	 0.7150
BJ	 0.9810	 0.7170
BK	 0.9390	 0.6160
BL	 0.9540	 0.6780
BM	 0.9930	 0.7350
BN	 0.9640	 0.6860
BO	 0.9610	 0.6480
BP	 0.9840	 0.7130
BQ	 0.9760	 0.7080
BR	 0.9880	 0.7150
BS	 0.9860	 0.7170
BT	 0.9800	 0.7000
BU	 0.9730	 0.6850
BV	 0.9650	 0.6940
BW	 0.8890	 0.6320
BY	 0.9820	 0.7110
BZ	 0.9510	 0.6520
Ba	 0.9550	 0.6820
Bb	 0.9770	 0.7160
Bc	 0.9790	 0.7140
Bd	 0.9750	 0.7040
Be	 0.9980	 0.7350
Bf	 0.9980	 0.7240
Bg	 0.9780	 0.6780
Bi	 0.9720	 0.7230
Bj	 0.9540	 0.6970
Bk	 0.9510	 0.6740
Bl	 0.9410	 0.6410
H	 0.8240	 0.6120