



wwPDB EM Validation Summary Report ⓘ

Aug 3, 2026 – 12:54 pm BST

PDB ID : 9SRD / pdb_00009srd
EMDB ID : EMD-55138
Title : Cryo-EM structure of P. abyssi 70S ribosome in complex with hibernation factor HibA (HibA-uL5 conformation)
Authors : Madru, C.; Bourgeois, G.; Mechulam, Y.; Schmitt, E.
Deposited on : 2025-09-24
Resolution : 2.10 Å(reported)
Based on initial model : .

This is a wwPDB EM Validation Summary 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:

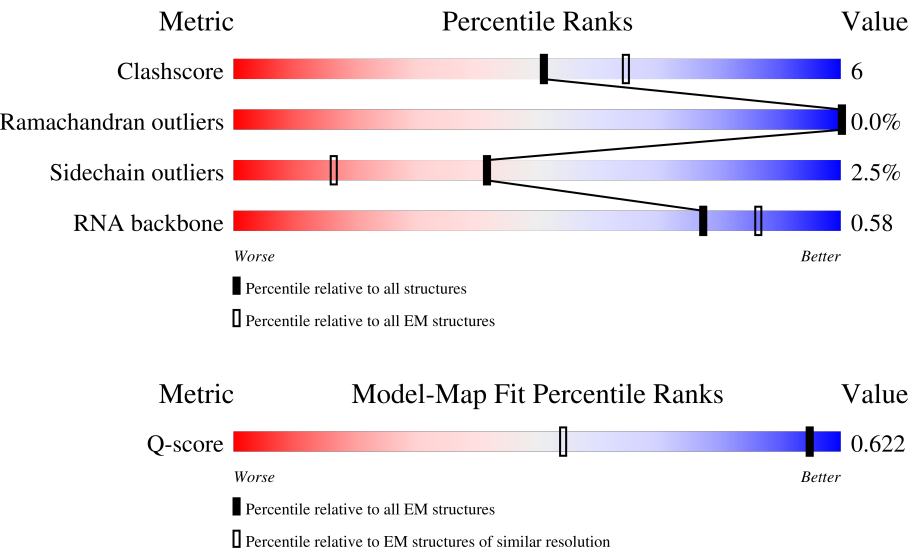
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

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

The reported resolution of this entry is 2.10 Å.

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



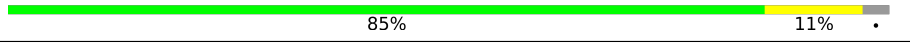
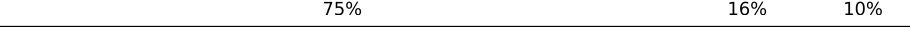
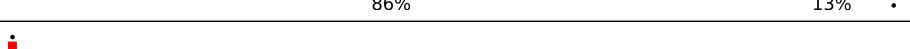
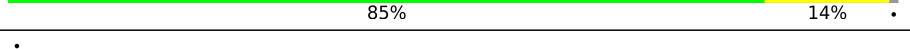
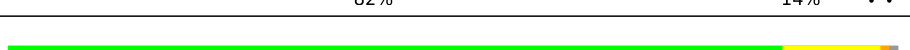
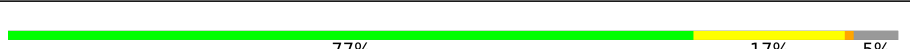
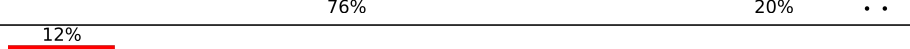
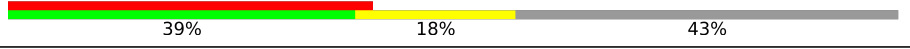
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2317 (1.60 - 2.60)

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

Mol	Chain	Length	Quality of chain
1	1	3018	
2	2	1512	
3	3	128	

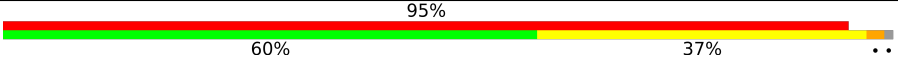
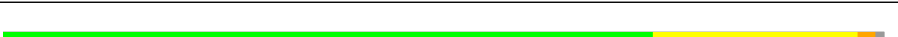
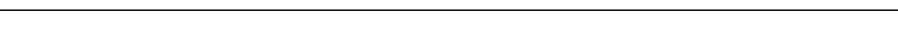
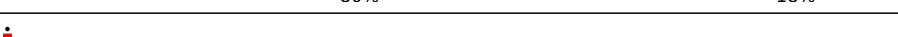
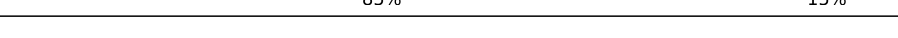
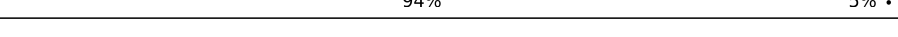
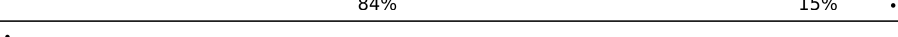
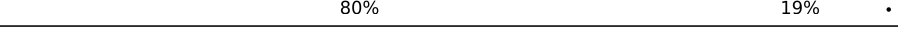
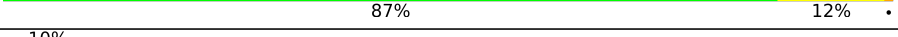
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Mol	Chain	Length	Quality of chain
4	AA	199	
5	AB	202	
6	AC	63	
7	AD	180	
8	AE	243	
9	AF	236	
10	AG	125	
11	AH	215	
12	AI	130	
13	AJ	127	
14	AK	135	
15	AL	102	
16	AM	137	
17	AN	147	
18	AP	56	
19	AQ	158	
20	AR	113	
21	AS	67	
22	AU	150	
23	AV	99	
23	B6	99	
24	AW	65	
25	AX	71	
26	AY	51	
27	AZ	210	

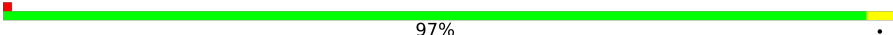
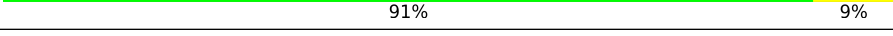
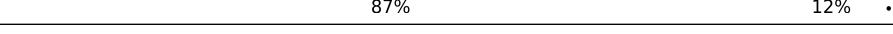
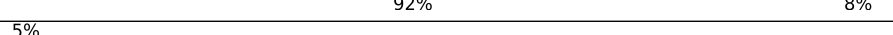
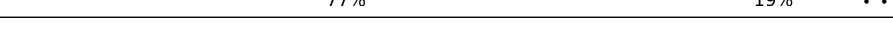
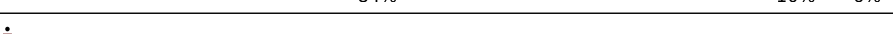
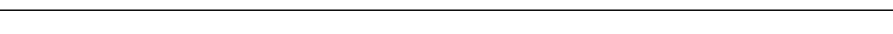
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Mol	Chain	Length	Quality of chain
28	A0	37	 89% 8%
29	A3	123	 95% 60% 37%
29	B4	123	 21% 66% 32%
29	BG	123	 92% 7%
30	AT	132	 80% 18%
31	AO	148	 74% 20% 7%
32	BB	239	 90% 9%
33	BY	155	 90% 9%
34	BO	203	 80% 17%
35	BC	361	 89% 10%
36	B5	82	 73% 23%
36	BK	82	 84% 13%
37	BL	147	 88% 11%
38	Bf	51	 80% 18%
39	BU	121	 85% 15%
40	Bb	130	 94% 5%
41	Be	62	 84% 15%
42	BE	188	 76% 21%
43	Ba	94	 80% 19%
44	BT	86	 87% 12%
45	BW	68	 10% 88% 12%
46	Bi	83	 90% 8%
47	BI	142	 88% 12%
48	BR	97	 85% 14%
49	BQ	151	 81% 18%

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Mol	Chain	Length	Quality of chain
50	BV	67	 87% 7% 6%
51	Bj	94	 97%
52	BD	255	 87% 12%
53	BF	184	 85% 14%
54	BZ	99	 86% 13%
55	BP	120	 87% 13%
56	BM	194	 91% 9%
57	BS	155	 87% 12%
58	Bd	91	 92% 8%
59	BN	181	 5% 77% 19%
60	Bg	51	 84% 10% 6%
61	Bc	87	 86% 13%
62	BJ	141	 90% 9%
63	Bl	77	 77% 22%
64	Bk	65	 89% 8%
65	H	392	 42% 63% 31%

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 170227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called rRNA 23S.

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

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

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

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

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

- Molecule 4 is a protein called 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	29	Total	C	N	O	S	0	0
			227	141	44	37	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		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 Dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	H	377	Total	C	N	O	S	0	0
			3009	1922	525	552	10		

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

Mol	Chain	Residues	Atoms		AltConf
66	1	167	Total	Mg	0
			167	167	
66	2	69	Total	Mg	0
			69	69	
66	3	1	Total	Mg	0
			1	1	
66	AK	1	Total	Mg	0
			1	1	
66	AN	1	Total	Mg	0
			1	1	
66	BB	1	Total	Mg	0
			1	1	
66	Bb	1	Total	Mg	0
			1	1	
66	BD	1	Total	Mg	0
			1	1	
66	BM	1	Total	Mg	0
			1	1	
66	BS	1	Total	Mg	0
			1	1	

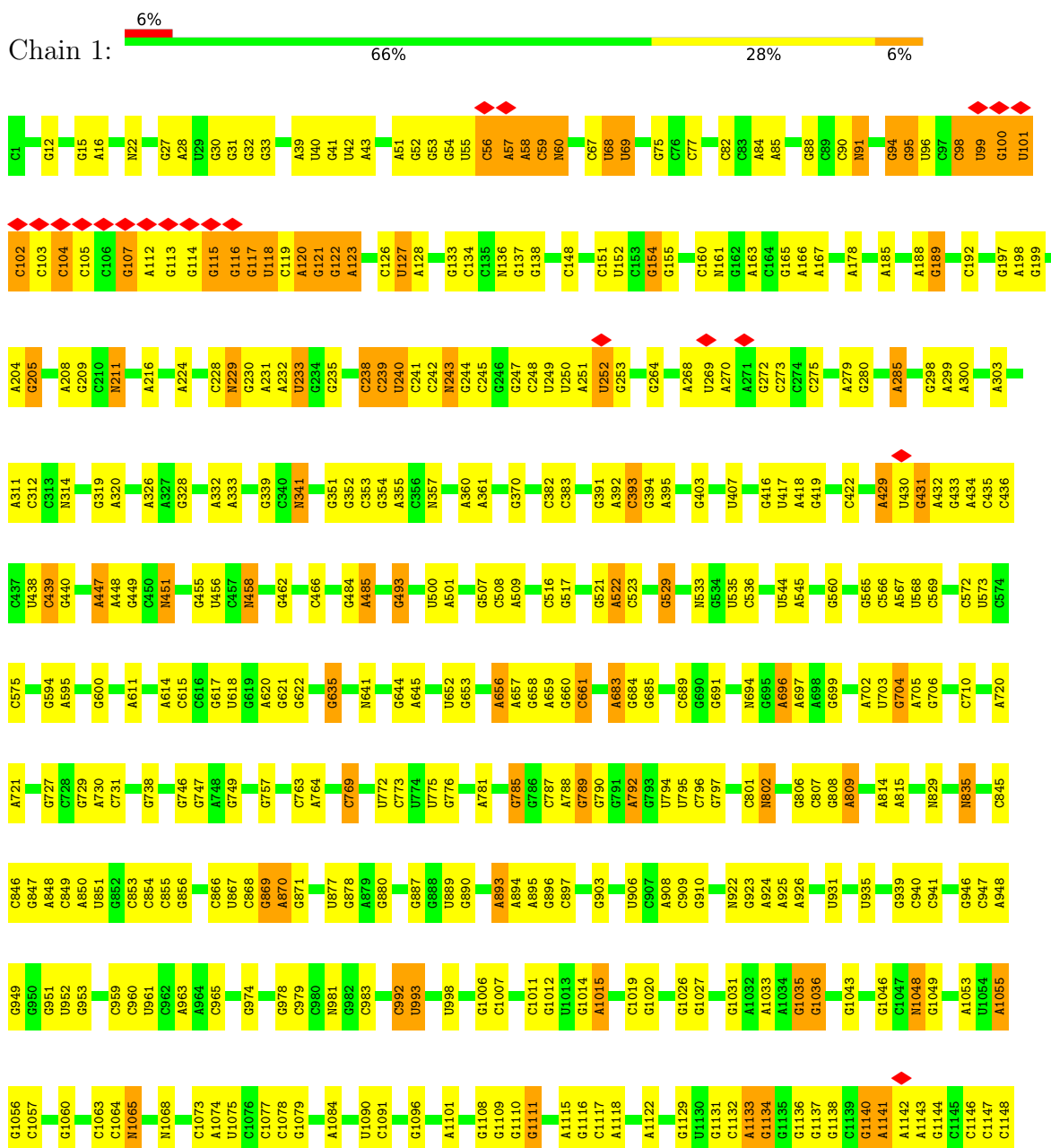
- Molecule 67 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

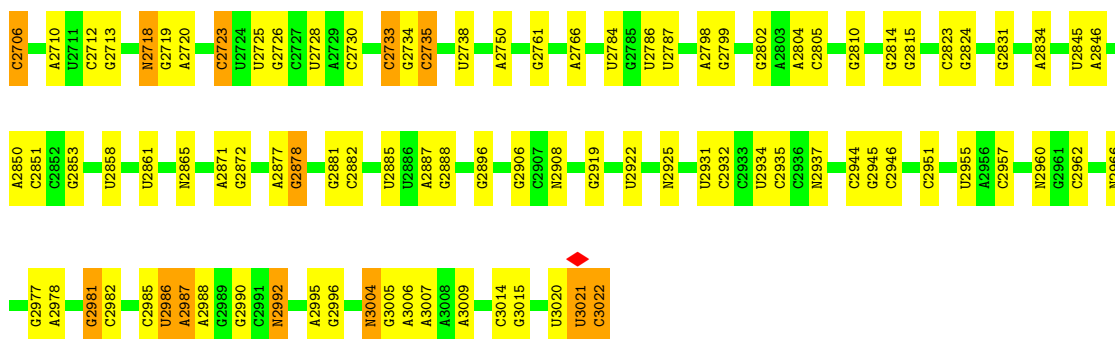
3 Residue-property plots

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

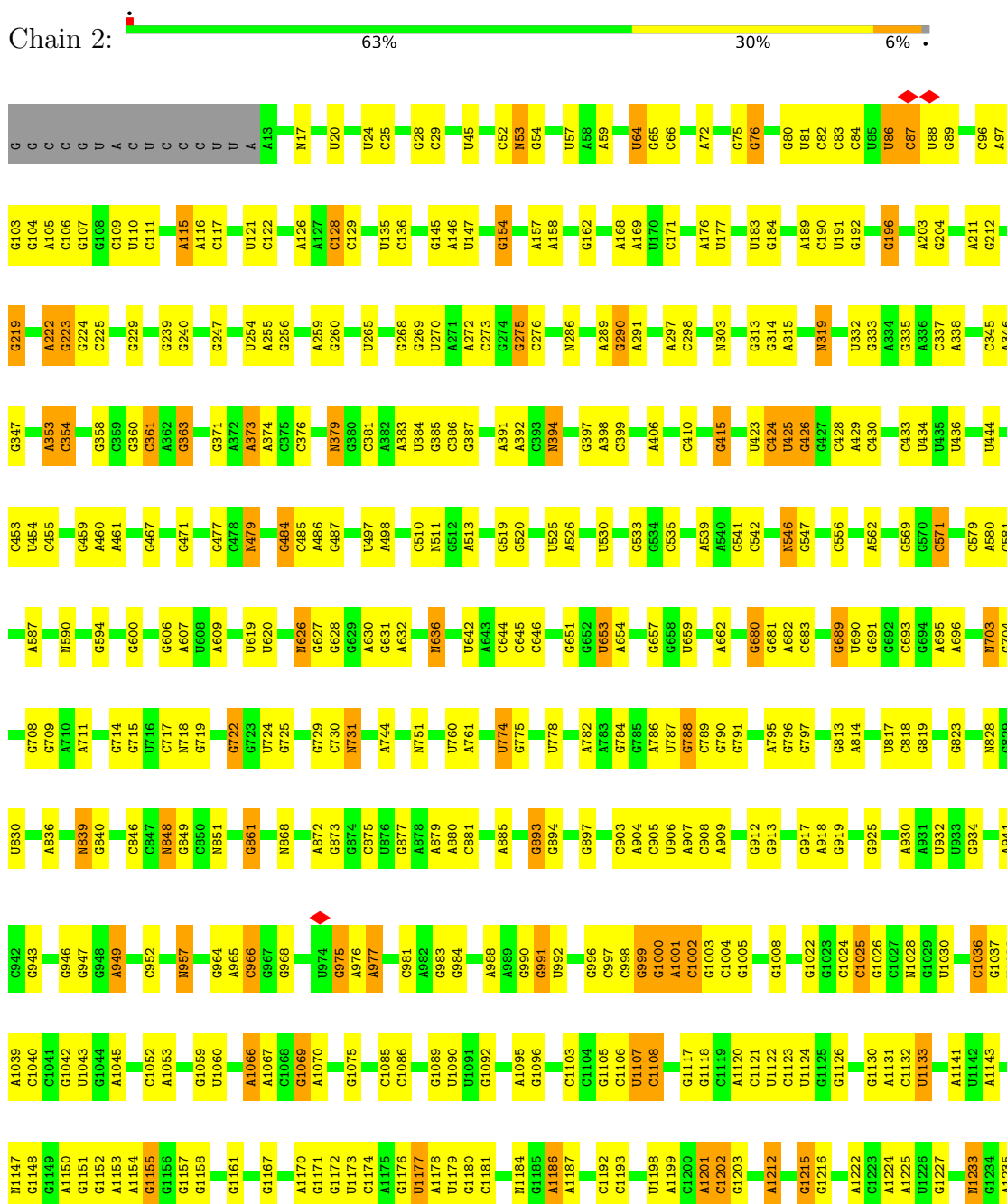
• Molecule 1: rRNA 23S

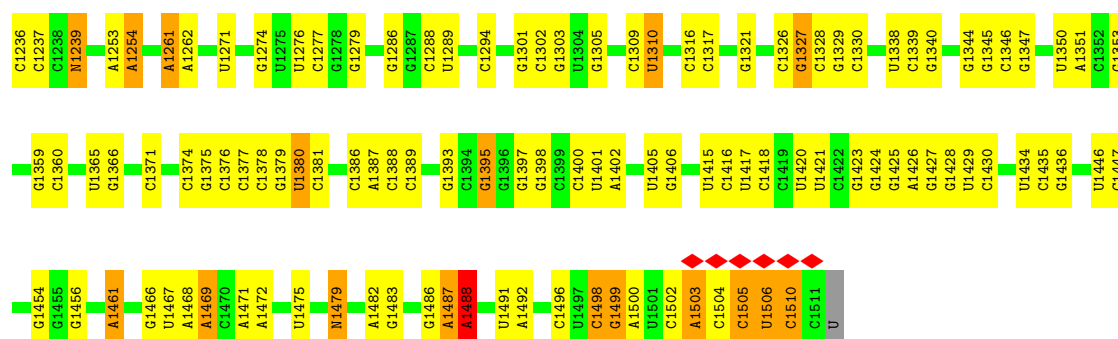


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A2593	N2495	C2401	G2341	U2232	G2108	A1976	A1841	U1715	A1613	G1477	U1349	G1285	C1153
G2496	G2496	G2402	G2342	G2233	A2109	A1977	A1842	A1730	C1616	G1478	A1350	U1288	C1154
A2497	A2497	U2403	G2343	U2234	A2110	G1986	A1943	U1731	N1617	C1479	A1351	G1289	U1159
A2498	A2498	U2404	G2344	G2234	G2111	U1987	A1944	G1732	G1618	C1480	C1352	N1283	G1160
A2499	A2499	C2405	G2345	C2242	A2112	G1988	C1947	A1733	C1619	G1481	A1353	G1294	A1161
U2503	U2503	A2406	G2346	G2243	U2118	G1993	G1851	G1734	G1620	A1484	G1354	G1295	A1162
A2504	A2504	U2407	G2347	G2244	A2119	C1994	G1852	G1735	N1621	A1489	C1355	G1296	A1163
U2505	U2505	G2408	G2348	C2247	G2120	U1996	G1853	G1739	A1625	C1490	C1356	G1299	C1164
C2506	C2506	U2409	G2349	N2248	A2121	A1997	U1856	U1741	C1626	G1498	C1357	U1299	G1168
G2510	G2510	G2410	G2350	N2249	U2128	A1998	U1857	U1742	G1630	G1499	C1358	U1300	G1169
A2514	A2514	A2411	G2351	G2253	G2129	C1999	U1862	A1743	C1633	C1509	C1359	A1301	A1170
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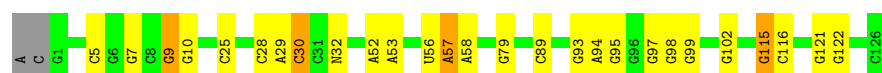


• Molecule 2: rRNA 16S

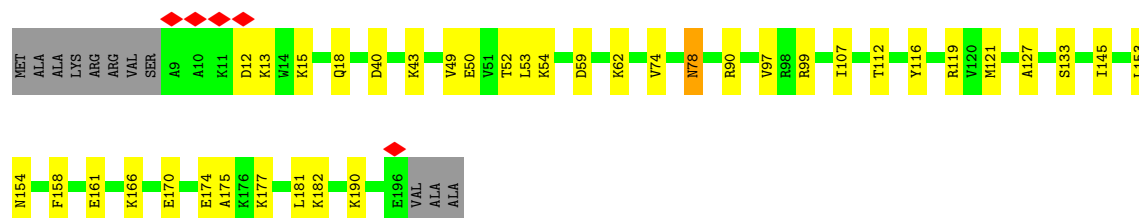
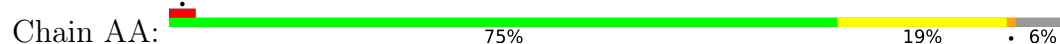




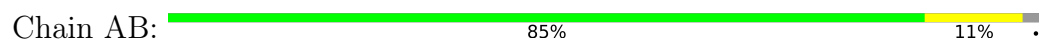
• Molecule 3: rRNA 5S



• Molecule 4: 30S ribosomal protein S3Ae



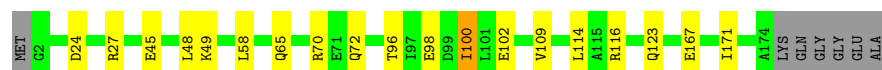
• Molecule 5: 30S ribosomal protein S2



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

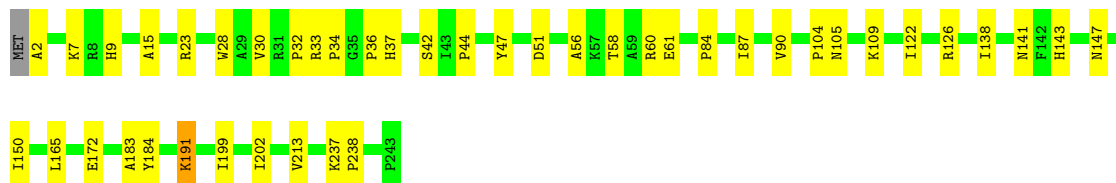


• Molecule 7: 30S ribosomal protein S4



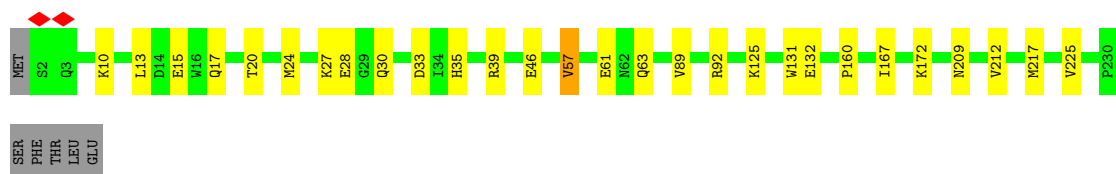
- Molecule 8: 30S ribosomal protein S4e

Chain AE:  82% 17%



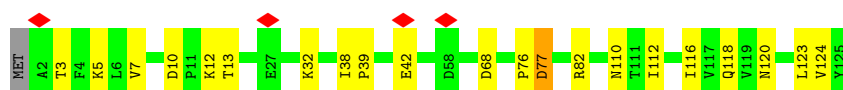
- Molecule 9: 30S ribosomal protein S5

Chain AF:  85% 11% .



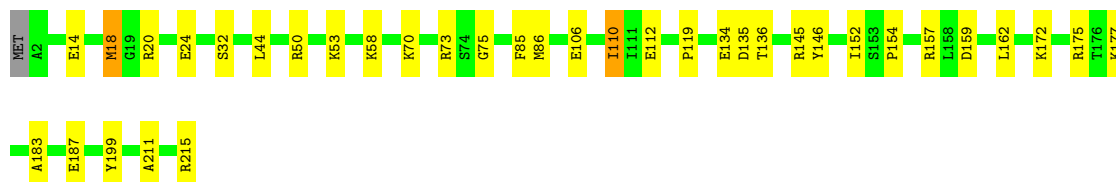
- Molecule 10: 30S ribosomal protein S6e

Chain AG:  82% 16% ..



- Molecule 11: 30S ribosomal protein S7

Chain AH:  83% 16% .



- Molecule 12: 30S ribosomal protein S8

Chain AI:  86% 13% .

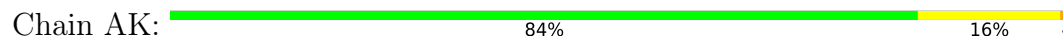


- Molecule 13: 30S ribosomal protein S8e

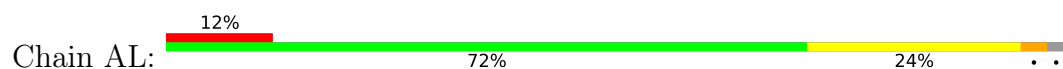
Chain AJ:  85% 13% ..



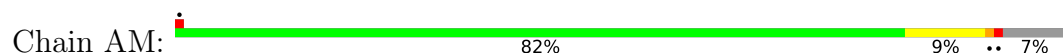
- Molecule 14: 30S ribosomal protein S9



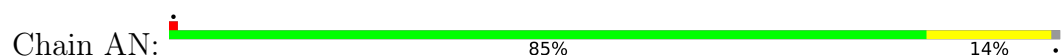
- Molecule 15: 30S ribosomal protein S10



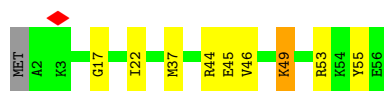
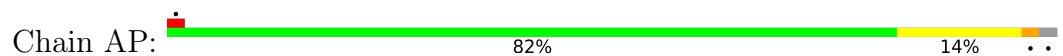
- Molecule 16: 30S ribosomal protein S11



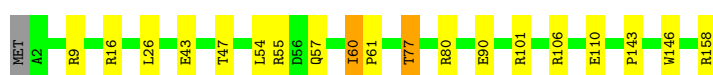
- Molecule 17: 30S ribosomal protein S12



- Molecule 18: 30S ribosomal protein S14 type Z



- Molecule 19: 30S ribosomal protein S15



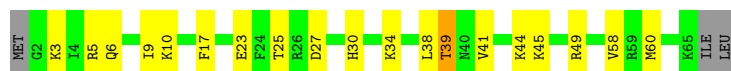
- Molecule 20: 30S ribosomal protein S17

Chain AR:  77% 17% 5%



- Molecule 21: 30S ribosomal protein S17e

Chain AS:  67% 27% 6%



- Molecule 22: 30S ribosomal protein S19e

Chain AU:  87% 12% 1%



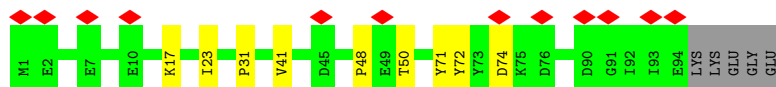
- Molecule 23: 30S ribosomal protein S24e

Chain AV:  76% 20% 4%



- Molecule 23: 30S ribosomal protein S24e

Chain B6:  12% 86% 9% 5%



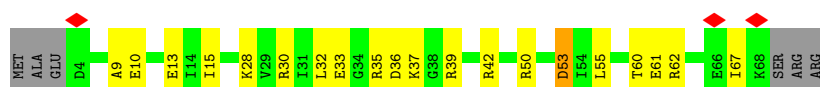
- Molecule 24: 30S ribosomal protein S27e

Chain AW:  69% 22% 6%

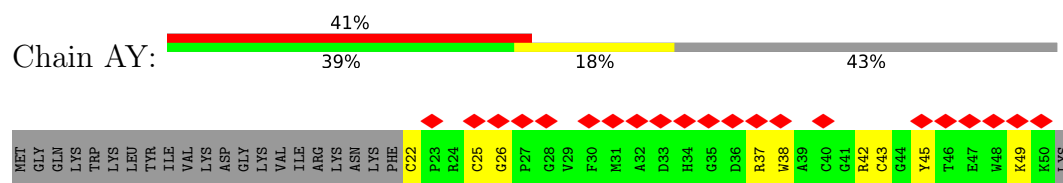


- Molecule 25: 30S ribosomal protein S28e

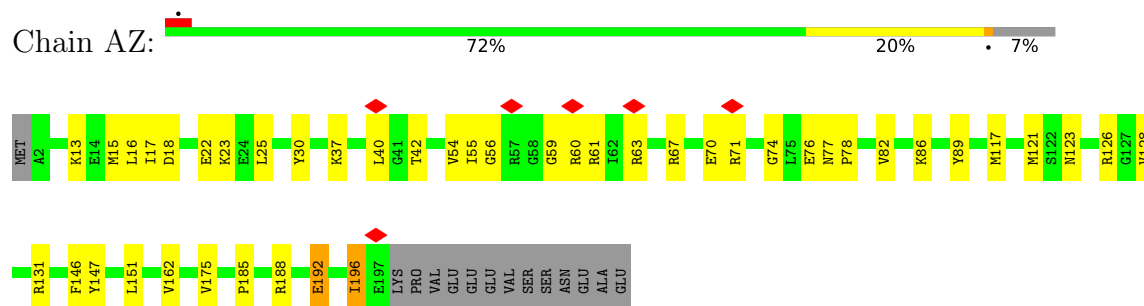
Chain AX:  63% 27% 8%



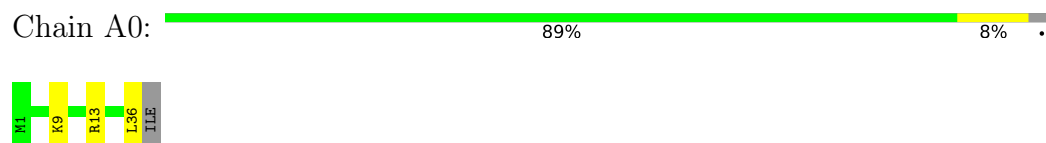
- Molecule 26: 30S ribosomal protein S27ae



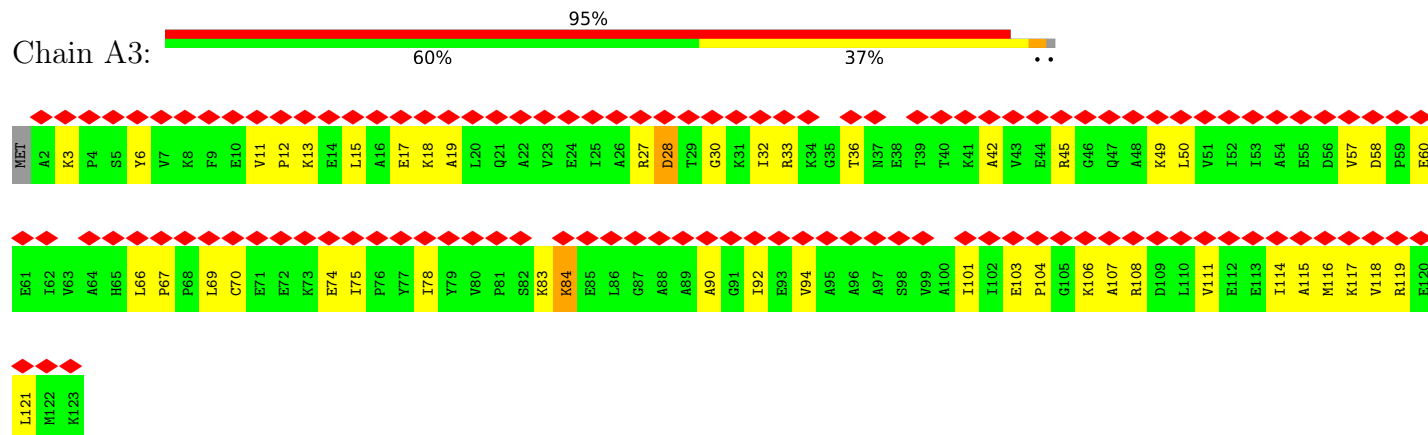
- Molecule 27: 30S ribosomal protein S3



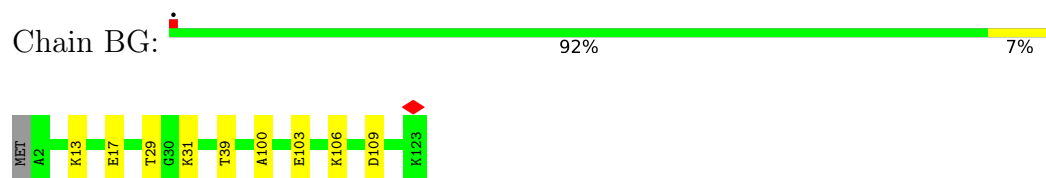
- Molecule 28: Small ribosomal subunit protein eS32



- Molecule 29: 50S ribosomal protein L7Ae

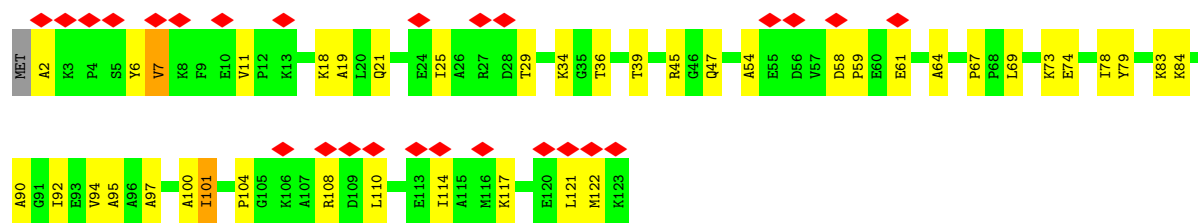


- Molecule 29: 50S ribosomal protein L7Ae

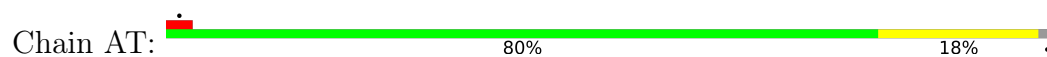


- Molecule 29: 50S ribosomal protein L7Ae

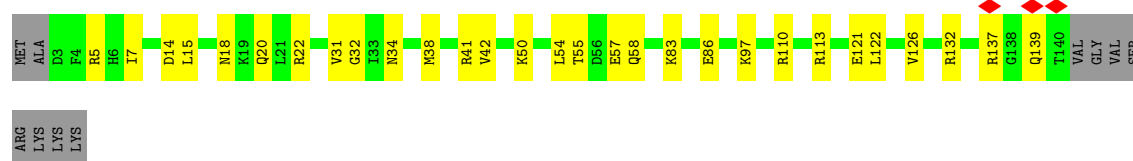
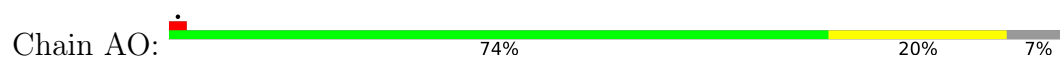




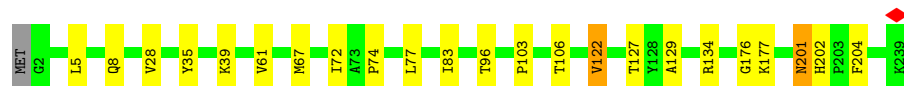
- Molecule 30: 30S ribosomal protein S19



- Molecule 31: 30S ribosomal protein S13



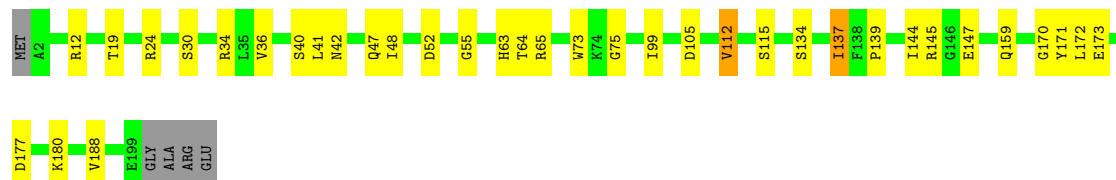
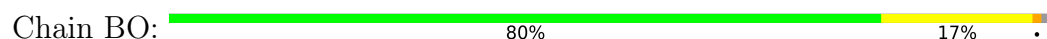
- Molecule 32: Large ribosomal subunit protein uL2



- Molecule 33: Large ribosomal subunit protein uL30

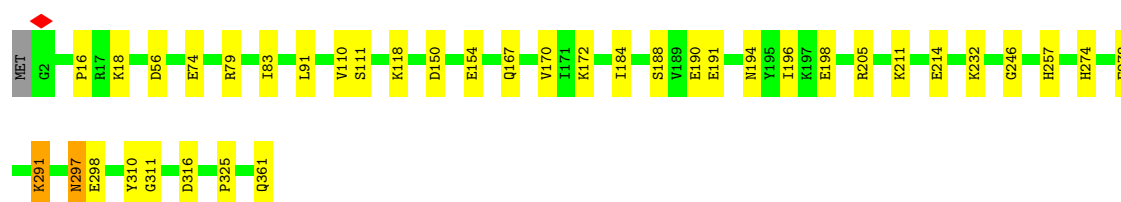


- Molecule 34: Large ribosomal subunit protein uL18



- Molecule 35: Large ribosomal subunit protein uL3

Chain BC:  89% 10% .



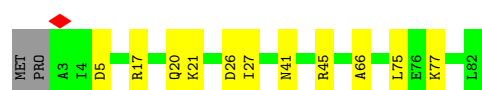
- Molecule 36: Large ribosomal subunit protein eL14

Chain B5:  73% 23% ..



- Molecule 36: Large ribosomal subunit protein eL14

Chain BK:  84% 13% .



- Molecule 37: Large ribosomal subunit protein uL15

Chain BL:  88% 11% .



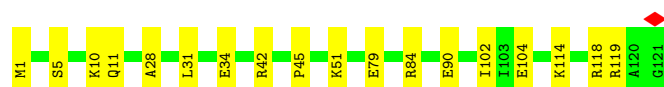
- Molecule 38: Large ribosomal subunit protein eL39

Chain Bf:  80% 18% .



- Molecule 39: Large ribosomal subunit protein uL24

Chain BU:  85% 15%



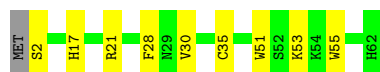
- Molecule 40: Large ribosomal subunit protein eL32

Chain Bb:  94% 5% .



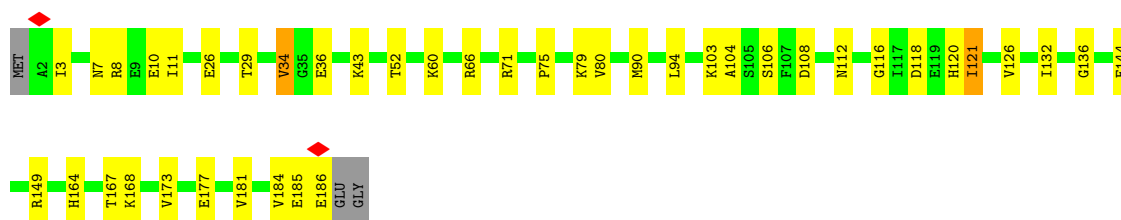
- Molecule 41: Large ribosomal subunit protein eL37

Chain Be: 84% 15% .



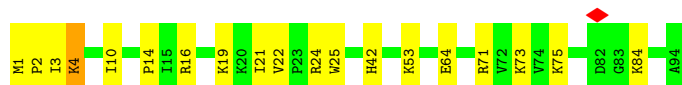
- Molecule 42: Large ribosomal subunit protein uL5

Chain BE: 76% 21% ..



- Molecule 43: Large ribosomal subunit protein eL31

Chain Ba: 80% 19% .



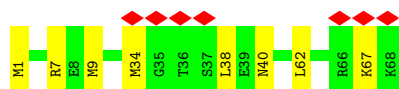
- Molecule 44: Large ribosomal subunit protein uL23

Chain BT: 87% 12% .



- Molecule 45: Large ribosomal subunit protein uL29

Chain BW: 10% 88% 12%



- Molecule 46: Large ribosomal subunit protein eL43

Chain Bi: 90% 8% .



- Molecule 47: Large ribosomal subunit protein uL13

Chain BI:  88% 12%



- Molecule 48: Large ribosomal subunit protein eL21

Chain BR:  85% 14%



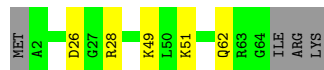
- Molecule 49: Large ribosomal subunit protein eL19

Chain BQ:  81% 18%



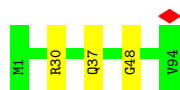
- Molecule 50: Large ribosomal subunit protein eL24

Chain BV:  87% 7% 6%



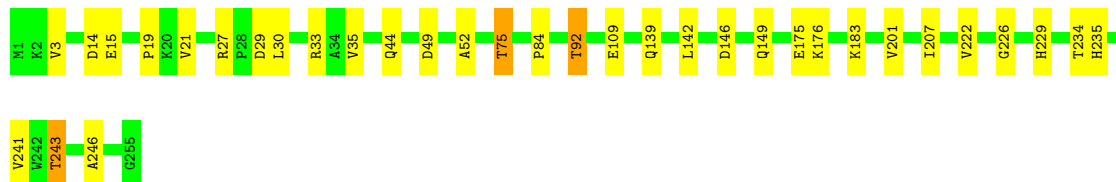
- Molecule 51: Large ribosomal subunit protein eL42

Chain Bj:  97%



- Molecule 52: Large ribosomal subunit protein uL4

Chain BD:  87% 12%

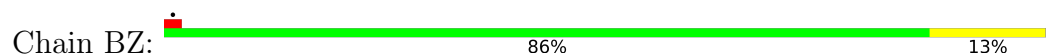


- Molecule 53: Large ribosomal subunit protein uL6

Chain BF:  85% 14%



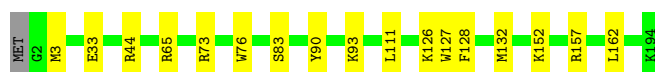
- Molecule 54: Large ribosomal subunit protein eL30



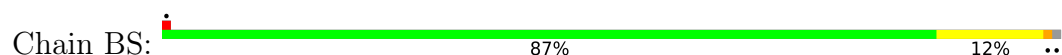
- Molecule 55: Large ribosomal subunit protein eL18



- Molecule 56: Large ribosomal subunit protein eL15



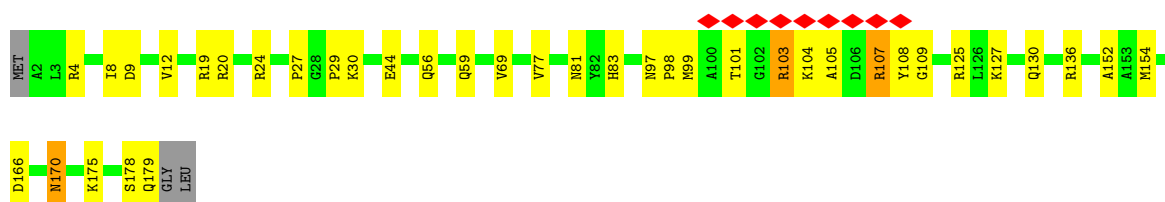
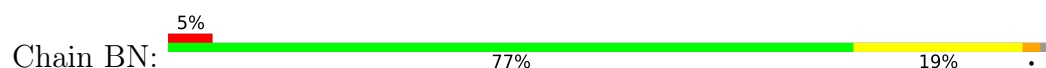
- Molecule 57: Large ribosomal subunit protein uL22



- Molecule 58: Large ribosomal subunit protein eL34



- Molecule 59: Large ribosomal subunit protein uL16



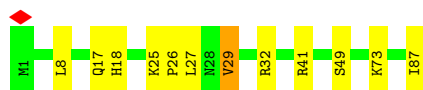
- Molecule 60: Large ribosomal subunit protein eL40

Chain Bg:  84% 10% 6%



- Molecule 61: Large ribosomal subunit protein eL33

Chain Bc:  86% 13% .



- Molecule 62: Large ribosomal subunit protein uL14

Chain BJ:  90% 9% .



- Molecule 63: Large ribosomal subunit protein eL20

Chain Bl:  77% 22% .



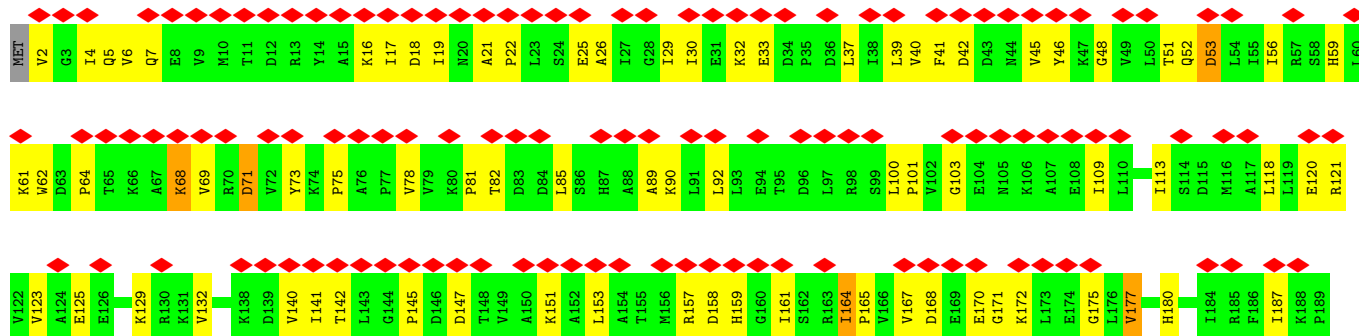
- Molecule 64: C2H2-type domain-containing protein

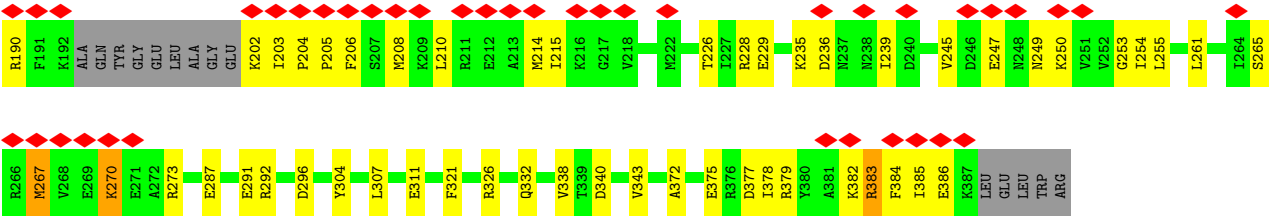
Chain Bk:  89% 8% .



- Molecule 65: Dehydrogenase

Chain H:  42% 63% 31% . .





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	207000	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)	300	Depositor
Maximum defocus (nm)	800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00125	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: OMU, LHH, MG, 6MZ, B8H, ZN, OMG, 5MC, A2M, UR3, 4AC, OMC, MA6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.26	1/70601 (0.0%)	0.32	4/110066 (0.0%)
2	2	0.23	1/34435 (0.0%)	0.27	0/53681
3	3	0.20	0/2995	0.25	0/4669
4	AA	0.14	0/1557	0.25	0/2087
5	AB	0.15	0/1602	0.26	0/2165
6	AC	0.16	0/463	0.27	0/628
7	AD	0.15	0/1476	0.21	0/1980
8	AE	0.16	0/2032	0.27	0/2742
9	AF	0.18	0/1838	0.27	0/2478
10	AG	0.13	0/993	0.29	0/1329
11	AH	0.14	0/1762	0.26	0/2366
12	AI	0.18	0/1055	0.27	0/1415
13	AJ	0.15	0/995	0.23	0/1327
14	AK	0.16	0/1089	0.28	0/1459
15	AL	0.16	0/817	0.29	0/1097
16	AM	0.16	0/973	0.34	1/1311 (0.1%)
17	AN	0.17	0/1165	0.26	0/1547
18	AP	0.18	0/465	0.31	0/613
19	AQ	0.15	0/1333	0.24	0/1791
20	AR	0.16	0/907	0.31	0/1225
21	AS	0.15	0/548	0.25	0/725
22	AU	0.15	0/1253	0.25	0/1689
23	AV	0.14	0/826	0.23	0/1108
23	B6	0.11	0/808	0.24	0/1086
24	AW	0.15	0/476	0.25	0/641
25	AX	0.19	0/518	0.33	0/694
26	AY	0.10	0/235	0.27	0/315
27	AZ	0.14	0/1563	0.26	0/2099
28	A0	0.20	0/349	0.27	0/451
29	A3	0.12	0/945	0.30	0/1274
29	B4	0.14	0/945	0.32	0/1274
29	BG	0.16	0/944	0.27	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	AT	0.14	0/1077	0.26	0/1439
31	AO	0.14	0/1135	0.26	0/1526
32	BB	0.22	0/1882	0.32	0/2538
33	BY	0.19	0/1254	0.27	0/1677
34	BO	0.15	0/1645	0.25	0/2209
35	BC	0.21	0/2933	0.29	0/3943
36	B5	0.16	0/619	0.29	0/830
36	BK	0.16	0/611	0.28	0/819
37	BL	0.19	0/1167	0.32	0/1552
38	Bf	0.21	0/443	0.27	0/589
39	BU	0.18	0/1027	0.27	0/1368
40	Bb	0.20	0/1120	0.27	0/1494
41	Be	0.22	0/514	0.29	0/676
42	BE	0.15	0/1509	0.28	0/2022
43	Ba	0.19	0/793	0.27	0/1064
44	BT	0.18	0/705	0.26	0/945
45	BW	0.16	0/566	0.23	0/747
46	Bi	0.19	0/630	0.31	0/839
47	BI	0.20	0/1166	0.26	0/1559
48	BR	0.20	0/819	0.29	0/1098
49	BQ	0.20	0/1281	0.27	0/1689
50	BV	0.20	0/547	0.25	0/729
51	Bj	0.18	0/807	0.26	0/1070
52	BD	0.20	0/2069	0.30	0/2787
53	BF	0.17	0/1485	0.27	0/2003
54	BZ	0.17	0/759	0.28	0/1023
55	BP	0.19	0/984	0.26	0/1314
56	BM	0.23	0/1627	0.30	0/2170
57	BS	0.20	0/1275	0.31	0/1715
58	Bd	0.19	0/778	0.28	0/1036
59	BN	0.18	0/1483	0.28	0/1992
60	Bg	0.16	0/396	0.25	0/526
61	Bc	0.19	0/693	0.30	0/926
62	BJ	0.20	0/1080	0.28	0/1456
63	Bl	0.16	0/669	0.27	0/886
64	Bk	0.22	0/538	0.28	0/709
65	H	0.16	0/3053	0.39	3/4117 (0.1%)
All	All	0.22	2/179102 (0.0%)	0.30	8/263688 (0.0%)

All (2) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1036	C	O3'-P	-7.02	1.50	1.61
1	1	96	U	C1'-N1	5.75	1.57	1.48

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	126	C	P-O3'-C3'	-15.70	96.65	120.20
1	1	126	C	OP1-P-O3'	-8.35	82.94	108.00
65	H	383	ARG	N-CA-C	6.30	120.58	113.01
16	AM	52	ARG	N-CA-C	5.98	117.79	111.28
65	H	377	ASP	CA-C-N	-5.92	115.08	122.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	65181	0	32948	579	0
2	2	32291	0	16342	301	0
3	3	2703	0	1375	17	0
4	AA	1531	0	1623	24	0
5	AB	1571	0	1630	16	0
6	AC	449	0	435	7	0
7	AD	1452	0	1521	13	0
8	AE	1983	0	2060	25	0
9	AF	1808	0	1879	20	0
10	AG	977	0	1037	14	0
11	AH	1725	0	1780	28	0
12	AI	1034	0	1069	14	0
13	AJ	986	0	1070	11	0
14	AK	1073	0	1133	14	0
15	AL	809	0	859	18	0
16	AM	955	0	981	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	AN	1148	0	1248	12	0
18	AP	455	0	475	7	0
19	AQ	1305	0	1388	16	0
20	AR	884	0	906	11	0
21	AS	541	0	573	15	0
22	AU	1223	0	1263	12	0
23	AV	808	0	832	15	0
23	B6	790	0	806	5	0
24	AW	470	0	495	8	0
25	AX	516	0	544	13	0
26	AY	227	0	207	7	0
27	AZ	1541	0	1624	32	0
28	A0	343	0	407	1	0
29	A3	933	0	982	38	0
29	B4	933	0	982	25	0
29	BG	932	0	982	5	0
30	AT	1057	0	1131	15	0
31	AO	1116	0	1152	19	0
32	BB	1838	0	1903	17	0
33	BY	1235	0	1314	10	0
34	BO	1607	0	1638	24	0
35	BC	2870	0	3021	21	0
36	B5	614	0	671	15	0
36	BK	607	0	663	8	0
37	BL	1149	0	1218	16	0
38	Bf	435	0	494	8	0
39	BU	1011	0	1078	13	0
40	Bb	1095	0	1190	4	0
41	Be	503	0	533	8	0
42	BE	1485	0	1539	27	0
43	Ba	778	0	851	13	0
44	BT	696	0	758	8	0
45	BW	565	0	628	6	0
46	Bi	620	0	668	4	0
47	BI	1148	0	1237	13	0
48	BR	797	0	835	11	0
49	BQ	1265	0	1392	21	0
50	BV	532	0	523	4	0
51	Bj	789	0	842	2	0
52	BD	2026	0	2131	23	0
53	BF	1456	0	1514	16	0
54	BZ	749	0	796	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BP	971	0	1039	10	0
56	BM	1588	0	1683	12	0
57	BS	1247	0	1280	10	0
58	Bd	759	0	825	7	0
59	BN	1452	0	1491	26	0
60	Bg	387	0	397	3	0
61	Bc	684	0	748	8	0
62	BJ	1066	0	1133	9	0
63	Bl	659	0	702	10	0
64	Bk	528	0	575	3	0
65	H	3009	0	3133	92	0
66	1	167	0	0	0	0
66	2	69	0	0	0	0
66	3	1	0	0	0	0
66	AK	1	0	0	0	0
66	AN	1	0	0	0	0
66	BB	1	0	0	0	0
66	BD	1	0	0	0	0
66	BM	1	0	0	0	0
66	BS	1	0	0	0	0
66	Bb	1	0	0	0	0
67	AC	2	0	0	0	0
67	AF	1	0	0	0	0
67	AP	1	0	0	0	0
67	AR	1	0	0	0	0
67	AW	1	0	0	0	0
67	BV	1	0	0	0	0
67	Bd	1	0	0	0	0
67	Be	1	0	0	0	0
67	Bg	1	0	0	0	0
67	Bi	1	0	0	0	0
67	Bj	1	0	0	0	0
67	Bk	1	0	0	0	0
All	All	170227	0	124182	1619	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1619 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:107:G:N2	1:1:112:A:N7	1.85	1.20
1:1:107:G:N2	1:1:112:A:C8	2.14	1.15
1:1:100:G:N2	1:1:119:C:O2	1.82	1.12
1:1:117:G:O2'	1:1:118:U:OP1	1.67	1.12
1:1:2585:4AC:H5	1:1:2597:G:H1	1.12	1.09

There are no symmetry-related clashes.

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	
4	AA	186/199 (94%)	182 (98%)	4 (2%)	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%)	234 (98%)	6 (2%)	0	100	100
9	AF	227/236 (96%)	222 (98%)	5 (2%)	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%)	123 (97%)	4 (3%)	0	100	100
13	AJ	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
14	AK	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
15	AL	98/102 (96%)	95 (97%)	3 (3%)	0	100	100
16	AM	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
17	AN	144/147 (98%)	144 (100%)	0	0	100	100
18	AP	53/56 (95%)	53 (100%)	0	0	100	100
19	AQ	155/158 (98%)	152 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AR	105/113 (93%)	103 (98%)	2 (2%)	0	100	100
21	AS	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
22	AU	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
23	AV	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
23	B6	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
24	AW	59/65 (91%)	55 (93%)	4 (7%)	0	100	100
25	AX	63/71 (89%)	62 (98%)	1 (2%)	0	100	100
26	AY	27/51 (53%)	23 (85%)	4 (15%)	0	100	100
27	AZ	194/210 (92%)	184 (95%)	10 (5%)	0	100	100
28	A0	34/37 (92%)	34 (100%)	0	0	100	100
29	A3	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
29	B4	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
29	BG	120/123 (98%)	120 (100%)	0	0	100	100
30	AT	128/132 (97%)	128 (100%)	0	0	100	100
31	AO	136/148 (92%)	127 (93%)	9 (7%)	0	100	100
32	BB	236/239 (99%)	229 (97%)	6 (2%)	1 (0%)	30	28
33	BY	152/155 (98%)	151 (99%)	1 (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%)	77 (98%)	2 (2%)	0	100	100
36	BK	78/82 (95%)	74 (95%)	4 (5%)	0	100	100
37	BL	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
38	Bf	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
39	BU	119/121 (98%)	119 (100%)	0	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%)	180 (98%)	3 (2%)	0	100	100
43	Ba	92/94 (98%)	92 (100%)	0	0	100	100
44	BT	84/86 (98%)	84 (100%)	0	0	100	100
45	BW	66/68 (97%)	66 (100%)	0	0	100	100
46	Bi	80/83 (96%)	76 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	92 (100%)	0	0	100	100
52	BD	253/255 (99%)	249 (98%)	4 (2%)	0	100	100
53	BF	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
54	BZ	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
55	BP	118/120 (98%)	118 (100%)	0	0	100	100
56	BM	191/194 (98%)	188 (98%)	3 (2%)	0	100	100
57	BS	152/155 (98%)	148 (97%)	4 (3%)	0	100	100
58	Bd	89/91 (98%)	89 (100%)	0	0	100	100
59	BN	176/181 (97%)	172 (98%)	4 (2%)	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%)	60 (98%)	1 (2%)	0	100	100
65	H	373/392 (95%)	349 (94%)	23 (6%)	1 (0%)	36	36
All	All	8537/8861 (96%)	8347 (98%)	188 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
65	H	206	PHE
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	
4	AA	160/167 (96%)	156 (98%)	4 (2%)	42	48
5	AB	168/173 (97%)	164 (98%)	4 (2%)	43	49
6	AC	50/55 (91%)	49 (98%)	1 (2%)	48	56
7	AD	156/160 (98%)	155 (99%)	1 (1%)	78	86
8	AE	213/214 (100%)	211 (99%)	2 (1%)	70	78
9	AF	192/198 (97%)	190 (99%)	2 (1%)	68	76
10	AG	107/108 (99%)	102 (95%)	5 (5%)	23	24
11	AH	183/184 (100%)	180 (98%)	3 (2%)	55	64
12	AI	106/107 (99%)	104 (98%)	2 (2%)	50	58
13	AJ	101/103 (98%)	99 (98%)	2 (2%)	48	56
14	AK	111/111 (100%)	107 (96%)	4 (4%)	31	34
15	AL	89/91 (98%)	84 (94%)	5 (6%)	19	18
16	AM	94/104 (90%)	89 (95%)	5 (5%)	20	19
17	AN	120/121 (99%)	118 (98%)	2 (2%)	53	62
18	AP	45/46 (98%)	43 (96%)	2 (4%)	25	26
19	AQ	142/143 (99%)	140 (99%)	2 (1%)	59	67
20	AR	96/102 (94%)	93 (97%)	3 (3%)	35	39
21	AS	58/61 (95%)	56 (97%)	2 (3%)	32	35
22	AU	126/127 (99%)	124 (98%)	2 (2%)	55	64
23	AV	88/90 (98%)	86 (98%)	2 (2%)	44	51
23	B6	86/90 (96%)	86 (100%)	0	100	100
24	AW	53/56 (95%)	49 (92%)	4 (8%)	12	10
25	AX	55/60 (92%)	51 (93%)	4 (7%)	13	10
26	AY	22/42 (52%)	22 (100%)	0	100	100
27	AZ	155/168 (92%)	150 (97%)	5 (3%)	34	38
28	A0	34/35 (97%)	33 (97%)	1 (3%)	37	42
29	A3	98/99 (99%)	91 (93%)	7 (7%)	13	11
29	B4	98/99 (99%)	94 (96%)	4 (4%)	27	29
29	BG	98/99 (99%)	98 (100%)	0	100	100
30	AT	113/114 (99%)	110 (97%)	3 (3%)	39	45
31	AO	115/123 (94%)	110 (96%)	5 (4%)	26	27
32	BB	188/189 (100%)	185 (98%)	3 (2%)	55	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BY	132/133 (99%)	131 (99%)	1 (1%)	73	81
34	BO	167/170 (98%)	162 (97%)	5 (3%)	36	41
35	BC	306/307 (100%)	298 (97%)	8 (3%)	40	46
36	B5	65/66 (98%)	61 (94%)	4 (6%)	16	14
36	BK	64/66 (97%)	63 (98%)	1 (2%)	55	64
37	BL	118/118 (100%)	116 (98%)	2 (2%)	53	62
38	Bf	46/47 (98%)	45 (98%)	1 (2%)	45	53
39	BU	109/109 (100%)	108 (99%)	1 (1%)	70	78
40	Bb	117/118 (99%)	114 (97%)	3 (3%)	40	46
41	Be	52/53 (98%)	51 (98%)	1 (2%)	50	58
42	BE	158/160 (99%)	152 (96%)	6 (4%)	29	32
43	Ba	84/84 (100%)	81 (96%)	3 (4%)	31	34
44	BT	77/77 (100%)	74 (96%)	3 (4%)	28	31
45	BW	63/63 (100%)	62 (98%)	1 (2%)	55	64
46	Bi	61/62 (98%)	60 (98%)	1 (2%)	55	64
47	BI	122/122 (100%)	121 (99%)	1 (1%)	73	81
48	BR	86/87 (99%)	85 (99%)	1 (1%)	63	72
49	BQ	132/133 (99%)	131 (99%)	1 (1%)	73	81
50	BV	54/58 (93%)	54 (100%)	0	100	100
51	Bj	83/84 (99%)	83 (100%)	0	100	100
52	BD	212/212 (100%)	208 (98%)	4 (2%)	50	58
53	BF	156/157 (99%)	153 (98%)	3 (2%)	50	58
54	BZ	79/80 (99%)	77 (98%)	2 (2%)	42	48
55	BP	102/102 (100%)	100 (98%)	2 (2%)	48	56
56	BM	160/161 (99%)	160 (100%)	0	100	100
57	BS	130/131 (99%)	128 (98%)	2 (2%)	57	65
58	Bd	82/82 (100%)	82 (100%)	0	100	100
59	BN	149/151 (99%)	146 (98%)	3 (2%)	48	56
60	Bg	37/39 (95%)	37 (100%)	0	100	100
61	Bc	74/74 (100%)	72 (97%)	2 (3%)	39	45
62	BJ	108/109 (99%)	107 (99%)	1 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	Bl	72/72 (100%)	67 (93%)	5 (7%)	14	12
64	Bk	55/57 (96%)	54 (98%)	1 (2%)	51	60
65	H	327/338 (97%)	305 (93%)	22 (7%)	15	12
All	All	7359/7521 (98%)	7177 (98%)	182 (2%)	42	48

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BE	94	LEU
57	BS	155	ARG
43	Ba	1	MET
49	BQ	108	LYS
63	Bl	2	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 161 such sidechains are listed below:

Mol	Chain	Res	Type
51	Bj	6	GLN
59	BN	56	GLN
52	BD	139	GLN
55	BP	10	ASN
59	BN	170	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3016/3018 (99%)	444 (14%)	22 (0%)
2	2	1495/1512 (98%)	176 (11%)	2 (0%)
3	3	125/128 (97%)	12 (9%)	0
All	All	4636/4658 (99%)	632 (13%)	24 (0%)

5 of 632 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	12	G
1	1	28	A
1	1	39	A
1	1	51	A
1	1	52	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1364	C
1	1	2367	G
1	1	2341	G
1	1	2455	A
1	1	866	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	4AC	1	2545	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	751	2	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
1	OMG	1	789	1	23,26,27	1.25	3 (13%)	33,38,41	1.97	6 (18%)
2	4AC	2	839	2	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	533	1	21,24,25	1.01	2 (9%)	29,34,37	1.32	4 (13%)
1	A2M	1	2173	1	22,25,26	1.43	4 (18%)	31,36,39	2.07	8 (25%)
2	OMG	2	467	2	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
2	5MC	2	875	2	18,22,23	0.93	2 (11%)	26,32,35	1.17	3 (11%)
1	OMG	1	2138	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	OMU	1	2784	1	19,22,23	1.23	3 (15%)	26,31,34	1.74	5 (19%)
1	4AC	1	1293	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	1873	1	21,24,25	1.07	2 (9%)	29,34,37	1.32	4 (13%)
1	OMG	1	2678	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	7 (21%)
1	4AC	1	2925	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	590	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	5MC	2	1498	2	18,22,23	0.92	2 (11%)	26,32,35	1.25	4 (15%)
1	5MC	1	2162	1	18,22,23	0.93	2 (11%)	26,32,35	1.14	3 (11%)
1	4AC	1	1885	1	21,24,25	1.04	2 (9%)	29,34,37	1.23	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LHH	1	616	1	22,25,26	0.31	0	29,35,38	0.46	0
2	4AC	2	626	2	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
2	4AC	2	319	2	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1780	1	21,24,25	1.04	2 (9%)	29,34,37	1.60	4 (13%)
1	5MC	1	2093	1	18,22,23	0.94	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	1	1554	1	21,24,25	1.02	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	229	1	21,24,25	1.06	2 (9%)	29,34,37	1.30	3 (10%)
1	4AC	1	314	1	21,24,25	1.05	2 (9%)	29,34,37	1.26	4 (13%)
1	4AC	1	2001	1	21,24,25	1.07	2 (9%)	29,34,37	1.50	4 (13%)
1	4AC	1	2642	1	21,24,25	1.02	2 (9%)	29,34,37	1.30	4 (13%)
2	OMU	2	1380	2	19,22,23	1.30	3 (15%)	26,31,34	1.75	4 (15%)
1	5MC	1	2198	1	18,22,23	0.93	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	1	2992	1	21,24,25	1.04	2 (9%)	29,34,37	0.88	1 (3%)
2	4AC	2	546	2	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
2	4AC	2	1239	2	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	OMG	1	2144	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
2	OMC	2	846	2	19,22,23	0.81	0	26,31,34	0.80	0
2	4AC	2	851	2	21,24,25	1.06	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1065	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
1	5MC	1	2183	1	18,22,23	0.94	2 (11%)	26,32,35	1.12	2 (7%)
1	OMG	1	923	1,66	23,26,27	1.21	3 (13%)	33,38,41	1.98	7 (21%)
1	5MC	1	2163	1	18,22,23	0.93	2 (11%)	26,32,35	1.11	2 (7%)
2	4AC	2	1233	2	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
2	OMG	2	657	2	23,26,27	1.24	3 (13%)	33,38,41	1.97	6 (18%)
2	OMU	2	1177	2	19,22,23	1.24	3 (15%)	26,31,34	1.71	4 (15%)
2	UR3	2	1467	2	19,22,23	0.94	0	26,32,35	1.45	2 (7%)
1	4AC	1	1594	1,66	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
2	5MC	2	535	2	18,22,23	0.93	2 (11%)	26,32,35	1.14	2 (7%)
1	4AC	1	1938	1	21,24,25	1.06	2 (9%)	29,34,37	1.31	4 (13%)
2	LHH	2	1041	2	22,25,26	0.31	0	29,35,38	0.49	0
2	OMG	2	680	2	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	4AC	1	3004	1	21,24,25	1.05	2 (9%)	29,34,37	1.27	4 (13%)
2	4AC	2	394	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	1147	2	21,24,25	1.02	2 (9%)	29,34,37	1.44	4 (13%)
1	4AC	1	2960	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	2495	1	21,24,25	1.05	2 (9%)	29,34,37	1.29	4 (13%)
2	LHH	2	250	2	22,25,26	0.31	0	29,35,38	0.49	0
1	4AC	1	1222	1,66	21,24,25	1.04	2 (9%)	29,34,37	1.26	4 (13%)
2	5MC	2	1505	2	18,22,23	0.94	2 (11%)	26,32,35	1.59	5 (19%)
1	4AC	1	2570	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	829	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	161	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1617	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	OMC	1	1948	1	19,22,23	0.81	0	26,31,34	0.77	0
2	OMU	2	787	2	19,22,23	1.25	3 (15%)	26,31,34	1.85	5 (19%)
1	4AC	1	1068	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
2	5MC	2	1025	2	18,22,23	0.95	2 (11%)	26,32,35	1.15	3 (11%)
1	4AC	1	1755	1	21,24,25	1.04	2 (9%)	29,34,37	1.67	5 (17%)
1	4AC	1	1550	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2062	1	21,24,25	1.03	2 (9%)	29,34,37	1.27	4 (13%)
1	4AC	1	91	1	21,24,25	1.01	2 (9%)	29,34,37	1.40	4 (13%)
2	OMG	2	873	2	23,26,27	1.22	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	1048	1	21,24,25	1.06	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	17	2	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	OMU	2	64	2	19,22,23	1.24	3 (15%)	26,31,34	1.70	5 (19%)
2	4AC	2	479	2	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	243	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	OMG	2	519	2	23,26,27	1.21	3 (13%)	33,38,41	1.98	6 (18%)
1	4AC	1	1460	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	1184	2	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
2	OMU	2	774	2	19,22,23	1.23	3 (15%)	26,31,34	1.71	5 (19%)
2	4AC	2	703	2	21,24,25	1.01	2 (9%)	29,34,37	1.58	4 (13%)
2	OMU	2	830	2	19,22,23	1.27	3 (15%)	26,31,34	1.72	5 (19%)
2	4AC	2	303	2	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2937	1,66	21,24,25	1.02	2 (9%)	29,34,37	1.52	4 (13%)
2	4AC	2	379	2	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	835	1	21,24,25	1.05	2 (9%)	29,34,37	1.30	4 (13%)
2	OMC	2	1376	2	19,22,23	0.81	0	26,31,34	0.77	0
1	4AC	1	1667	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	2966	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	2548	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	2585	1	21,24,25	1.08	2 (9%)	29,34,37	1.76	6 (20%)
2	B8H	2	938	2	19,22,23	0.57	0	22,32,35	0.62	0
1	4AC	1	2136	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	1934	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2608	1	21,24,25	1.07	2 (9%)	29,34,37	1.80	6 (20%)
1	4AC	1	1878	1	21,24,25	1.04	2 (9%)	29,34,37	1.50	4 (13%)
1	4AC	1	1621	1	21,24,25	1.04	2 (9%)	29,34,37	1.24	4 (13%)
2	4AC	2	511	2	21,24,25	1.04	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	694	1	21,24,25	1.01	2 (9%)	29,34,37	1.27	4 (13%)
2	4AC	2	286	2	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
2	4AC	2	718	2	21,24,25	1.02	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	1	451	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
2	5MC	2	1202	2	18,22,23	0.96	2 (11%)	26,32,35	1.28	4 (15%)
1	4AC	1	1695	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	MA6	2	1487	2	23,26,27	1.45	5 (21%)	34,38,41	2.11	10 (29%)
1	4AC	1	641	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	1962	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
2	5MC	2	1496	2	18,22,23	0.92	2 (11%)	26,32,35	1.13	3 (11%)
1	4AC	1	2865	1	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	1	2908	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1662	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
2	OMU	2	20	2	19,22,23	1.27	3 (15%)	26,31,34	1.83	5 (19%)
2	4AC	2	848	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	53	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	802	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1765	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
2	OMC	2	1040	2	19,22,23	0.83	0	26,31,34	0.90	1 (3%)
1	4AC	1	22	1	21,24,25	1.04	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	1557	1	21,24,25	1.02	2 (9%)	29,34,37	1.27	4 (13%)
1	4AC	1	136	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
2	4AC	2	636	2	21,24,25	1.03	2 (9%)	29,34,37	1.47	4 (13%)
2	OMG	2	934	2	23,26,27	1.20	3 (13%)	33,38,41	1.99	6 (18%)
1	4AC	1	341	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	2718	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	211	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
3	4AC	3	32	3	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
2	6MZ	2	1469	2,66	22,25,26	1.47	4 (18%)	30,36,39	2.20	9 (30%)
1	OMG	1	2147	1	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
1	4AC	1	458	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	A2M	2	373	2	22,25,26	1.45	4 (18%)	31,36,39	2.06	8 (25%)
1	4AC	1	2249	1	21,24,25	1.06	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	731	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	981	1	21,24,25	1.04	2 (9%)	29,34,37	1.23	4 (13%)
2	4AC	2	1479	2	21,24,25	1.01	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	2027	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	1243	1	21,24,25	1.05	2 (9%)	29,34,37	1.29	4 (13%)
1	4AC	1	2329	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	OMC	2	129	2	19,22,23	0.83	0	26,31,34	0.84	0
2	OMC	2	773	2	19,22,23	0.82	0	26,31,34	0.77	0
1	4AC	1	60	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
2	4AC	2	828	2	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
1	OMC	1	615	1	19,22,23	0.80	0	26,31,34	0.76	0
1	4AC	1	2083	1	21,24,25	1.09	2 (9%)	29,34,37	1.25	3 (10%)
2	5MC	2	1374	2	18,22,23	0.93	2 (11%)	26,32,35	1.11	2 (7%)
1	A2M	1	1055	1	22,25,26	1.44	4 (18%)	31,36,39	2.10	8 (25%)
2	4AC	2	868	2	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	1	357	1	21,24,25	1.01	2 (9%)	29,34,37	1.29	5 (17%)
2	OMG	2	913	2	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
2	4AC	2	1028	2	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	5MC	1	2733	1	18,22,23	0.97	2 (11%)	26,32,35	1.25	4 (15%)
1	4AC	1	2287	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
2	5MC	2	693	2	18,22,23	0.92	2 (11%)	26,32,35	1.15	3 (11%)
1	5MC	1	2203	1	18,22,23	0.93	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	1	922	1	21,24,25	1.06	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	1867	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
1	OMG	1	328	1	23,26,27	1.22	3 (13%)	33,38,41	1.99	6 (18%)
2	OMG	2	1069	2	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
2	OMG	2	471	2	23,26,27	1.23	3 (13%)	33,38,41	1.94	6 (18%)
2	4AC	2	957	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MA6	2	1488	2	23,26,27	1.44	5 (21%)	34,38,41	2.13	10 (29%)

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
1	4AC	1	2545	1	-	0/11/29/30	0/2/2/2
2	4AC	2	751	2	-	0/11/29/30	0/2/2/2
1	OMG	1	789	1	-	3/9/27/28	0/3/3/3
2	4AC	2	839	2	-	0/11/29/30	0/2/2/2
1	4AC	1	533	1	-	0/11/29/30	0/2/2/2
1	A2M	1	2173	1	-	0/9/27/28	0/3/3/3
2	OMG	2	467	2	-	0/9/27/28	0/3/3/3
2	5MC	2	875	2	-	0/7/25/26	0/2/2/2
1	OMG	1	2138	1	-	0/9/27/28	0/3/3/3
1	OMU	1	2784	1	-	0/9/27/28	0/2/2/2
1	4AC	1	1293	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1873	1	-	0/11/29/30	0/2/2/2
1	OMG	1	2678	1	-	0/9/27/28	0/3/3/3
1	4AC	1	2925	1	-	0/11/29/30	0/2/2/2
2	4AC	2	590	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1498	2	-	4/7/25/26	0/2/2/2
1	5MC	1	2162	1	-	0/7/25/26	0/2/2/2
1	4AC	1	1885	1	-	0/11/29/30	0/2/2/2
1	LHH	1	616	1	-	0/13/31/32	0/2/2/2
2	4AC	2	626	2	-	0/11/29/30	0/2/2/2
2	4AC	2	319	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1780	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2093	1	-	0/7/25/26	0/2/2/2
1	4AC	1	1554	1	-	0/11/29/30	0/2/2/2
1	4AC	1	229	1	-	0/11/29/30	0/2/2/2
1	4AC	1	314	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2001	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2642	1	-	0/11/29/30	0/2/2/2
2	OMU	2	1380	2	-	0/9/27/28	0/2/2/2
1	5MC	1	2198	1	-	0/7/25/26	0/2/2/2
1	4AC	1	2992	1	-	3/11/29/30	0/2/2/2
2	4AC	2	546	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1239	2	-	0/11/29/30	0/2/2/2
1	OMG	1	2144	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	2	846	2	-	0/9/27/28	0/2/2/2
2	4AC	2	851	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1065	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2183	1	-	0/7/25/26	0/2/2/2
1	OMG	1	923	1,66	-	0/9/27/28	0/3/3/3
1	5MC	1	2163	1	-	0/7/25/26	0/2/2/2
2	4AC	2	1233	2	-	0/11/29/30	0/2/2/2
2	OMG	2	657	2	-	0/9/27/28	0/3/3/3
2	OMU	2	1177	2	-	1/9/27/28	0/2/2/2
2	UR3	2	1467	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1594	1,66	-	0/11/29/30	0/2/2/2
2	5MC	2	535	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1938	1	-	0/11/29/30	0/2/2/2
2	LHH	2	1041	2	-	0/13/31/32	0/2/2/2
2	OMG	2	680	2	-	0/9/27/28	0/3/3/3
1	4AC	1	3004	1	-	0/11/29/30	0/2/2/2
2	4AC	2	394	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1147	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2960	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2495	1	-	0/11/29/30	0/2/2/2
2	LHH	2	250	2	-	0/13/31/32	0/2/2/2
1	4AC	1	1222	1,66	-	0/11/29/30	0/2/2/2
2	5MC	2	1505	2	-	4/7/25/26	0/2/2/2
1	4AC	1	2570	1	-	0/11/29/30	0/2/2/2
1	4AC	1	829	1	-	0/11/29/30	0/2/2/2
1	4AC	1	161	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1617	1	-	0/11/29/30	0/2/2/2
1	OMC	1	1948	1	-	0/9/27/28	0/2/2/2
2	OMU	2	787	2	-	2/9/27/28	0/2/2/2
1	4AC	1	1068	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1025	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1755	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1550	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2062	1	-	0/11/29/30	0/2/2/2
1	4AC	1	91	1	-	0/11/29/30	0/2/2/2
2	OMG	2	873	2	-	1/9/27/28	0/3/3/3
1	4AC	1	1048	1	-	0/11/29/30	0/2/2/2
2	4AC	2	17	2	-	0/11/29/30	0/2/2/2
2	OMU	2	64	2	-	0/9/27/28	0/2/2/2
2	4AC	2	479	2	-	0/11/29/30	0/2/2/2
1	4AC	1	243	1	-	0/11/29/30	0/2/2/2
2	OMG	2	519	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	1460	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1184	2	-	0/11/29/30	0/2/2/2
2	OMU	2	774	2	-	0/9/27/28	0/2/2/2
2	4AC	2	703	2	-	0/11/29/30	0/2/2/2
2	OMU	2	830	2	-	0/9/27/28	0/2/2/2
2	4AC	2	303	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2937	1,66	-	1/11/29/30	0/2/2/2
2	4AC	2	379	2	-	0/11/29/30	0/2/2/2
1	4AC	1	835	1	-	0/11/29/30	0/2/2/2
2	OMC	2	1376	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1667	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2966	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2548	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2585	1	-	3/11/29/30	0/2/2/2
2	B8H	2	938	2	-	0/7/25/26	0/2/2/2
1	4AC	1	2136	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1934	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2608	1	-	3/11/29/30	0/2/2/2
1	4AC	1	1878	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1621	1	-	0/11/29/30	0/2/2/2
2	4AC	2	511	2	-	0/11/29/30	0/2/2/2
1	4AC	1	694	1	-	0/11/29/30	0/2/2/2
2	4AC	2	286	2	-	0/11/29/30	0/2/2/2
2	4AC	2	718	2	-	0/11/29/30	0/2/2/2
1	4AC	1	451	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1202	2	-	2/7/25/26	0/2/2/2
1	4AC	1	1695	1	-	0/11/29/30	0/2/2/2
2	MA6	2	1487	2	-	0/11/29/30	0/3/3/3
1	4AC	1	641	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1962	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1496	2	-	0/7/25/26	0/2/2/2
1	4AC	1	2865	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2908	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1662	1	-	0/11/29/30	0/2/2/2
2	OMU	2	20	2	-	5/9/27/28	0/2/2/2
2	4AC	2	848	2	-	0/11/29/30	0/2/2/2
2	4AC	2	53	2	-	0/11/29/30	0/2/2/2
1	4AC	1	802	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1765	1	-	0/11/29/30	0/2/2/2
2	OMC	2	1040	2	-	0/9/27/28	0/2/2/2
1	4AC	1	22	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	1557	1	-	0/11/29/30	0/2/2/2
1	4AC	1	136	1	-	0/11/29/30	0/2/2/2
2	4AC	2	636	2	-	0/11/29/30	0/2/2/2
2	OMG	2	934	2	-	2/9/27/28	0/3/3/3
1	4AC	1	341	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2718	1	-	0/11/29/30	0/2/2/2
1	4AC	1	211	1	-	0/11/29/30	0/2/2/2
3	4AC	3	32	3	-	0/11/29/30	0/2/2/2
2	6MZ	2	1469	2,66	-	0/9/27/28	0/3/3/3
1	OMG	1	2147	1	-	3/9/27/28	0/3/3/3
1	4AC	1	458	1	-	0/11/29/30	0/2/2/2
2	A2M	2	373	2	-	0/9/27/28	0/3/3/3
1	4AC	1	2249	1	-	0/11/29/30	0/2/2/2
2	4AC	2	731	2	-	0/11/29/30	0/2/2/2
1	4AC	1	981	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1479	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2027	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1243	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2329	1	-	0/11/29/30	0/2/2/2
2	OMC	2	129	2	-	0/9/27/28	0/2/2/2
2	OMC	2	773	2	-	0/9/27/28	0/2/2/2
1	4AC	1	60	1	-	0/11/29/30	0/2/2/2
2	4AC	2	828	2	-	0/11/29/30	0/2/2/2
1	OMC	1	615	1	-	0/9/27/28	0/2/2/2
1	4AC	1	2083	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1374	2	-	0/7/25/26	0/2/2/2
1	A2M	1	1055	1	-	0/9/27/28	0/3/3/3
2	4AC	2	868	2	-	0/11/29/30	0/2/2/2
1	4AC	1	357	1	-	0/11/29/30	0/2/2/2
2	OMG	2	913	2	-	1/9/27/28	0/3/3/3
2	4AC	2	1028	2	-	0/11/29/30	0/2/2/2
1	5MC	1	2733	1	-	4/7/25/26	0/2/2/2
1	4AC	1	2287	1	-	0/11/29/30	0/2/2/2
2	5MC	2	693	2	-	0/7/25/26	0/2/2/2
1	5MC	1	2203	1	-	0/7/25/26	0/2/2/2
1	4AC	1	922	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1867	1	-	0/11/29/30	0/2/2/2
1	OMG	1	328	1	-	0/9/27/28	0/3/3/3
2	OMG	2	1069	2	-	2/9/27/28	0/3/3/3
2	OMG	2	471	2	-	0/9/27/28	0/3/3/3
2	4AC	2	957	2	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MA6	2	1488	2	-	2/11/29/30	0/3/3/3

The worst 5 of 332 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1469	6MZ	C5-C4	4.50	1.47	1.39
2	2	1487	MA6	C5-C4	4.30	1.47	1.39
2	2	373	A2M	C5-C4	4.28	1.47	1.39
1	1	2173	A2M	C5-C4	4.28	1.47	1.39
2	2	1488	MA6	C5-C4	4.23	1.46	1.39

The worst 5 of 643 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	657	OMG	C5-C4-N3	-6.46	117.99	128.46
1	1	1055	A2M	C5-C4-N3	-6.34	118.48	126.75
1	1	2173	A2M	C5-C4-N3	-6.28	118.56	126.75
2	2	373	A2M	C5-C4-N3	-6.25	118.60	126.75
2	2	471	OMG	C5-C4-N3	-6.23	118.36	128.46

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2147	OMG	O4'-C4'-C5'-O5'
1	1	2147	OMG	C3'-C4'-C5'-O5'
1	1	2585	4AC	O4'-C1'-N1-C2
1	1	2585	4AC	O4'-C1'-N1-C6
1	1	2608	4AC	O4'-C1'-N1-C2

There are no ring outliers.

72 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2545	4AC	1	0
1	1	789	OMG	1	0
2	2	839	4AC	1	0
1	1	1293	4AC	1	0
2	2	626	4AC	1	0
2	2	319	4AC	1	0
1	1	1780	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	229	4AC	1	0
1	1	2001	4AC	2	0
2	2	1380	OMU	2	0
1	1	2198	5MC	1	0
1	1	2992	4AC	1	0
2	2	546	4AC	2	0
2	2	1239	4AC	1	0
2	2	846	OMC	1	0
1	1	1065	4AC	1	0
2	2	1233	4AC	1	0
2	2	1177	OMU	2	0
1	1	1594	4AC	1	0
2	2	680	OMG	1	0
1	1	3004	4AC	1	0
2	2	394	4AC	1	0
1	1	2495	4AC	1	0
1	1	2570	4AC	1	0
1	1	1617	4AC	2	0
2	2	1025	5MC	1	0
1	1	1755	4AC	2	0
1	1	1550	4AC	1	0
1	1	91	4AC	2	0
1	1	1048	4AC	1	0
2	2	64	OMU	1	0
2	2	479	4AC	1	0
1	1	243	4AC	1	0
1	1	1460	4AC	1	0
2	2	774	OMU	1	0
2	2	703	4AC	6	0
2	2	379	4AC	1	0
1	1	835	4AC	1	0
2	2	1376	OMC	2	0
1	1	1667	4AC	3	0
1	1	2548	4AC	1	0
1	1	2585	4AC	3	0
1	1	1934	4AC	1	0
1	1	2608	4AC	3	0
1	1	1878	4AC	1	0
1	1	451	4AC	1	0
2	2	1202	5MC	1	0
1	1	1695	4AC	1	0
2	2	1487	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1662	4AC	1	0
2	2	848	4AC	1	0
2	2	53	4AC	1	0
1	1	802	4AC	2	0
2	2	636	4AC	3	0
1	1	341	4AC	1	0
1	1	2718	4AC	1	0
1	1	211	4AC	1	0
2	2	1469	6MZ	1	0
1	1	458	4AC	1	0
2	2	373	A2M	1	0
2	2	731	4AC	1	0
2	2	1479	4AC	1	0
1	1	2027	4AC	1	0
2	2	129	OMC	1	0
1	1	60	4AC	2	0
1	1	615	OMC	1	0
1	1	1055	A2M	1	0
1	1	2287	4AC	2	0
1	1	1867	4AC	1	0
2	2	1069	OMG	1	0
2	2	957	4AC	1	0
2	2	1488	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

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

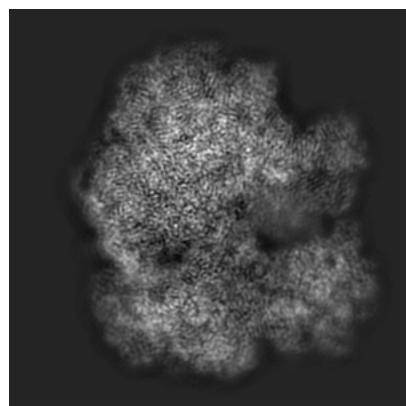
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55138. These allow visual inspection of the internal detail of the map and identification of artifacts.

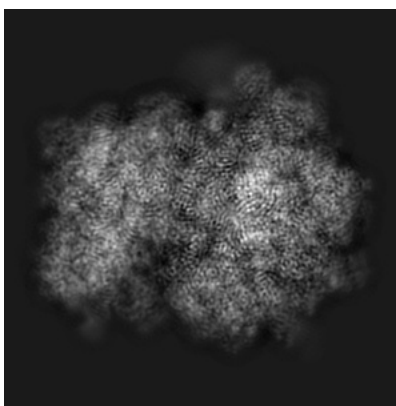
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

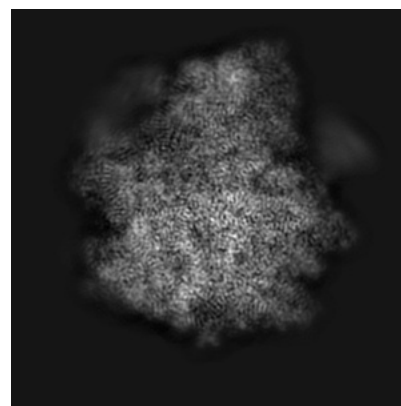
6.1.1 Primary map



X

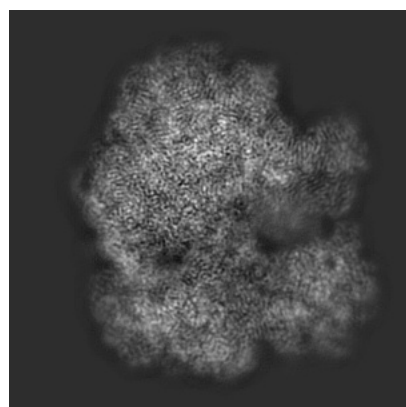


Y

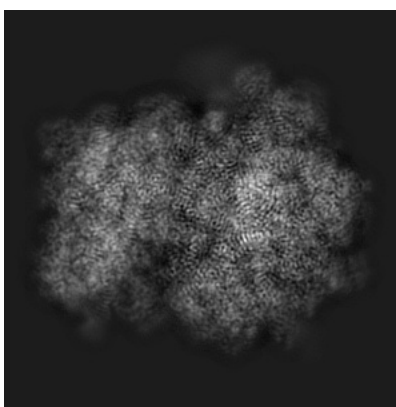


Z

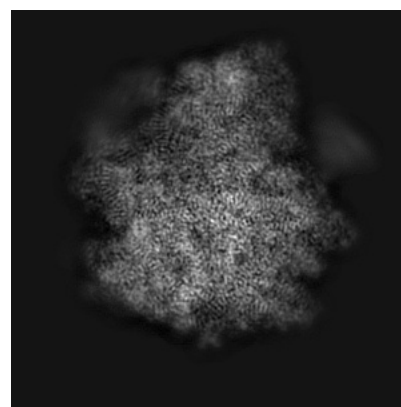
6.1.2 Raw map



X



Y

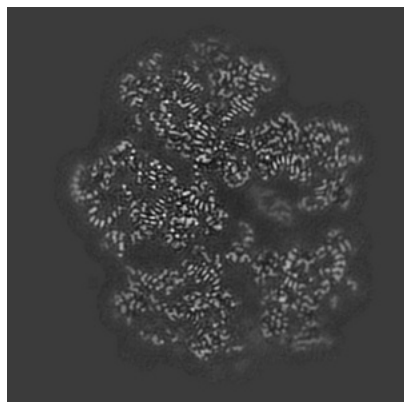


Z

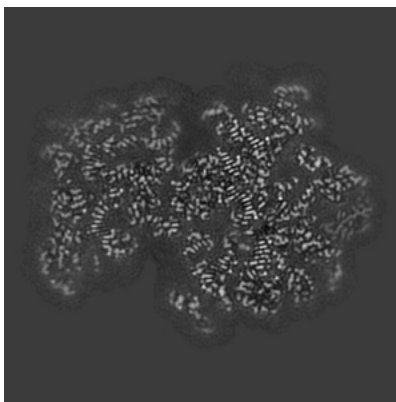
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

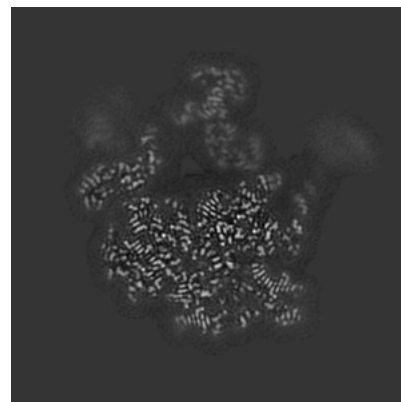
6.2.1 Primary map



X Index: 180

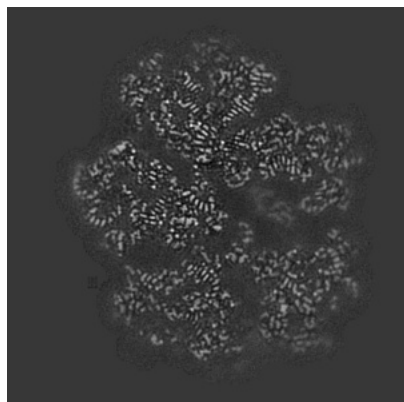


Y Index: 180

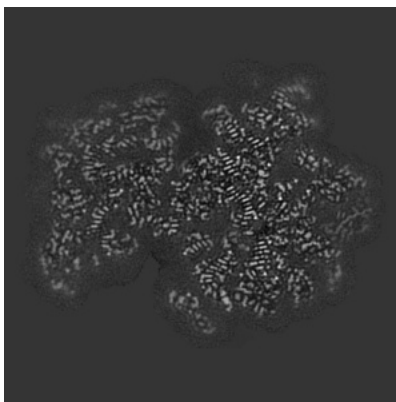


Z Index: 180

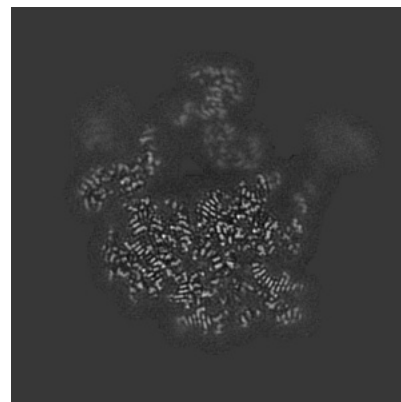
6.2.2 Raw map



X Index: 180



Y Index: 180

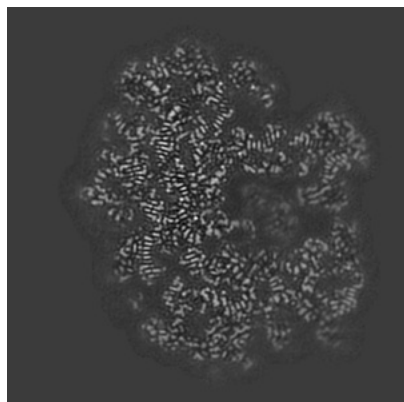


Z Index: 180

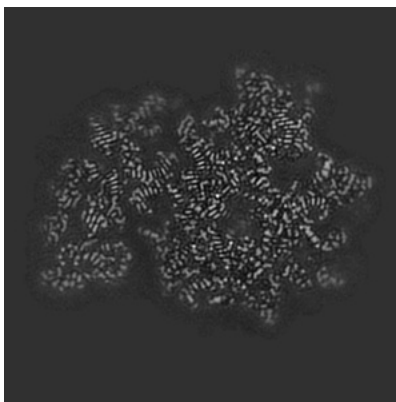
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

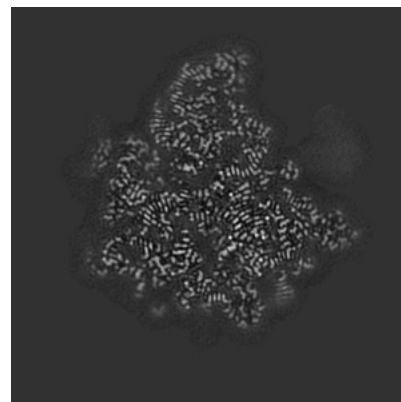
6.3.1 Primary map



X Index: 195

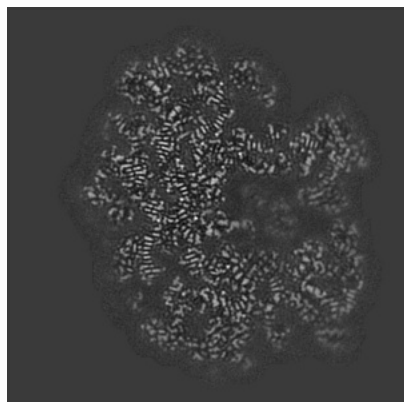


Y Index: 166

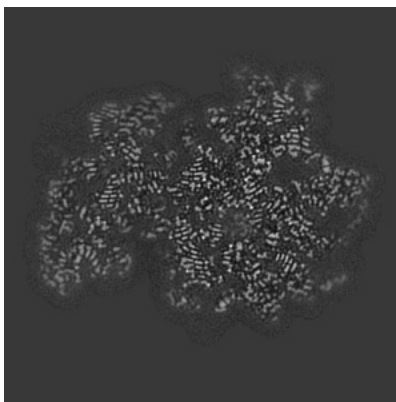


Z Index: 228

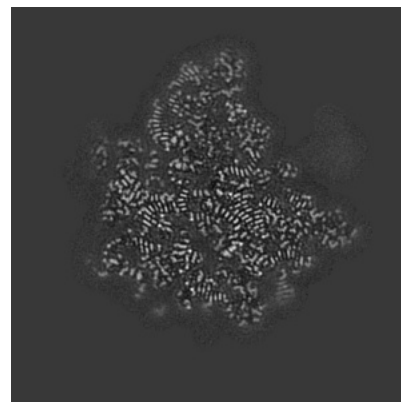
6.3.2 Raw map



X Index: 195



Y Index: 171

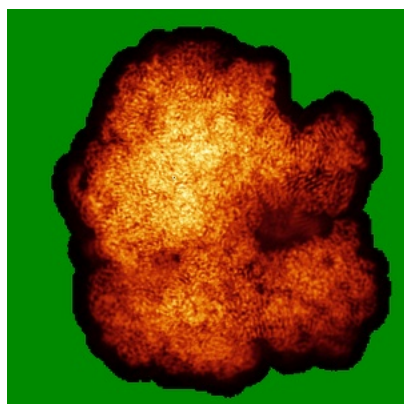


Z Index: 229

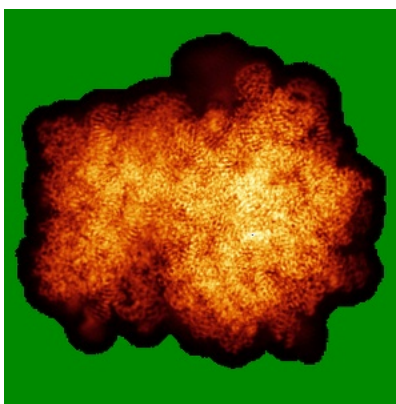
The images above show the largest variance slices of the map in three orthogonal directions.

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

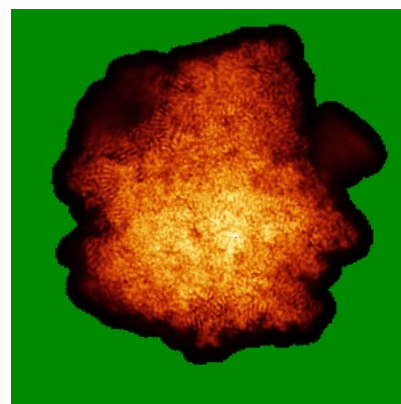
6.4.1 Primary map



X

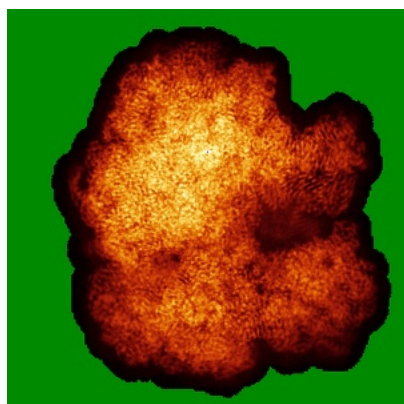


Y

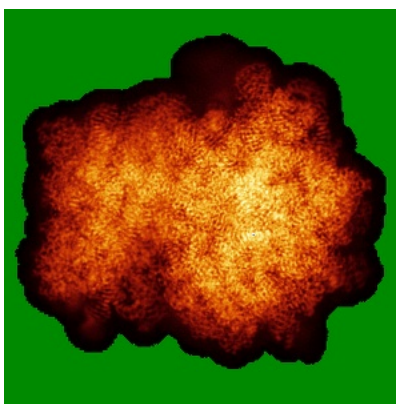


Z

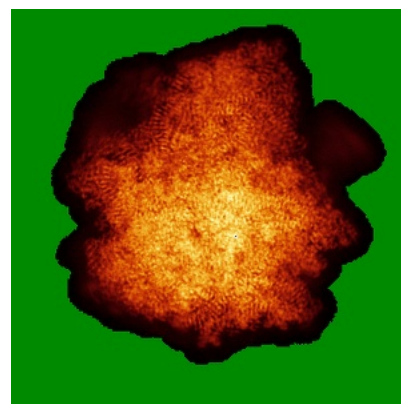
6.4.2 Raw map



X



Y

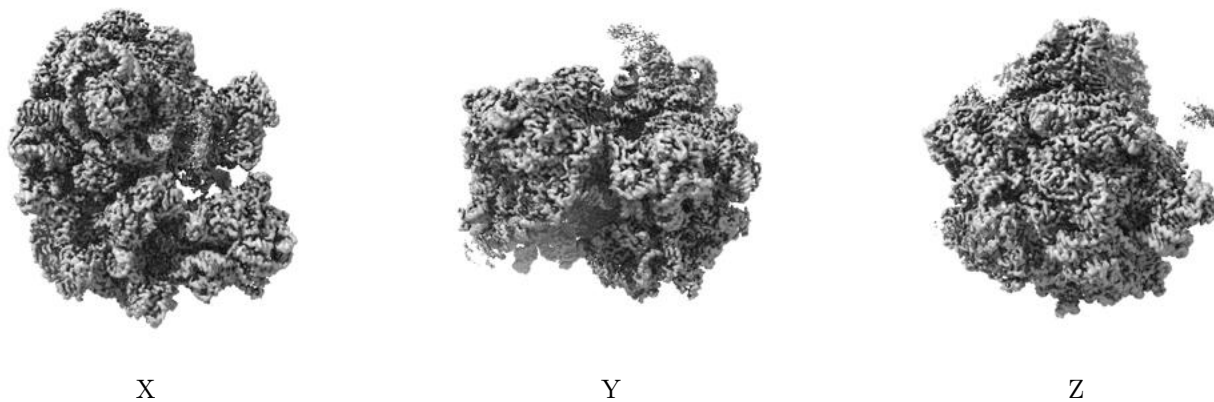


Z

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

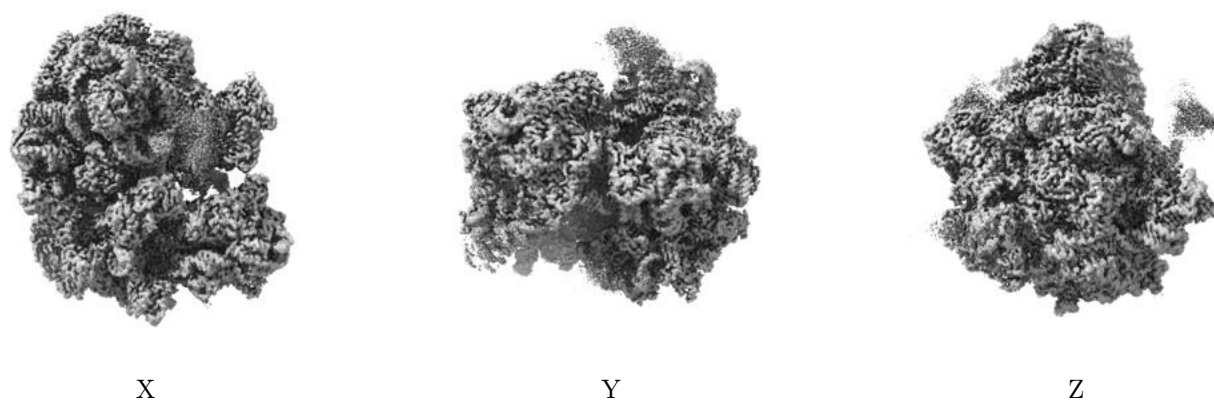
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00125. 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.

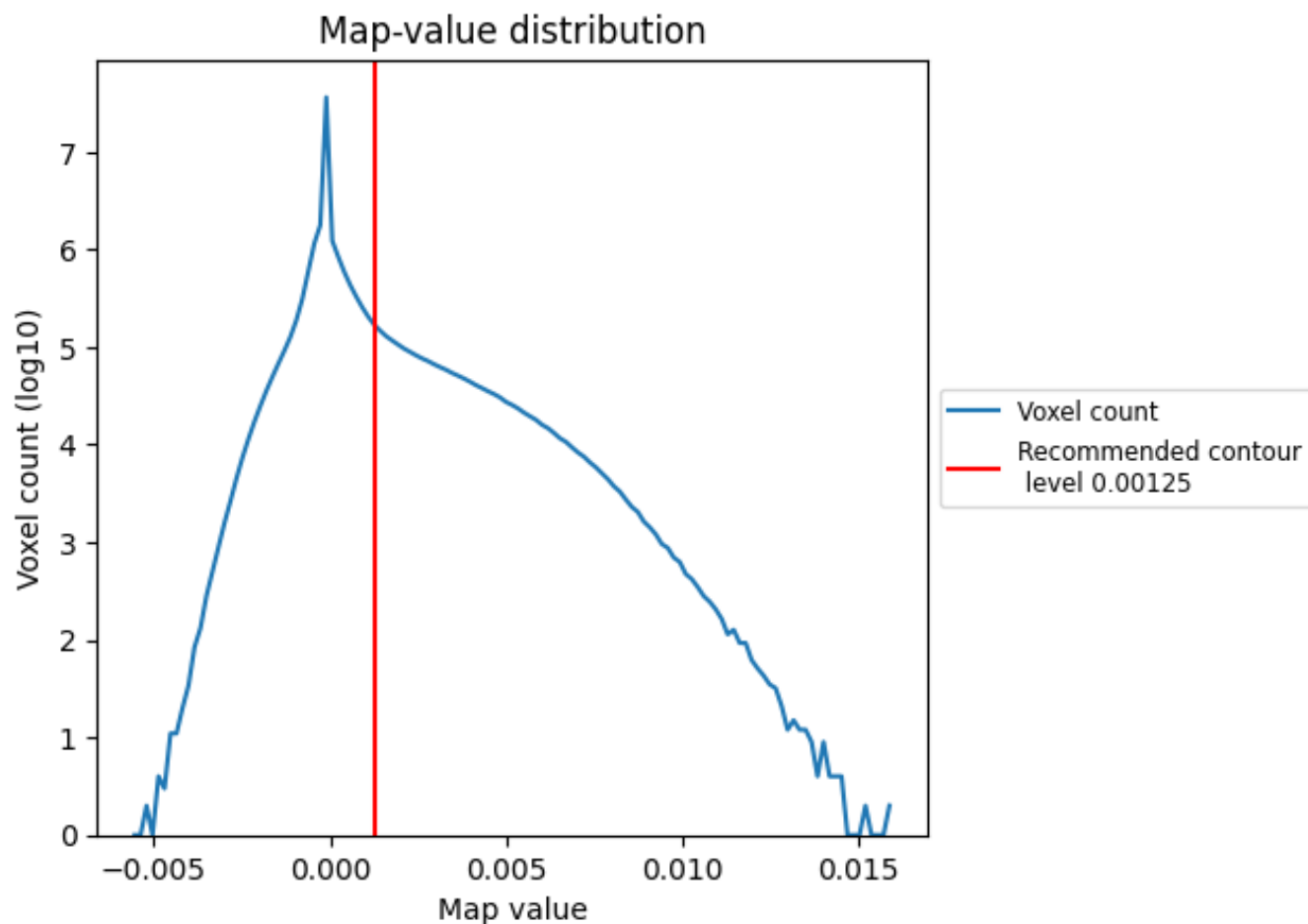
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

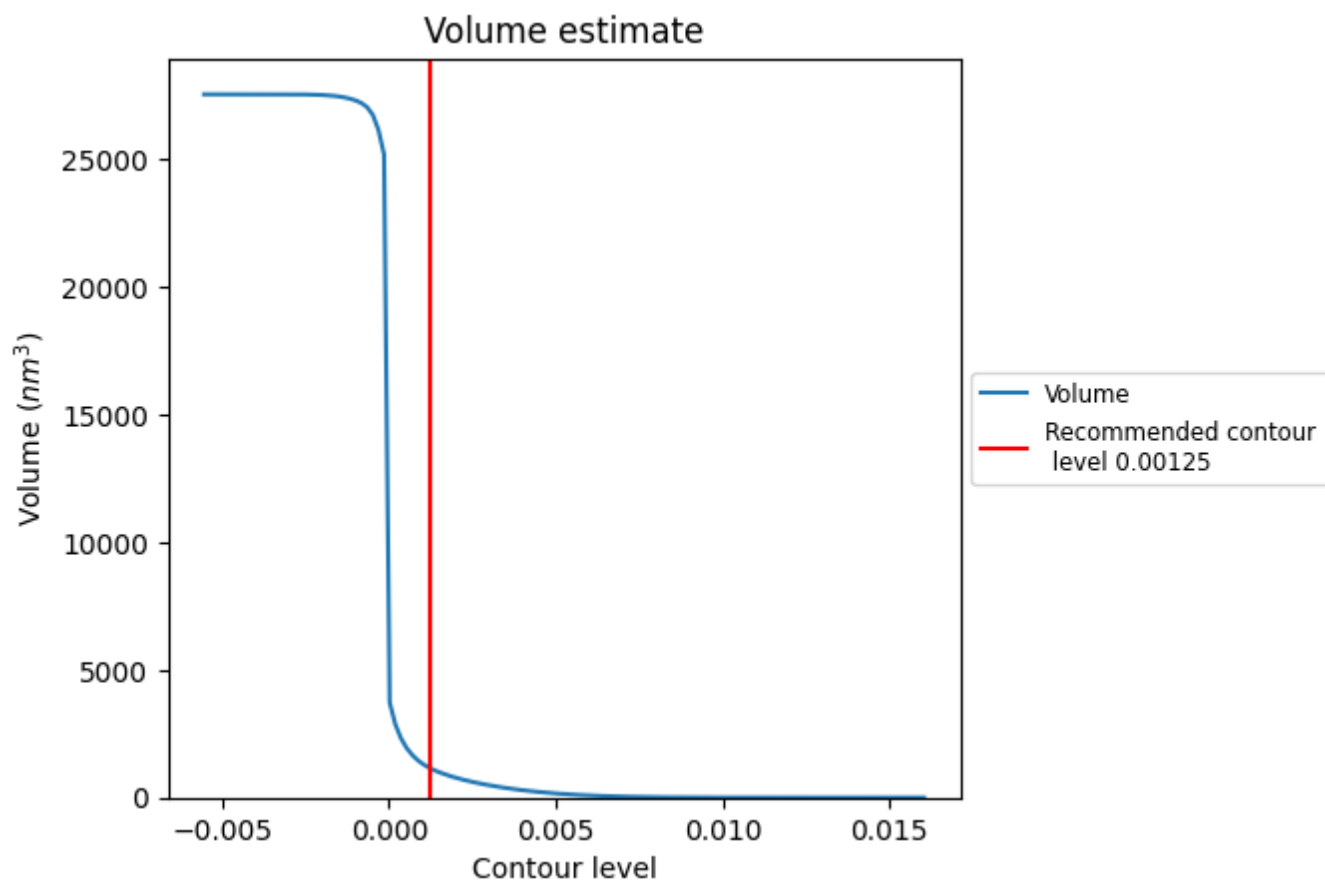
This section contains the results of statistical analysis of the map.

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.

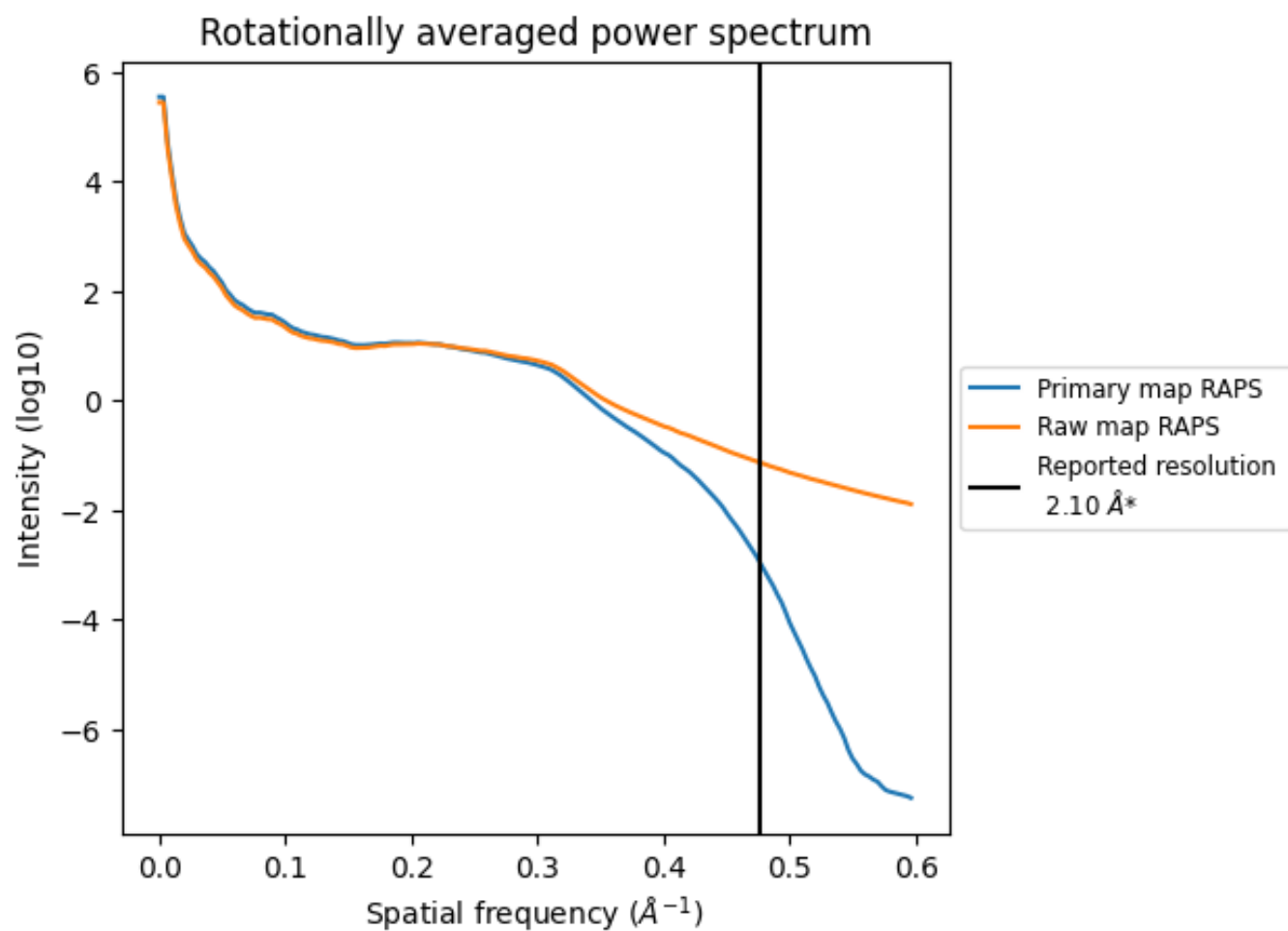
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1139 nm^3 ; this corresponds to an approximate mass of 1029 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

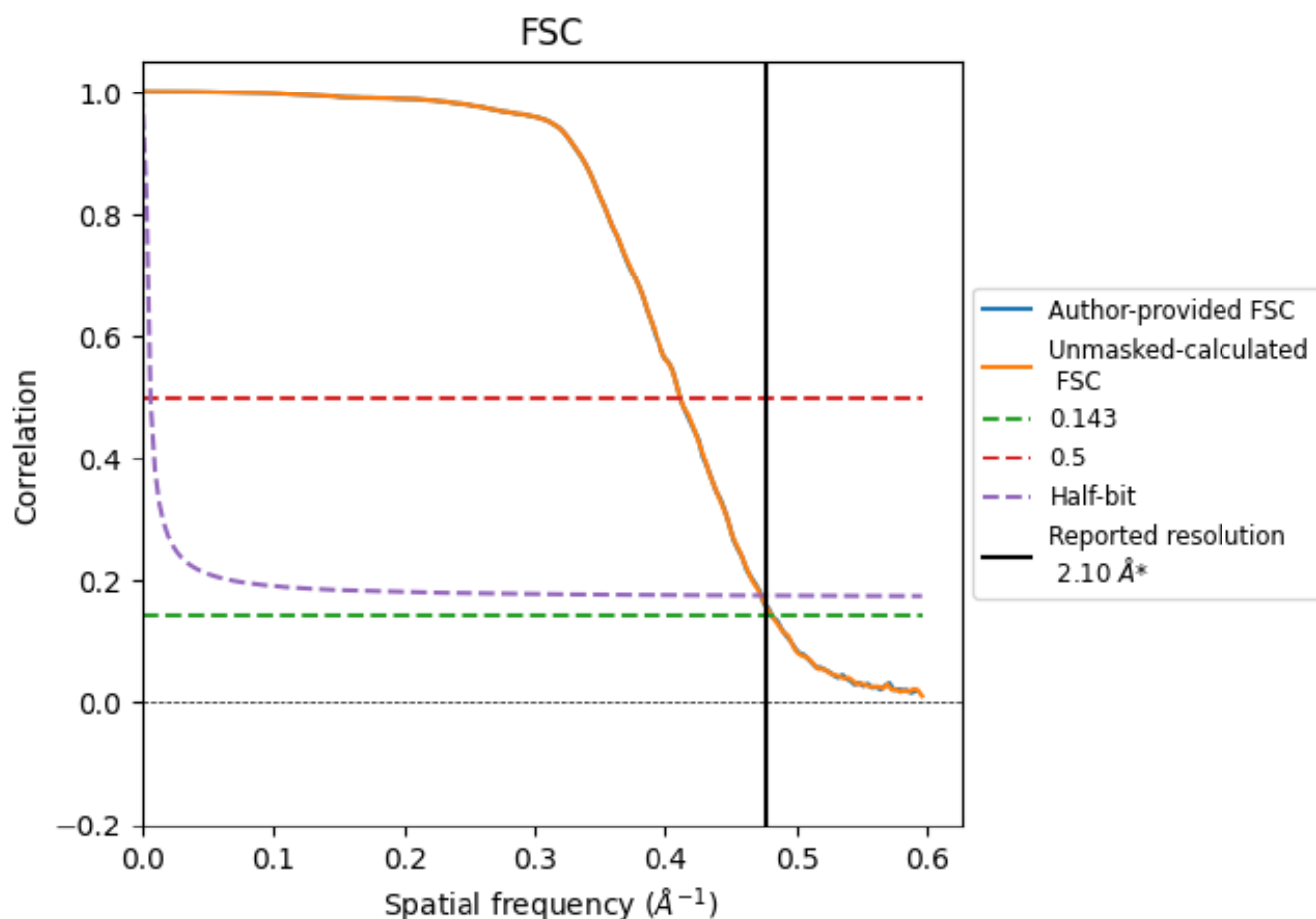


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

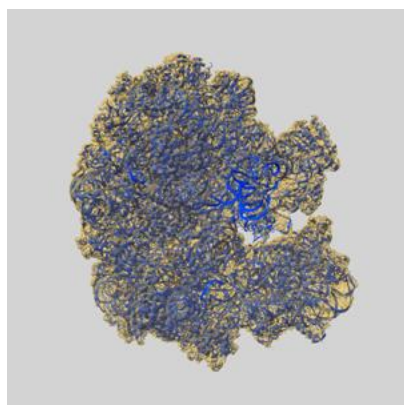
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.08	2.43	2.11
Unmasked-calculated*	2.08	2.43	2.12

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

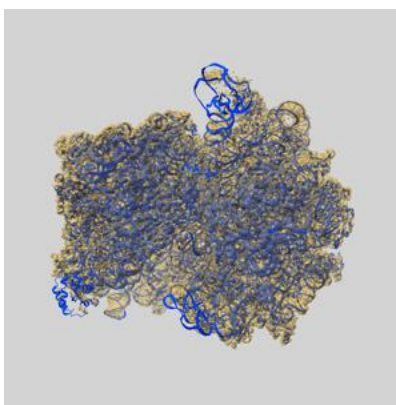
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-55138 and PDB model 9SRD. Per-residue inclusion information can be found in section 3 on page 17.

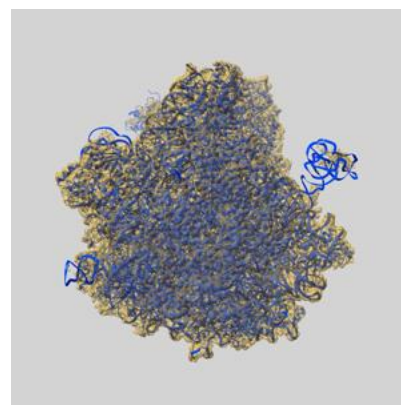
9.1 Map-model overlay ⓘ



X



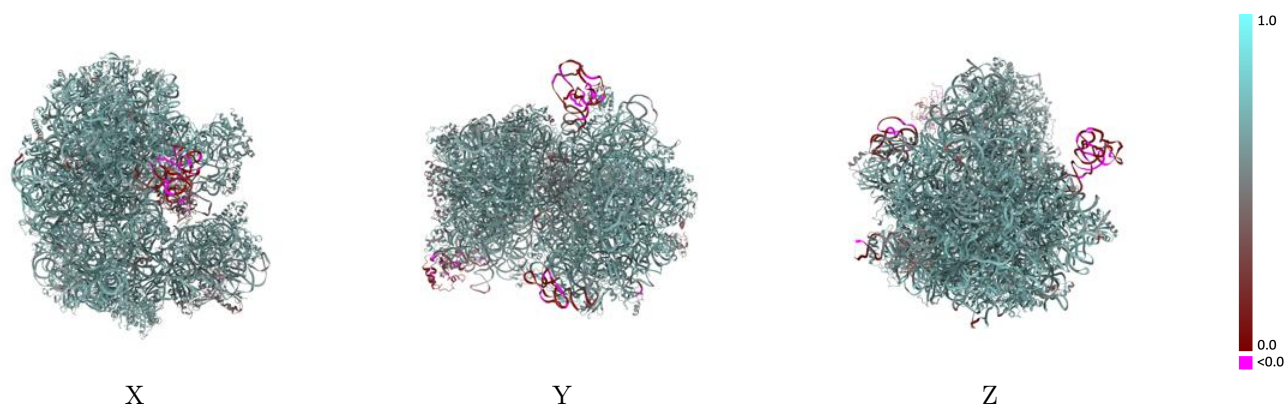
Y



Z

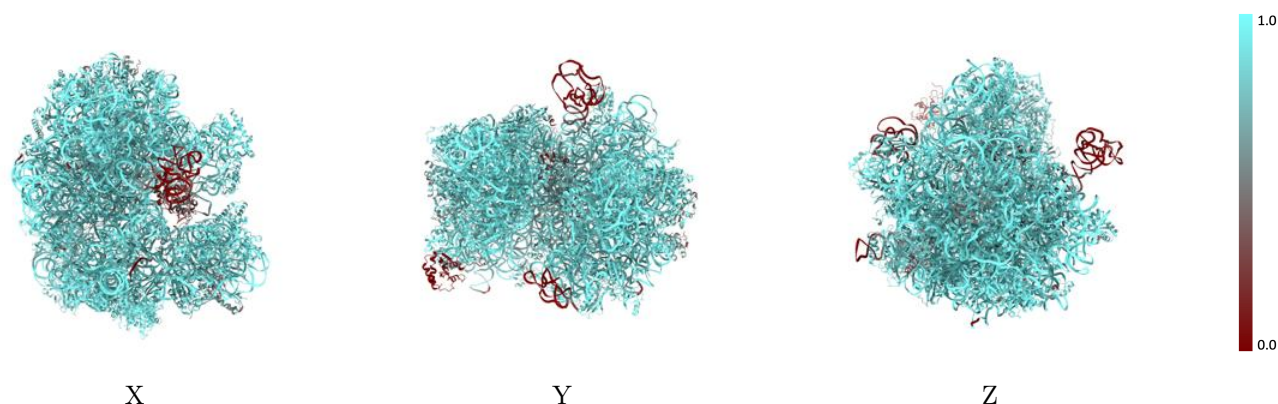
The images above show the 3D surface view of the map at the recommended contour level 0.00125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



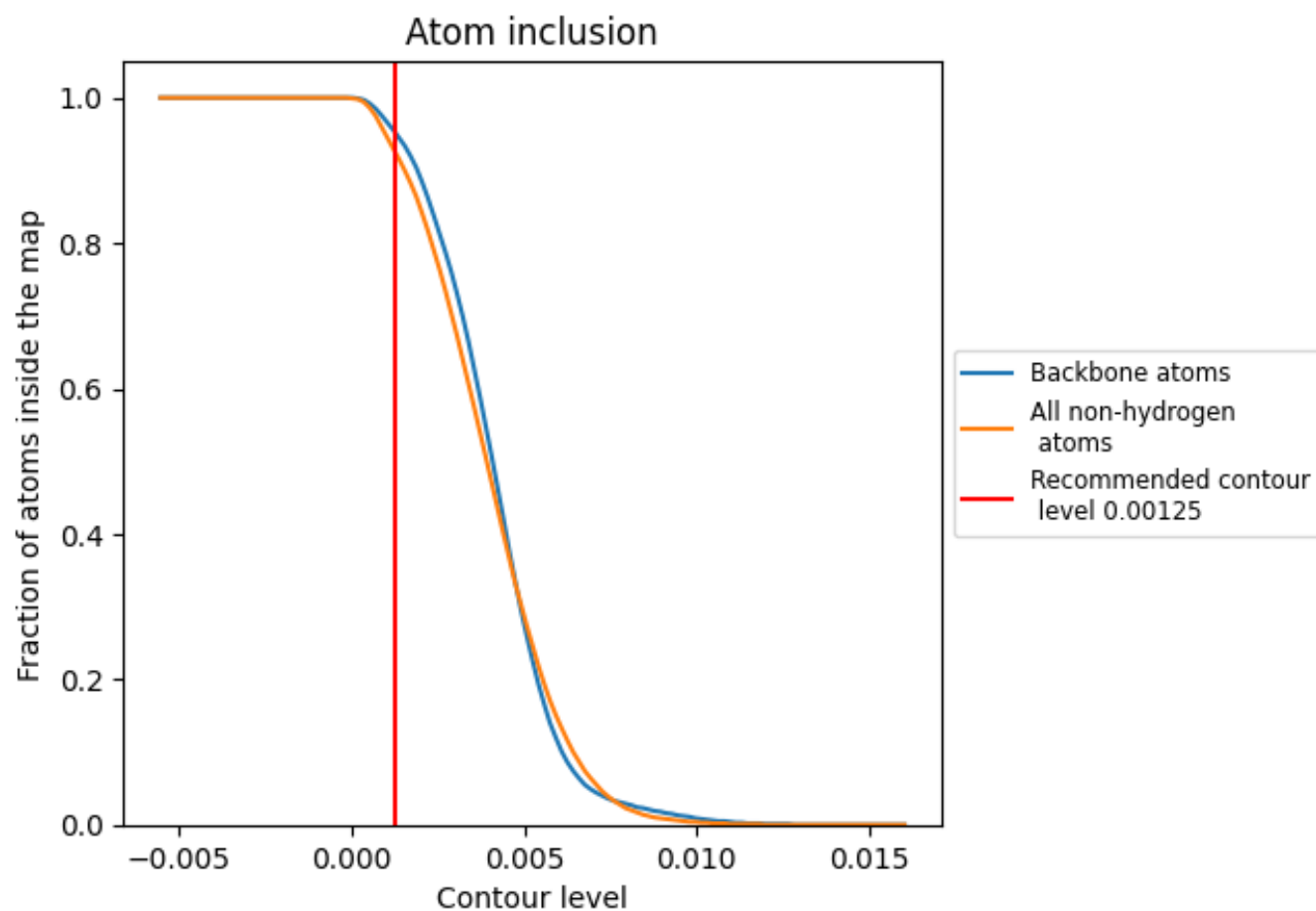
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.00125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.6220
1	 0.9380	 0.6260
2	 0.9820	 0.6300
3	 0.9930	 0.6230
A0	 0.9370	 0.6750
A3	 0.0610	 0.1700
AA	 0.8560	 0.5930
AB	 0.9310	 0.6050
AC	 0.9230	 0.6260
AD	 0.9430	 0.6360
AE	 0.9420	 0.6230
AF	 0.9300	 0.6310
AG	 0.8190	 0.5470
AH	 0.9060	 0.6020
AI	 0.9550	 0.6530
AJ	 0.9170	 0.6330
AK	 0.9210	 0.5980
AL	 0.7630	 0.5090
AM	 0.9140	 0.6230
AN	 0.9220	 0.6420
AO	 0.9110	 0.5930
AP	 0.8940	 0.5950
AQ	 0.9210	 0.6270
AR	 0.9360	 0.6450
AS	 0.8820	 0.5560
AT	 0.8750	 0.5810
AU	 0.9380	 0.6170
AV	 0.9070	 0.6030
AW	 0.8910	 0.5760
AX	 0.8480	 0.5710
AY	 0.1880	 0.1240
AZ	 0.8230	 0.5440
B4	 0.5690	 0.4650
B5	 0.9400	 0.6200
B6	 0.6350	 0.6090



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Chain	Atom inclusion	Q-score
BB	 0.9680	 0.6850
BC	 0.9590	 0.6760
BD	 0.9720	 0.6730
BE	 0.8700	 0.5700
BF	 0.9160	 0.6180
BG	 0.9150	 0.6260
BI	 0.9550	 0.6700
BJ	 0.9570	 0.6790
BK	 0.9190	 0.5900
BL	 0.9220	 0.6350
BM	 0.9860	 0.6940
BN	 0.9140	 0.6360
BO	 0.9290	 0.6120
BP	 0.9620	 0.6620
BQ	 0.9390	 0.6610
BR	 0.9620	 0.6690
BS	 0.9680	 0.6740
BT	 0.9490	 0.6500
BU	 0.9540	 0.6490
BV	 0.9530	 0.6680
BW	 0.8530	 0.5920
BY	 0.9600	 0.6650
BZ	 0.9060	 0.6070
Ba	 0.9120	 0.6390
Bb	 0.9570	 0.6770
Bc	 0.9440	 0.6640
Bd	 0.9610	 0.6540
Be	 0.9920	 0.6890
Bf	 0.9880	 0.6720
Bg	 0.9650	 0.6490
Bi	 0.9430	 0.6790
Bj	 0.9350	 0.6550
Bk	 0.9330	 0.6450
Bl	 0.8920	 0.6140
H	 0.5110	 0.4780