



wwPDB EM Validation Summary Report ⓘ

Jul 13, 2026 – 12:19 pm BST

PDB ID : 9T7H / pdb_00009t7h
EMDB ID : EMD-55636
Title : Cryo-EM structure of P. abyssi 70S ribosome in complex with hibernation factor HibA (L1 stalk conformation)
Authors : Madru, C.M.; Bourgeois, G.B.; Mechulam, Y.M.; Schmitt, E.S.
Deposited on : 2025-11-10
Resolution : 2.10 Å(reported)

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

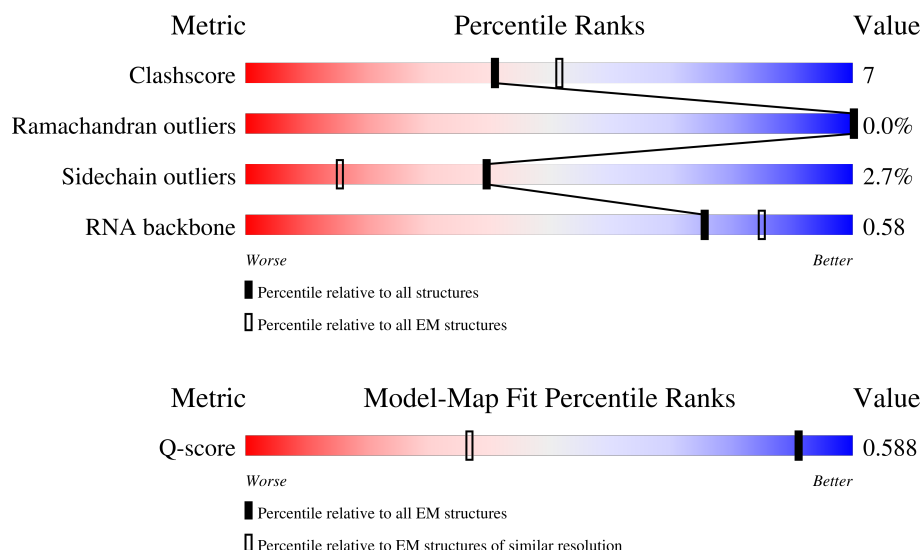
1 Overall quality at a glance i

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	

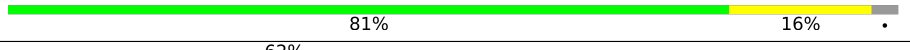
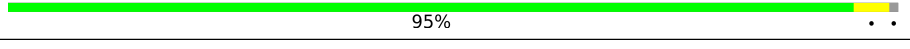
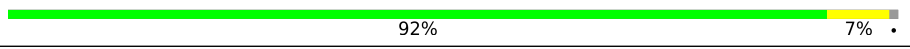
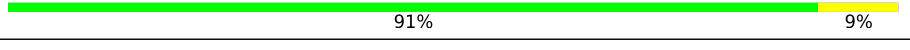
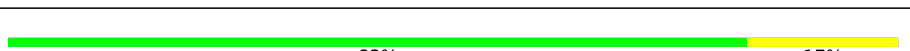
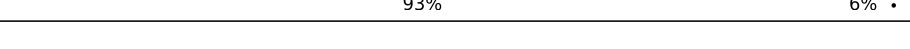
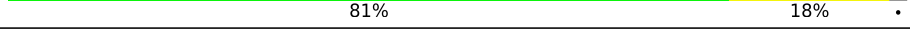
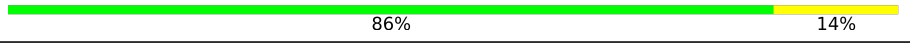
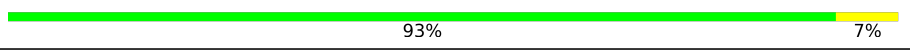
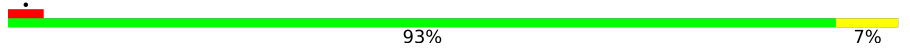
Continued on next page...

Continued from previous page...

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

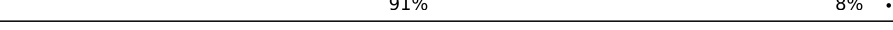
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
50	BQ	151	 86% 13% .
51	BV	67	 82% 12% 6%
52	Bj	94	 90% 10%
53	BD	255	 85% 13% .
54	BF	184	 82% 16% ..
55	BZ	99	 82% 17% .
56	BP	120	 88% 12%
57	BM	194	 91% 8% .
58	BS	155	 86% 12% ..
59	Bd	91	 91% 8% .
60	BN	181	 80% 17% ..
61	Bg	51	 78% 16% 6%
62	Bc	87	 89% 10% .
63	BJ	141	 91% 8% .
64	Bl	77	 79% 21%
65	Bk	65	 88% 9% .
66	BA	219	 36% 52% 44% ..

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 171964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

- Molecule 4 is a protein called Dehydrogenase.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	29	Total	C	N	O	S	0	0
			227	141	44	37	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 66 is a protein called Large ribosomal subunit protein uL1.

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

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	1	165	Total	Mg	0
			165	165	
67	2	61	Total	Mg	0
			61	61	
67	3	1	Total	Mg	0
			1	1	
67	AD	1	Total	Mg	0
			1	1	
67	AE	1	Total	Mg	0
			1	1	
67	AF	1	Total	Mg	0
			1	1	
67	AK	1	Total	Mg	0
			1	1	
67	AN	1	Total	Mg	0
			1	1	
67	AR	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
67	AU	1	Total 1	Mg 1	0
67	AT	1	Total 1	Mg 1	0
67	BB	2	Total 2	Mg 2	0
67	Bb	1	Total 1	Mg 1	0
67	BD	1	Total 1	Mg 1	0
67	BM	1	Total 1	Mg 1	0
67	BS	1	Total 1	Mg 1	0

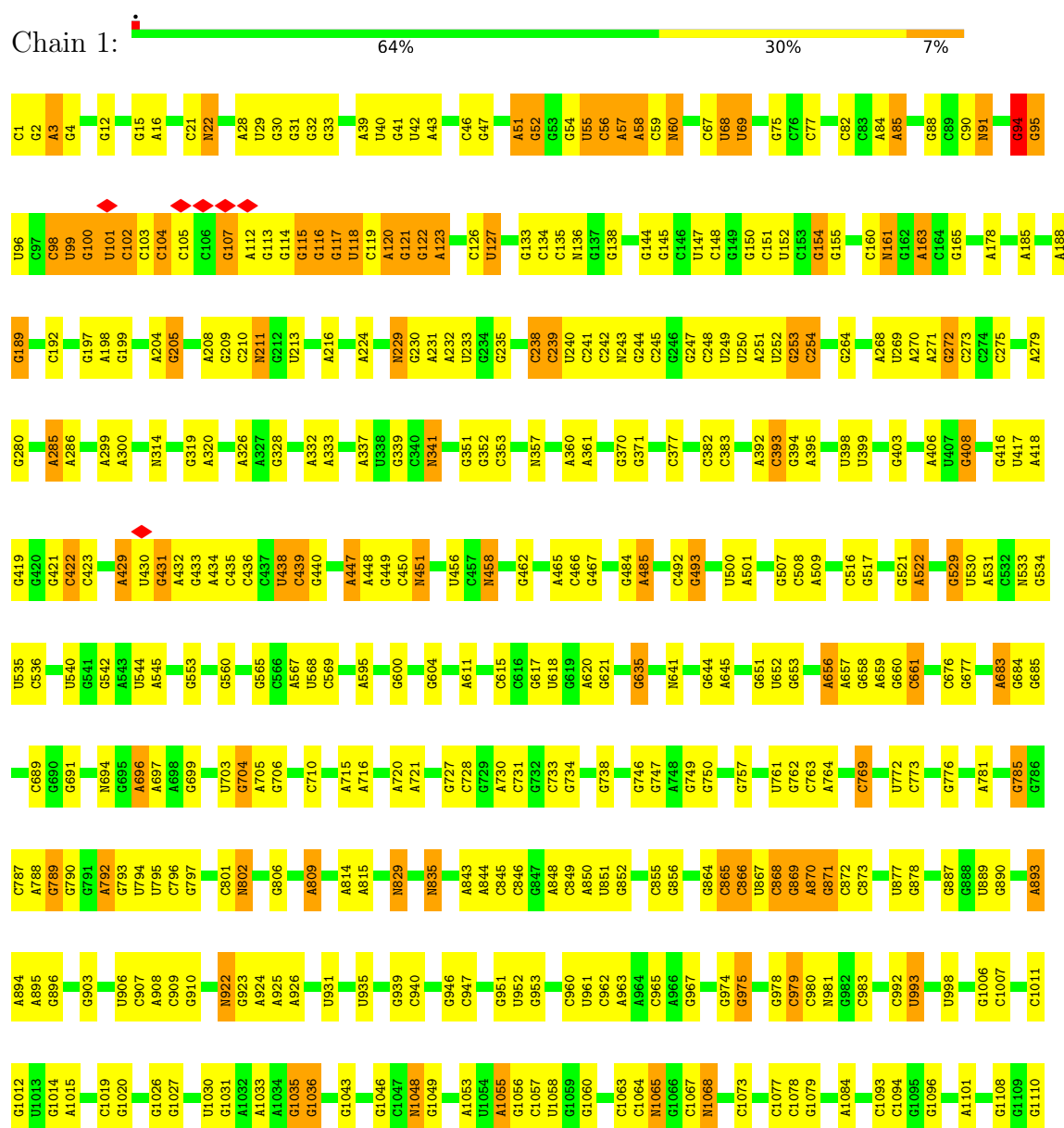
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

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

• Molecule 1: rRNA 23S

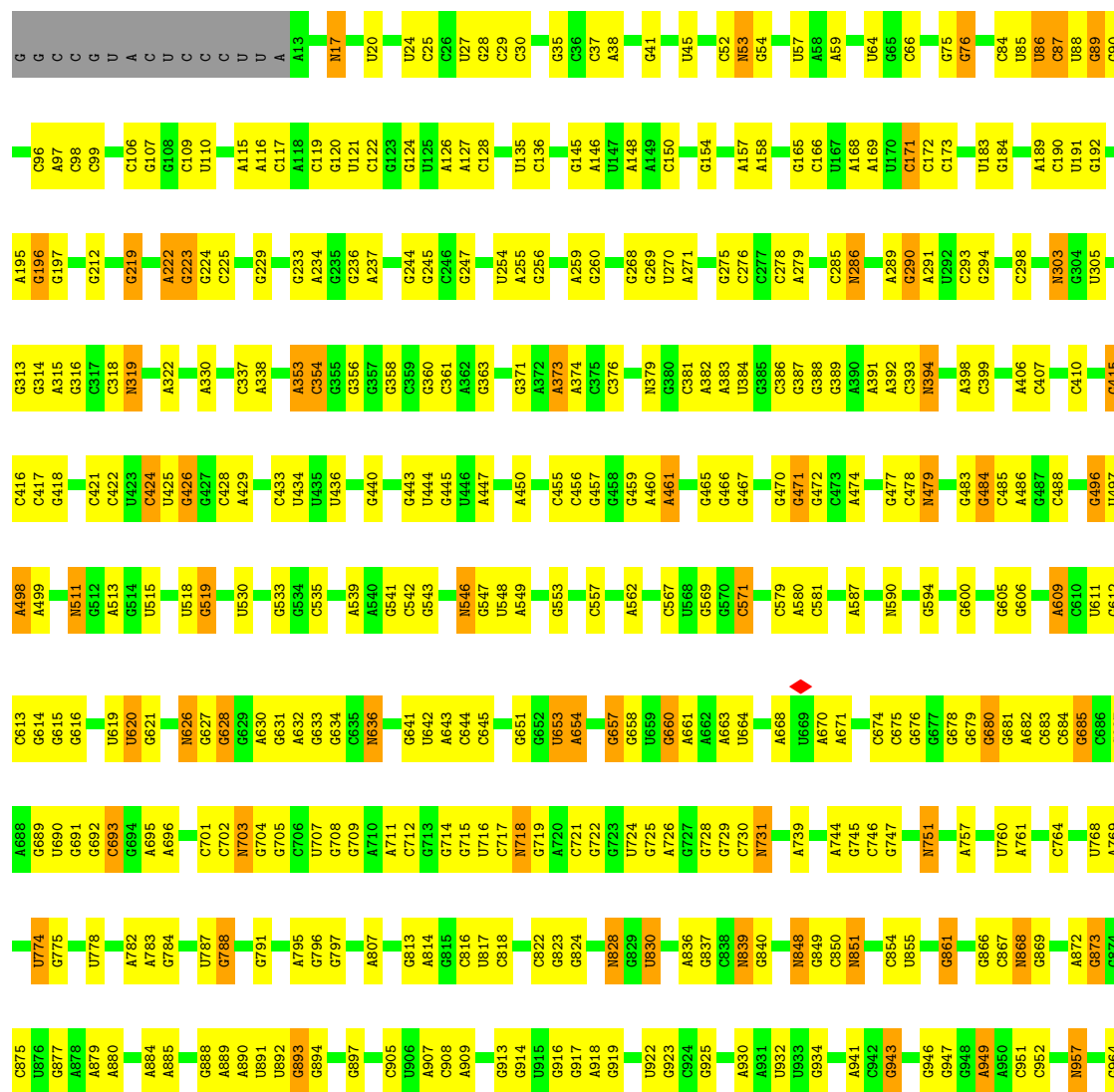


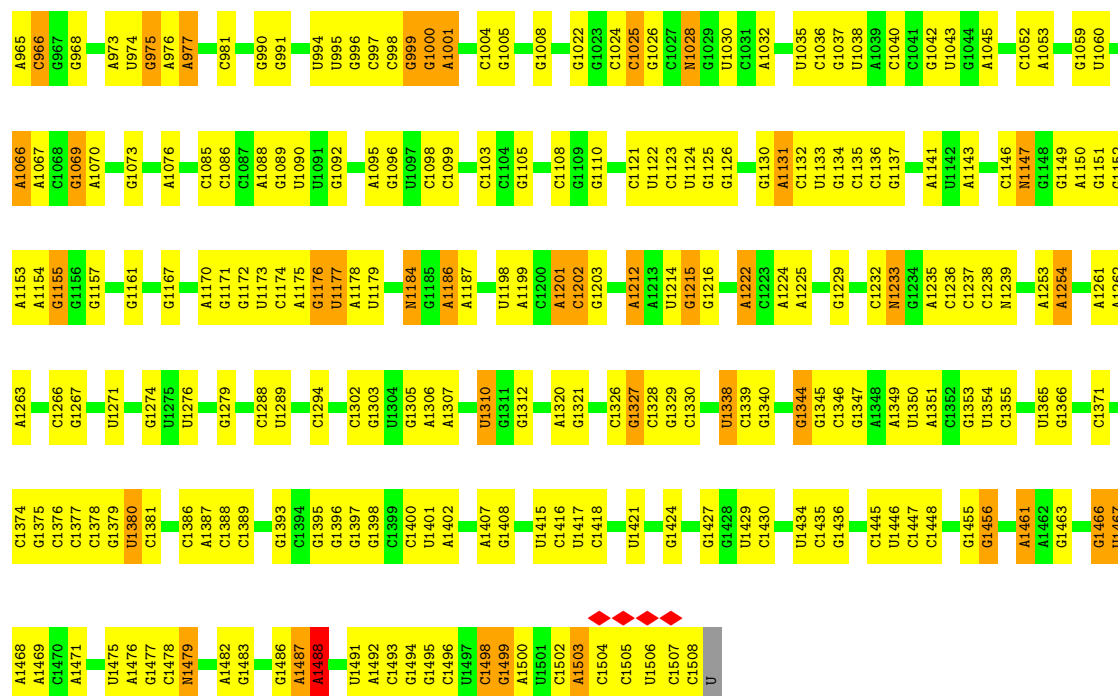




• Molecule 2: rRNA 16S

Chain 2: 57% 35% 7% .





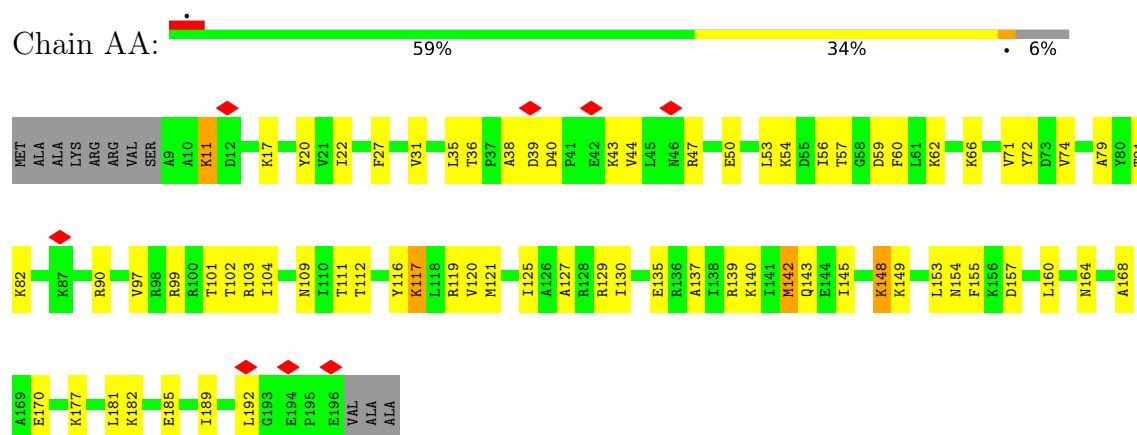
• Molecule 3: rRNA 5S



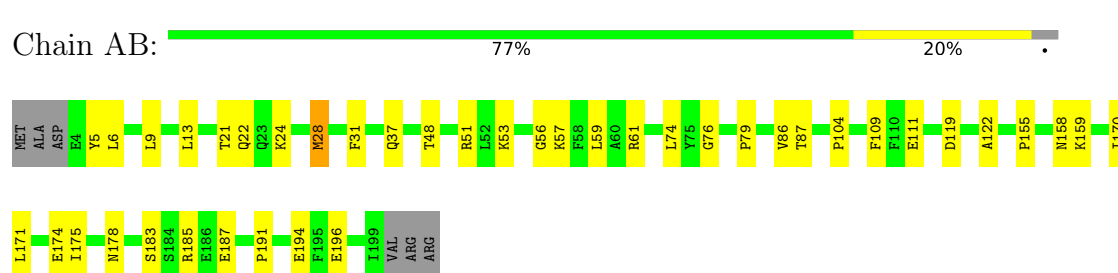
• Molecule 4: Dehydrogenase



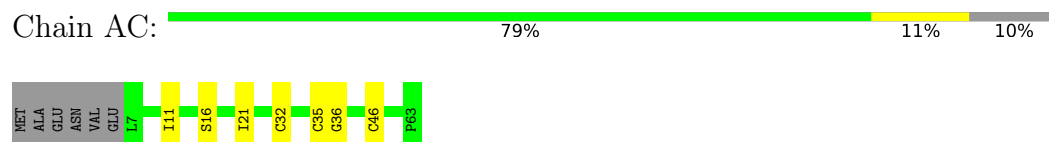
- Molecule 5: 30S ribosomal protein S3Ae



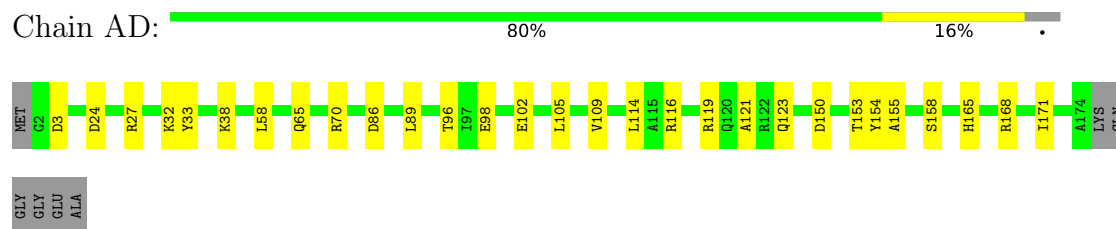
- Molecule 6: 30S ribosomal protein S2



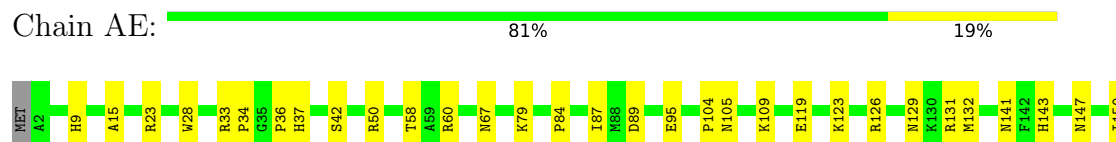
- Molecule 7: Zn-ribbon RNA-binding protein involved in translation



- Molecule 8: 30S ribosomal protein S4



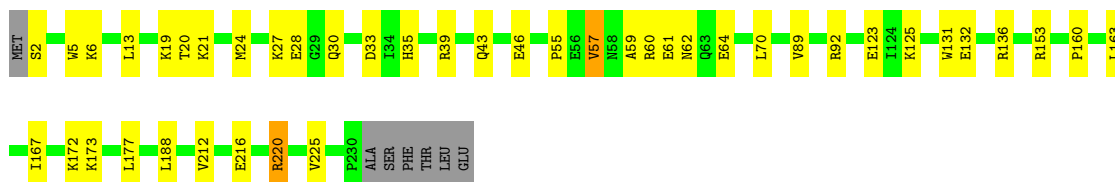
- Molecule 9: 30S ribosomal protein S4e





- Molecule 10: 30S ribosomal protein S5

Chain AF: 79% 17% ..



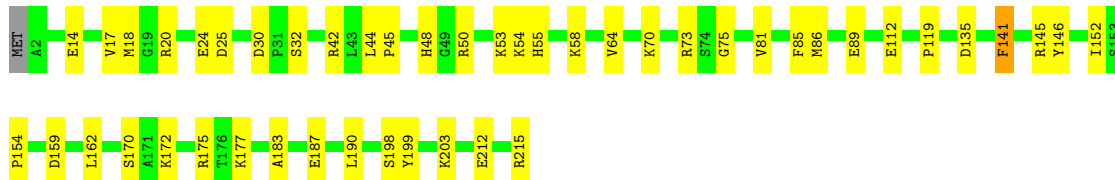
- Molecule 11: 30S ribosomal protein S6e

Chain AG: 74% 23% ..



- Molecule 12: 30S ribosomal protein S7

Chain AH: 78% 21%



- Molecule 13: 30S ribosomal protein S8

Chain AI: 84% 15% ..



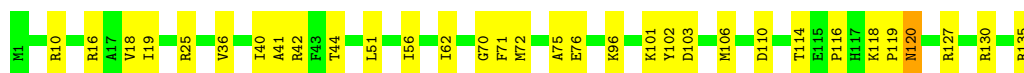
- Molecule 14: 30S ribosomal protein S8e

Chain AJ: 75% 20% ..

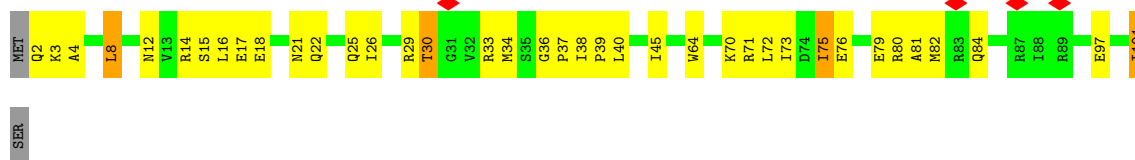


- Molecule 15: 30S ribosomal protein S9

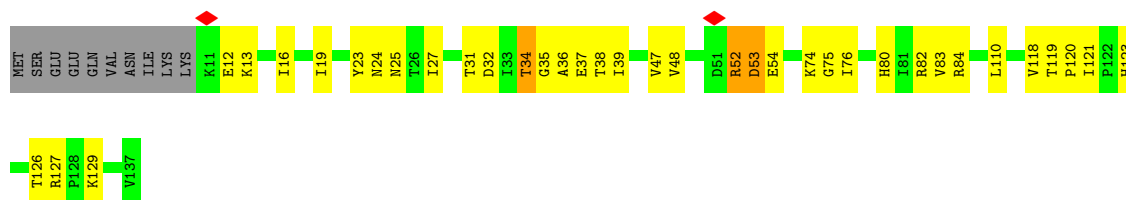
Chain AK: 76% 23%



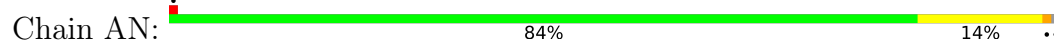
- Molecule 16: 30S ribosomal protein S10



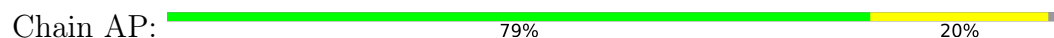
- Molecule 17: 30S ribosomal protein S11



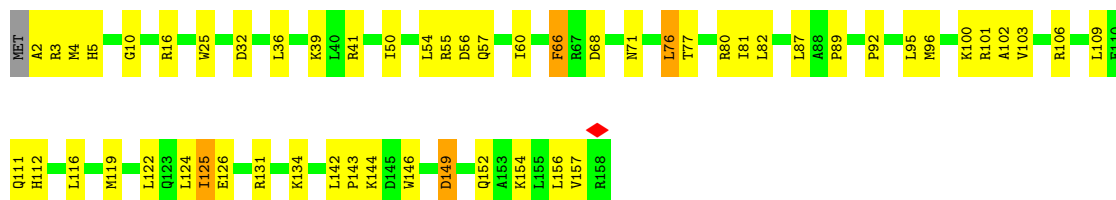
- Molecule 18: 30S ribosomal protein S12



- Molecule 19: 30S ribosomal protein S14 type Z



- Molecule 20: 30S ribosomal protein S15



- Molecule 21: 30S ribosomal protein S17

Chain AR:  80% 14% 5%



- Molecule 22: 30S ribosomal protein S17e

Chain AS:  73% 22% 5%



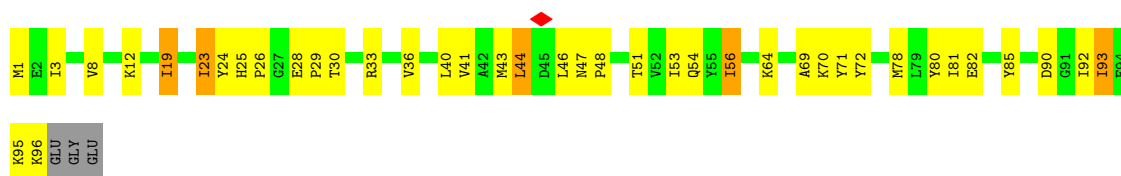
- Molecule 23: 30S ribosomal protein S19e

Chain AU:  83% 16% 1%



- Molecule 24: 30S ribosomal protein S24e

Chain AV:  57% 35% 5%



- Molecule 24: 30S ribosomal protein S24e

Chain B6:  77% 18% 5%



- Molecule 25: 30S ribosomal protein S27e

Chain AW:  68% 25% 6%

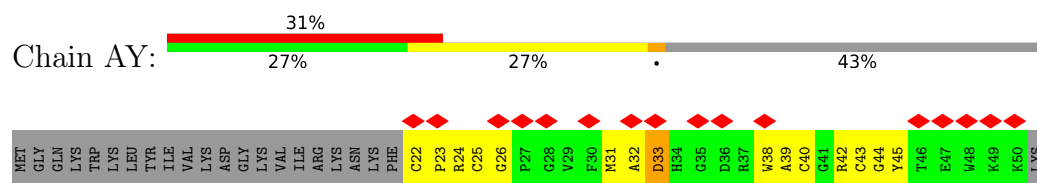


- Molecule 26: 30S ribosomal protein S28e

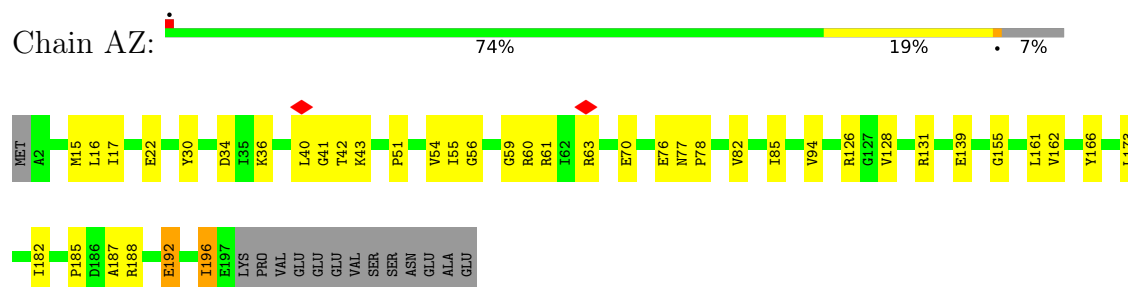
Chain AX:  59% 30% 8%



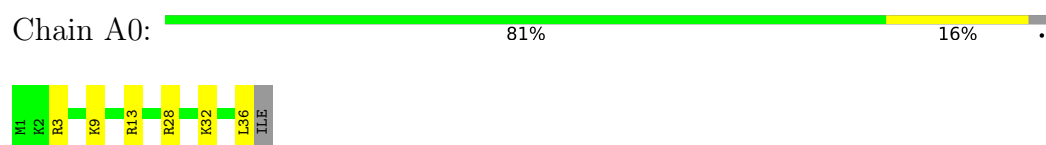
- Molecule 27: 30S ribosomal protein S27ae



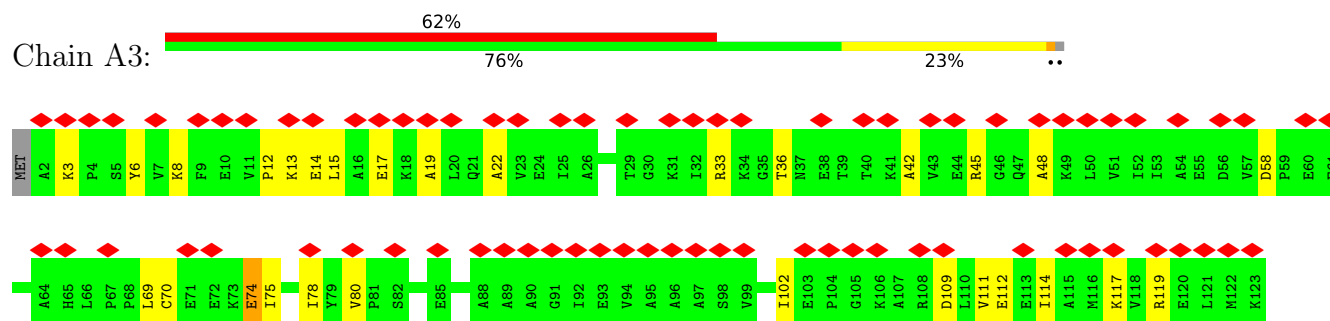
- Molecule 28: 30S ribosomal protein S3



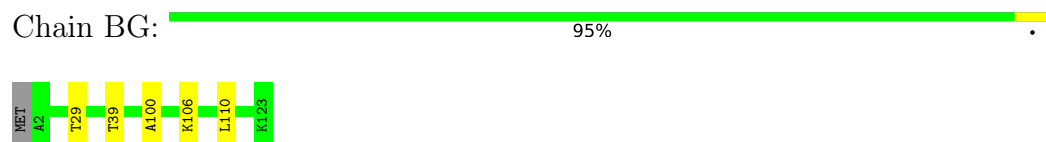
- Molecule 29: Small ribosomal subunit protein eS32



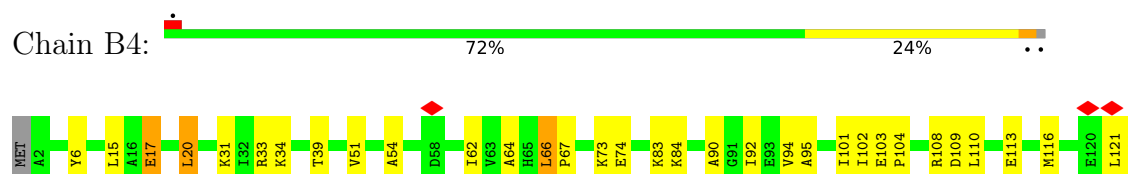
- Molecule 30: 50S ribosomal protein L7Ae



- Molecule 30: 50S ribosomal protein L7Ae



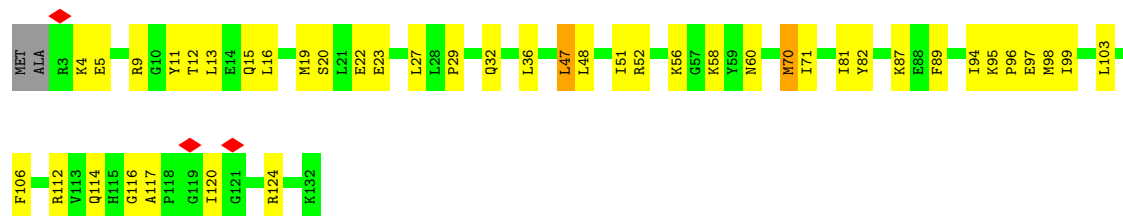
- Molecule 30: 50S ribosomal protein L7Ae



K123

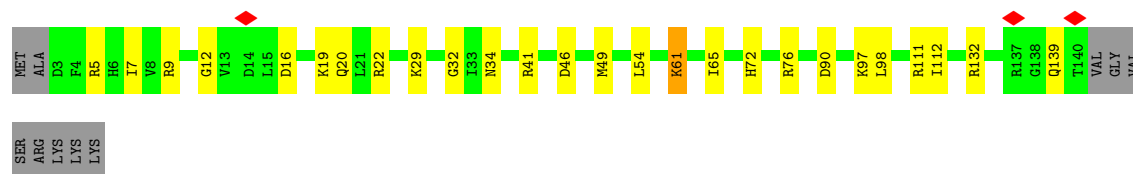
- Molecule 31: 30S ribosomal protein S19

Chain AT:  66% 31% ..



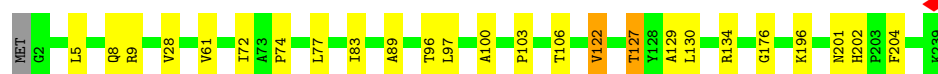
- Molecule 32: 30S ribosomal protein S13

Chain AO:  76% 17% 7%

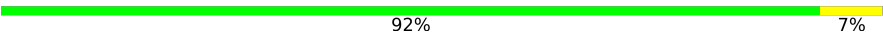


- Molecule 33: Large ribosomal subunit protein uL2

Chain BB:  89% 10% .



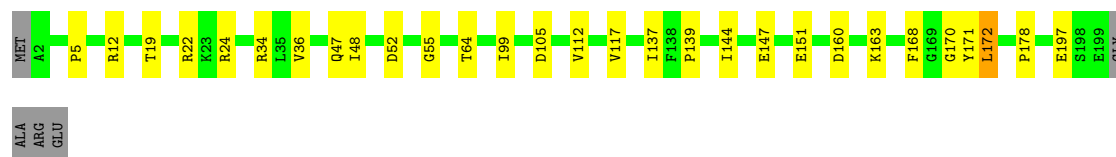
- Molecule 34: Large ribosomal subunit protein uL30

Chain BY:  92% 7% .



- Molecule 35: Large ribosomal subunit protein uL18

Chain BO:  83% 14% .



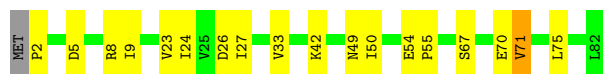
- Molecule 36: Large ribosomal subunit protein uL3

Chain BC:  91% 9%



- Molecule 37: Large ribosomal subunit protein eL14

Chain B5:  77% 21% ..



- Molecule 37: Large ribosomal subunit protein eL14

Chain BK:  87% 11% .



- Molecule 38: Large ribosomal subunit protein uL15

Chain BL:  85% 15%



- Molecule 39: Large ribosomal subunit protein eL39

Chain Bf:  86% 10% ..

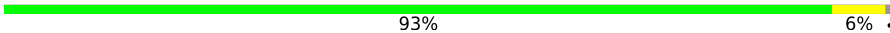


- Molecule 40: Large ribosomal subunit protein uL24

Chain BU:  83% 17%



- Molecule 41: Large ribosomal subunit protein eL32

Chain Bb:  93% 6% .



- Molecule 42: Large ribosomal subunit protein eL37

Chain Be:  81% 18%



- Molecule 43: Large ribosomal subunit protein uL5

Chain BE:  70% 26%

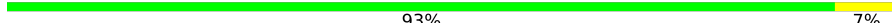


- Molecule 44: Large ribosomal subunit protein eL31

Chain Ba:  86% 14%

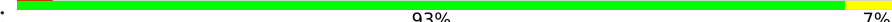


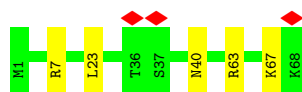
- Molecule 45: Large ribosomal subunit protein uL23

Chain BT:  93% 7%



- Molecule 46: Large ribosomal subunit protein uL29

Chain BW:  93% 7%



- Molecule 47: Large ribosomal subunit protein eL43

Chain Bi:  93% 6%

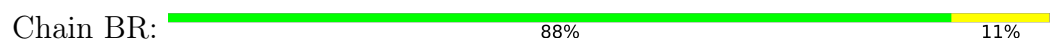


- Molecule 48: Large ribosomal subunit protein uL13

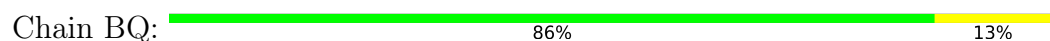
Chain BI:  89% 11%



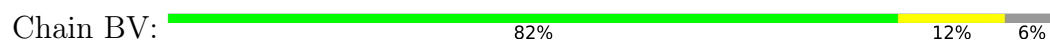
- Molecule 49: Large ribosomal subunit protein eL21



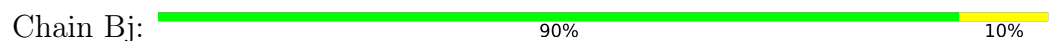
- Molecule 50: Large ribosomal subunit protein eL19



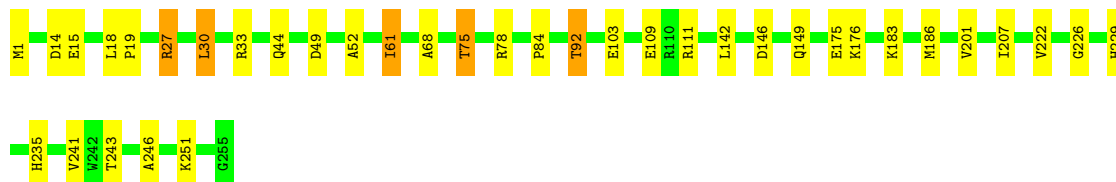
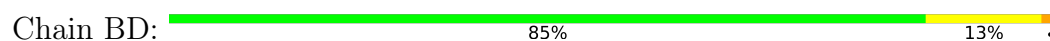
- Molecule 51: Large ribosomal subunit protein eL24



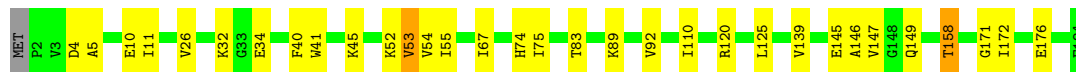
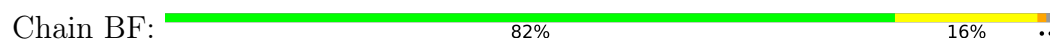
- Molecule 52: Large ribosomal subunit protein eL42



- Molecule 53: Large ribosomal subunit protein uL4



- Molecule 54: Large ribosomal subunit protein uL6



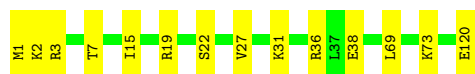
- Molecule 55: Large ribosomal subunit protein eL30

Chain BZ:  82% 17% .



- Molecule 56: Large ribosomal subunit protein eL18

Chain BP:  88% 12%



- Molecule 57: Large ribosomal subunit protein eL15

Chain BM:  91% 8%



- Molecule 58: Large ribosomal subunit protein uL22

Chain BS:  86% 12% ..



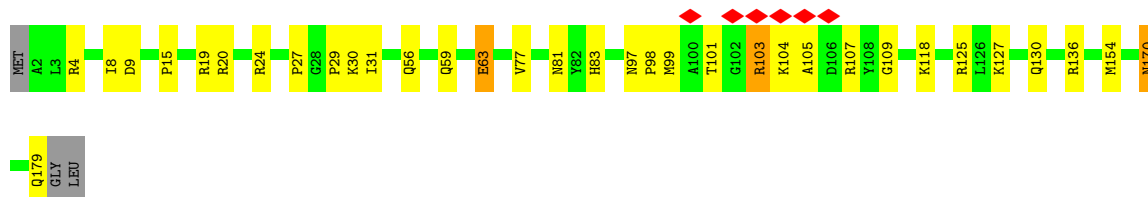
- Molecule 59: Large ribosomal subunit protein eL34

Chain Bd:  91% 8%



- Molecule 60: Large ribosomal subunit protein uL16

Chain BN:  80% 17% ..



- Molecule 61: Large ribosomal subunit protein eL40

Chain Bg:  78% 16% 6%





- Molecule 62: Large ribosomal subunit protein eL33

Chain Bc: 89% 10%



- Molecule 63: Large ribosomal subunit protein uL14

Chain BJ: 91% 8%



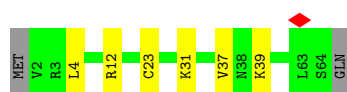
- Molecule 64: Large ribosomal subunit protein eL20

Chain Bl: 79% 21%



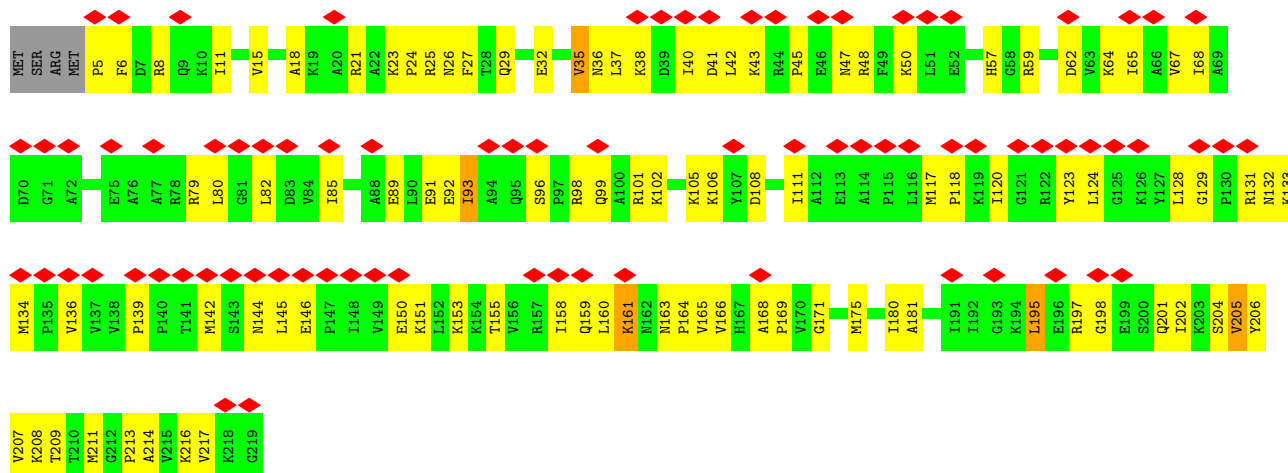
- Molecule 65: C2H2-type domain-containing protein

Chain Bk: 88% 9%



- Molecule 66: Large ribosomal subunit protein uL1

Chain BA: 36% 52% 44%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170000	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	0.015	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0008	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	2/70601 (0.0%)	0.31	0/110066
2	2	0.18	0/34435	0.26	0/53681
3	3	0.18	0/2995	0.25	0/4669
4	H	0.13	0/3120	0.31	0/4209
5	AA	0.11	0/1557	0.27	0/2087
6	AB	0.12	0/1602	0.24	0/2165
7	AC	0.12	0/463	0.27	0/628
8	AD	0.12	0/1476	0.21	0/1980
9	AE	0.14	0/2032	0.27	0/2742
10	AF	0.15	0/1838	0.26	0/2478
11	AG	0.12	0/993	0.30	0/1329
12	AH	0.11	0/1762	0.23	0/2366
13	AI	0.15	0/1055	0.26	0/1415
14	AJ	0.14	0/995	0.24	0/1327
15	AK	0.13	0/1089	0.31	0/1459
16	AL	0.13	0/817	0.30	0/1097
17	AM	0.12	0/973	0.30	0/1311
18	AN	0.15	0/1165	0.29	0/1547
19	AP	0.15	0/465	0.29	0/613
20	AQ	0.11	0/1333	0.28	0/1791
21	AR	0.14	0/907	0.29	0/1225
22	AS	0.12	0/548	0.25	0/725
23	AU	0.11	0/1253	0.22	0/1689
24	AV	0.14	0/826	0.29	0/1108
24	B6	0.10	0/808	0.23	0/1086
25	AW	0.11	0/476	0.24	0/641
26	AX	0.14	0/518	0.28	0/694
27	AY	0.09	0/235	0.27	0/315
28	AZ	0.13	0/1563	0.26	0/2099
29	A0	0.16	0/349	0.25	0/451
30	A3	0.11	0/945	0.31	0/1274
30	B4	0.12	0/945	0.32	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	BG	0.13	0/944	0.25	0/1274
31	AT	0.12	0/1077	0.26	0/1439
32	AO	0.12	0/1135	0.29	0/1526
33	BB	0.19	0/1882	0.29	0/2538
34	BY	0.16	0/1254	0.26	0/1677
35	BO	0.15	0/1645	0.26	0/2209
36	BC	0.17	0/2933	0.28	0/3943
37	B5	0.14	0/619	0.28	0/830
37	BK	0.14	0/611	0.29	0/819
38	BL	0.17	0/1167	0.31	0/1552
39	Bf	0.18	0/443	0.25	0/589
40	BU	0.15	0/1027	0.25	0/1368
41	Bb	0.17	0/1120	0.26	0/1494
42	Be	0.20	0/514	0.28	0/676
43	BE	0.14	0/1509	0.28	0/2022
44	Ba	0.16	0/793	0.26	0/1064
45	BT	0.17	0/705	0.28	0/945
46	BW	0.13	0/566	0.22	0/747
47	Bi	0.15	0/630	0.28	0/839
48	BI	0.18	0/1166	0.25	0/1559
49	BR	0.17	0/819	0.24	0/1098
50	BQ	0.17	0/1281	0.24	0/1689
51	BV	0.18	0/547	0.28	0/729
52	Bj	0.16	0/807	0.24	0/1070
53	BD	0.17	0/2069	0.28	0/2787
54	BF	0.15	0/1485	0.27	0/2003
55	BZ	0.15	0/759	0.27	0/1023
56	BP	0.16	0/984	0.25	0/1314
57	BM	0.19	0/1627	0.29	0/2170
58	BS	0.19	0/1275	0.30	0/1715
59	Bd	0.21	0/778	0.37	0/1036
60	BN	0.16	0/1483	0.26	0/1992
61	Bg	0.13	0/396	0.23	0/526
62	Bc	0.17	0/693	0.29	0/926
63	BJ	0.17	0/1080	0.27	0/1456
64	Bl	0.15	0/669	0.25	0/886
65	Bk	0.19	0/538	0.27	0/709
66	BA	0.11	0/1700	0.28	0/2288
All	All	0.19	2/180869 (0.0%)	0.28	0/266068

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	94	G	O3'-P	-6.15	1.51	1.61
1	1	96	U	C1'-N1	5.73	1.57	1.48

There are no bond angle outliers.

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	32949	665	0
2	2	32291	0	16340	427	0
3	3	2703	0	1375	23	0
4	H	3074	0	3190	100	0
5	AA	1531	0	1623	50	0
6	AB	1571	0	1630	25	0
7	AC	449	0	435	5	0
8	AD	1452	0	1521	20	0
9	AE	1983	0	2060	30	0
10	AF	1808	0	1879	34	0
11	AG	977	0	1037	19	0
12	AH	1725	0	1780	33	0
13	AI	1034	0	1069	15	0
14	AJ	986	0	1070	22	0
15	AK	1073	0	1133	23	0
16	AL	809	0	859	31	0
17	AM	955	0	981	33	0
18	AN	1148	0	1248	13	0
19	AP	455	0	475	11	0
20	AQ	1305	0	1388	41	0
21	AR	884	0	906	11	0
22	AS	541	0	573	10	0
23	AU	1223	0	1263	19	0
24	AV	808	0	832	26	0
24	B6	790	0	806	12	0
25	AW	470	0	495	13	0
26	AX	516	0	544	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AY	227	0	207	11	0
28	AZ	1541	0	1624	26	0
29	A0	343	0	407	4	0
30	A3	933	0	982	19	0
30	B4	933	0	982	21	0
30	BG	932	0	982	3	0
31	AT	1057	0	1131	27	0
32	AO	1116	0	1152	19	0
33	BB	1838	0	1903	17	0
34	BY	1235	0	1314	10	0
35	BO	1607	0	1638	16	0
36	BC	2870	0	3020	18	0
37	B5	614	0	671	12	0
37	BK	607	0	663	7	0
38	BL	1149	0	1218	16	0
39	Bf	435	0	494	4	0
40	BU	1011	0	1078	14	0
41	Bb	1095	0	1190	6	0
42	Be	503	0	533	11	0
43	BE	1485	0	1539	32	0
44	Ba	778	0	851	9	0
45	BT	696	0	758	3	0
46	BW	565	0	628	3	0
47	Bi	620	0	668	2	0
48	BI	1148	0	1237	11	0
49	BR	797	0	835	7	0
50	BQ	1265	0	1391	13	0
51	BV	532	0	523	7	0
52	Bj	789	0	842	7	0
53	BD	2026	0	2131	27	0
54	BF	1456	0	1514	18	0
55	BZ	749	0	796	11	0
56	BP	971	0	1039	10	0
57	BM	1588	0	1683	10	0
58	BS	1247	0	1280	11	0
59	Bd	759	0	825	10	0
60	BN	1452	0	1491	26	0
61	Bg	387	0	397	5	0
62	Bc	684	0	748	7	0
63	BJ	1066	0	1133	7	0
64	Bl	659	0	702	11	0
65	Bk	528	0	575	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	BA	1675	0	1787	86	0
67	1	165	0	0	0	0
67	2	61	0	0	0	0
67	3	1	0	0	0	0
67	AD	1	0	0	0	0
67	AE	1	0	0	0	0
67	AF	1	0	0	0	0
67	AK	1	0	0	0	0
67	AN	1	0	0	0	0
67	AR	1	0	0	0	0
67	AT	1	0	0	0	0
67	AU	1	0	0	0	0
67	BB	2	0	0	0	0
67	BD	1	0	0	0	0
67	BM	1	0	0	0	0
67	BS	1	0	0	0	0
67	Bb	1	0	0	0	0
68	AC	2	0	0	0	0
68	AF	1	0	0	0	0
68	AP	1	0	0	0	0
68	AR	1	0	0	0	0
68	AW	1	0	0	0	0
68	BV	1	0	0	0	0
68	Bd	1	0	0	0	0
68	Be	1	0	0	0	0
68	Bg	1	0	0	0	0
68	Bi	1	0	0	0	0
68	Bj	1	0	0	0	0
68	Bk	1	0	0	0	0
All	All	171964	0	126023	2034	0

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

The worst 5 of 2034 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
1:1:117:G:O2'	1:1:118:U:OP1	1.67	1.12
1:1:100:G:N2	1:1:119:C:O2	1.82	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2585:4AC:H5	1:1:2597:G:H1	1.13	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	H	384/392 (98%)	368 (96%)	15 (4%)	1 (0%)	36	36
5	AA	186/199 (94%)	181 (97%)	5 (3%)	0	100	100
6	AB	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
7	AC	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
8	AD	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
9	AE	240/243 (99%)	234 (98%)	6 (2%)	0	100	100
10	AF	227/236 (96%)	221 (97%)	6 (3%)	0	100	100
11	AG	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
12	AH	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
13	AI	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
14	AJ	123/127 (97%)	121 (98%)	2 (2%)	0	100	100
15	AK	133/135 (98%)	129 (97%)	3 (2%)	1 (1%)	16	12
16	AL	98/102 (96%)	95 (97%)	3 (3%)	0	100	100
17	AM	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
18	AN	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
19	AP	53/56 (95%)	53 (100%)	0	0	100	100
20	AQ	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
21	AR	105/113 (93%)	102 (97%)	3 (3%)	0	100	100
22	AS	62/67 (92%)	60 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	AU	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
24	AV	94/99 (95%)	90 (96%)	4 (4%)	0	100	100
24	B6	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
25	AW	59/65 (91%)	55 (93%)	4 (7%)	0	100	100
26	AX	63/71 (89%)	63 (100%)	0	0	100	100
27	AY	27/51 (53%)	23 (85%)	4 (15%)	0	100	100
28	AZ	194/210 (92%)	186 (96%)	8 (4%)	0	100	100
29	A0	34/37 (92%)	34 (100%)	0	0	100	100
30	A3	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
30	B4	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
30	BG	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
31	AT	128/132 (97%)	128 (100%)	0	0	100	100
32	AO	136/148 (92%)	130 (96%)	6 (4%)	0	100	100
33	BB	236/239 (99%)	229 (97%)	6 (2%)	1 (0%)	30	28
34	BY	152/155 (98%)	150 (99%)	2 (1%)	0	100	100
35	BO	196/203 (97%)	195 (100%)	1 (0%)	0	100	100
36	BC	358/361 (99%)	349 (98%)	8 (2%)	1 (0%)	36	36
37	B5	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
37	BK	78/82 (95%)	75 (96%)	3 (4%)	0	100	100
38	BL	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
39	Bf	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
40	BU	119/121 (98%)	119 (100%)	0	0	100	100
41	Bb	127/130 (98%)	127 (100%)	0	0	100	100
42	Be	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
43	BE	183/188 (97%)	181 (99%)	2 (1%)	0	100	100
44	Ba	92/94 (98%)	92 (100%)	0	0	100	100
45	BT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
46	BW	66/68 (97%)	66 (100%)	0	0	100	100
47	Bi	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
48	BI	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
49	BR	94/97 (97%)	94 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BQ	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
51	BV	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
52	Bj	92/94 (98%)	92 (100%)	0	0	100	100
53	BD	253/255 (99%)	249 (98%)	4 (2%)	0	100	100
54	BF	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
55	BZ	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
56	BP	118/120 (98%)	118 (100%)	0	0	100	100
57	BM	191/194 (98%)	189 (99%)	2 (1%)	0	100	100
58	BS	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
59	Bd	89/91 (98%)	89 (100%)	0	0	100	100
60	BN	176/181 (97%)	171 (97%)	5 (3%)	0	100	100
61	Bg	46/51 (90%)	46 (100%)	0	0	100	100
62	Bc	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
63	BJ	138/141 (98%)	138 (100%)	0	0	100	100
64	Bl	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
65	Bk	61/65 (94%)	61 (100%)	0	0	100	100
66	BA	213/219 (97%)	207 (97%)	6 (3%)	0	100	100
All	All	8761/9080 (96%)	8568 (98%)	189 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	AK	120	ASN
4	H	268	VAL
36	BC	347	VAL
33	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	H	332/338 (98%)	311 (94%)	21 (6%)	16	14
5	AA	160/167 (96%)	151 (94%)	9 (6%)	19	18
6	AB	168/173 (97%)	163 (97%)	5 (3%)	36	41
7	AC	50/55 (91%)	50 (100%)	0	100	100
8	AD	156/160 (98%)	155 (99%)	1 (1%)	78	86
9	AE	213/214 (100%)	212 (100%)	1 (0%)	81	88
10	AF	192/198 (97%)	190 (99%)	2 (1%)	68	76
11	AG	107/108 (99%)	104 (97%)	3 (3%)	38	43
12	AH	183/184 (100%)	179 (98%)	4 (2%)	45	53
13	AI	106/107 (99%)	104 (98%)	2 (2%)	50	58
14	AJ	101/103 (98%)	94 (93%)	7 (7%)	14	12
15	AK	111/111 (100%)	108 (97%)	3 (3%)	39	45
16	AL	89/91 (98%)	85 (96%)	4 (4%)	24	25
17	AM	94/104 (90%)	88 (94%)	6 (6%)	16	14
18	AN	120/121 (99%)	116 (97%)	4 (3%)	33	37
19	AP	45/46 (98%)	45 (100%)	0	100	100
20	AQ	142/143 (99%)	134 (94%)	8 (6%)	19	18
21	AR	96/102 (94%)	93 (97%)	3 (3%)	35	39
22	AS	58/61 (95%)	56 (97%)	2 (3%)	32	35
23	AU	126/127 (99%)	126 (100%)	0	100	100
24	AV	88/90 (98%)	78 (89%)	10 (11%)	5	3
24	B6	86/90 (96%)	85 (99%)	1 (1%)	63	72
25	AW	53/56 (95%)	51 (96%)	2 (4%)	29	32
26	AX	55/60 (92%)	49 (89%)	6 (11%)	6	4
27	AY	22/42 (52%)	20 (91%)	2 (9%)	9	6
28	AZ	155/168 (92%)	151 (97%)	4 (3%)	40	46
29	A0	34/35 (97%)	33 (97%)	1 (3%)	37	42
30	A3	98/99 (99%)	96 (98%)	2 (2%)	48	56
30	B4	98/99 (99%)	91 (93%)	7 (7%)	13	11
30	BG	98/99 (99%)	98 (100%)	0	100	100
31	AT	113/114 (99%)	109 (96%)	4 (4%)	32	35
32	AO	115/123 (94%)	113 (98%)	2 (2%)	53	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BB	188/189 (100%)	185 (98%)	3 (2%)	55	64
34	BY	132/133 (99%)	132 (100%)	0	100	100
35	BO	167/170 (98%)	161 (96%)	6 (4%)	31	34
36	BC	306/307 (100%)	304 (99%)	2 (1%)	76	83
37	B5	65/66 (98%)	62 (95%)	3 (5%)	24	25
37	BK	64/66 (97%)	63 (98%)	1 (2%)	55	64
38	BL	118/118 (100%)	116 (98%)	2 (2%)	53	62
39	Bf	46/47 (98%)	44 (96%)	2 (4%)	26	27
40	BU	109/109 (100%)	108 (99%)	1 (1%)	70	78
41	Bb	117/118 (99%)	116 (99%)	1 (1%)	70	78
42	Be	52/53 (98%)	52 (100%)	0	100	100
43	BE	158/160 (99%)	148 (94%)	10 (6%)	16	14
44	Ba	84/84 (100%)	83 (99%)	1 (1%)	63	72
45	BT	77/77 (100%)	74 (96%)	3 (4%)	28	31
46	BW	63/63 (100%)	61 (97%)	2 (3%)	34	38
47	Bi	61/62 (98%)	60 (98%)	1 (2%)	55	64
48	BI	122/122 (100%)	121 (99%)	1 (1%)	73	81
49	BR	86/87 (99%)	84 (98%)	2 (2%)	44	51
50	BQ	132/133 (99%)	129 (98%)	3 (2%)	44	51
51	BV	54/58 (93%)	54 (100%)	0	100	100
52	Bj	83/84 (99%)	82 (99%)	1 (1%)	63	72
53	BD	212/212 (100%)	206 (97%)	6 (3%)	38	43
54	BF	156/157 (99%)	152 (97%)	4 (3%)	40	46
55	BZ	79/80 (99%)	78 (99%)	1 (1%)	61	69
56	BP	102/102 (100%)	101 (99%)	1 (1%)	68	76
57	BM	160/161 (99%)	159 (99%)	1 (1%)	78	86
58	BS	130/131 (99%)	128 (98%)	2 (2%)	57	65
59	Bd	82/82 (100%)	81 (99%)	1 (1%)	63	72
60	BN	149/151 (99%)	146 (98%)	3 (2%)	48	56
61	Bg	37/39 (95%)	37 (100%)	0	100	100
62	Bc	74/74 (100%)	73 (99%)	1 (1%)	59	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	BJ	108/109 (99%)	106 (98%)	2 (2%)	50	58
64	Bl	72/72 (100%)	70 (97%)	2 (3%)	38	43
65	Bk	55/57 (96%)	55 (100%)	0	100	100
66	BA	182/186 (98%)	173 (95%)	9 (5%)	22	22
All	All	7546/7707 (98%)	7342 (97%)	204 (3%)	40	45

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	AT	70	MET
43	BE	120	HIS
66	BA	136	VAL
33	BB	106	THR
37	B5	71	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
50	BQ	67	HIS
59	Bd	35	HIS
51	BV	57	GLN
54	BF	156	GLN
60	BN	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3016/3018 (99%)	427 (14%)	19 (0%)
2	2	1495/1512 (98%)	175 (11%)	2 (0%)
3	3	125/128 (97%)	13 (10%)	0
All	All	4636/4658 (99%)	615 (13%)	21 (0%)

5 of 615 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	3	A
1	1	12	G
1	1	28	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	39	A
1	1	51	A

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2397	G
1	1	2986	U
2	2	653	U
1	1	3021	U
1	1	2733	5MC

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	458	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
2	4AC	2	751	2	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2136	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	1243	1	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
2	4AC	2	590	2	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	5MC	1	2733	1	18,22,23	0.96	2 (11%)	26,32,35	1.26	3 (11%)
2	OMC	2	773	2	19,22,23	0.82	0	26,31,34	0.83	0
1	4AC	1	1938	1	21,24,25	1.04	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	161	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1962	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2642	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
2	4AC	2	303	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1873	1	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
2	5MC	2	1374	2	18,22,23	0.92	2 (11%)	26,32,35	1.13	2 (7%)

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	1.47	4 (17%)	34,38,41	2.10	9 (26%)
1	4AC	1	229	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
2	OMG	2	471	2	23,26,27	1.22	3 (13%)	33,38,41	1.92	6 (18%)
1	LHH	1	616	1	22,25,26	0.31	0	29,35,38	0.47	0
2	4AC	2	718	2	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	UR3	2	1467	2	19,22,23	0.94	0	26,32,35	1.43	2 (7%)
2	B8H	2	938	2	19,22,23	0.53	0	22,32,35	0.61	0
2	4AC	2	1479	2	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	17	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
2	6MZ	2	1469	2,67	22,25,26	1.48	4 (18%)	30,36,39	2.19	9 (30%)
1	OMG	1	923	67,1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	2083	1	21,24,25	1.04	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	1	922	1	21,24,25	1.05	2 (9%)	29,34,37	1.44	4 (13%)
1	4AC	1	2287	1	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
1	OMG	1	2678	1	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	357	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	2249	1	21,24,25	1.05	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	2960	1	21,24,25	1.00	2 (9%)	29,34,37	1.32	4 (13%)
1	OMG	1	789	1	23,26,27	1.25	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	2966	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	5MC	1	2093	1	18,22,23	0.94	2 (11%)	26,32,35	1.14	2 (7%)
2	4AC	2	828	2	21,24,25	1.00	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	2001	1	21,24,25	1.06	2 (9%)	29,34,37	1.48	4 (13%)
2	OMG	2	680	2	23,26,27	1.23	3 (13%)	33,38,41	1.99	6 (18%)
2	4AC	2	379	2	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
2	OMG	2	913	2	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	2027	1	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	2585	1	21,24,25	1.06	2 (9%)	29,34,37	1.75	5 (17%)
2	5MC	2	1498	2	18,22,23	0.94	2 (11%)	26,32,35	1.27	4 (15%)
1	4AC	1	835	1	21,24,25	1.03	2 (9%)	29,34,37	1.34	4 (13%)
2	OMG	2	467	2	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	1557	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
2	OMU	2	1380	2	19,22,23	1.29	3 (15%)	26,31,34	1.74	4 (15%)
1	4AC	1	2608	1	21,24,25	1.06	2 (9%)	29,34,37	1.73	5 (17%)
1	OMC	1	615	1	19,22,23	0.80	0	26,31,34	0.83	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	2	1069	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	4AC	2	703	2	21,24,25	1.03	1 (4%)	29,34,37	1.46	4 (13%)
1	4AC	1	2548	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	5MC	2	1505	2	18,22,23	0.98	2 (11%)	26,32,35	1.13	3 (11%)
1	4AC	1	1617	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	OMG	1	2144	1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
1	4AC	1	2062	1	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
1	A2M	1	2173	1	22,25,26	1.44	4 (18%)	31,36,39	2.05	8 (25%)
2	4AC	2	636	2	21,24,25	1.02	1 (4%)	29,34,37	1.40	4 (13%)
1	4AC	1	3004	1	21,24,25	1.03	2 (9%)	29,34,37	1.28	4 (13%)
1	A2M	1	1055	1	22,25,26	1.45	4 (18%)	31,36,39	2.07	9 (29%)
1	5MC	1	2183	1	18,22,23	0.94	2 (11%)	26,32,35	1.15	2 (7%)
1	4AC	1	2865	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	546	2,67	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
2	5MC	2	1025	2	18,22,23	0.94	2 (11%)	26,32,35	1.16	3 (11%)
1	4AC	1	341	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1885	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
2	OMU	2	830	2	19,22,23	1.25	3 (15%)	26,31,34	1.69	4 (15%)
1	4AC	1	829	1	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)
2	MA6	2	1487	2	23,26,27	1.47	4 (17%)	34,38,41	2.10	10 (29%)
1	OMC	1	1948	1	19,22,23	0.82	0	26,31,34	0.79	0
1	4AC	1	1048	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	694	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1460	1	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	641	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
2	5MC	2	875	2	18,22,23	0.95	2 (11%)	26,32,35	1.18	3 (11%)
2	OMC	2	129	2	19,22,23	0.81	0	26,31,34	0.83	0
1	4AC	1	1780	1	21,24,25	1.04	2 (9%)	29,34,37	1.50	4 (13%)
1	4AC	1	2908	1	21,24,25	1.01	2 (9%)	29,34,37	1.32	4 (13%)
2	OMG	2	657	2	23,26,27	1.23	3 (13%)	33,38,41	1.93	5 (15%)
2	LHH	2	1041	2	22,25,26	0.32	0	29,35,38	0.48	0
1	4AC	1	1695	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	802	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	981	1	21,24,25	1.01	2 (9%)	29,34,37	1.29	4 (13%)
1	4AC	1	1662	1	21,24,25	0.99	2 (9%)	29,34,37	1.39	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	1	91	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	848	2	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
2	OMU	2	64	2	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
2	4AC	2	1147	2	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
2	5MC	2	1496	2	18,22,23	0.93	2 (11%)	26,32,35	1.17	3 (11%)
1	4AC	1	136	1	21,24,25	1.01	2 (9%)	29,34,37	1.30	4 (13%)
1	4AC	1	2925	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	1550	1	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
2	4AC	2	1233	2	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	1	2570	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
2	4AC	2	731	2	21,24,25	1.01	2 (9%)	29,34,37	1.46	4 (13%)
2	5MC	2	693	2	18,22,23	0.94	2 (11%)	26,32,35	1.17	3 (11%)
1	4AC	1	1554	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	511	2	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	1667	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	OMC	2	846	2	19,22,23	0.81	0	26,31,34	0.81	0
2	OMG	2	873	2	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	4AC	1	1594	67,1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	1	2992	1	21,24,25	1.04	2 (9%)	29,34,37	0.86	2 (6%)
2	OMG	2	519	2	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
2	4AC	2	1184	2	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
3	4AC	3	32	3	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	OMG	1	328	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
2	4AC	2	868	2	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
1	5MC	1	2203	1	18,22,23	0.93	2 (11%)	26,32,35	1.14	2 (7%)
1	4AC	1	1755	1	21,24,25	1.09	2 (9%)	29,34,37	1.63	5 (17%)
1	4AC	1	1222	67,1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
2	OMU	2	20	2	19,22,23	1.25	3 (15%)	26,31,34	1.78	5 (19%)
1	4AC	1	533	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	2937	67,1	21,24,25	1.03	2 (9%)	29,34,37	1.57	4 (13%)
2	OMG	2	934	2	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
2	4AC	2	851	2	21,24,25	1.02	2 (9%)	29,34,37	1.29	4 (13%)
1	5MC	1	2163	1	18,22,23	0.94	2 (11%)	26,32,35	1.14	3 (11%)
1	4AC	1	243	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	60	1	21,24,25	1.02	2 (9%)	29,34,37	1.39	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4AC	2	394	2	21,24,25	1.00	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	1	2495	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
2	OMU	2	1177	2	19,22,23	1.22	3 (15%)	26,31,34	1.70	5 (19%)
1	4AC	1	2718	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
1	OMG	1	2138	1	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
1	4AC	1	2329	1	21,24,25	1.02	2 (9%)	29,34,37	1.37	4 (13%)
2	OMC	2	1376	2	19,22,23	0.80	0	26,31,34	0.77	0
1	4AC	1	2545	1	21,24,25	1.01	2 (9%)	29,34,37	1.35	4 (13%)
1	4AC	1	22	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	1	451	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	OMU	1	2784	1	19,22,23	1.22	3 (15%)	26,31,34	1.71	5 (19%)
2	5MC	2	1202	2	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
2	4AC	2	839	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1867	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1065	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	5MC	1	2198	1	18,22,23	0.91	2 (11%)	26,32,35	1.15	2 (7%)
2	4AC	2	53	2	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
2	A2M	2	373	2	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
2	4AC	2	957	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1878	1	21,24,25	1.02	2 (9%)	29,34,37	1.46	4 (13%)
2	4AC	2	626	2	21,24,25	1.02	1 (4%)	29,34,37	1.44	4 (13%)
2	OMU	2	787	2	19,22,23	1.24	2 (10%)	26,31,34	1.82	5 (19%)
2	OMC	2	1040	2	19,22,23	1.08	2 (10%)	26,31,34	0.85	0
1	4AC	1	1621	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	1	1765	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	5MC	1	2162	1	18,22,23	0.95	2 (11%)	26,32,35	1.21	3 (11%)
1	OMG	1	2147	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
1	4AC	1	314	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
2	4AC	2	1239	2	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
2	4AC	2	1028	2	21,24,25	1.01	2 (9%)	29,34,37	1.36	4 (13%)
2	4AC	2	479	2	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
2	4AC	2	286	2	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	1	1068	1	21,24,25	1.04	2 (9%)	29,34,37	1.37	4 (13%)
2	LHH	2	250	2	22,25,26	0.32	0	29,35,38	0.43	0
1	4AC	1	211	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5MC	2	535	2	18,22,23	0.93	2 (11%)	26,32,35	1.14	2 (7%)
2	4AC	2	319	2	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
2	OMU	2	774	2	19,22,23	1.21	2 (10%)	26,31,34	1.73	5 (19%)
1	4AC	1	1934	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	1	1293	1	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	458	1	-	0/11/29/30	0/2/2/2
2	4AC	2	751	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2136	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1243	1	-	0/11/29/30	0/2/2/2
2	4AC	2	590	2	-	0/11/29/30	0/2/2/2
1	5MC	1	2733	1	-	4/7/25/26	0/2/2/2
2	OMC	2	773	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1938	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	1962	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2642	1	-	0/11/29/30	0/2/2/2
2	4AC	2	303	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1873	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1374	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1488	2	-	1/11/29/30	0/3/3/3
1	4AC	1	229	1	-	0/11/29/30	0/2/2/2
2	OMG	2	471	2	-	0/9/27/28	0/3/3/3
1	LHH	1	616	1	-	0/13/31/32	0/2/2/2
2	4AC	2	718	2	-	0/11/29/30	0/2/2/2
2	UR3	2	1467	2	-	0/7/25/26	0/2/2/2
2	B8H	2	938	2	-	1/7/25/26	0/2/2/2
2	4AC	2	1479	2	-	0/11/29/30	0/2/2/2
2	4AC	2	17	2	-	0/11/29/30	0/2/2/2
2	6MZ	2	1469	2,67	-	0/9/27/28	0/3/3/3
1	OMG	1	923	67,1	-	1/9/27/28	0/3/3/3
1	4AC	1	2083	1	-	0/11/29/30	0/2/2/2
1	4AC	1	922	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2287	1	-	0/11/29/30	0/2/2/2
1	OMG	1	2678	1	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	357	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2249	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2960	1	-	0/11/29/30	0/2/2/2
1	OMG	1	789	1	-	3/9/27/28	0/3/3/3
1	4AC	1	2966	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2093	1	-	0/7/25/26	0/2/2/2
2	4AC	2	828	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2001	1	-	0/11/29/30	0/2/2/2
2	OMG	2	680	2	-	1/9/27/28	0/3/3/3
2	4AC	2	379	2	-	0/11/29/30	0/2/2/2
2	OMG	2	913	2	-	0/9/27/28	0/3/3/3
1	4AC	1	2027	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2585	1	-	3/11/29/30	0/2/2/2
2	5MC	2	1498	2	-	4/7/25/26	0/2/2/2
1	4AC	1	835	1	-	0/11/29/30	0/2/2/2
2	OMG	2	467	2	-	0/9/27/28	0/3/3/3
1	4AC	1	1557	1	-	0/11/29/30	0/2/2/2
2	OMU	2	1380	2	-	0/9/27/28	0/2/2/2
1	4AC	1	2608	1	-	3/11/29/30	0/2/2/2
1	OMC	1	615	1	-	0/9/27/28	0/2/2/2
2	OMG	2	1069	2	-	1/9/27/28	0/3/3/3
2	4AC	2	703	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2548	1	-	0/11/29/30	0/2/2/2
2	5MC	2	1505	2	-	4/7/25/26	0/2/2/2
1	4AC	1	1617	1	-	0/11/29/30	0/2/2/2
1	OMG	1	2144	1	-	1/9/27/28	0/3/3/3
1	4AC	1	2062	1	-	0/11/29/30	0/2/2/2
1	A2M	1	2173	1	-	0/9/27/28	0/3/3/3
2	4AC	2	636	2	-	0/11/29/30	0/2/2/2
1	4AC	1	3004	1	-	0/11/29/30	0/2/2/2
1	A2M	1	1055	1	-	0/9/27/28	0/3/3/3
1	5MC	1	2183	1	-	0/7/25/26	0/2/2/2
1	4AC	1	2865	1	-	0/11/29/30	0/2/2/2
2	4AC	2	546	2,67	-	0/11/29/30	0/2/2/2
2	5MC	2	1025	2	-	0/7/25/26	0/2/2/2
1	4AC	1	341	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1885	1	-	0/11/29/30	0/2/2/2
2	OMU	2	830	2	-	0/9/27/28	0/2/2/2
1	4AC	1	829	1	-	0/11/29/30	0/2/2/2
2	MA6	2	1487	2	-	0/11/29/30	0/3/3/3
1	OMC	1	1948	1	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	1	1048	1	-	0/11/29/30	0/2/2/2
1	4AC	1	694	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1460	1	-	0/11/29/30	0/2/2/2
1	4AC	1	641	1	-	0/11/29/30	0/2/2/2
2	5MC	2	875	2	-	0/7/25/26	0/2/2/2
2	OMC	2	129	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1780	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2908	1	-	0/11/29/30	0/2/2/2
2	OMG	2	657	2	-	0/9/27/28	0/3/3/3
2	LHH	2	1041	2	-	0/13/31/32	0/2/2/2
1	4AC	1	1695	1	-	0/11/29/30	0/2/2/2
1	4AC	1	802	1	-	0/11/29/30	0/2/2/2
1	4AC	1	981	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1662	1	-	0/11/29/30	0/2/2/2
1	4AC	1	91	1	-	0/11/29/30	0/2/2/2
2	4AC	2	848	2	-	0/11/29/30	0/2/2/2
2	OMU	2	64	2	-	2/9/27/28	0/2/2/2
2	4AC	2	1147	2	-	0/11/29/30	0/2/2/2
2	5MC	2	1496	2	-	0/7/25/26	0/2/2/2
1	4AC	1	136	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2925	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1550	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1233	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2570	1	-	0/11/29/30	0/2/2/2
2	4AC	2	731	2	-	0/11/29/30	0/2/2/2
2	5MC	2	693	2	-	0/7/25/26	0/2/2/2
1	4AC	1	1554	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	1667	1	-	0/11/29/30	0/2/2/2
2	OMC	2	846	2	-	0/9/27/28	0/2/2/2
2	OMG	2	873	2	-	1/9/27/28	0/3/3/3
1	4AC	1	1594	67,1	-	0/11/29/30	0/2/2/2
1	4AC	1	2992	1	-	2/11/29/30	0/2/2/2
2	OMG	2	519	2	-	0/9/27/28	0/3/3/3
2	4AC	2	1184	2	-	0/11/29/30	0/2/2/2
3	4AC	3	32	3	-	0/11/29/30	0/2/2/2
1	OMG	1	328	1	-	0/9/27/28	0/3/3/3
2	4AC	2	868	2	-	0/11/29/30	0/2/2/2
1	5MC	1	2203	1	-	0/7/25/26	0/2/2/2
1	4AC	1	1755	1	-	2/11/29/30	0/2/2/2
1	4AC	1	1222	67,1	-	0/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	2	20	2	-	6/9/27/28	0/2/2/2
1	4AC	1	533	1	-	0/11/29/30	0/2/2/2
1	4AC	1	2937	67,1	-	1/11/29/30	0/2/2/2
2	OMG	2	934	2	-	2/9/27/28	0/3/3/3
2	4AC	2	851	2	-	0/11/29/30	0/2/2/2
1	5MC	1	2163	1	-	0/7/25/26	0/2/2/2
1	4AC	1	243	1	-	0/11/29/30	0/2/2/2
1	4AC	1	60	1	-	0/11/29/30	0/2/2/2
2	4AC	2	394	2	-	0/11/29/30	0/2/2/2
1	4AC	1	2495	1	-	0/11/29/30	0/2/2/2
2	OMU	2	1177	2	-	0/9/27/28	0/2/2/2
1	4AC	1	2718	1	-	0/11/29/30	0/2/2/2
1	OMG	1	2138	1	-	0/9/27/28	0/3/3/3
1	4AC	1	2329	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	2545	1	-	0/11/29/30	0/2/2/2
1	4AC	1	22	1	-	0/11/29/30	0/2/2/2
1	4AC	1	451	1	-	0/11/29/30	0/2/2/2
1	OMU	1	2784	1	-	0/9/27/28	0/2/2/2
2	5MC	2	1202	2	-	0/7/25/26	0/2/2/2
2	4AC	2	839	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1867	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1065	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2198	1	-	0/7/25/26	0/2/2/2
2	4AC	2	53	2	-	0/11/29/30	0/2/2/2
2	A2M	2	373	2	-	0/9/27/28	0/3/3/3
2	4AC	2	957	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1878	1	-	0/11/29/30	0/2/2/2
2	4AC	2	626	2	-	0/11/29/30	0/2/2/2
2	OMU	2	787	2	-	4/9/27/28	0/2/2/2
2	OMC	2	1040	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1621	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1765	1	-	0/11/29/30	0/2/2/2
1	5MC	1	2162	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2147	1	-	2/9/27/28	0/3/3/3
1	4AC	1	314	1	-	0/11/29/30	0/2/2/2
2	4AC	2	1239	2	-	0/11/29/30	0/2/2/2
2	4AC	2	1028	2	-	0/11/29/30	0/2/2/2
2	4AC	2	479	2	-	0/11/29/30	0/2/2/2
2	4AC	2	286	2	-	0/11/29/30	0/2/2/2
1	4AC	1	1068	1	-	0/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LHH	2	250	2	-	0/13/31/32	0/2/2/2
1	4AC	1	211	1	-	0/11/29/30	0/2/2/2
2	5MC	2	535	2	-	0/7/25/26	0/2/2/2
2	4AC	2	319	2	-	0/11/29/30	0/2/2/2
2	OMU	2	774	2	-	0/9/27/28	0/2/2/2
1	4AC	1	1934	1	-	0/11/29/30	0/2/2/2
1	4AC	1	1293	1	-	0/11/29/30	0/2/2/2

The worst 5 of 327 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1488	MA6	C5-C4	4.60	1.47	1.39
2	2	1469	6MZ	C5-C4	4.55	1.47	1.39
2	2	373	A2M	C5-C4	4.42	1.47	1.39
2	2	1487	MA6	C5-C4	4.41	1.47	1.39
1	1	1055	A2M	C5-C4	4.28	1.47	1.39

The worst 5 of 637 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	680	OMG	C5-C4-N3	-6.70	117.59	128.46
2	2	657	OMG	C5-C4-N3	-6.41	118.06	128.46
2	2	373	A2M	C5-C4-N3	-6.32	118.51	126.75
1	1	2173	A2M	C5-C4-N3	-6.32	118.51	126.75
1	1	1055	A2M	C5-C4-N3	-6.28	118.56	126.75

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

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

There are no ring outliers.

89 monomers are involved in 134 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	458	4AC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	751	4AC	1	0
1	1	2136	4AC	1	0
1	1	161	4AC	1	0
2	2	303	4AC	1	0
2	2	1488	MA6	1	0
1	1	229	4AC	1	0
2	2	471	OMG	3	0
2	2	718	4AC	2	0
2	2	1467	UR3	1	0
2	2	1479	4AC	1	0
2	2	17	4AC	1	0
1	1	922	4AC	1	0
1	1	2287	4AC	2	0
1	1	2249	4AC	1	0
1	1	2960	4AC	1	0
1	1	789	OMG	3	0
2	2	828	4AC	1	0
2	2	680	OMG	3	0
1	1	2585	4AC	3	0
1	1	835	4AC	1	0
2	2	1380	OMU	2	0
1	1	2608	4AC	3	0
2	2	1069	OMG	1	0
2	2	703	4AC	5	0
1	1	1617	4AC	3	0
1	1	2144	OMG	1	0
2	2	636	4AC	1	0
1	1	1055	A2M	1	0
2	2	546	4AC	2	0
2	2	1025	5MC	1	0
1	1	341	4AC	1	0
1	1	1885	4AC	1	0
2	2	830	OMU	1	0
1	1	829	4AC	1	0
2	2	1487	MA6	2	0
1	1	1048	4AC	1	0
1	1	1460	4AC	1	0
1	1	1780	4AC	1	0
1	1	2908	4AC	1	0
2	2	657	OMG	1	0
1	1	802	4AC	2	0
1	1	1662	4AC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	91	4AC	2	0
2	2	848	4AC	1	0
2	2	1147	4AC	2	0
1	1	1550	4AC	1	0
2	2	1233	4AC	1	0
2	2	731	4AC	2	0
2	2	693	5MC	1	0
2	2	511	4AC	3	0
1	1	1667	4AC	4	0
2	2	873	OMG	1	0
1	1	1594	4AC	1	0
1	1	2992	4AC	1	0
2	2	519	OMG	2	0
2	2	1184	4AC	1	0
3	3	32	4AC	1	0
2	2	868	4AC	1	0
1	1	1755	4AC	3	0
2	2	851	4AC	1	0
1	1	2163	5MC	3	0
1	1	60	4AC	1	0
2	2	394	4AC	2	0
2	2	1177	OMU	2	0
1	1	2718	4AC	1	0
2	2	1376	OMC	2	0
1	1	22	4AC	1	0
1	1	451	4AC	3	0
2	2	1202	5MC	1	0
2	2	839	4AC	1	0
1	1	1867	4AC	1	0
1	1	1065	4AC	2	0
1	1	2198	5MC	1	0
2	2	53	4AC	1	0
2	2	373	A2M	2	0
2	2	957	4AC	1	0
1	1	1878	4AC	2	0
2	2	626	4AC	3	0
1	1	1765	4AC	1	0
1	1	2162	5MC	2	0
2	2	1028	4AC	1	0
2	2	479	4AC	2	0
2	2	286	4AC	1	0
1	1	1068	4AC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	211	4AC	1	0
2	2	319	4AC	2	0
2	2	774	OMU	1	0
1	1	1934	4AC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 254 ligands modelled in this entry, 254 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

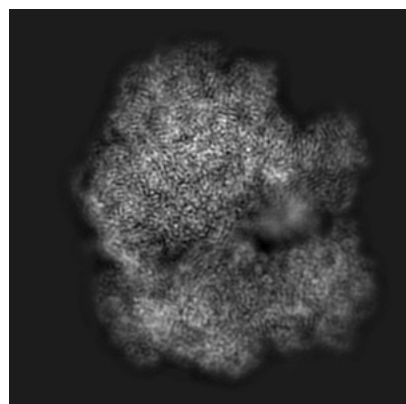
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55636. These allow visual inspection of the internal detail of the map and identification of artifacts.

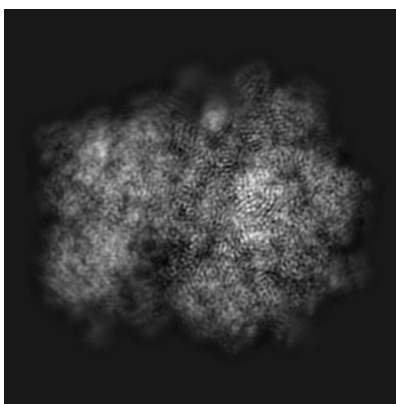
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

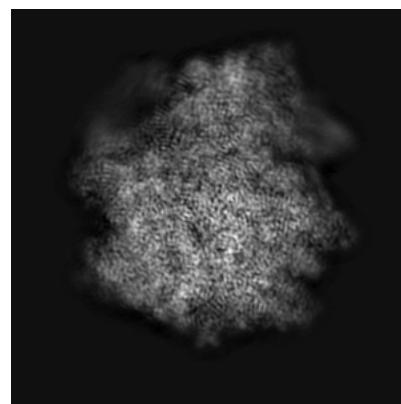
6.1.1 Primary map



X

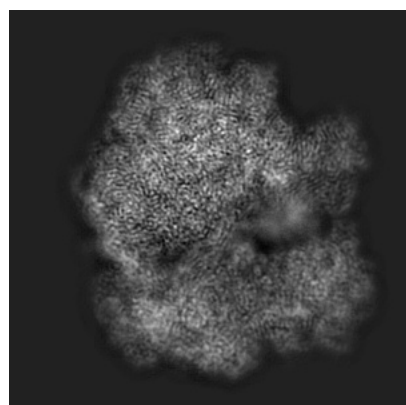


Y

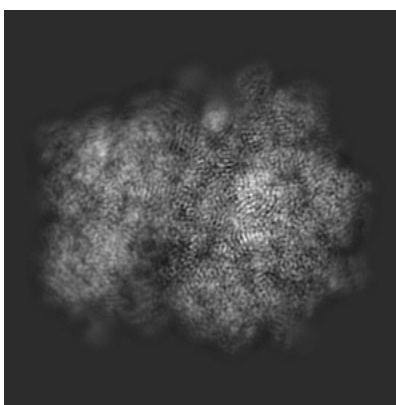


Z

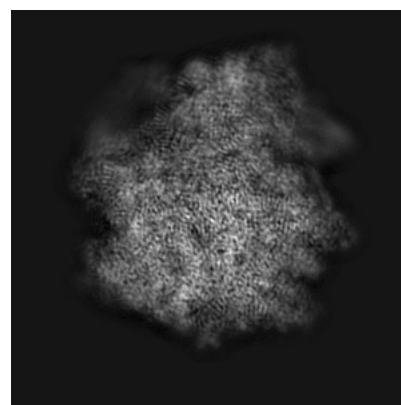
6.1.2 Raw map



X



Y

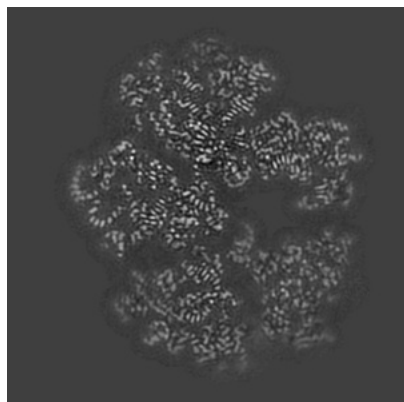


Z

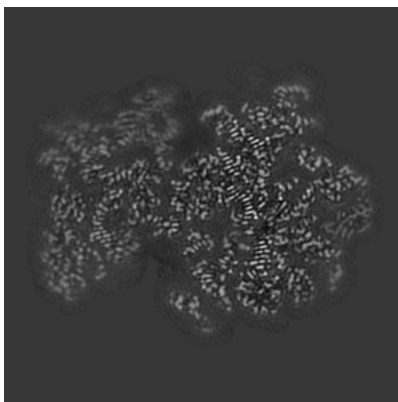
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

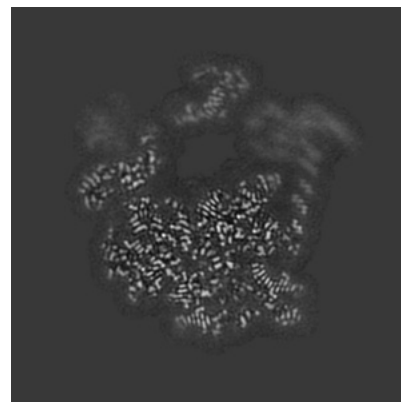
6.2.1 Primary map



X Index: 180

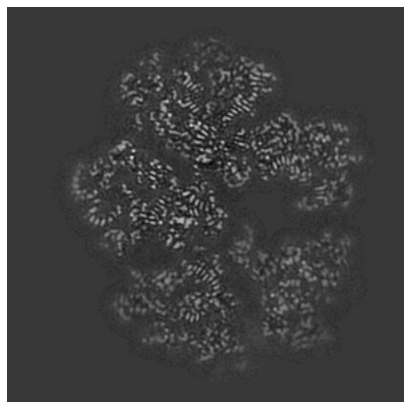


Y Index: 180

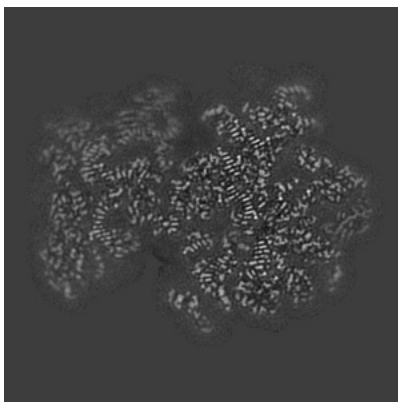


Z Index: 180

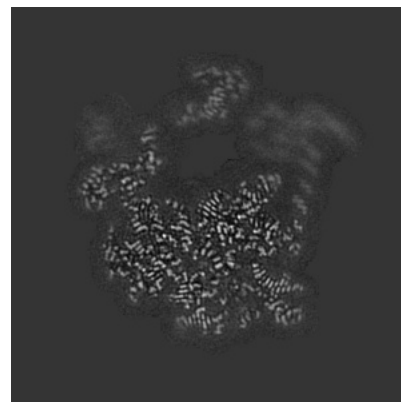
6.2.2 Raw map



X Index: 180



Y Index: 180

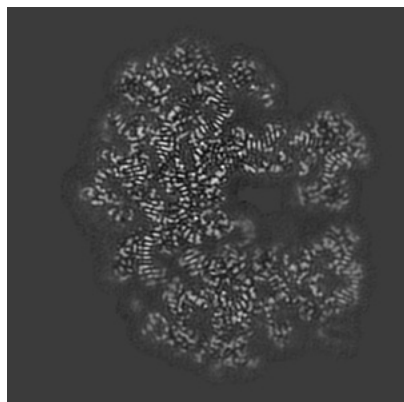


Z Index: 180

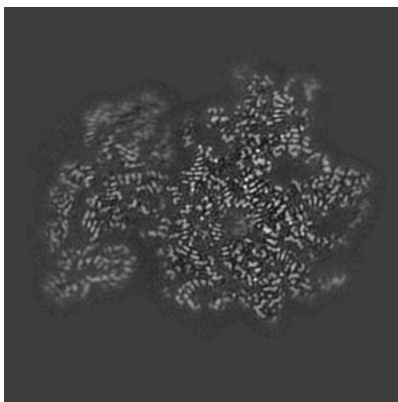
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

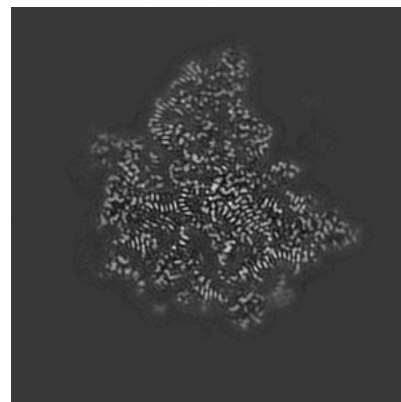
6.3.1 Primary map



X Index: 195

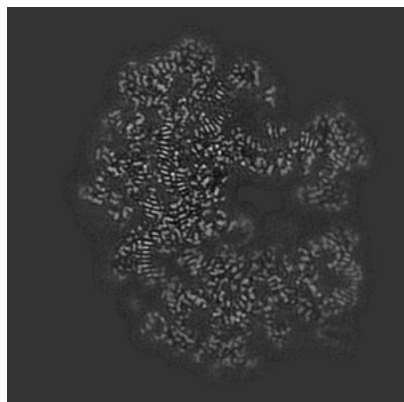


Y Index: 170

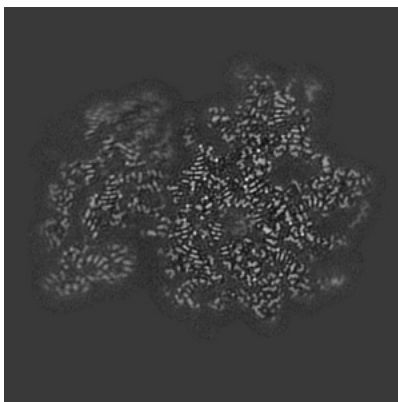


Z Index: 232

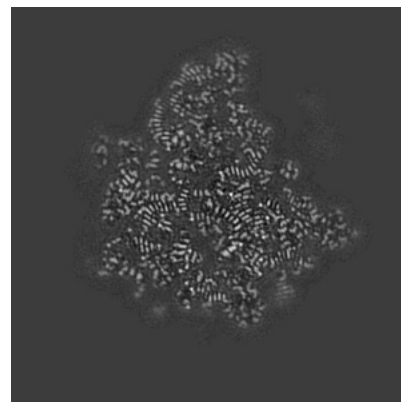
6.3.2 Raw map



X Index: 197



Y Index: 170

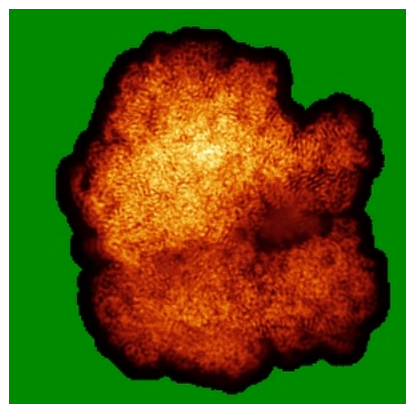


Z Index: 229

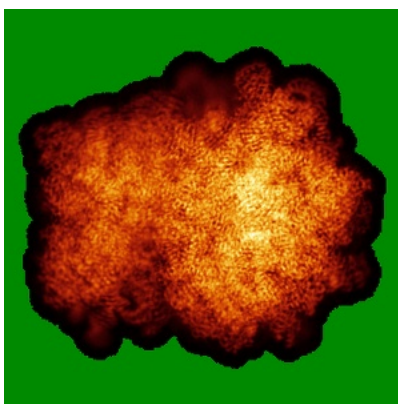
The images above show the largest variance slices of the map in three orthogonal directions.

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

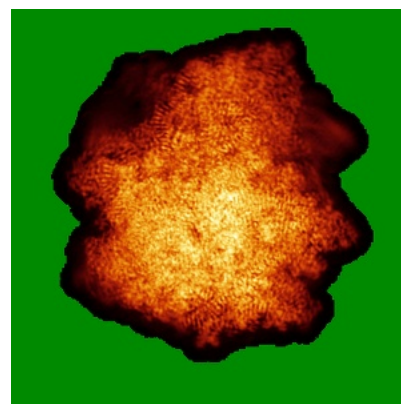
6.4.1 Primary map



X

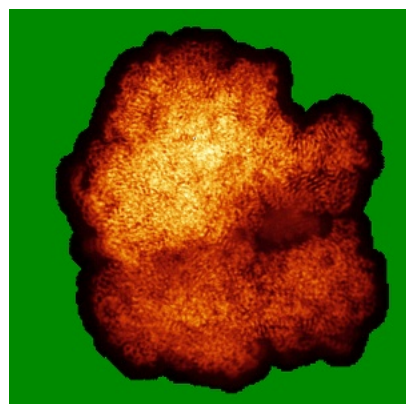


Y

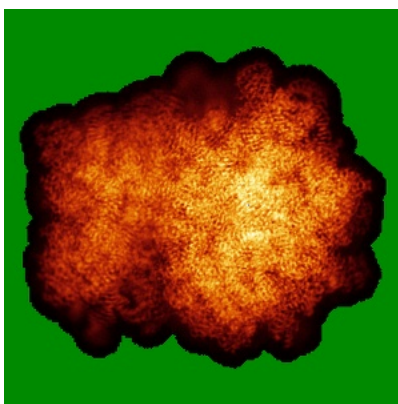


Z

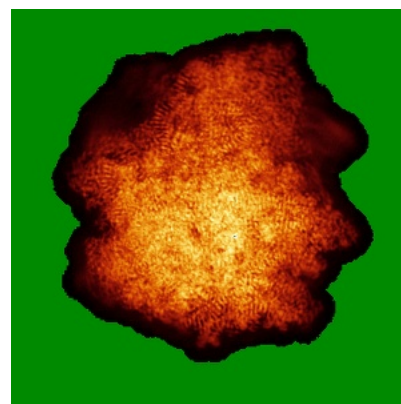
6.4.2 Raw map



X



Y

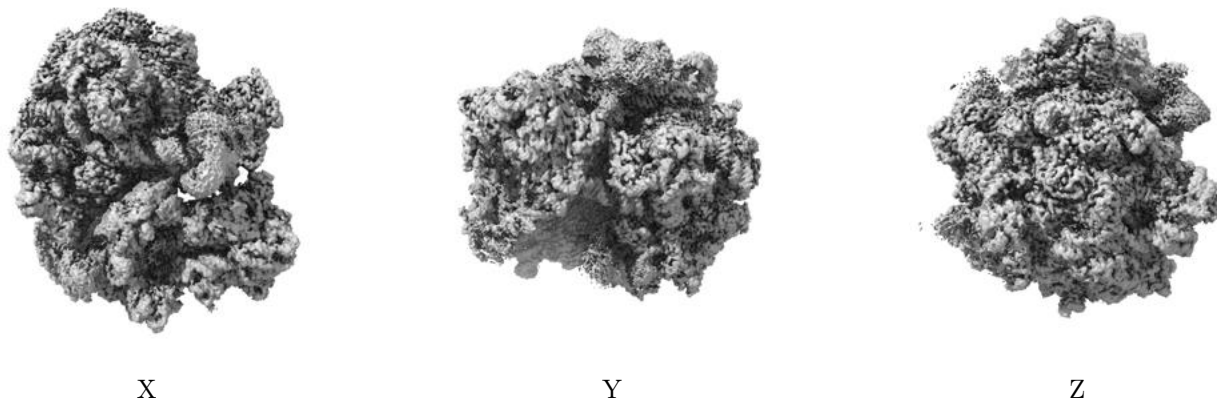


Z

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.

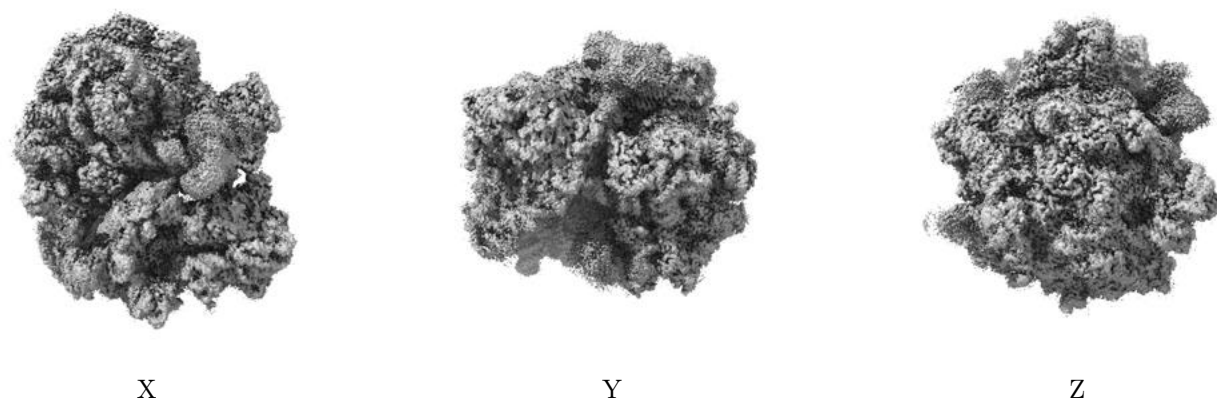
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0008. 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.

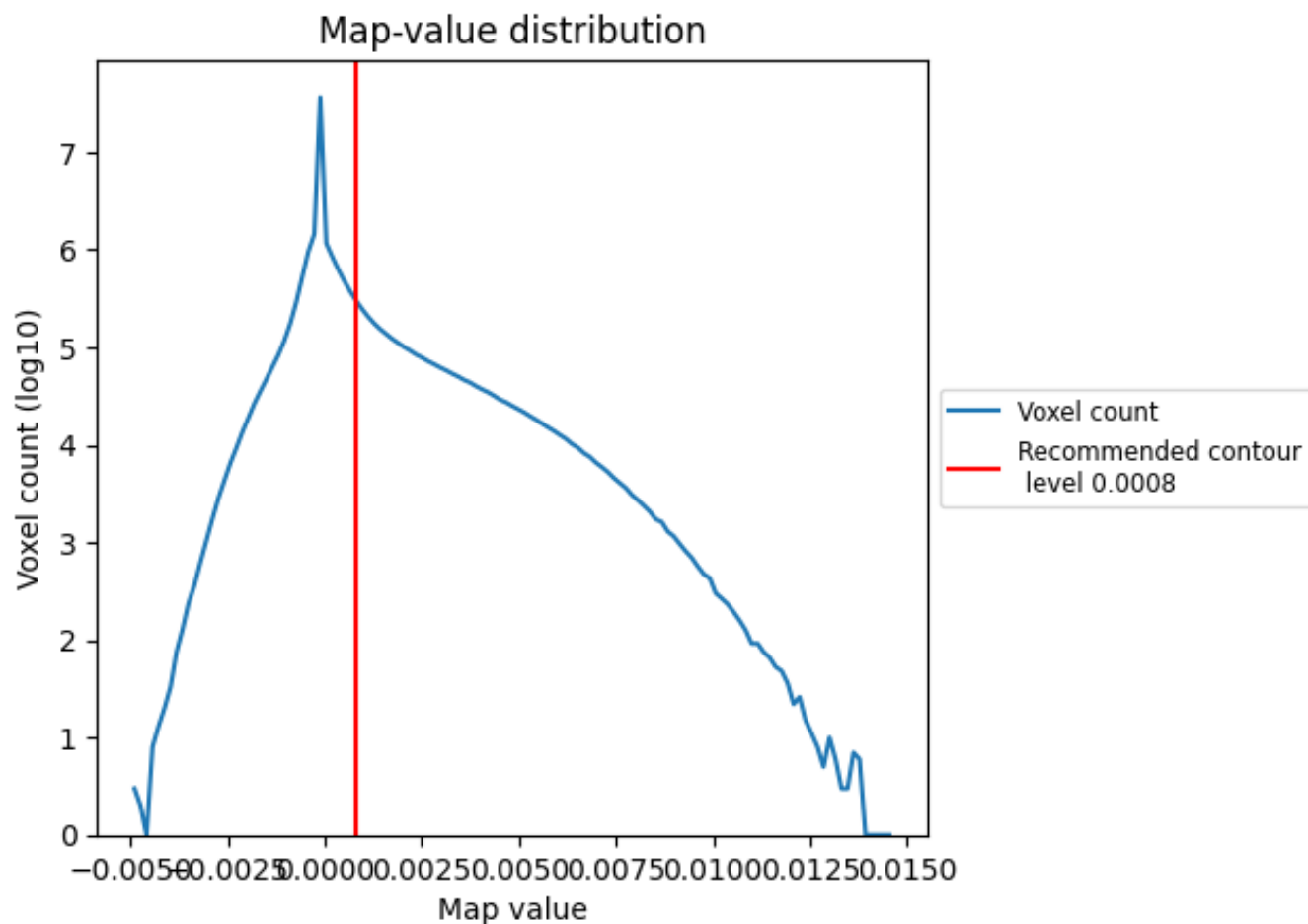
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

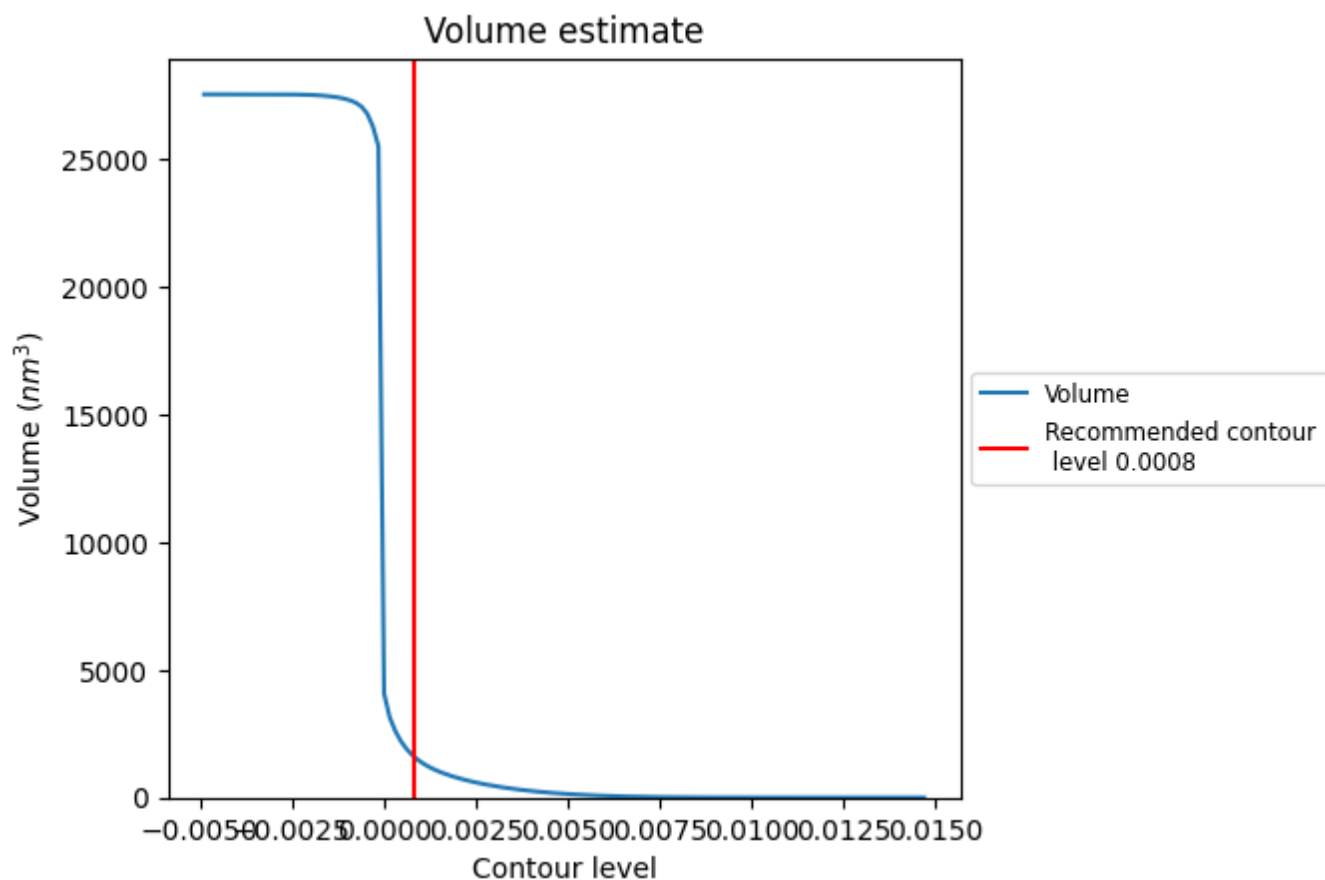
This section contains the results of statistical analysis of the map.

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.

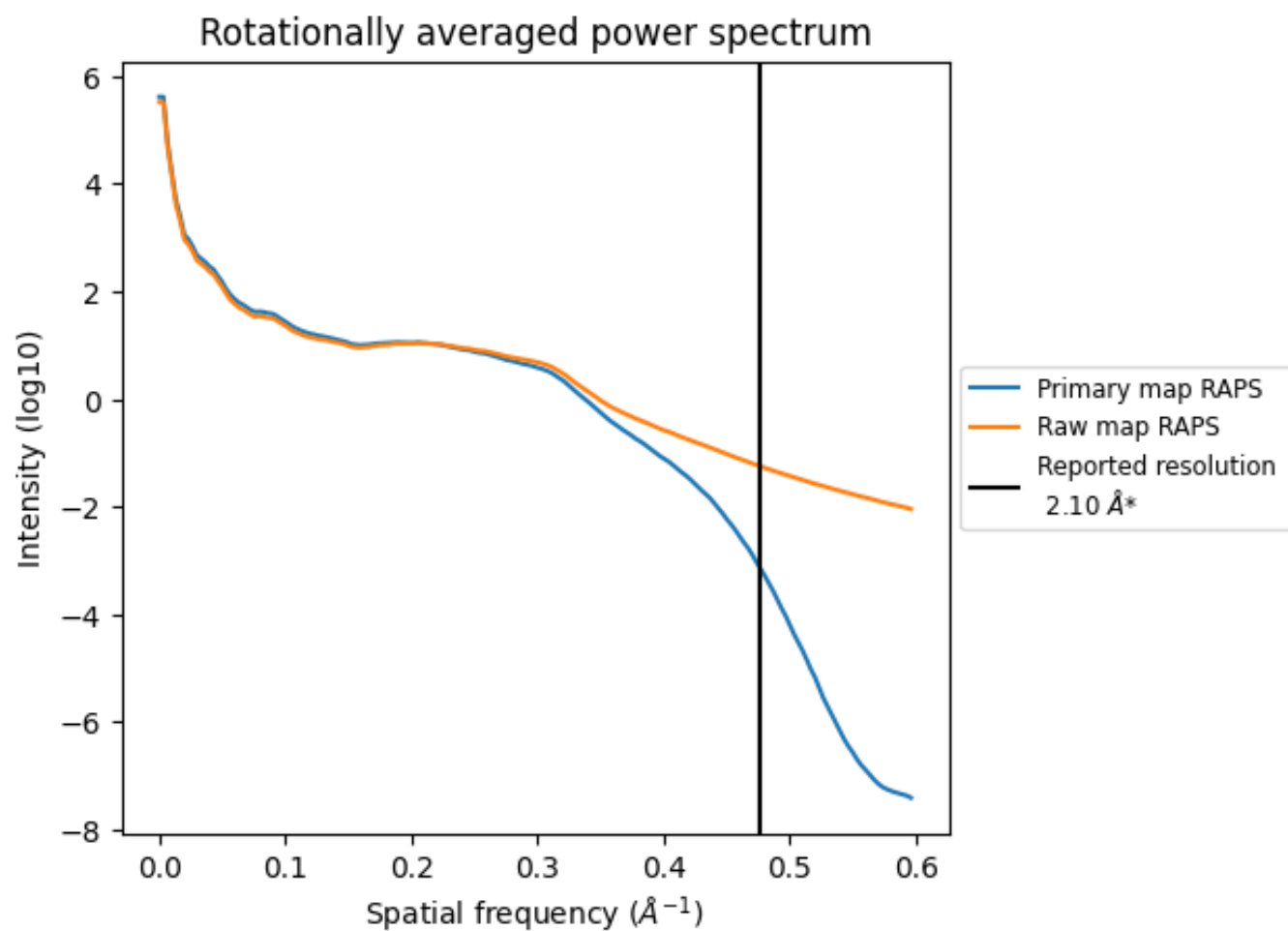
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1631 nm^3 ; this corresponds to an approximate mass of 1474 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 ⓘ

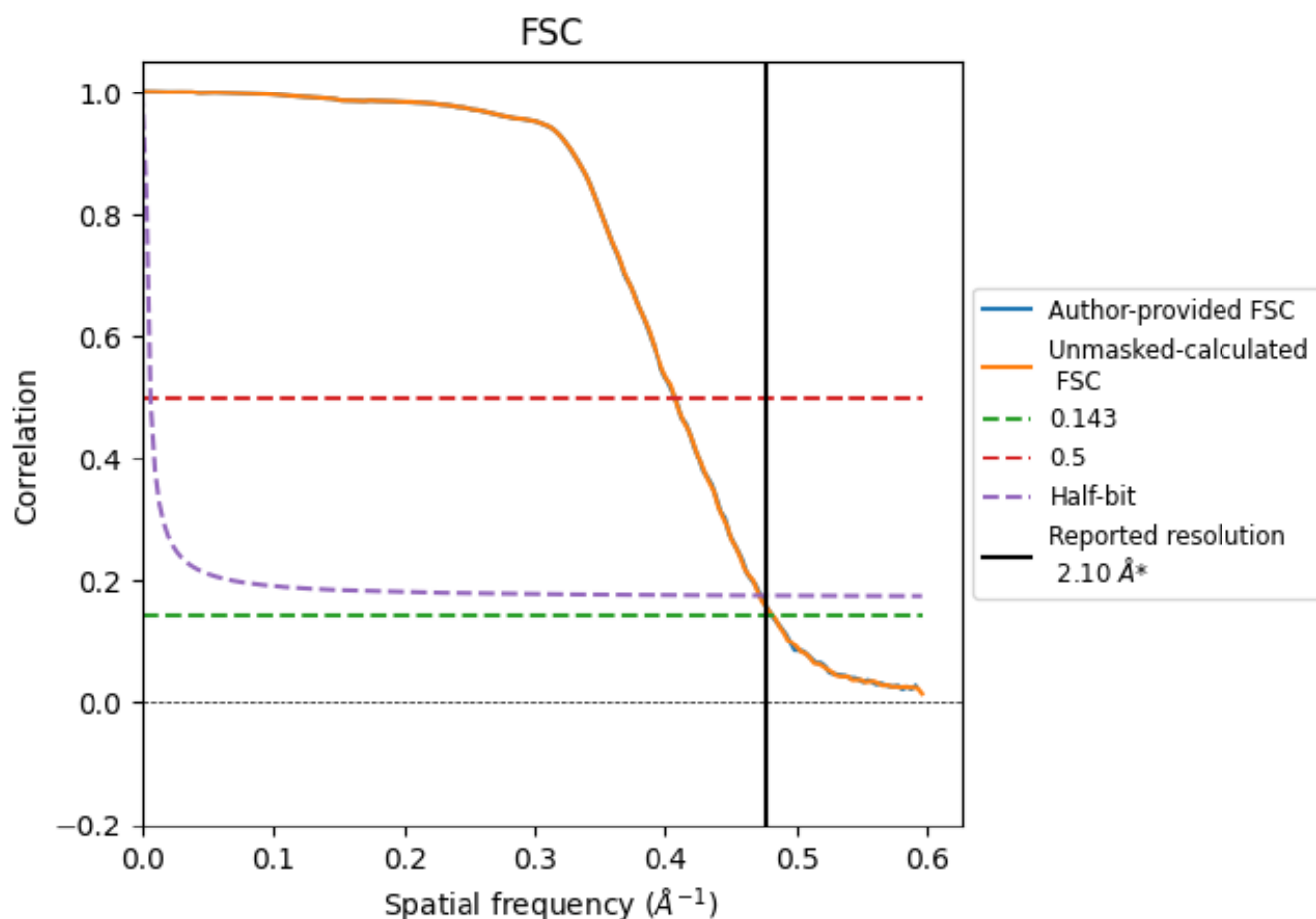


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

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](#)

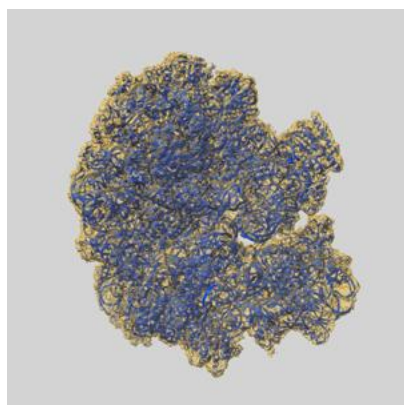
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.08	2.46	2.12
Unmasked-calculated*	2.08	2.46	2.12

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

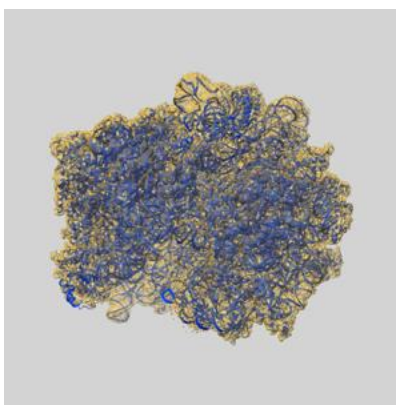
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55636 and PDB model 9T7H. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

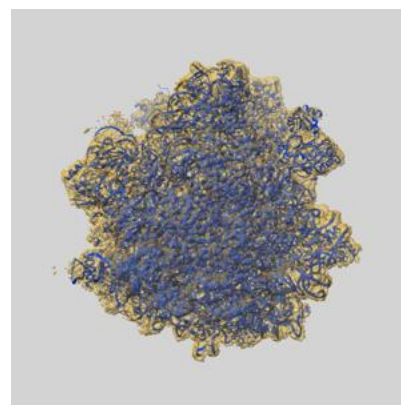
9.1 Map-model overlay [i](#)



X



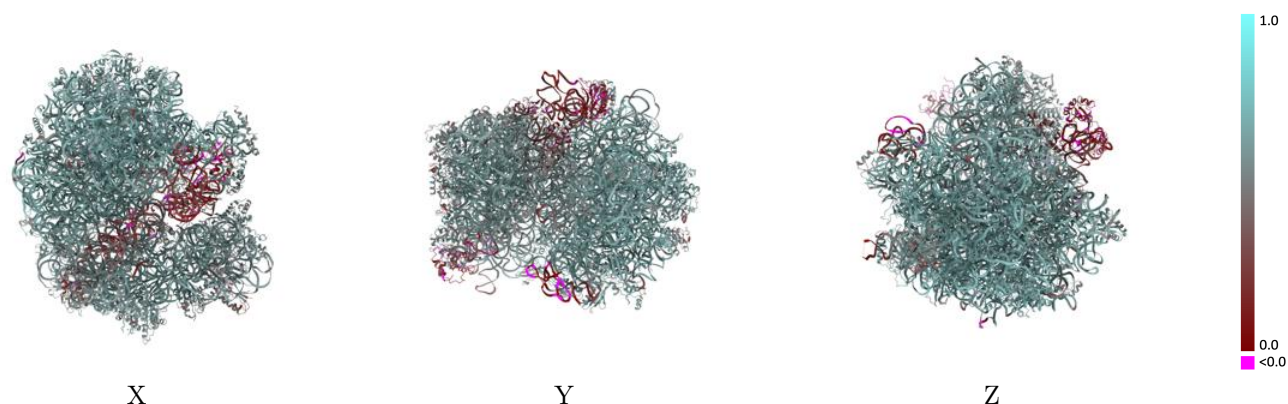
Y



Z

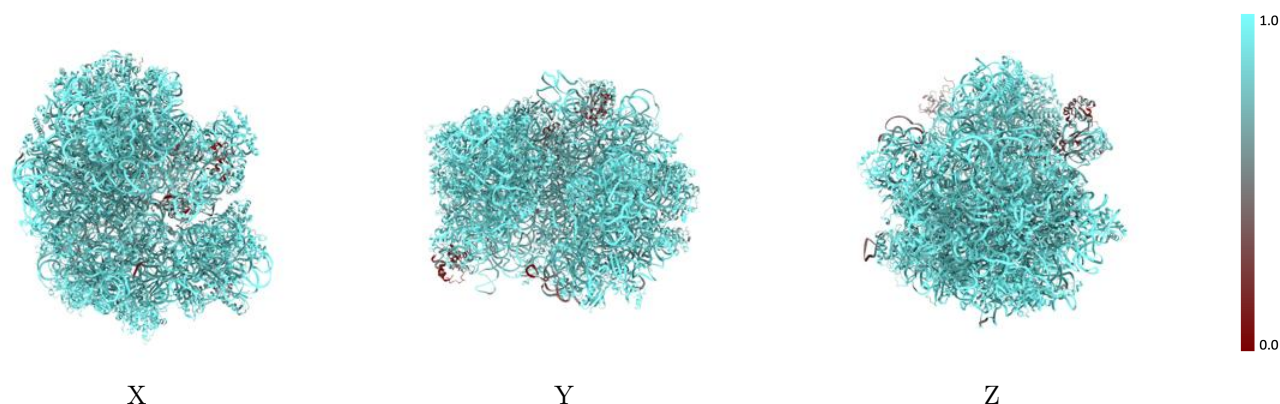
The images above show the 3D surface view of the map at the recommended contour level 0.0008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



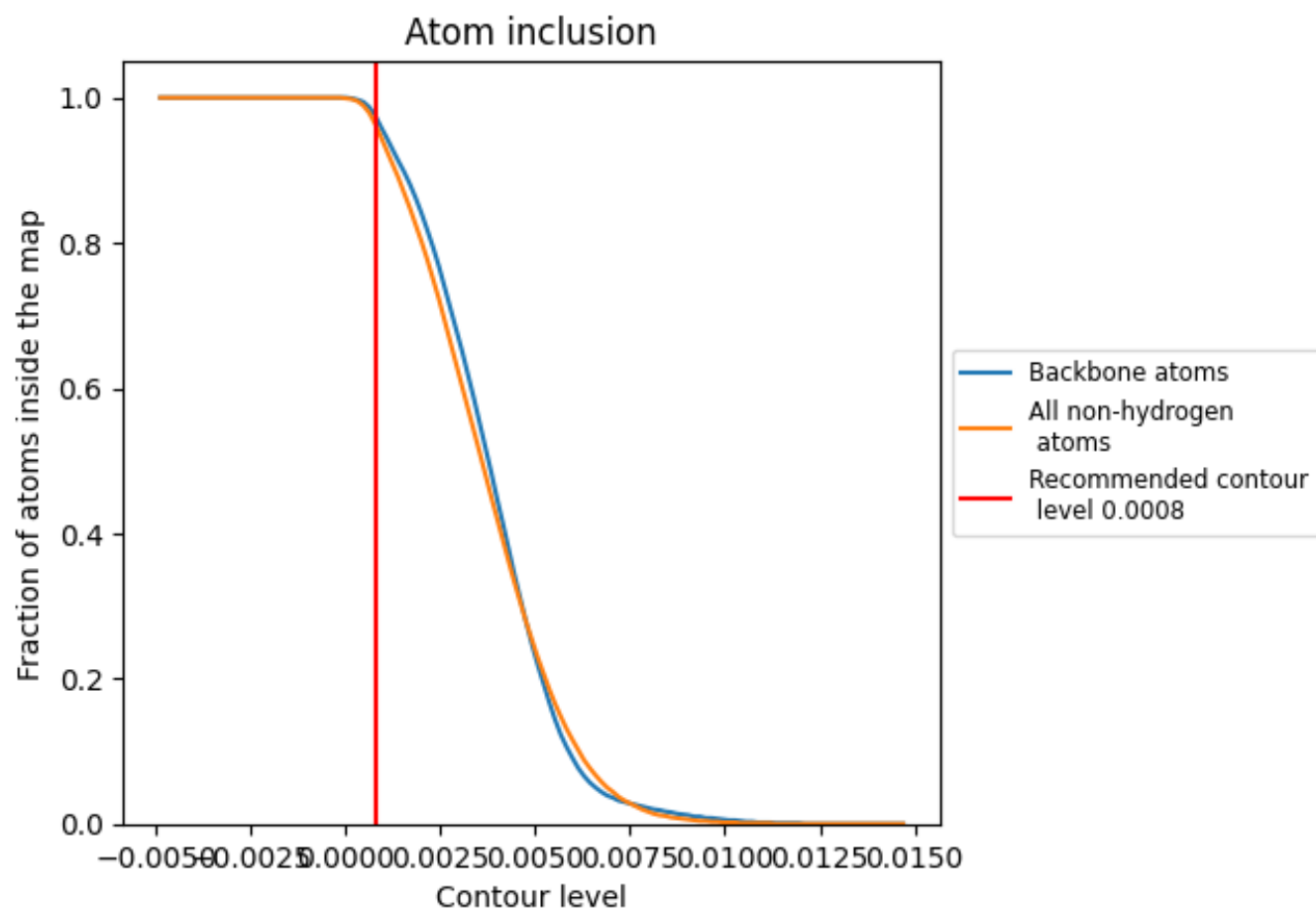
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0008).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.0008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9610	 0.5880
1	 0.9810	 0.6170
2	 0.9880	 0.5750
3	 0.9990	 0.6260
A0	 0.9590	 0.6450
A3	 0.3360	 0.1760
AA	 0.8060	 0.3140
AB	 0.9640	 0.5600
AC	 0.9710	 0.5850
AD	 0.9740	 0.5880
AE	 0.9820	 0.5840
AF	 0.9770	 0.6080
AG	 0.9120	 0.5450
AH	 0.9710	 0.5790
AI	 0.9790	 0.6040
AJ	 0.9720	 0.6140
AK	 0.9770	 0.5800
AL	 0.8960	 0.4860
AM	 0.8820	 0.4380
AN	 0.9640	 0.5860
AO	 0.9420	 0.5510
AP	 0.9520	 0.5840
AQ	 0.9170	 0.4170
AR	 0.9710	 0.5930
AS	 0.9700	 0.5350
AT	 0.9390	 0.5330
AU	 0.9790	 0.5740
AV	 0.9680	 0.5040
AW	 0.9540	 0.3650
AX	 0.9590	 0.5500
AY	 0.3810	 0.1020
AZ	 0.9120	 0.5200
B4	 0.8390	 0.4420
B5	 0.9950	 0.6030
B6	 0.8530	 0.6070



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BA	 0.5150	 0.1550
BB	 0.9830	 0.6640
BC	 0.9790	 0.6580
BD	 0.9880	 0.6580
BE	 0.9510	 0.5540
BF	 0.9710	 0.6110
BG	 0.9730	 0.6170
BI	 0.9800	 0.6640
BJ	 0.9720	 0.6580
BK	 0.9760	 0.5840
BL	 0.9680	 0.6280
BM	 0.9940	 0.6810
BN	 0.9580	 0.6330
BO	 0.9780	 0.5970
BP	 0.9880	 0.6560
BQ	 0.9740	 0.6450
BR	 0.9840	 0.6600
BS	 0.9880	 0.6700
BT	 0.9770	 0.6450
BU	 0.9890	 0.6390
BV	 0.9710	 0.6570
BW	 0.9260	 0.5940
BY	 0.9880	 0.6560
BZ	 0.9580	 0.5760
Ba	 0.9630	 0.6300
Bb	 0.9770	 0.6580
Bc	 0.9810	 0.6560
Bd	 0.9790	 0.6450
Be	 1.0000	 0.6770
Bf	 0.9950	 0.6650
Bg	 0.9970	 0.6400
Bi	 0.9730	 0.6590
Bj	 0.9680	 0.6540
Bk	 0.9710	 0.6310
Bl	 0.9720	 0.6050
H	 0.6720	 0.3420