



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 10:53 pm BST

PDB ID : 8A98
EMDB ID : EMD-15272
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :
snoRNA MUTANT
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.
Deposited on : 2022-06-28
Resolution : 2.46 Å (reported)
Based on initial models : 5T2A, 6AZ3, 6AZ1

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

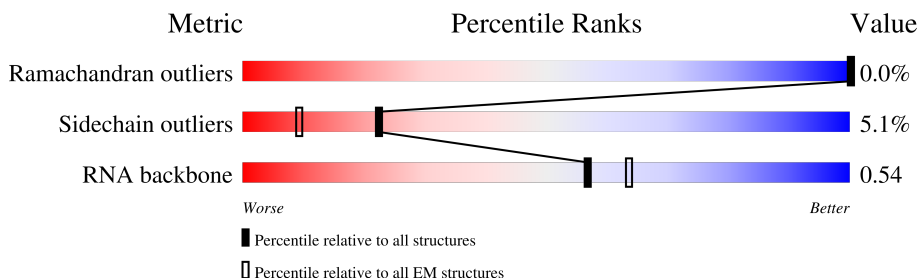
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 Å.

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





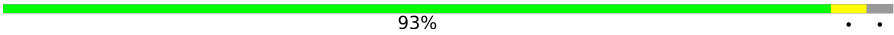
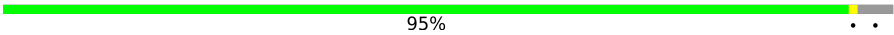
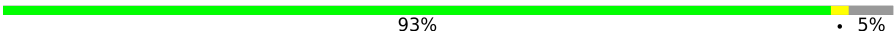








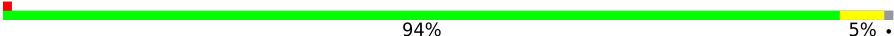




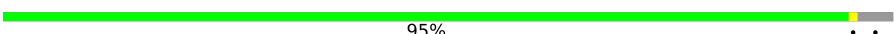
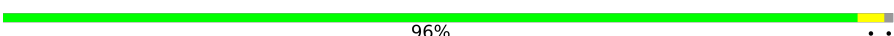
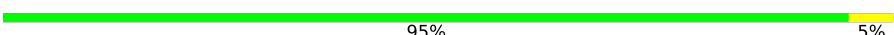
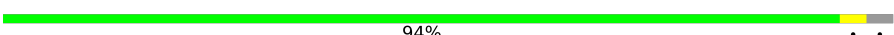



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	SW	152	
2	SZ	137	
3	SY	164	
4	SX	161	
5	SV	143	
6	SU	173	
7	ST	151	
8	SS	57	






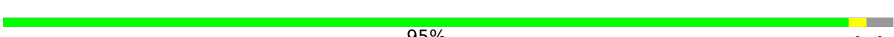




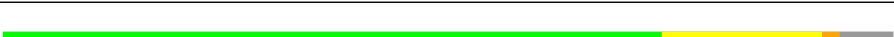


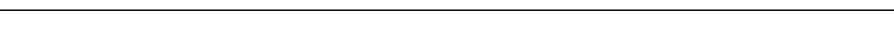
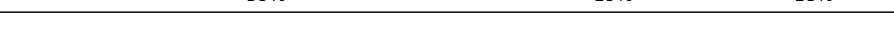
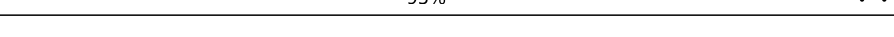


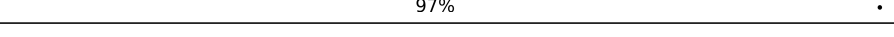
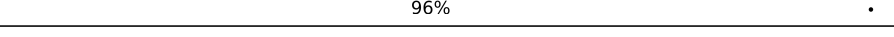

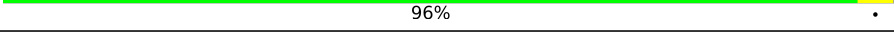

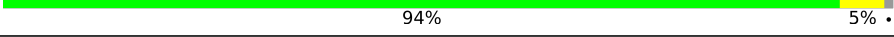

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Mol	Chain	Length	Quality of chain
9	SR	153	
10	SB	246	
11	SC	219	
12	SD	190	
13	SE	273	
14	SK	220	
15	S4	19	
16	Sg	312	
17	Sa	120	
18	Sc	86	
19	Se	66	
20	S1	2204	
21	SQ	141	
22	SP	143	
23	SO	144	
24	SN	168	
25	Sd	87	
26	SM	116	
27	SL	149	
28	SJ	130	
29	SI	200	
30	SH	190	
31	SG	249	
32	SF	265	
33	SA	264	





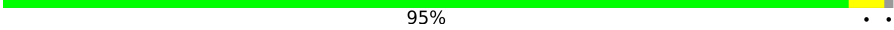
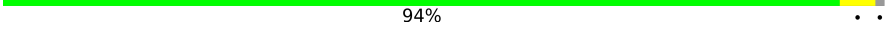





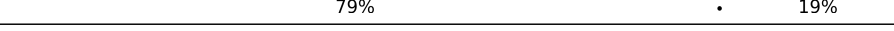




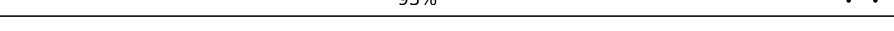


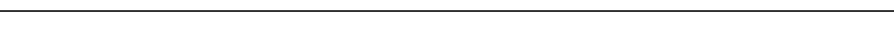

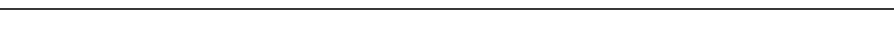
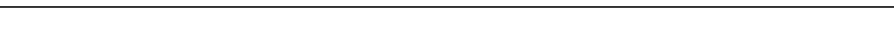


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Mol	Chain	Length	Quality of chain
34	Sb	112	
35	Sh	235	
36	f	133	
37	d	104	
38	c	252	
39	a	127	
40	b	70	
41	1	1782	
42	2	1526	
43	4	183	
44	7	171	
45	B	419	
46	8	123	
47	5	135	
48	A	260	
49	O	305	
50	G	264	
51	H	222	
52	M	204	
53	I	220	
54	P	198	
55	Q	254	
56	R	179	
57	E	190	
58	6	73	

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Mol	Chain	Length	Quality of chain
59	T	166	 91% 8%
60	S	159	 92%
61	K	175	 83% 5% 13%
62	D	188	 81% 15%
63	L	145	 95%
64	Y	134	 94%
65	Z	147	 92% 5%
66	F	195	 70% 27%
67	h	168	 70% 5% 25%
68	g	144	 92%
69	J	139	 88% 5% 7%
70	V	145	 79% 19%
71	W	143	 80% 17%
72	U	129	 79% 8% 13%
73	i	105	 85% 6% 10%
74	p	106	 84% 7% 9%
75	o	92	 93%
76	X	124	 51% 48%
77	k	83	 82% 6% 12%
78	l	51	 96%
79	n	34	 88% 9%
80	C	373	 94%
81	3	216	 52% 19% 25%
82	e	188	 84% 7% 8%
83	j	83	 93%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 197779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SW	105	Total	C	N	O	S	0	0
			787	506	152	125	4		

- Molecule 2 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SZ	122	Total	C	N	O	S	1	0
			967	620	184	160	3		

- Molecule 3 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SY	83	Total	C	N	O	S	0	0
			604	371	110	119	4		

- Molecule 4 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SX	139	Total	C	N	O	S	0	0
			1071	682	204	181	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SX	37	SER	THR	conflict	UNP E9AEE8

- Molecule 5 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SV	113	Total	C	N	O	S	0	0
			843	535	159	145	4		

- Molecule 6 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SU	148	Total	C	N	O	S	0	0
			1170	739	235	191	5		

- Molecule 7 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	ST	141	Total	C	N	O	S	0	0
			1145	723	228	186	8		

- Molecule 8 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SS	55	Total	C	N	O	S	0	0
			428	265	87	72	4		

- Molecule 9 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SR	119	Total	C	N	O	S	0	0
			892	567	167	154	4		

- Molecule 10 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SB	209	Total	C	N	O	S	2	0
			1643	1046	297	288	12		

- Molecule 11 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SC	212	Total	C	N	O	S	2	0
			1619	1028	296	282	13		

- Molecule 12 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SD	182	Total	C	N	O	S	1	0
			1513	951	308	246	8		

- Molecule 13 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SE	260	Total	C	N	O	S	2	0
			2056	1304	396	347	9		

- Molecule 14 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SK	180	Total	C	N	O	S	0	0
			1424	895	300	227	2		

- Molecule 15 is a RNA chain called E-site_tRNA_chain_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S4	19	Total	C	N	O	P	0	0
			404	181	76	129	18		

- Molecule 16 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Sg	300	Total	C	N	O	S	0	0
			2251	1415	399	424	13		

- Molecule 17 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Sa	71	Total	C	N	O	S	0	0
			541	345	93	100	3		

- Molecule 18 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Sc	84	Total	C	N	O	S	0	0
			638	396	123	111	8		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Se	52	Total	C	N	O	S	0	0
			404	253	87	63	1		

- Molecule 20 is a RNA chain called SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S1	1727	Total	C	N	O	P	0	0
			36928	16523	6655	12024	1726		

- Molecule 21 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SQ	28	Total	C	N	O	S	0	0
			179	111	33	33	2		

- Molecule 22 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SP	142	Total	C	N	O	S	3	0
			1115	704	222	186	3		

- Molecule 23 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SO	136	Total	C	N	O	S	1	0
			1012	625	197	182	8		

- Molecule 24 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SN	101	Total	C	N	O	S	0	0
			813	521	143	142	7		

- Molecule 25 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Sd	65	Total	C	N	O	S	0	0
			466	286	94	82	4		

- Molecule 26 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SM	102	Total	C	N	O	S	1	0
			811	506	149	154	2		

- Molecule 27 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SL	143	Total	C	N	O	S	0	0
			1130	727	209	191	3		

- Molecule 28 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SJ	129	Total	C	N	O	S	0	0
			1014	643	188	175	8		

- Molecule 29 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SI	200	Total	C	N	O	S	0	0
			1613	1026	307	272	8		

- Molecule 30 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SH	184	Total	C	N	O	S	0	0
			1437	894	277	259	7		

- Molecule 31 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SG	233	Total	C	N	O	S	1	0
			1809	1131	370	305	3		

- Molecule 32 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SF	220	Total	C	N	O	S	0	0
			1656	1063	299	284	10		

- Molecule 33 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SA	225	Total	C	N	O	S	2	0
			1834	1148	353	322	11		

- Molecule 34 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sb	100	Total	C	N	O	S	0	0
			779	484	162	126	7		

- Molecule 35 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sh	94	Total	C	N	O	S	0	0
			657	406	125	124	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	122	Total	C	N	O	S	0	0
			988	621	196	167	4		

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	90	Total	C	N	O	S	0	0
			625	388	114	118	5		

- Molecule 38 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	227	Total	C	N	O	S	0	0
			1779	1134	340	294	11		

- Molecule 39 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a	123	Total	C	N	O	S	0	0
			955	597	199	157	2		

- Molecule 40 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	b	66	Total	C	N	O	0	0
			520	318	120	82		

- Molecule 41 is a RNA chain called LSUa_rRNA_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1	1579	Total	C	N	O	P	0	0
			33802	15099	6193	10932	1578		

- Molecule 42 is a RNA chain called LSub_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	2	1047	Total	C	N	O	P	0	0
			22358	10009	4022	7280	1047		

- Molecule 43 is a RNA chain called SR2_chain_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	4	183	Total	C	N	O	P	0	0
			3906	1742	706	1275	183		

- Molecule 44 is a RNA chain called 5.8S_rRNA_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	7	160	Total	C	N	O	P	0	0
			3399	1520	599	1121	159		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	87	U	A	conflict	GB 1207899567

- Molecule 45 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	B	402	Total	C	N	O	S	7	0
			3200	2019	636	532	13		

- Molecule 46 is a RNA chain called 5S_rRNA_chain_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	8	118	Total	C	N	O	P	0	0
			2511	1123	448	822	118		

- Molecule 47 is a RNA chain called SR4_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	111	Total	C	N	O	P	0	0
			2373	1058	431	773	111		

- Molecule 48 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	255	Total	C	N	O	S	5	0
			1973	1229	407	326	11		

- Molecule 49 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O	252	Total	C	N	O	S	3	0
			1970	1259	373	333	5		

- Molecule 50 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	G	233	Total	C	N	O	S	2	0
			1850	1160	370	313	7		

- Molecule 51 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	H	221	Total	C	N	O	S	1	0
			1771	1121	352	291	7		

- Molecule 52 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	M	203	Total	C	N	O	S	0	0
			1714	1080	362	264	8		

- Molecule 53 is a protein called eL13_chain_I.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	I	205	Total	C	N	O	S	0	0
			1593	993	318	274	8		

- Molecule 54 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	P	197	Total	C	N	O	S	0	0
			1539	968	307	258	6		

- Molecule 55 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Q	189	Total	C	N	O	S	0	0
			1482	916	319	241	6		

- Molecule 56 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	R	178	Total	C	N	O	S	0	0
			1447	921	277	244	5		

- Molecule 57 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	E	186	Total	C	N	O	S	0	0
			1439	911	267	255	6		

- Molecule 58 is a RNA chain called SR6_chain_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	71	Total	C	N	O	P	0	0
			1484	663	267	483	71		

- Molecule 59 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	T	153	Total	C	N	O	S	0	0
			1233	770	244	208	11		

- Molecule 60 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	S	152	Total	C	N	O	S	0	0
			1203	764	236	200	3		

- Molecule 61 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	K	153	Total	C	N	O	S	0	0
			1193	746	234	206	7		

- Molecule 62 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	D	159	Total	C	N	O	S	0	0
			1140	723	212	197	8		

- Molecule 63 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	L	144	Total	C	N	O	S	0	0
			1124	707	226	185	6		

- Molecule 64 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Y	132	Total	C	N	O	S	1	0
			1046	667	211	165	3		

- Molecule 65 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Z	139	Total	C	N	O	S	0	0
			1052	642	221	184	5		

- Molecule 66 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	F	142	Total	C	N	O	S	0	0
			1045	665	194	184	2		

- Molecule 67 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	h	126	Total	C	N	O	S	1	0
			1016	626	222	162	6		

- Molecule 68 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	g	138	Total	C	N	O	S	0	0
			1101	684	233	179	5		

- Molecule 69 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	J	129	Total	C	N	O	S	0	0
			968	614	183	165	6		

- Molecule 70 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	V	118	Total	C	N	O	S	0	0
			939	595	176	165	3		

- Molecule 71 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	W	118	Total	C	N	O	S	0	0
			948	591	197	156	4		

- Molecule 72 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	U	112	Total	C	N	O	S	0	0
			879	572	154	151	2		

- Molecule 73 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	i	95	Total	C	N	O	S	0	0
			738	467	148	121	2		

- Molecule 74 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	p	96	Total	C	N	O	S	0	0
			722	460	144	116	2		

- Molecule 75 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o	90	Total	C	N	O	S	0	0
			696	432	144	114	6		

- Molecule 76 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	X	65	Total	C	N	O	S	0	0
			553	362	106	81	4		

- Molecule 77 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	k	73	Total	C	N	O	S	0	0
			546	342	104	97	3		

- Molecule 78 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	l	50	Total	C	N	O	S	0	0
			440	285	91	63	1		

- Molecule 79 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	n	33	Total	C	N	O	S	0	0
			259	161	60	37	1		

- Molecule 80 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	C	366	Total	C	N	O	S	0	0
			2797	1745	554	483	15		

- Molecule 81 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	3	161	Total	C	N	O	P	0	0
			3419	1529	596	1133	161		

- Molecule 82 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	173	Total	C	N	O	S	0	0
			1298	821	254	220	3		

- Molecule 83 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	j	80	Total	C	N	O	S	0	0
			662	403	151	102	6		

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	SS	1	Total	Mg	0
			1	1	
84	S1	23	Total	Mg	0
			23	23	
84	SL	1	Total	Mg	0
			1	1	
84	1	61	Total	Mg	0
			61	61	
84	2	31	Total	Mg	0
			31	31	
84	4	3	Total	Mg	0
			3	3	
84	7	4	Total	Mg	0
			4	4	
84	8	1	Total	Mg	0
			1	1	
84	5	1	Total	Mg	0
			1	1	
84	6	1	Total	Mg	0
			1	1	
84	T	1	Total	Mg	0
			1	1	
84	J	1	Total	Mg	0
			1	1	
84	3	1	Total	Mg	0
			1	1	

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	Sc	1	Total 1	Zn 1	0
85	Sb	1	Total 1	Zn 1	0
85	o	1	Total 1	Zn 1	0
85	j	1	Total 1	Zn 1	0

- Molecule 86 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
86	1	5	Total 5	Na 5	0
86	2	3	Total 3	Na 3	0

- Molecule 87 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
87	1	2	Total 2	K 2	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms		AltConf
88	SZ	1	Total 1	O 1	0
88	SY	1	Total 1	O 1	0
88	SX	7	Total 7	O 7	0
88	ST	5	Total 5	O 5	0
88	SS	1	Total 1	O 1	0
88	SR	2	Total 2	O 2	0
88	SB	3	Total 3	O 3	0
88	SC	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
88	SD	1	Total 1	O 1	0
88	SE	1	Total 1	O 1	0
88	SK	1	Total 1	O 1	0
88	S4	1	Total 1	O 1	0
88	Sg	3	Total 3	O 3	0
88	Sa	1	Total 1	O 1	0
88	Sc	2	Total 2	O 2	0
88	S1	237	Total 237	O 237	0
88	SP	3	Total 3	O 3	0
88	SO	2	Total 2	O 2	0
88	SN	3	Total 3	O 3	0
88	Sd	1	Total 1	O 1	0
88	SH	4	Total 4	O 4	0
88	SF	2	Total 2	O 2	0
88	Sb	2	Total 2	O 2	0
88	f	16	Total 16	O 16	0
88	d	3	Total 3	O 3	0
88	c	4	Total 4	O 4	0
88	a	3	Total 3	O 3	0
88	1	918	Total 918	O 918	0
88	2	536	Total 536	O 536	0

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Mol	Chain	Residues	Atoms		AltConf
88	4	73	Total 73	O 73	0
88	7	85	Total 85	O 85	0
88	B	29	Total 29	O 29	0
88	8	17	Total 17	O 17	0
88	5	37	Total 37	O 37	0
88	A	30	Total 30	O 30	0
88	G	4	Total 4	O 4	0
88	H	9	Total 9	O 9	0
88	M	28	Total 28	O 28	0
88	I	21	Total 21	O 21	0
88	P	12	Total 12	O 12	0
88	Q	6	Total 6	O 6	0
88	R	1	Total 1	O 1	0
88	E	1	Total 1	O 1	0
88	6	3	Total 3	O 3	0
88	T	14	Total 14	O 14	0
88	S	4	Total 4	O 4	0
88	K	1	Total 1	O 1	0
88	L	17	Total 17	O 17	0
88	h	12	Total 12	O 12	0
88	g	9	Total 9	O 9	0

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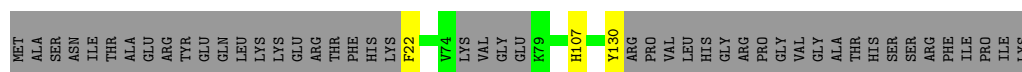
Mol	Chain	Residues	Atoms		AltConf
88	J	1	Total 1	O 1	0
88	V	6	Total 6	O 6	0
88	W	2	Total 2	O 2	0
88	i	1	Total 1	O 1	0
88	p	13	Total 13	O 13	0
88	o	2	Total 2	O 2	0
88	X	2	Total 2	O 2	0
88	k	2	Total 2	O 2	0
88	l	6	Total 6	O 6	0
88	C	21	Total 21	O 21	0
88	3	31	Total 31	O 31	0
88	e	9	Total 9	O 9	0
88	j	13	Total 13	O 13	0

3 Residue-property plots [i](#)


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

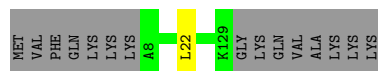
- Molecule 1: Putative 40S ribosomal protein S15

Chain SW: 



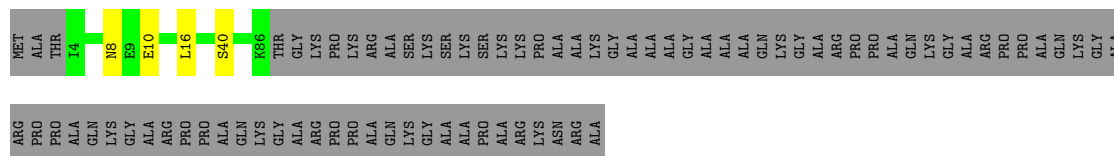
- Molecule 2: 40S ribosomal protein S24

Chain SZ: 




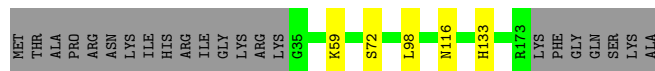
- Molecule 3: Putative 40S ribosomal protein S21

Chain SY: 




- Molecule 4: 40S ribosomal protein S19-like protein

Chain SX: 




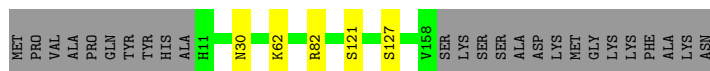
- Molecule 5: Putative 40S ribosomal protein S17

Chain SV: 



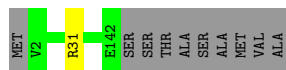
- Molecule 6: Putative 40S ribosomal protein S11

Chain SU:  83% 14%



- Molecule 7: Putative 40S ribosomal protein S13

Chain ST:  93% 7%



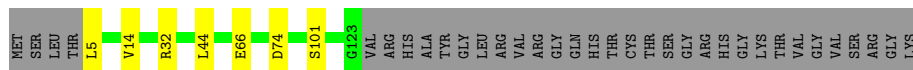
- Molecule 8: Putative ribosomal protein S29

Chain SS:  93%




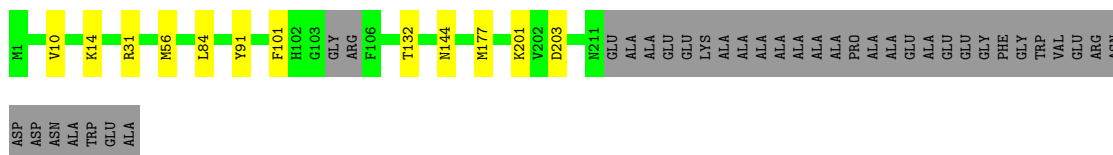
- Molecule 9: Putative 40S ribosomal protein S18

Chain SR:  73% 5% 22%



- Molecule 10: 40S ribosomal protein SA

Chain SB:  80% 5% 15%



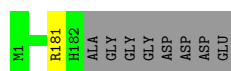
- Molecule 11: Putative 40S ribosomal protein S3

Chain SC:  93%



- Molecule 12: Putative 40S ribosomal protein S9

Chain SD:  95%



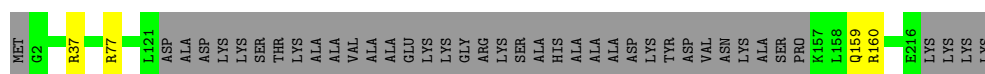
- Molecule 13: 40S ribosomal protein S4

Chain SE: 93% 5%



- Molecule 14: 40S ribosomal protein S8

Chain SK: 80% 18%



- Molecule 15: E-site_tRNA_chain_S4

Chain S4: 68% 32%



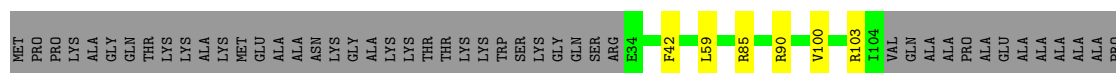
- Molecule 16: Small ribosomal subunit protein RACK1

Chain Sg: 87% 9%



- Molecule 17: 40S ribosomal protein S25

Chain Sa: 54% 5% 41%



- Molecule 18: Putative 40S ribosomal protein S27-1

Chain Sc: 90% 8%



Chain SH:  94% . .




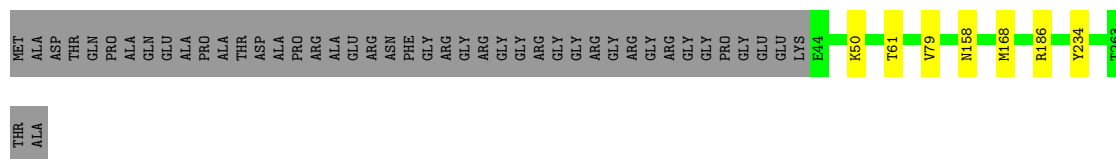
- Molecule 31: 40S ribosomal protein S6

Chain SG:  91% . 6%




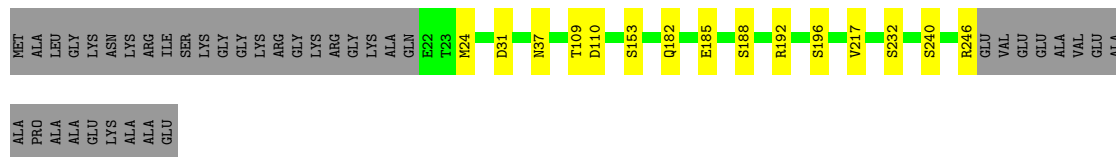
- Molecule 32: 40S ribosomal protein S2

Chain SF:  80% . 17%



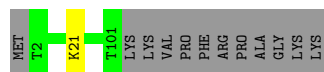
- Molecule 33: 40S ribosomal protein S3a

Chain SA:  80% 6% 15%



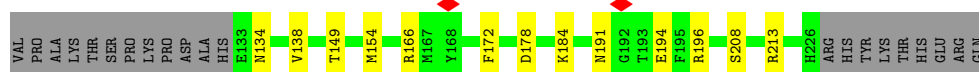
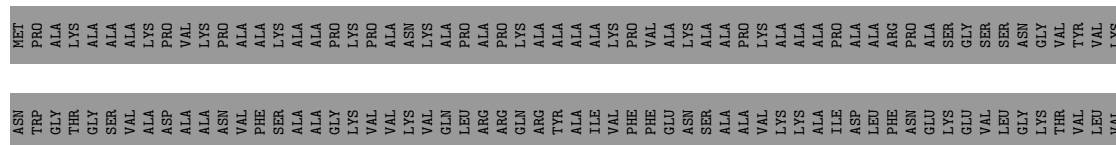
- Molecule 34: 40S ribosomal protein S26

Chain Sb:  88% . 11%



- Molecule 35: Putative RNA binding protein

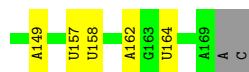
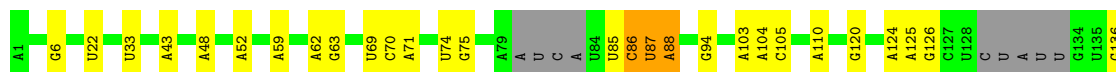
Chain Sh:  34% 6% 60%





- Molecule 44: 5.8S_rRNA_chain_7

Chain 7: 74% 18% • 6%



- Molecule 45: Putative ribosomal protein L3

Chain B: 93% • •



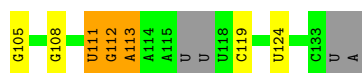
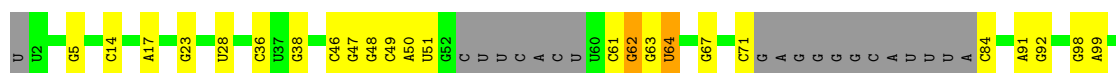
- Molecule 46: 5S_rRNA_chain_8

Chain 8: 82% 14% •



- Molecule 47: SR4_chain_5

Chain 5: 59% 19% • 18%



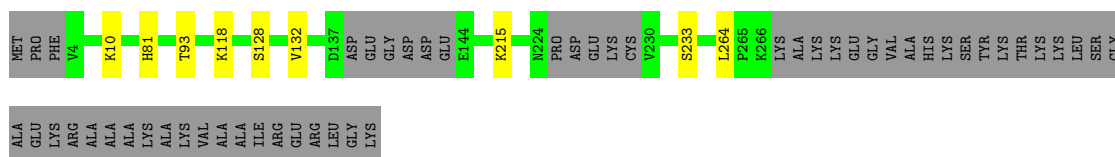
- Molecule 48: Putative 60S ribosomal protein L2

Chain A: 95% • •



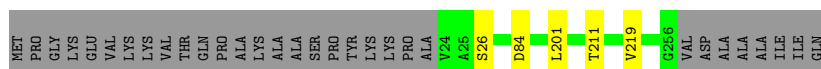
- Molecule 49: Putative 60S ribosomal protein L5

Chain O: 80% • 17%



- Molecule 50: 60S ribosomal protein L7a

Chain G: 86% 12%



- Molecule 51: Putative 60S ribosomal protein L13a

Chain H: 97% 1%



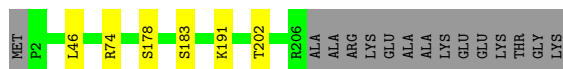
- Molecule 52: Ribosomal protein L15

Chain M: 96% 1%



- Molecule 53: eL13_chain_I

Chain I: 90% 7%



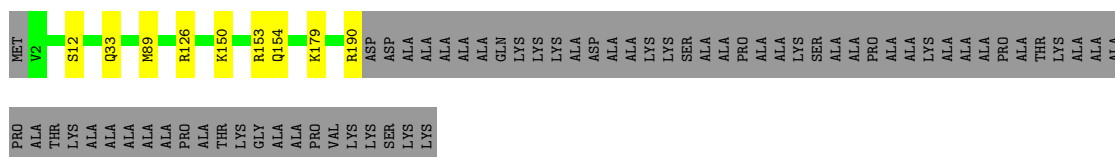
- Molecule 54: 60S ribosomal protein L18

Chain P: 96% 1%



- Molecule 55: Putative 60S ribosomal protein L19

Chain Q: 71% 26%




- Molecule 56: 60S ribosomal protein L18a

Chain R:  94% 5%



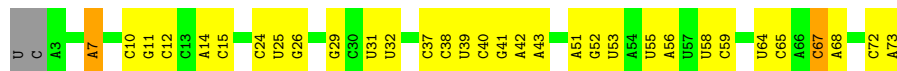
- Molecule 57: Putative 60S ribosomal protein L9

Chain E:  91% 7%




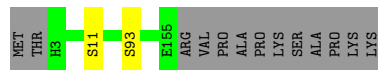
- Molecule 58: SR6_chain_6

Chain 6:  53% 41%



- Molecule 59: Putative 60S ribosomal protein L17

Chain T:  91% 8%




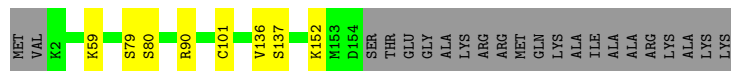
- Molecule 60: Putative 60S ribosomal protein L21

Chain S:  92%




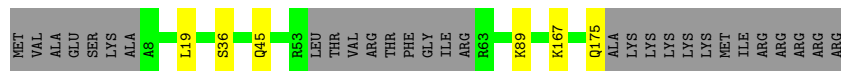
- Molecule 61: Putative 40S ribosomal protein L14

Chain K:  83% 5% 13%



- Molecule 62: 60S ribosomal protein L11

Chain D:  81% 15%



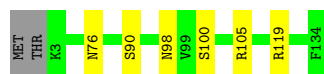
- Molecule 63: Putative 60S ribosomal protein L27A/L29

Chain L:  95%



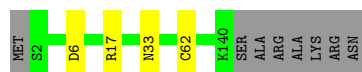
- Molecule 64: 60S ribosomal protein L27

Chain Y:  94%



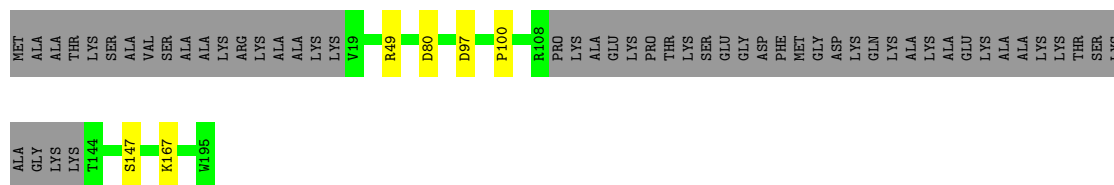
- Molecule 65: Putative 60S ribosomal protein L28

Chain Z:  92%



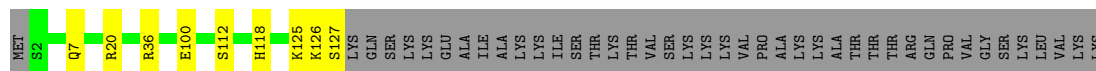
- Molecule 66: Putative 60S ribosomal protein L6

Chain F:  70%



- Molecule 67: Putative 60S ribosomal protein L34

Chain h:  70%




- Molecule 68: Putative ribosomal protein l35a

Chain g:  92%




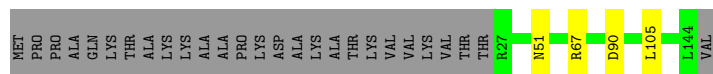
- Molecule 69: Putative 60S ribosomal protein L23

Chain J:  88%




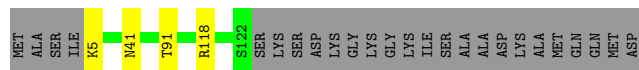
- Molecule 70: Putative 60S ribosomal protein L23a

Chain V:  79% 19%




- Molecule 71: Putative 60S ribosomal protein L26

Chain W:  80% 17%




- Molecule 72: Putative 60S ribosomal protein L22

Chain U:  79% 8% 13%




- Molecule 73: Putative 60S Ribosomal protein L36

Chain i:  85% 6% 10%



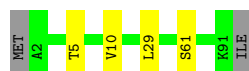
- Molecule 74: Putative 60S ribosomal protein L44

Chain p:  84% 7% 9%



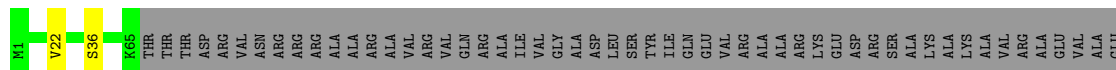
- Molecule 75: 60S ribosomal protein L37a

Chain o:  93%



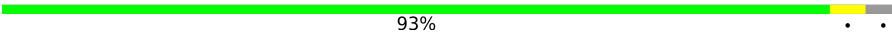
- Molecule 76: Putative ribosomal protein L24

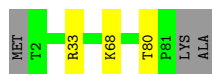
Chain X:  51% 48%



NET	THR	ARG	ALA	GLY	M1	K11	I14	E23	S24	R25	K31	R32	K46	K47	N57	R74	M81	S88	L114	M115	K116	E151	THR	THR	GLU	GLY	ASN	LYS	HIS	LYS	H160	S172	V181	GLN
-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	-----

- Molecule 83: Ribosomal protein L37

Chain j:  93% . .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	345376	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.367	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: 1MA, G7M, C4J, OMU, ZN, OMG, NA, K, MG, PSU, A2M, MA6, 5MC, OMC

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	SW	0.34	0/804	0.50	0/1090
2	SZ	0.27	0/988	0.51	0/1322
3	SY	0.25	0/610	0.54	0/829
4	SX	0.36	0/1100	0.53	0/1485
5	SV	0.31	0/850	0.50	0/1141
6	SU	0.28	0/1196	0.54	0/1613
7	ST	0.28	0/1168	0.58	0/1567
8	SS	0.37	0/433	0.60	0/578
9	SR	0.35	0/908	0.53	0/1232
10	SB	0.27	0/1679	0.52	0/2273
11	SC	0.31	0/1647	0.53	0/2208
12	SD	0.26	0/1541	0.58	0/2066
13	SE	0.27	0/2100	0.54	0/2830
14	SK	0.27	0/1445	0.59	0/1937
15	S4	0.57	0/450	1.03	0/698
16	Sg	0.33	0/2306	0.56	0/3144
17	Sa	0.34	0/546	0.56	0/738
18	Sc	0.29	0/651	0.57	0/877
19	Se	0.26	0/410	0.59	0/544
20	S1	0.60	0/40111	0.91	99/62469 (0.2%)
21	SQ	0.24	0/178	0.49	0/242
22	SP	0.29	0/1144	0.56	0/1533
23	SO	0.34	0/1027	0.57	0/1382
24	SN	0.34	0/836	0.55	0/1134
25	Sd	0.31	0/468	0.60	0/630
26	SM	0.30	0/821	0.55	0/1112
27	SL	0.35	0/1151	0.50	0/1547
28	SJ	0.28	0/1031	0.52	0/1382
29	SI	0.26	0/1643	0.53	0/2215
30	SH	0.34	0/1459	0.54	0/1958
31	SG	0.27	0/1833	0.58	0/2458
32	SF	0.28	0/1692	0.51	0/2294

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SA	0.27	0/1862	0.55	0/2505
34	Sb	0.29	0/796	0.57	0/1070
35	Sh	0.27	0/664	0.56	0/904
36	f	0.42	0/1008	0.62	0/1351
37	d	0.39	0/635	0.49	0/871
38	c	0.40	0/1812	0.57	0/2440
39	a	0.36	0/965	0.58	0/1295
40	b	0.34	0/531	0.56	0/712
41	1	0.91	0/37000	1.00	89/57678 (0.2%)
42	2	0.87	0/23546	1.03	78/36681 (0.2%)
43	4	0.82	0/4341	0.95	3/6767 (0.0%)
44	7	0.92	0/3669	0.98	7/5710 (0.1%)
45	B	0.39	0/3283	0.61	0/4421
46	8	0.62	0/2806	0.85	3/4367 (0.1%)
47	5	0.88	0/2650	1.04	10/4123 (0.2%)
48	A	0.39	0/2029	0.65	0/2722
49	O	0.34	0/2007	0.54	0/2696
50	G	0.35	0/1883	0.60	0/2535
51	H	0.39	0/1810	0.60	1/2435 (0.0%)
52	M	0.42	0/1754	0.64	0/2342
53	I	0.36	0/1626	0.56	0/2186
54	P	0.40	0/1564	0.60	0/2092
55	Q	0.37	0/1500	0.61	0/2000
56	R	0.41	0/1481	0.55	0/1997
57	E	0.31	0/1458	0.58	0/1971
58	6	0.70	0/1658	1.04	9/2580 (0.3%)
59	T	0.41	0/1257	0.59	0/1683
60	S	0.38	0/1230	0.58	0/1658
61	K	0.34	0/1212	0.55	0/1634
62	D	0.31	0/1159	0.54	0/1565
63	L	0.41	0/1151	0.59	0/1538
64	Y	0.36	0/1070	0.57	0/1437
65	Z	0.33	0/1066	0.60	0/1431
66	F	0.36	0/1065	0.58	1/1451 (0.1%)
67	h	0.45	2/1035 (0.2%)	0.63	0/1378
68	g	0.45	0/1124	0.64	0/1511
69	J	0.40	0/985	0.60	0/1329
70	V	0.37	0/954	0.56	0/1284
71	W	0.35	0/962	0.62	0/1284
72	U	0.34	0/892	0.51	0/1192
73	i	0.34	0/750	0.55	0/1003
74	p	0.41	0/733	0.61	0/977
75	o	0.44	0/708	0.68	0/944

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	X	0.38	0/574	0.61	0/774
77	k	0.36	0/554	0.58	0/751
78	l	0.40	0/453	0.58	0/606
79	n	0.43	0/263	0.71	0/348
80	C	0.39	0/2847	0.60	0/3836
81	3	0.79	0/3792	1.09	27/5895 (0.5%)
82	e	0.42	0/1314	0.61	0/1761
83	j	0.44	0/676	0.73	0/902
All	All	0.65	2/206390 (0.0%)	0.84	327/303151 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	36[A]	ARG	C-O	5.13	1.33	1.23
67	h	36[B]	ARG	C-O	5.13	1.33	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	214	C	P-O3'-C3'	-12.86	104.27	119.70
42	2	508	A	P-O3'-C3'	-12.19	105.07	119.70
41	1	487	A	P-O3'-C3'	-10.88	106.65	119.70
20	S1	232	C	P-O3'-C3'	-10.87	106.66	119.70
42	2	497	G	P-O3'-C3'	-10.59	107.00	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SW	101/152 (66%)	97 (96%)	4 (4%)	0	100	100
2	SZ	121/137 (88%)	116 (96%)	5 (4%)	0	100	100
3	SY	81/164 (49%)	79 (98%)	2 (2%)	0	100	100
4	SX	137/161 (85%)	129 (94%)	8 (6%)	0	100	100
5	SV	109/143 (76%)	105 (96%)	4 (4%)	0	100	100
6	SU	146/173 (84%)	139 (95%)	7 (5%)	0	100	100
7	ST	139/151 (92%)	131 (94%)	8 (6%)	0	100	100
8	SS	53/57 (93%)	49 (92%)	4 (8%)	0	100	100
9	SR	117/153 (76%)	115 (98%)	2 (2%)	0	100	100
10	SB	207/246 (84%)	199 (96%)	8 (4%)	0	100	100
11	SC	212/219 (97%)	206 (97%)	6 (3%)	0	100	100
12	SD	181/190 (95%)	174 (96%)	7 (4%)	0	100	100
13	SE	260/273 (95%)	256 (98%)	4 (2%)	0	100	100
14	SK	176/220 (80%)	173 (98%)	3 (2%)	0	100	100
16	Sg	294/312 (94%)	269 (92%)	25 (8%)	0	100	100
17	Sa	69/120 (58%)	65 (94%)	4 (6%)	0	100	100
18	Sc	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
19	Se	48/66 (73%)	43 (90%)	5 (10%)	0	100	100
21	SQ	24/141 (17%)	24 (100%)	0	0	100	100
22	SP	143/143 (100%)	141 (99%)	2 (1%)	0	100	100
23	SO	135/144 (94%)	130 (96%)	5 (4%)	0	100	100
24	SN	99/168 (59%)	94 (95%)	5 (5%)	0	100	100
25	Sd	63/87 (72%)	57 (90%)	6 (10%)	0	100	100
26	SM	101/116 (87%)	99 (98%)	2 (2%)	0	100	100
27	SL	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
28	SJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
29	SI	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
30	SH	180/190 (95%)	175 (97%)	5 (3%)	0	100	100
31	SG	232/249 (93%)	229 (99%)	3 (1%)	0	100	100
32	SF	218/265 (82%)	214 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	SA	225/264 (85%)	224 (100%)	1 (0%)	0	100	100
34	Sb	98/112 (88%)	94 (96%)	4 (4%)	0	100	100
35	Sh	92/235 (39%)	85 (92%)	7 (8%)	0	100	100
36	f	120/133 (90%)	116 (97%)	4 (3%)	0	100	100
37	d	88/104 (85%)	85 (97%)	3 (3%)	0	100	100
38	c	225/252 (89%)	218 (97%)	7 (3%)	0	100	100
39	a	121/127 (95%)	115 (95%)	6 (5%)	0	100	100
40	b	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
45	B	407/419 (97%)	397 (98%)	10 (2%)	0	100	100
48	A	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
49	O	249/305 (82%)	235 (94%)	14 (6%)	0	100	100
50	G	233/264 (88%)	225 (97%)	8 (3%)	0	100	100
51	H	220/222 (99%)	219 (100%)	1 (0%)	0	100	100
52	M	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
53	I	203/220 (92%)	192 (95%)	11 (5%)	0	100	100
54	P	195/198 (98%)	188 (96%)	7 (4%)	0	100	100
55	Q	187/254 (74%)	184 (98%)	3 (2%)	0	100	100
56	R	176/179 (98%)	174 (99%)	2 (1%)	0	100	100
57	E	184/190 (97%)	174 (95%)	10 (5%)	0	100	100
59	T	151/166 (91%)	148 (98%)	3 (2%)	0	100	100
60	S	150/159 (94%)	143 (95%)	7 (5%)	0	100	100
61	K	151/175 (86%)	145 (96%)	6 (4%)	0	100	100
62	D	155/188 (82%)	146 (94%)	9 (6%)	0	100	100
63	L	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
64	Y	131/134 (98%)	128 (98%)	3 (2%)	0	100	100
65	Z	137/147 (93%)	134 (98%)	3 (2%)	0	100	100
66	F	138/195 (71%)	135 (98%)	3 (2%)	0	100	100
67	h	125/168 (74%)	119 (95%)	6 (5%)	0	100	100
68	g	136/144 (94%)	131 (96%)	4 (3%)	1 (1%)	19	24
69	J	127/139 (91%)	125 (98%)	2 (2%)	0	100	100
70	V	116/145 (80%)	114 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	W	116/143 (81%)	113 (97%)	3 (3%)	0	100	100
72	U	108/129 (84%)	105 (97%)	3 (3%)	0	100	100
73	i	91/105 (87%)	88 (97%)	3 (3%)	0	100	100
74	p	94/106 (89%)	81 (86%)	13 (14%)	0	100	100
75	o	88/92 (96%)	78 (89%)	10 (11%)	0	100	100
76	X	63/124 (51%)	61 (97%)	2 (3%)	0	100	100
77	k	71/83 (86%)	69 (97%)	2 (3%)	0	100	100
78	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
79	n	31/34 (91%)	28 (90%)	3 (10%)	0	100	100
80	C	364/373 (98%)	354 (97%)	10 (3%)	0	100	100
82	e	169/188 (90%)	159 (94%)	9 (5%)	1 (1%)	22	28
83	j	78/83 (94%)	76 (97%)	2 (3%)	0	100	100
All	All	10720/12433 (86%)	10343 (96%)	375 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
82	e	47	LYS
68	g	20	LYS

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	
1	SW	74/130 (57%)	71 (96%)	3 (4%)	26	39
2	SZ	100/118 (85%)	99 (99%)	1 (1%)	73	83
3	SY	63/116 (54%)	59 (94%)	4 (6%)	15	20
4	SX	107/131 (82%)	102 (95%)	5 (5%)	22	32
5	SV	83/126 (66%)	80 (96%)	3 (4%)	30	44
6	SU	121/152 (80%)	116 (96%)	5 (4%)	26	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	ST	122/132 (92%)	121 (99%)	1 (1%)	79	88
8	SS	42/49 (86%)	40 (95%)	2 (5%)	21	31
9	SR	86/130 (66%)	79 (92%)	7 (8%)	9	11
10	SB	175/202 (87%)	163 (93%)	12 (7%)	13	16
11	SC	168/184 (91%)	158 (94%)	10 (6%)	16	22
12	SD	160/164 (98%)	159 (99%)	1 (1%)	84	91
13	SE	215/225 (96%)	209 (97%)	6 (3%)	38	54
14	SK	138/176 (78%)	134 (97%)	4 (3%)	37	52
16	Sg	235/265 (89%)	207 (88%)	28 (12%)	4	3
17	Sa	58/95 (61%)	52 (90%)	6 (10%)	6	5
18	Sc	68/76 (90%)	61 (90%)	7 (10%)	6	5
19	Se	40/54 (74%)	38 (95%)	2 (5%)	20	29
21	SQ	15/120 (12%)	15 (100%)	0	100	100
22	SP	114/117 (97%)	107 (94%)	7 (6%)	15	21
23	SO	101/113 (89%)	95 (94%)	6 (6%)	16	23
24	SN	85/128 (66%)	76 (89%)	9 (11%)	5	5
25	Sd	46/75 (61%)	41 (89%)	5 (11%)	5	4
26	SM	94/104 (90%)	90 (96%)	4 (4%)	25	37
27	SL	114/120 (95%)	112 (98%)	2 (2%)	54	68
28	SJ	108/111 (97%)	104 (96%)	4 (4%)	29	43
29	SI	174/186 (94%)	164 (94%)	10 (6%)	17	23
30	SH	150/159 (94%)	145 (97%)	5 (3%)	33	47
31	SG	180/208 (86%)	174 (97%)	6 (3%)	33	47
32	SF	170/208 (82%)	163 (96%)	7 (4%)	26	39
33	SA	198/222 (89%)	183 (92%)	15 (8%)	11	13
34	Sb	80/93 (86%)	79 (99%)	1 (1%)	65	78
35	Sh	59/177 (33%)	46 (78%)	13 (22%)	1	0
36	f	104/115 (90%)	102 (98%)	2 (2%)	52	67
37	d	60/89 (67%)	56 (93%)	4 (7%)	13	17
38	c	174/209 (83%)	169 (97%)	5 (3%)	37	52
39	a	93/118 (79%)	91 (98%)	2 (2%)	47	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	b	52/58 (90%)	50 (96%)	2 (4%)	28	41
45	B	331/351 (94%)	319 (96%)	12 (4%)	30	44
48	A	202/204 (99%)	195 (96%)	7 (4%)	31	45
49	O	191/242 (79%)	182 (95%)	9 (5%)	22	32
50	G	192/221 (87%)	187 (97%)	5 (3%)	41	57
51	H	183/188 (97%)	178 (97%)	5 (3%)	40	55
52	M	179/180 (99%)	172 (96%)	7 (4%)	27	41
53	I	165/183 (90%)	159 (96%)	6 (4%)	30	44
54	P	163/164 (99%)	156 (96%)	7 (4%)	25	37
55	Q	138/198 (70%)	129 (94%)	9 (6%)	14	18
56	R	155/159 (98%)	146 (94%)	9 (6%)	17	23
57	E	157/172 (91%)	143 (91%)	14 (9%)	8	8
59	T	131/143 (92%)	129 (98%)	2 (2%)	60	74
60	S	125/134 (93%)	120 (96%)	5 (4%)	27	39
61	K	121/145 (83%)	113 (93%)	8 (7%)	14	17
62	D	104/162 (64%)	98 (94%)	6 (6%)	17	23
63	L	113/114 (99%)	107 (95%)	6 (5%)	19	27
64	Y	106/116 (91%)	100 (94%)	6 (6%)	17	23
65	Z	106/118 (90%)	102 (96%)	4 (4%)	28	41
66	F	103/153 (67%)	98 (95%)	5 (5%)	21	30
67	h	105/146 (72%)	97 (92%)	8 (8%)	11	13
68	g	112/121 (93%)	108 (96%)	4 (4%)	30	44
69	J	102/111 (92%)	95 (93%)	7 (7%)	13	16
70	V	100/124 (81%)	96 (96%)	4 (4%)	27	39
71	W	102/122 (84%)	98 (96%)	4 (4%)	27	41
72	U	88/114 (77%)	78 (89%)	10 (11%)	4	4
73	i	75/88 (85%)	69 (92%)	6 (8%)	10	11
74	p	66/92 (72%)	59 (89%)	7 (11%)	5	5
75	o	70/74 (95%)	66 (94%)	4 (6%)	17	23
76	X	58/104 (56%)	56 (97%)	2 (3%)	32	46
77	k	56/74 (76%)	51 (91%)	5 (9%)	8	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	l	44/47 (94%)	43 (98%)	1 (2%)	45	61
79	n	24/32 (75%)	21 (88%)	3 (12%)	3	3
80	C	287/301 (95%)	272 (95%)	15 (5%)	19	27
82	e	128/158 (81%)	113 (88%)	15 (12%)	4	3
83	j	67/70 (96%)	64 (96%)	3 (4%)	23	34
All	All	8675/10380 (84%)	8229 (95%)	446 (5%)	22	28

5 of 446 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	A	93	LYS
83	j	33	ARG
56	R	89	TYR
82	e	81	MET
75	o	10	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
57	E	133	GLN
67	h	19	ASN
59	T	147	GLN
63	L	116	GLN
68	g	122	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	S4	17/19 (89%)	6 (35%)	0
20	S1	1699/2204 (77%)	353 (20%)	15 (0%)
41	1	1564/1782 (87%)	316 (20%)	24 (1%)
42	2	1035/1526 (67%)	215 (20%)	17 (1%)
43	4	182/183 (99%)	35 (19%)	2 (1%)
44	7	157/171 (91%)	24 (15%)	0
46	8	116/123 (94%)	13 (11%)	1 (0%)
47	5	107/135 (79%)	26 (24%)	3 (2%)
58	6	70/73 (95%)	29 (41%)	5 (7%)
81	3	156/216 (72%)	33 (21%)	3 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5103/6432 (79%)	1050 (20%)	70 (1%)

5 of 1050 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	S4	2	C
15	S4	5	G
15	S4	7	A
15	S4	69	G
15	S4	70	C

5 of 70 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
43	4	149	U
47	5	48	G
58	6	51	A
41	1	581	G
41	1	485	A

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

152 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	$\# Z > 2$
20	OMG	S1	1623	20	18,26,27	2.43	8 (44%)	19,38,41	1.56	4 (21%)
41	OMU	1	845	41	19,22,23	2.82	7 (36%)	26,31,34	1.77	4 (15%)
41	PSU	1	672	84,41	18,21,22	4.21	8 (44%)	22,30,33	1.91	5 (22%)
42	OMC	2	1397	42	19,22,23	2.72	8 (42%)	26,31,34	0.82	0
20	OMU	S1	2048	20	19,22,23	2.90	7 (36%)	26,31,34	1.79	5 (19%)
42	PSU	2	437	42	18,21,22	4.16	8 (44%)	22,30,33	1.88	5 (22%)
20	OMU	S1	29	20	19,22,23	3.00	8 (42%)	26,31,34	1.75	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	OMC	2	443	42	19,22,23	0.86	0	26,31,34	1.02	0
42	OMU	2	1359	42	19,22,23	2.88	8 (42%)	26,31,34	1.79	5 (19%)
42	OMG	2	1253	42	18,26,27	2.35	8 (44%)	19,38,41	1.61	6 (31%)
42	OMG	2	655	42	18,26,27	2.38	8 (44%)	19,38,41	1.63	4 (21%)
20	MA6	S1	2185	20	18,26,27	1.17	1 (5%)	19,38,41	3.11	2 (10%)
42	PSU	2	1265	42	18,21,22	4.46	7 (38%)	22,30,33	1.71	5 (22%)
20	OMC	S1	1866	20	19,22,23	2.80	8 (42%)	26,31,34	0.71	0
42	PSU	2	662	84,42	18,21,22	4.22	8 (44%)	22,30,33	1.80	5 (22%)
42	PSU	2	1194	42	18,21,22	4.21	8 (44%)	22,30,33	1.99	5 (22%)
20	OMU	S1	1621	20	19,22,23	2.94	8 (42%)	26,31,34	1.76	5 (19%)
41	OMC	1	695	41	19,22,23	2.72	8 (42%)	26,31,34	0.72	0
20	OMG	S1	600	20	18,26,27	2.52	8 (44%)	19,38,41	1.54	3 (15%)
42	A2M	2	1185	42	18,25,26	3.62	7 (38%)	18,36,39	3.71	4 (22%)
20	G7M	S1	1995	20	20,26,27	4.02	10 (50%)	17,39,42	1.00	1 (5%)
20	OMU	S1	8	20	19,22,23	2.97	8 (42%)	26,31,34	1.75	5 (19%)
41	OMG	1	1540	42,41	18,26,27	2.35	8 (44%)	19,38,41	1.69	5 (26%)
42	PSU	2	1303	42	18,21,22	4.47	8 (44%)	22,30,33	1.92	6 (27%)
20	OMG	S1	1550	20	18,26,27	2.49	8 (44%)	19,38,41	1.60	5 (26%)
44	A2M	7	43	44	18,25,26	3.70	7 (38%)	18,36,39	3.69	4 (22%)
20	OMU	S1	1833	20	19,22,23	3.02	8 (42%)	26,31,34	1.76	5 (19%)
41	PSU	1	1533	42,41	18,21,22	4.16	8 (44%)	22,30,33	2.06	5 (22%)
42	OMC	2	359	42	19,22,23	2.87	8 (42%)	26,31,34	0.66	0
20	PSU	S1	607	20	18,21,22	4.52	7 (38%)	22,30,33	1.75	5 (22%)
42	PSU	2	626	42	18,21,22	4.18	8 (44%)	22,30,33	1.75	3 (13%)
41	PSU	1	1664	41	18,21,22	4.20	8 (44%)	22,30,33	1.70	4 (18%)
20	A2M	S1	28	20	18,25,26	3.58	7 (38%)	18,36,39	3.74	4 (22%)
20	OMG	S1	2151	20	18,26,27	2.54	8 (44%)	19,38,41	1.62	4 (21%)
41	A2M	1	858	41	18,25,26	3.61	8 (44%)	18,36,39	3.89	4 (22%)
41	OMU	1	847	41	19,22,23	2.78	7 (36%)	26,31,34	1.88	5 (19%)
42	OMG	2	1229	42	18,26,27	2.39	8 (44%)	19,38,41	1.71	6 (31%)
42	A2M	2	527	42	18,25,26	3.78	8 (44%)	18,36,39	3.73	5 (27%)
41	OMC	1	1552	41	19,22,23	2.80	8 (42%)	26,31,34	0.78	0
42	A2M	2	95	42	18,25,26	3.64	7 (38%)	18,36,39	3.47	4 (22%)
20	5MC	S1	2061	20	18,22,23	0.98	2 (11%)	26,32,35	1.21	2 (7%)
41	OMG	1	1524	41	18,26,27	2.40	8 (44%)	19,38,41	1.74	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A2M	1	1539	84,87,42,41	18,25,26	3.63	7 (38%)	18,36,39	3.76	5 (27%)
42	OMC	2	1248	42	19,22,23	2.79	8 (42%)	26,31,34	0.91	1 (3%)
42	PSU	2	1413	42	18,21,22	4.19	8 (44%)	22,30,33	1.77	4 (18%)
42	OMG	2	534	42	18,26,27	2.38	8 (44%)	19,38,41	1.54	4 (21%)
20	PSU	S1	609	20	18,21,22	4.43	7 (38%)	22,30,33	1.82	5 (22%)
20	5MC	S1	1544	20	18,22,23	3.46	7 (38%)	26,32,35	1.05	1 (3%)
42	OMU	2	667	42	19,22,23	2.86	8 (42%)	26,31,34	1.81	5 (19%)
20	PSU	S1	1192	20	18,21,22	4.37	7 (38%)	22,30,33	1.63	4 (18%)
42	PSU	2	1060	42	18,21,22	4.32	8 (44%)	22,30,33	1.78	4 (18%)
42	PSU	2	1144	42	18,21,22	4.27	8 (44%)	22,30,33	1.93	4 (18%)
41	PSU	1	1017	41	18,21,22	4.13	8 (44%)	22,30,33	1.74	5 (22%)
42	PSU	2	500	42	18,21,22	1.40	2 (11%)	22,30,33	2.08	4 (18%)
41	OMG	1	1190	41	18,26,27	2.46	8 (44%)	19,38,41	1.73	5 (26%)
20	A2M	S1	98	20	18,25,26	3.60	8 (44%)	18,36,39	3.57	4 (22%)
20	PSU	S1	2046	20	18,21,22	4.34	7 (38%)	22,30,33	1.93	5 (22%)
41	PSU	1	239	41	18,21,22	4.34	7 (38%)	22,30,33	1.73	5 (22%)
41	PSU	1	870	84,41	18,21,22	4.24	8 (44%)	22,30,33	1.85	4 (18%)
41	OMU	1	1371	41	19,22,23	2.92	8 (42%)	26,31,34	2.09	6 (23%)
41	PSU	1	1528	41	18,21,22	4.25	8 (44%)	22,30,33	1.75	4 (18%)
42	A2M	2	665	42	18,25,26	3.64	7 (38%)	18,36,39	3.42	4 (22%)
20	PSU	S1	2202	20	18,21,22	4.43	7 (38%)	22,30,33	1.74	5 (22%)
42	PSU	2	593	42	18,21,22	4.18	9 (50%)	22,30,33	1.96	5 (22%)
44	A2M	7	162	41,44	18,25,26	3.64	8 (44%)	18,36,39	3.89	4 (22%)
20	PSU	S1	12	20	18,21,22	4.33	7 (38%)	22,30,33	1.98	5 (22%)
44	PSU	7	74	44	18,21,22	4.31	8 (44%)	22,30,33	1.85	5 (22%)
20	OMG	S1	1829	20	18,26,27	2.42	8 (44%)	19,38,41	1.52	4 (21%)
20	OMG	S1	1865	20	18,26,27	2.41	8 (44%)	19,38,41	1.69	5 (26%)
20	PSU	S1	1566	20	18,21,22	1.37	2 (11%)	22,30,33	2.00	5 (22%)
41	OMG	1	856	41	18,26,27	2.38	8 (44%)	19,38,41	1.63	5 (26%)
41	A2M	1	437	41	18,25,26	3.66	8 (44%)	18,36,39	3.83	4 (22%)
42	OMU	2	1077	42	19,22,23	2.90	8 (42%)	26,31,34	1.78	4 (15%)
20	OMU	S1	1979	20	19,22,23	2.86	8 (42%)	26,31,34	1.79	4 (15%)
20	A2M	S1	668	20	18,25,26	3.63	7 (38%)	18,36,39	3.75	4 (22%)
20	A2M	S1	2021	20	18,25,26	3.65	7 (38%)	18,36,39	3.70	4 (22%)
42	OMG	2	71	42	18,26,27	2.36	8 (44%)	19,38,41	1.61	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OMU	S1	1777	20	19,22,23	2.95	8 (42%)	26,31,34	1.74	5 (19%)
42	PSU	2	1403	42	18,21,22	4.23	9 (50%)	22,30,33	1.74	4 (18%)
42	A2M	2	628	42	18,25,26	3.68	9 (50%)	18,36,39	3.84	5 (27%)
42	OMC	2	1159	42	19,22,23	2.80	8 (42%)	26,31,34	0.81	0
20	OMU	S1	661	20	19,22,23	2.94	8 (42%)	26,31,34	1.71	4 (15%)
20	OMC	S1	38	20	19,22,23	2.92	8 (42%)	26,31,34	0.75	0
42	OMC	2	583	42	19,22,23	2.70	7 (36%)	26,31,34	0.78	0
42	PSU	2	1382	42	18,21,22	4.22	9 (50%)	22,30,33	1.79	5 (22%)
20	A2M	S1	512	20	18,25,26	0.97	1 (5%)	18,36,39	1.30	2 (11%)
20	OMG	S1	1647	20	18,26,27	2.40	8 (44%)	19,38,41	1.71	5 (26%)
42	A2M	2	572	42	18,25,26	3.69	7 (38%)	18,36,39	3.81	5 (27%)
20	MA6	S1	2184	20	18,26,27	1.16	2 (11%)	19,38,41	2.99	2 (10%)
42	OMU	2	560	42	19,22,23	2.88	7 (36%)	26,31,34	1.73	4 (15%)
41	A2M	1	697	41	18,25,26	3.68	7 (38%)	18,36,39	3.91	4 (22%)
41	PSU	1	1171	41	18,21,22	4.13	9 (50%)	22,30,33	1.77	5 (22%)
42	A2M	2	591	42	18,25,26	3.64	8 (44%)	18,36,39	3.67	4 (22%)
42	OMG	2	1046	42	18,26,27	2.50	8 (44%)	19,38,41	1.55	4 (21%)
42	A2M	2	1384	42	18,25,26	3.63	7 (38%)	18,36,39	3.57	4 (22%)
42	OMU	2	1419	42	19,22,23	2.87	8 (42%)	26,31,34	1.69	4 (15%)
81	OMU	3	13	81	19,22,23	2.87	7 (36%)	26,31,34	1.82	5 (19%)
42	PSU	2	1058	42	18,21,22	4.32	8 (44%)	22,30,33	1.75	4 (18%)
20	PSU	S1	1539	20	18,21,22	4.29	7 (38%)	22,30,33	1.75	4 (18%)
41	A2M	1	681	41	18,25,26	3.65	7 (38%)	18,36,39	3.53	4 (22%)
41	OMU	1	1659	41	19,22,23	2.80	7 (36%)	26,31,34	1.82	5 (19%)
42	PSU	2	78	42	18,21,22	4.25	9 (50%)	22,30,33	1.77	5 (22%)
42	OMG	2	641	42	18,26,27	2.39	8 (44%)	19,38,41	1.74	5 (26%)
41	PSU	1	1011	42,41	18,21,22	4.42	7 (38%)	22,30,33	1.91	5 (22%)
42	OMG	2	1231	42	18,26,27	2.37	8 (44%)	19,38,41	1.59	5 (26%)
41	PSU	1	940	41	18,21,22	4.25	8 (44%)	22,30,33	1.81	5 (22%)
43	OMG	4	74	43	18,26,27	2.29	8 (44%)	19,38,41	1.64	6 (31%)
20	PSU	S1	1657	20	18,21,22	4.29	7 (38%)	22,30,33	1.64	4 (18%)
42	5MC	2	524	84,42	18,22,23	3.24	7 (38%)	26,32,35	1.10	2 (7%)
20	OMC	S1	2140	20	19,22,23	2.96	8 (42%)	26,31,34	0.81	0
41	A2M	1	678	42,41	18,25,26	3.66	7 (38%)	18,36,39	3.53	4 (22%)
20	A2M	S1	897	20	18,25,26	3.66	9 (50%)	18,36,39	3.63	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	PSU	1	1181	41	18,21,22	4.28	7 (38%)	22,30,33	1.78	5 (22%)
41	OMC	1	1527	41	19,22,23	2.69	7 (36%)	26,31,34	0.72	0
41	PSU	1	422	41	18,21,22	4.31	8 (44%)	22,30,33	1.90	5 (22%)
41	1MA	1	677	84,41	16,25,26	1.10	2 (12%)	18,37,40	1.06	1 (5%)
44	PSU	7	69	44	18,21,22	4.28	8 (44%)	22,30,33	1.78	4 (18%)
42	A2M	2	1372	42	18,25,26	3.70	7 (38%)	18,36,39	3.74	4 (22%)
20	PSU	S1	1533	20	18,21,22	4.30	7 (38%)	22,30,33	1.84	5 (22%)
41	OMG	1	1626	41	18,26,27	2.35	8 (44%)	19,38,41	1.62	5 (26%)
42	OMC	2	1317	42	19,22,23	2.75	8 (42%)	26,31,34	0.87	1 (3%)
42	PSU	2	504	42	18,21,22	1.34	2 (11%)	22,30,33	2.14	4 (18%)
42	A2M	2	570	42,41	18,25,26	3.67	7 (38%)	18,36,39	3.45	5 (27%)
42	PSU	2	506	42	18,21,22	1.39	2 (11%)	22,30,33	2.11	5 (22%)
20	PSU	S1	33	20	18,21,22	4.48	7 (38%)	22,30,33	1.81	5 (22%)
20	PSU	S1	1156	20	18,21,22	4.48	7 (38%)	22,30,33	1.76	5 (22%)
42	PSU	2	1361	42	18,21,22	4.38	7 (38%)	22,30,33	1.93	5 (22%)
41	PSU	1	1402	41	18,21,22	4.13	9 (50%)	22,30,33	1.87	4 (18%)
20	A2M	S1	479	20	18,25,26	3.64	8 (44%)	18,36,39	3.75	4 (22%)
20	OMG	S1	1478	20	18,26,27	2.43	8 (44%)	19,38,41	1.69	5 (26%)
44	OMG	7	75	44	18,26,27	2.43	8 (44%)	19,38,41	1.62	5 (26%)
20	OMC	S1	18	20	19,22,23	2.89	8 (42%)	26,31,34	0.72	0
20	C4J	S1	1543	20	24,29,30	2.99	9 (37%)	29,42,45	1.46	5 (17%)
41	OMU	1	1107	41	19,22,23	2.80	8 (42%)	26,31,34	1.80	6 (23%)
20	PSU	S1	455	20	18,21,22	4.46	7 (38%)	22,30,33	1.90	5 (22%)
41	A2M	1	955	41	18,25,26	3.61	7 (38%)	18,36,39	3.49	4 (22%)
42	PSU	2	472	42	18,21,22	4.33	7 (38%)	22,30,33	1.79	5 (22%)
42	OMG	2	1078	42	18,26,27	2.36	8 (44%)	19,38,41	1.78	5 (26%)
42	A2M	2	382	42	18,25,26	3.63	7 (38%)	18,36,39	3.58	4 (22%)
42	PSU	2	510	42	18,21,22	1.41	3 (16%)	22,30,33	1.93	5 (22%)
20	PSU	S1	1841	20	18,21,22	4.37	7 (38%)	22,30,33	1.85	5 (22%)
42	PSU	2	597	42	18,21,22	4.16	8 (44%)	22,30,33	1.92	4 (18%)
42	PSU	2	1354	42	18,21,22	4.28	8 (44%)	22,30,33	1.90	5 (22%)
42	OMU	2	73	42	19,22,23	2.82	7 (36%)	26,31,34	1.70	5 (19%)
41	OMG	1	959	41	18,26,27	2.47	8 (44%)	19,38,41	1.71	4 (21%)
42	OMG	2	1360	42	18,26,27	2.40	8 (44%)	19,38,41	1.61	5 (26%)
42	PSU	2	1318	42	18,21,22	4.22	8 (44%)	22,30,33	1.73	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	PSU	2	1264	42	18,21,22	4.46	7 (38%)	22,30,33	1.84	5 (22%)
42	5MC	2	1308	42	18,22,23	3.48	7 (38%)	26,32,35	1.25	3 (11%)
20	PSU	S1	104	20	18,21,22	4.41	7 (38%)	22,30,33	1.78	5 (22%)
20	PSU	S1	1246	20	18,21,22	4.42	8 (44%)	22,30,33	1.71	4 (18%)
42	A2M	2	604	42,41	18,25,26	3.62	7 (38%)	18,36,39	3.80	4 (22%)

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
20	OMG	S1	1623	20	-	0/5/27/28	0/3/3/3
41	OMU	1	845	41	-	0/9/27/28	0/2/2/2
41	PSU	1	672	84,41	-	0/7/25/26	0/2/2/2
42	OMC	2	1397	42	-	0/9/27/28	0/2/2/2
20	OMU	S1	2048	20	-	0/9/27/28	0/2/2/2
42	PSU	2	437	42	-	0/7/25/26	0/2/2/2
20	OMU	S1	29	20	-	0/9/27/28	0/2/2/2
42	OMC	2	443	42	-	4/9/27/28	0/2/2/2
42	OMU	2	1359	42	-	1/9/27/28	0/2/2/2
42	OMG	2	1253	42	-	0/5/27/28	0/3/3/3
42	OMG	2	655	42	-	1/5/27/28	0/3/3/3
20	MA6	S1	2185	20	-	1/7/29/30	0/3/3/3
42	PSU	2	1265	42	-	2/7/25/26	0/2/2/2
20	OMC	S1	1866	20	-	0/9/27/28	0/2/2/2
42	PSU	2	662	84,42	-	0/7/25/26	0/2/2/2
42	PSU	2	1194	42	-	0/7/25/26	0/2/2/2
20	OMU	S1	1621	20	-	0/9/27/28	0/2/2/2
41	OMC	1	695	41	-	0/9/27/28	0/2/2/2
20	OMG	S1	600	20	-	2/5/27/28	0/3/3/3
42	A2M	2	1185	42	-	3/5/27/28	0/3/3/3
20	G7M	S1	1995	20	-	0/3/25/26	0/3/3/3
20	OMU	S1	8	20	-	6/9/27/28	0/2/2/2
41	OMG	1	1540	42,41	-	2/5/27/28	0/3/3/3
42	PSU	2	1303	42	-	2/7/25/26	0/2/2/2
20	OMG	S1	1550	20	-	2/5/27/28	0/3/3/3
44	A2M	7	43	44	-	0/5/27/28	0/3/3/3
20	OMU	S1	1833	20	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	1	1533	42,41	-	0/7/25/26	0/2/2/2
42	OMC	2	359	42	-	0/9/27/28	0/2/2/2
20	PSU	S1	607	20	-	6/7/25/26	0/2/2/2
42	PSU	2	626	42	-	0/7/25/26	0/2/2/2
41	PSU	1	1664	41	-	0/7/25/26	0/2/2/2
20	A2M	S1	28	20	-	0/5/27/28	0/3/3/3
20	OMG	S1	2151	20	-	0/5/27/28	0/3/3/3
41	A2M	1	858	41	-	0/5/27/28	0/3/3/3
41	OMU	1	847	41	-	0/9/27/28	0/2/2/2
42	OMG	2	1229	42	-	0/5/27/28	0/3/3/3
42	A2M	2	527	42	-	2/5/27/28	0/3/3/3
41	OMC	1	1552	41	-	0/9/27/28	0/2/2/2
42	A2M	2	95	42	-	1/5/27/28	0/3/3/3
20	5MC	S1	2061	20	-	0/7/25/26	0/2/2/2
41	OMG	1	1524	41	-	1/5/27/28	0/3/3/3
41	A2M	1	1539	84,87,42,41	-	0/5/27/28	0/3/3/3
42	OMC	2	1248	42	-	1/9/27/28	0/2/2/2
42	PSU	2	1413	42	-	0/7/25/26	0/2/2/2
42	OMG	2	534	42	-	2/5/27/28	0/3/3/3
20	PSU	S1	609	20	-	0/7/25/26	0/2/2/2
20	5MC	S1	1544	20	-	0/7/25/26	0/2/2/2
42	OMU	2	667	42	-	0/9/27/28	0/2/2/2
20	PSU	S1	1192	20	-	2/7/25/26	0/2/2/2
42	PSU	2	1060	42	-	1/7/25/26	0/2/2/2
42	PSU	2	1144	42	-	0/7/25/26	0/2/2/2
41	PSU	1	1017	41	-	0/7/25/26	0/2/2/2
42	PSU	2	500	42	-	3/7/25/26	0/2/2/2
41	OMG	1	1190	41	-	0/5/27/28	0/3/3/3
20	A2M	S1	98	20	-	1/5/27/28	0/3/3/3
20	PSU	S1	2046	20	-	0/7/25/26	0/2/2/2
41	PSU	1	239	41	-	2/7/25/26	0/2/2/2
41	PSU	1	870	84,41	-	0/7/25/26	0/2/2/2
41	OMU	1	1371	41	-	4/9/27/28	0/2/2/2
41	PSU	1	1528	41	-	0/7/25/26	0/2/2/2
42	A2M	2	665	42	-	3/5/27/28	0/3/3/3
20	PSU	S1	2202	20	-	1/7/25/26	0/2/2/2
42	PSU	2	593	42	-	0/7/25/26	0/2/2/2
44	A2M	7	162	41,44	-	1/5/27/28	0/3/3/3
20	PSU	S1	12	20	-	0/7/25/26	0/2/2/2
44	PSU	7	74	44	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OMG	S1	1829	20	-	2/5/27/28	0/3/3/3
20	OMG	S1	1865	20	-	0/5/27/28	0/3/3/3
20	PSU	S1	1566	20	-	0/7/25/26	0/2/2/2
41	OMG	1	856	41	-	0/5/27/28	0/3/3/3
41	A2M	1	437	41	-	1/5/27/28	0/3/3/3
42	OMU	2	1077	42	-	0/9/27/28	0/2/2/2
20	OMU	S1	1979	20	-	3/9/27/28	0/2/2/2
20	A2M	S1	668	20	-	3/5/27/28	0/3/3/3
20	A2M	S1	2021	20	-	3/5/27/28	0/3/3/3
42	OMG	2	71	42	-	0/5/27/28	0/3/3/3
20	OMU	S1	1777	20	-	0/9/27/28	0/2/2/2
42	PSU	2	1403	42	-	1/7/25/26	0/2/2/2
42	A2M	2	628	42	-	0/5/27/28	0/3/3/3
42	OMC	2	1159	42	-	0/9/27/28	0/2/2/2
20	OMU	S1	661	20	-	0/9/27/28	0/2/2/2
20	OMC	S1	38	20	-	0/9/27/28	0/2/2/2
42	OMC	2	583	42	-	0/9/27/28	0/2/2/2
42	PSU	2	1382	42	-	0/7/25/26	0/2/2/2
20	A2M	S1	512	20	-	3/5/27/28	0/3/3/3
20	OMG	S1	1647	20	-	0/5/27/28	0/3/3/3
42	A2M	2	572	42	-	0/5/27/28	0/3/3/3
20	MA6	S1	2184	20	-	0/7/29/30	0/3/3/3
42	OMU	2	560	42	-	1/9/27/28	0/2/2/2
41	A2M	1	697	41	-	1/5/27/28	0/3/3/3
41	PSU	1	1171	41	-	2/7/25/26	0/2/2/2
42	A2M	2	591	42	-	0/5/27/28	0/3/3/3
42	OMG	2	1046	42	-	2/5/27/28	0/3/3/3
42	A2M	2	1384	42	-	1/5/27/28	0/3/3/3
42	OMU	2	1419	42	-	1/9/27/28	0/2/2/2
81	OMU	3	13	81	-	0/9/27/28	0/2/2/2
42	PSU	2	1058	42	-	0/7/25/26	0/2/2/2
20	PSU	S1	1539	20	-	1/7/25/26	0/2/2/2
41	A2M	1	681	41	-	3/5/27/28	0/3/3/3
41	OMU	1	1659	41	-	0/9/27/28	0/2/2/2
42	PSU	2	78	42	-	2/7/25/26	0/2/2/2
42	OMG	2	641	42	-	0/5/27/28	0/3/3/3
41	PSU	1	1011	42,41	-	1/7/25/26	0/2/2/2
42	OMG	2	1231	42	-	0/5/27/28	0/3/3/3
41	PSU	1	940	41	-	0/7/25/26	0/2/2/2
43	OMG	4	74	43	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PSU	S1	1657	20	-	1/7/25/26	0/2/2/2
42	5MC	2	524	84,42	-	0/7/25/26	0/2/2/2
20	OMC	S1	2140	20	-	2/9/27/28	0/2/2/2
41	A2M	1	678	42,41	-	0/5/27/28	0/3/3/3
20	A2M	S1	897	20	-	2/5/27/28	0/3/3/3
41	PSU	1	1181	41	-	3/7/25/26	0/2/2/2
41	OMC	1	1527	41	-	1/9/27/28	0/2/2/2
41	PSU	1	422	41	-	0/7/25/26	0/2/2/2
41	1MA	1	677	84,41	-	0/3/25/26	0/3/3/3
44	PSU	7	69	44	-	2/7/25/26	0/2/2/2
42	A2M	2	1372	42	-	0/5/27/28	0/3/3/3
20	PSU	S1	1533	20	-	2/7/25/26	0/2/2/2
41	OMG	1	1626	41	-	0/5/27/28	0/3/3/3
42	OMC	2	1317	42	-	0/9/27/28	0/2/2/2
42	PSU	2	504	42	-	3/7/25/26	0/2/2/2
42	A2M	2	570	42,41	-	1/5/27/28	0/3/3/3
42	PSU	2	506	42	-	1/7/25/26	0/2/2/2
20	PSU	S1	33	20	-	2/7/25/26	0/2/2/2
20	PSU	S1	1156	20	-	0/7/25/26	0/2/2/2
42	PSU	2	1361	42	-	2/7/25/26	0/2/2/2
41	PSU	1	1402	41	-	2/7/25/26	0/2/2/2
20	A2M	S1	479	20	-	1/5/27/28	0/3/3/3
20	OMG	S1	1478	20	-	1/5/27/28	0/3/3/3
44	OMG	7	75	44	-	0/5/27/28	0/3/3/3
20	OMC	S1	18	20	-	0/9/27/28	0/2/2/2
20	C4J	S1	1543	20	-	2/16/34/35	0/2/2/2
41	OMU	1	1107	41	-	0/9/27/28	0/2/2/2
20	PSU	S1	455	20	-	0/7/25/26	0/2/2/2
41	A2M	1	955	41	-	0/5/27/28	0/3/3/3
42	PSU	2	472	42	-	0/7/25/26	0/2/2/2
42	OMG	2	1078	42	-	0/5/27/28	0/3/3/3
42	A2M	2	382	42	-	1/5/27/28	0/3/3/3
42	PSU	2	510	42	-	0/7/25/26	0/2/2/2
20	PSU	S1	1841	20	-	0/7/25/26	0/2/2/2
42	PSU	2	597	42	-	0/7/25/26	0/2/2/2
42	PSU	2	1354	42	-	0/7/25/26	0/2/2/2
42	OMU	2	73	42	-	0/9/27/28	0/2/2/2
41	OMG	1	959	41	-	2/5/27/28	0/3/3/3
42	OMG	2	1360	42	-	0/5/27/28	0/3/3/3
42	PSU	2	1318	42	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	PSU	2	1264	42	-	0/7/25/26	0/2/2/2
42	5MC	2	1308	42	-	6/7/25/26	0/2/2/2
20	PSU	S1	104	20	-	0/7/25/26	0/2/2/2
20	PSU	S1	1246	20	-	2/7/25/26	0/2/2/2
42	A2M	2	604	42,41	-	1/5/27/28	0/3/3/3

The worst 5 of 1107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	607	PSU	C6-C5	12.03	1.49	1.35
20	S1	33	PSU	C6-C5	11.67	1.48	1.35
20	S1	1156	PSU	C6-C5	11.66	1.48	1.35
20	S1	1246	PSU	C6-C5	11.62	1.48	1.35
41	1	1011	PSU	C6-C5	11.62	1.48	1.35

The worst 5 of 612 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	2185	MA6	N1-C6-N6	-12.06	104.36	117.06
20	S1	2184	MA6	N1-C6-N6	-11.54	104.91	117.06
41	1	858	A2M	C5-C6-N6	11.39	137.67	120.35
42	2	628	A2M	C5-C6-N6	11.38	137.65	120.35
41	1	697	A2M	C5-C6-N6	11.23	137.42	120.35

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	7	69	PSU	O4'-C1'-C5-C4
44	7	69	PSU	O4'-C1'-C5-C6
44	7	162	A2M	C1'-C2'-O2'-CM'
20	S1	33	PSU	C3'-C4'-C5'-O5'
20	S1	33	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 144 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
41	1	2
15	S4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S4	7:A	O3'	65:G	P	19.26
1	1	1097:A	O3'	1100:C	P	10.20
1	1	552:G	O3'	554:A	P	4.04

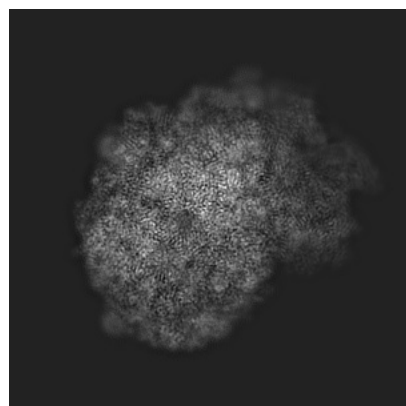
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15272. These allow visual inspection of the internal detail of the map and identification of artifacts.

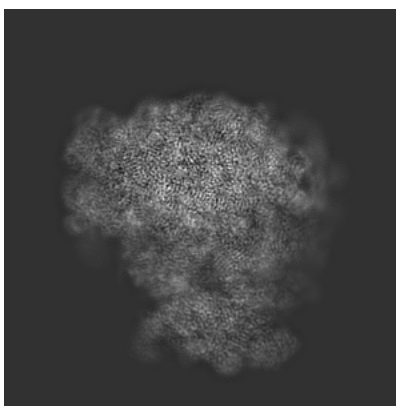
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

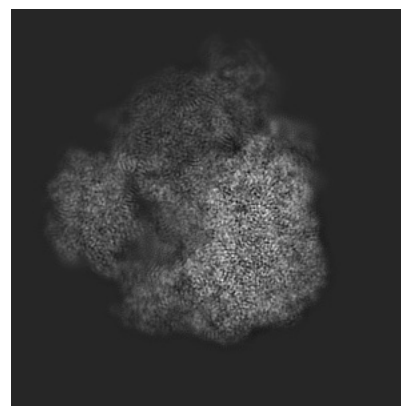
6.1.1 Primary map



X

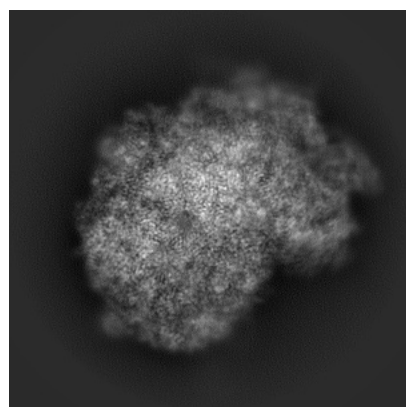


Y

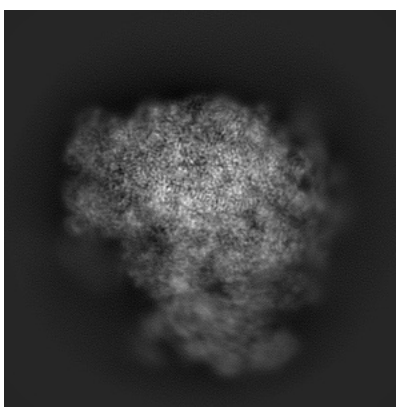


Z

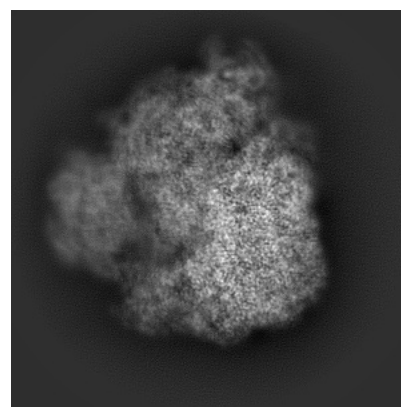
6.1.2 Raw map



X



Y

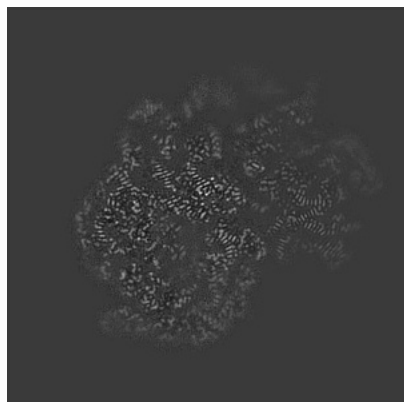


Z

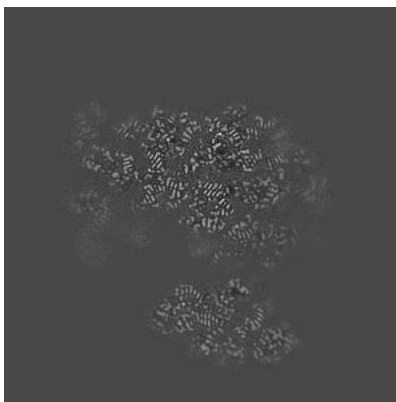
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

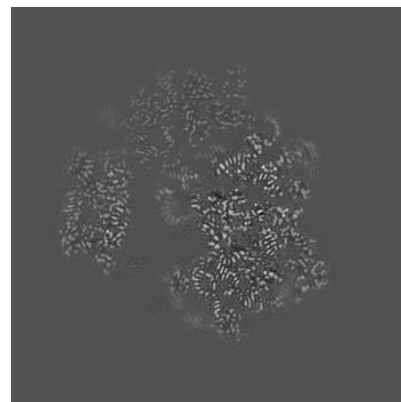
6.2.1 Primary map



X Index: 220

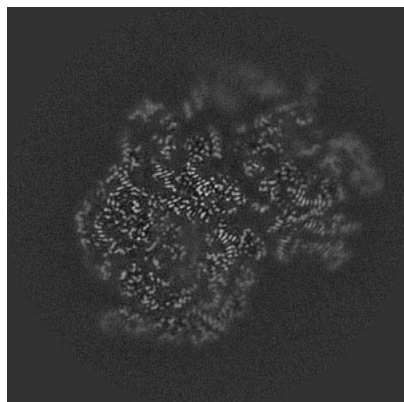


Y Index: 220

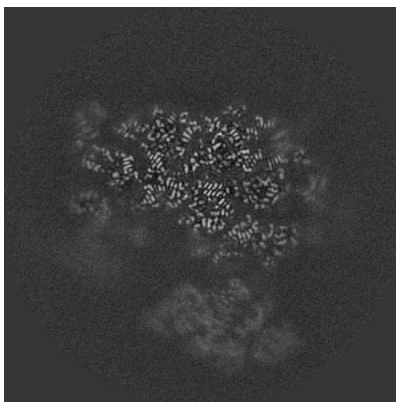


Z Index: 220

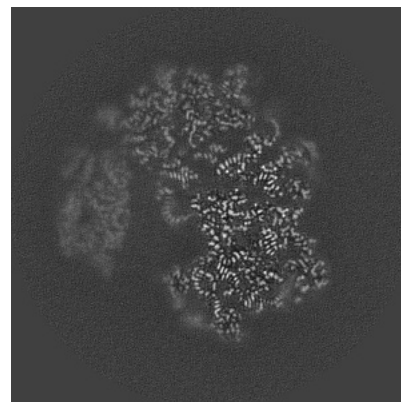
6.2.2 Raw map



X Index: 220



Y Index: 220

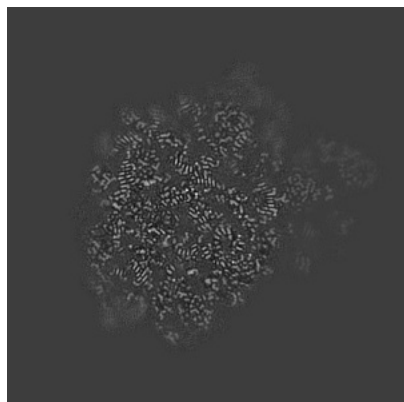


Z Index: 220

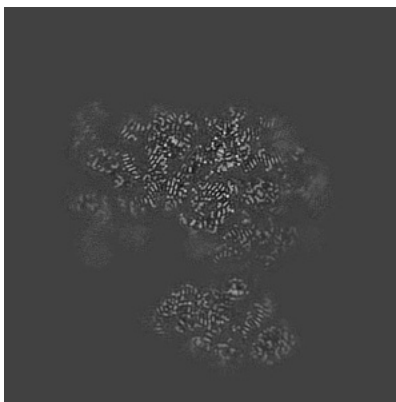
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

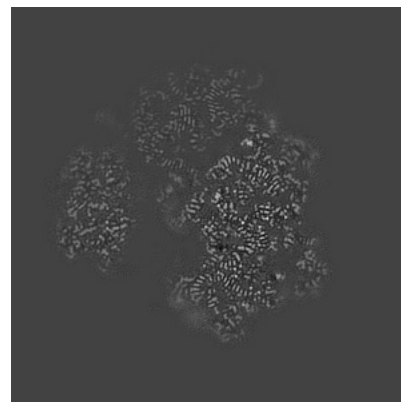
6.3.1 Primary map



X Index: 265

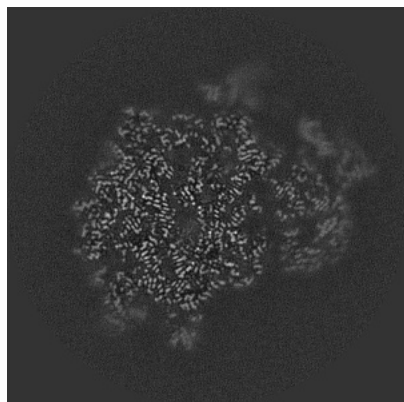


Y Index: 222

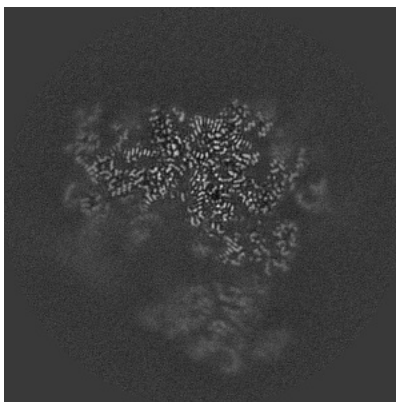


Z Index: 226

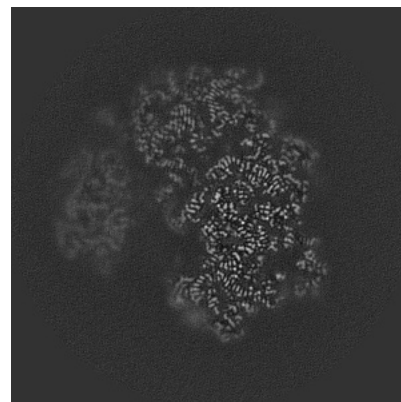
6.3.2 Raw map



X Index: 249



Y Index: 212

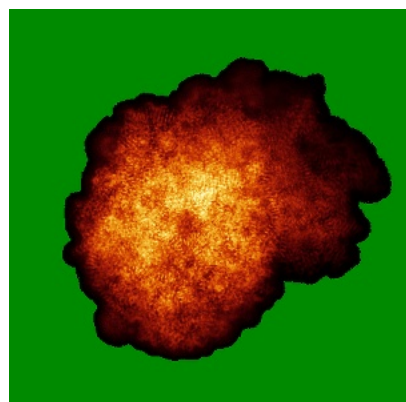


Z Index: 226

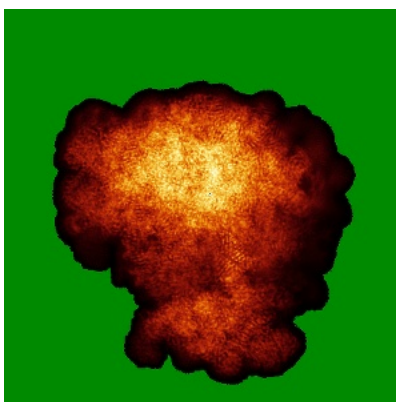
The images above show the largest variance slices of the map in three orthogonal directions.

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

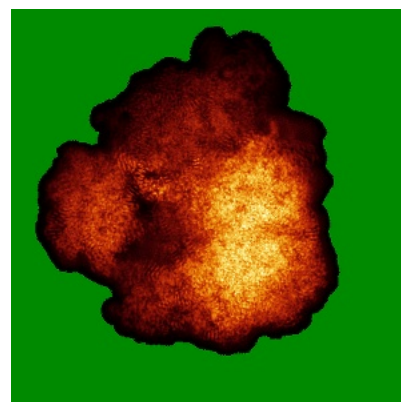
6.4.1 Primary map



X

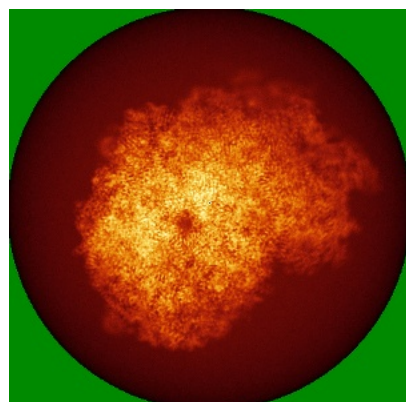


Y

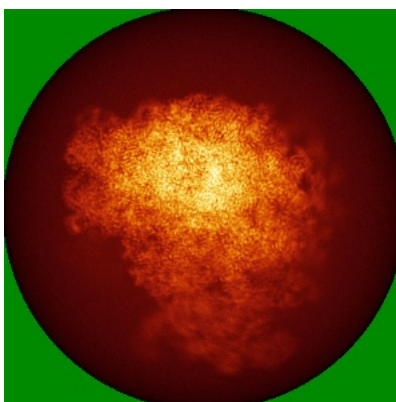


Z

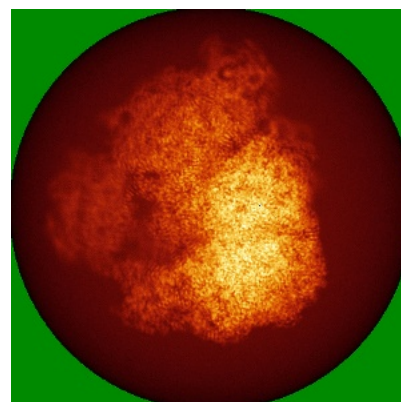
6.4.2 Raw map



X



Y

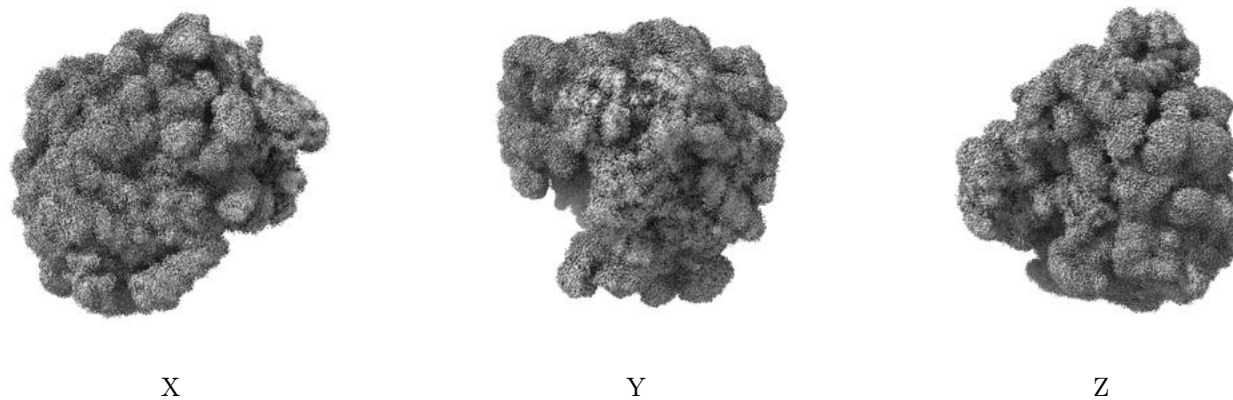


Z

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.

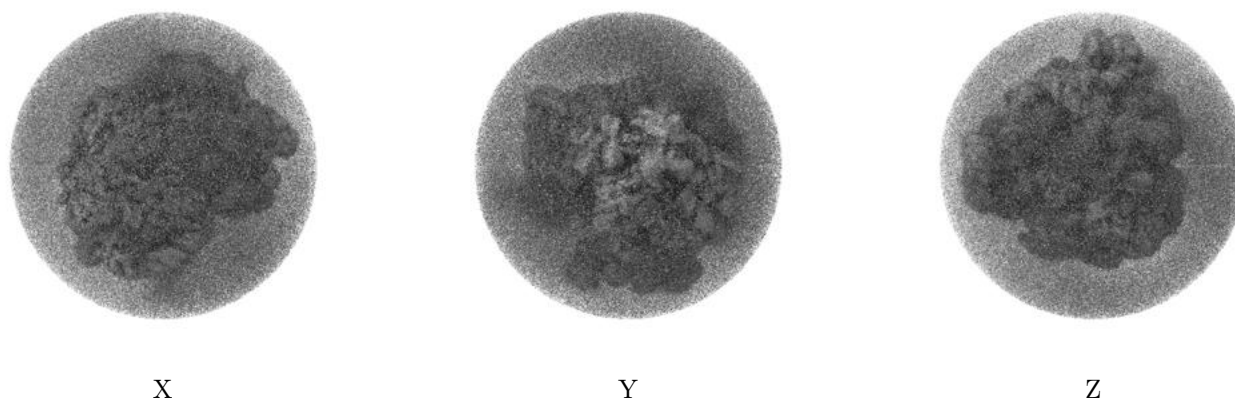
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

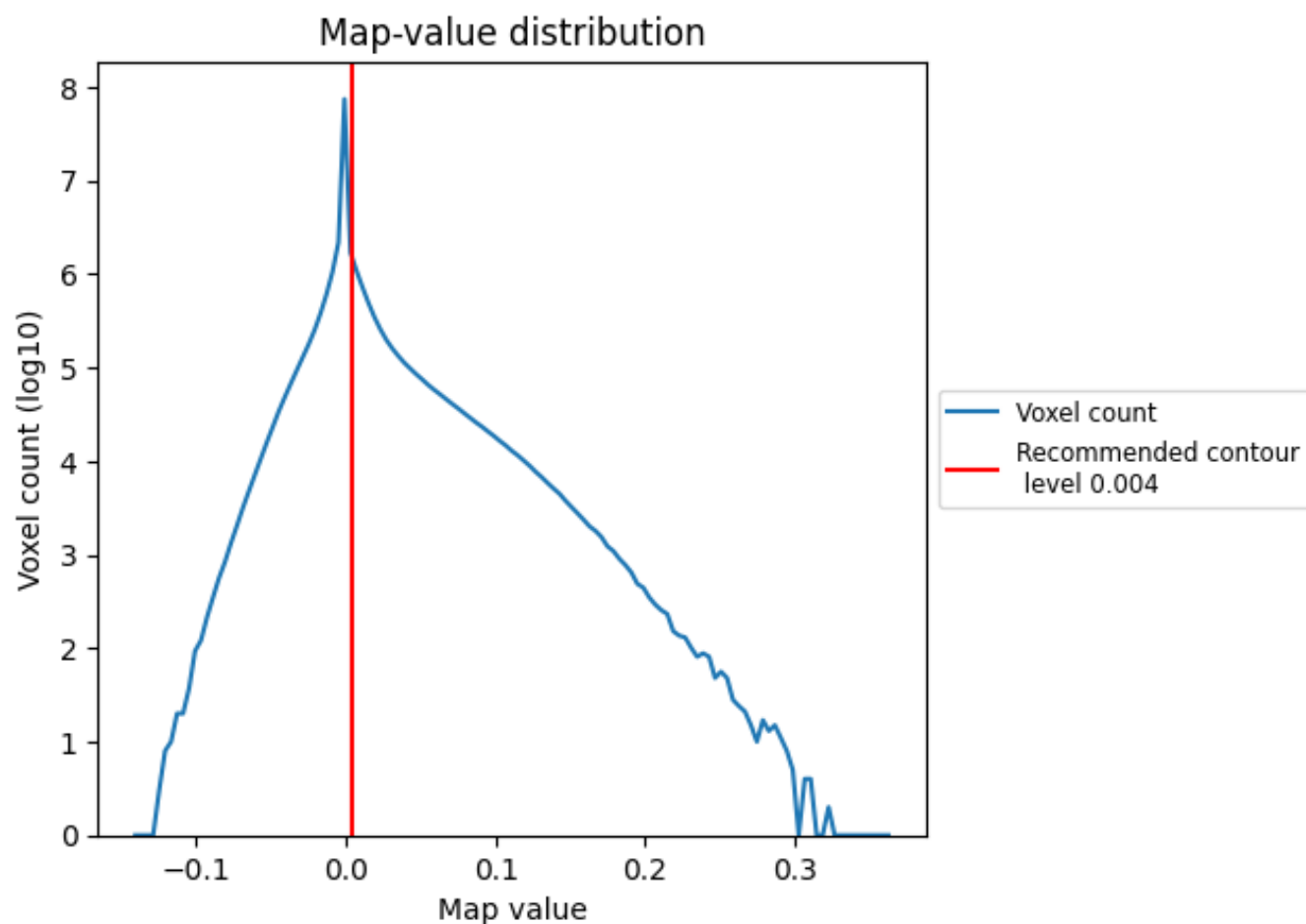
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

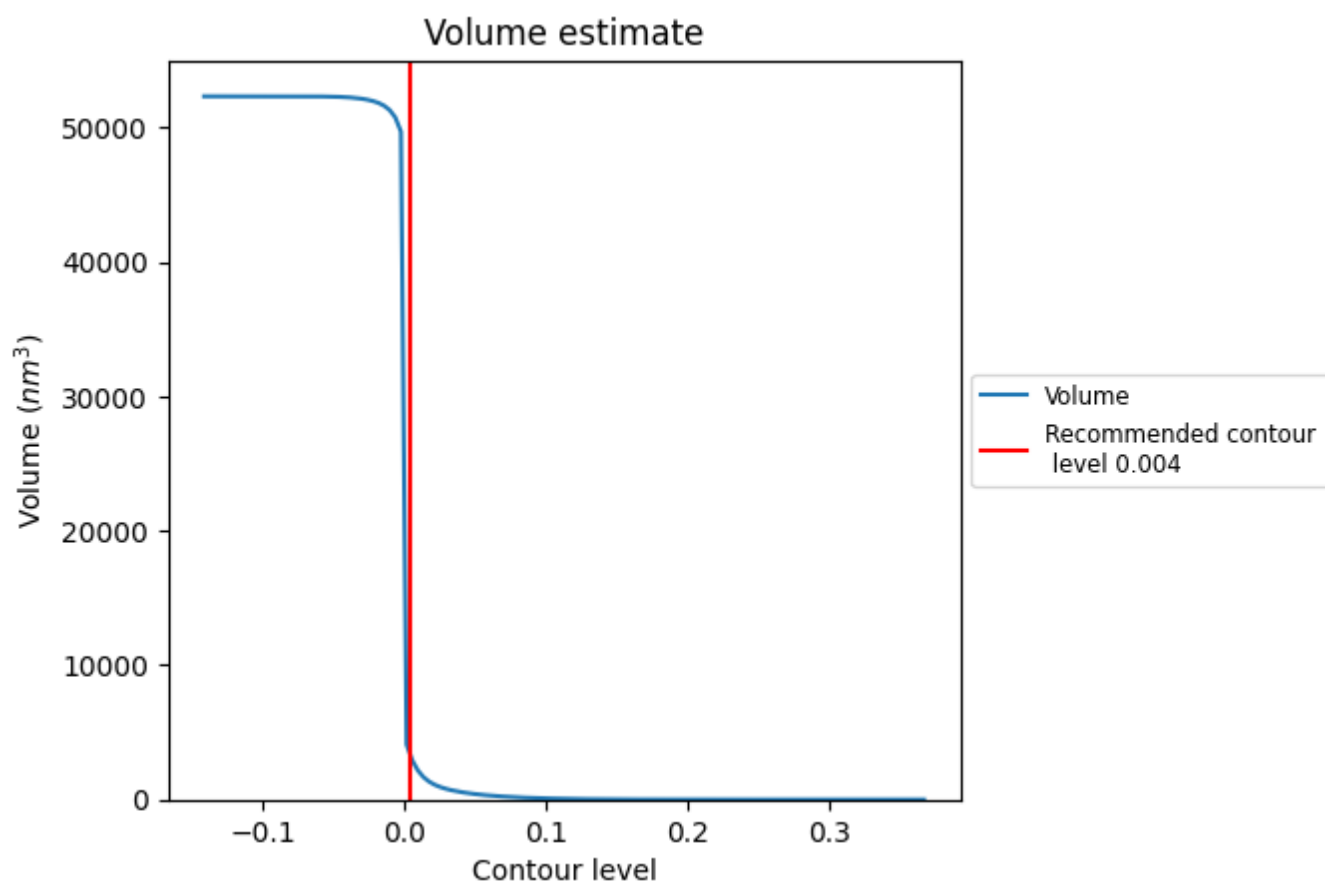
This section contains the results of statistical analysis of the map.

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.

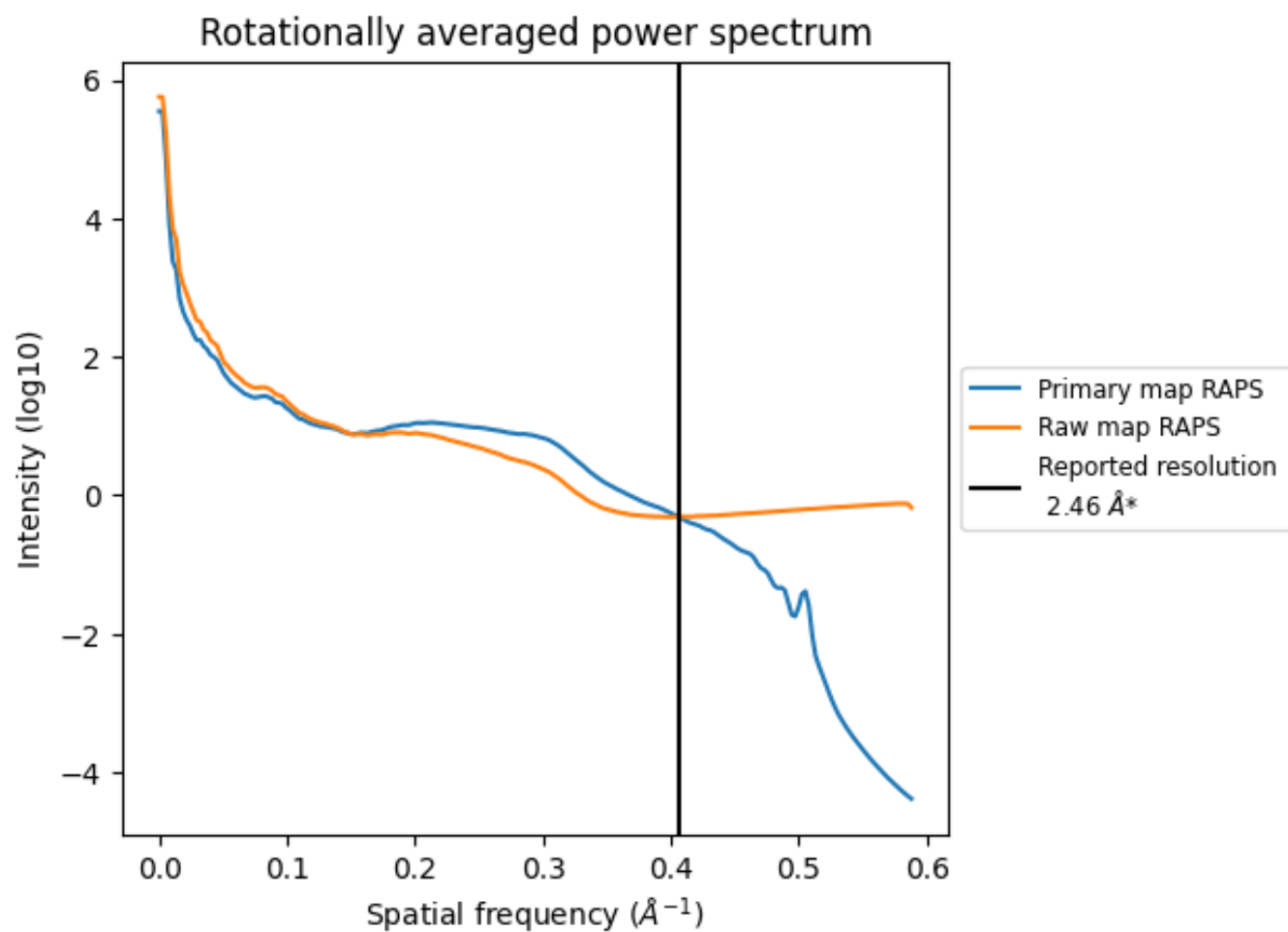
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3475 nm³; this corresponds to an approximate mass of 3139 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 ⓘ

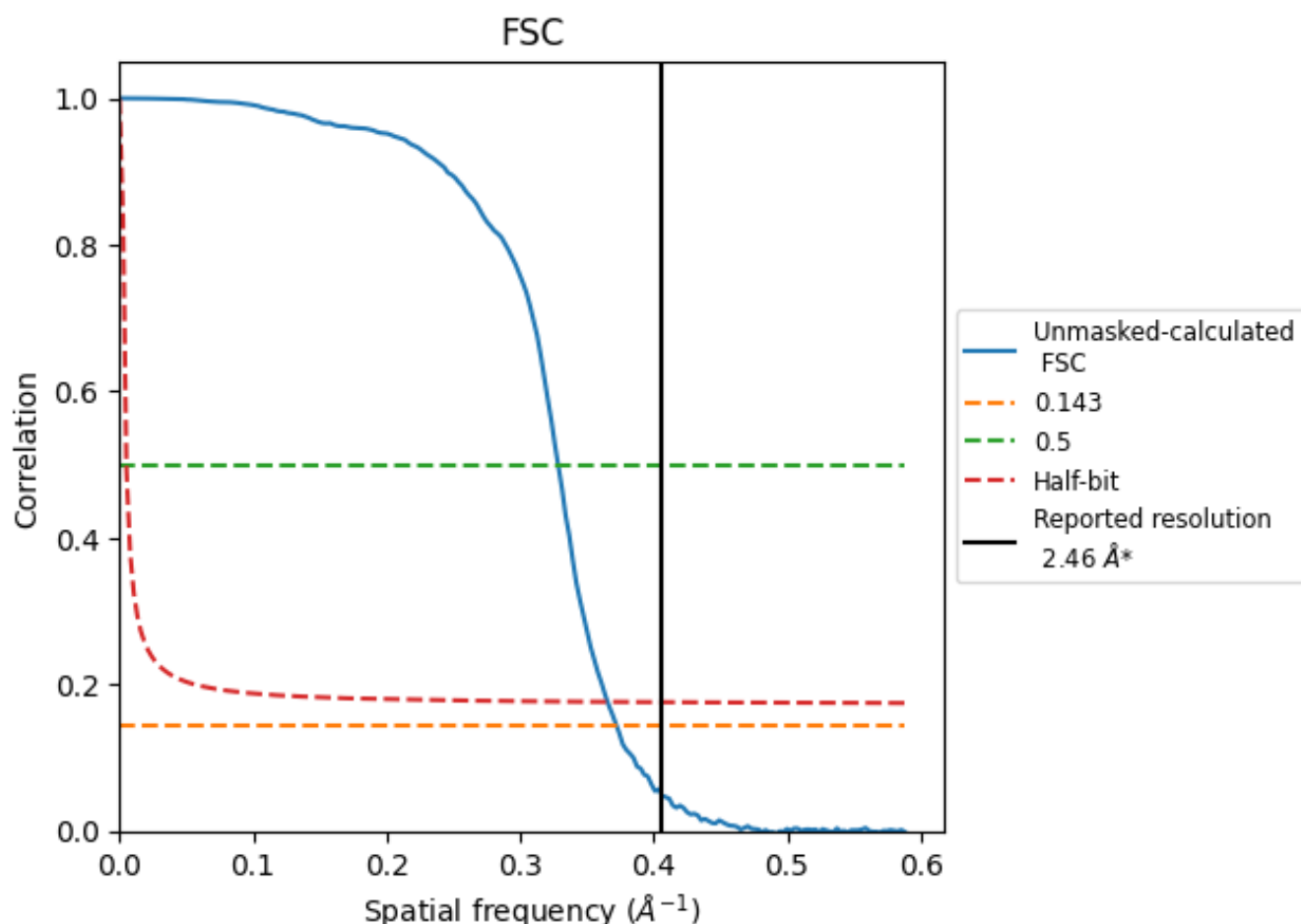


*Reported resolution corresponds to spatial frequency of 0.407 Å⁻¹

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 0.407 Å⁻¹

8.2 Resolution estimates [i](#)

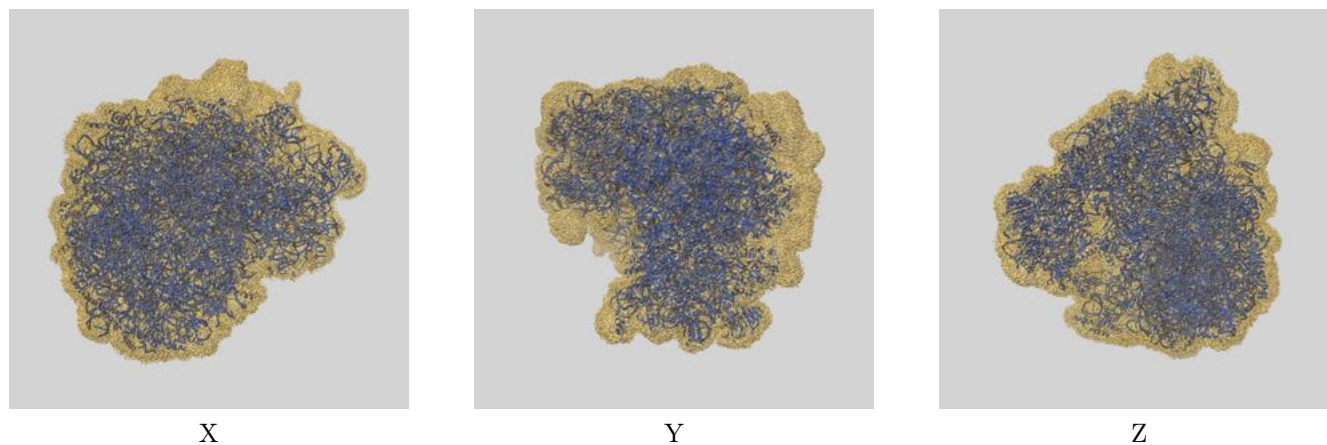
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.69	3.04	2.74

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

9 Map-model fit [i](#)

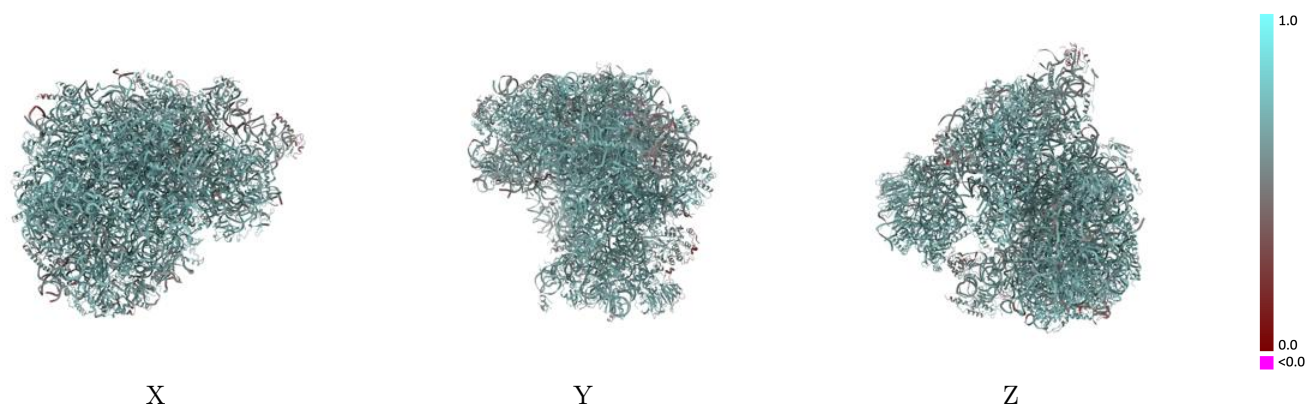
This section contains information regarding the fit between EMDB map EMD-15272 and PDB model 8A98. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



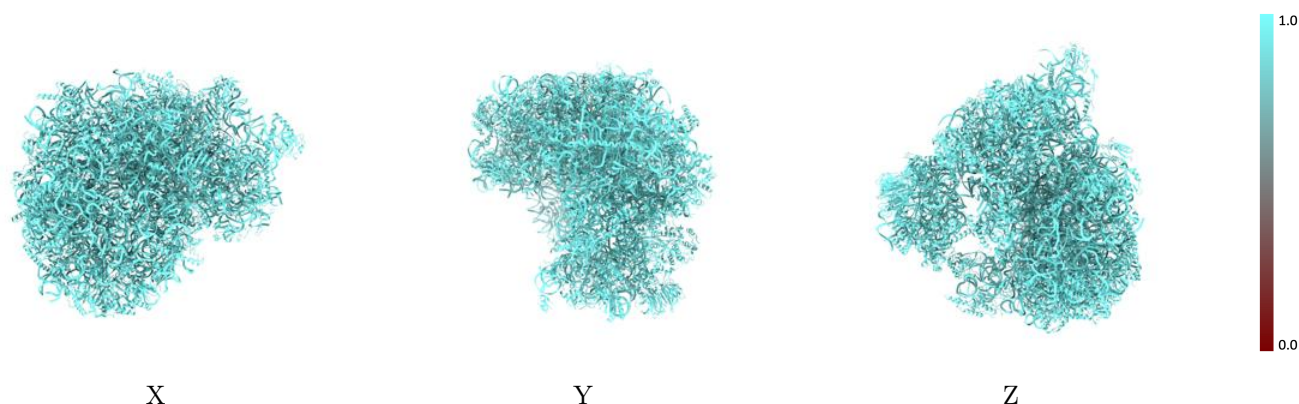
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



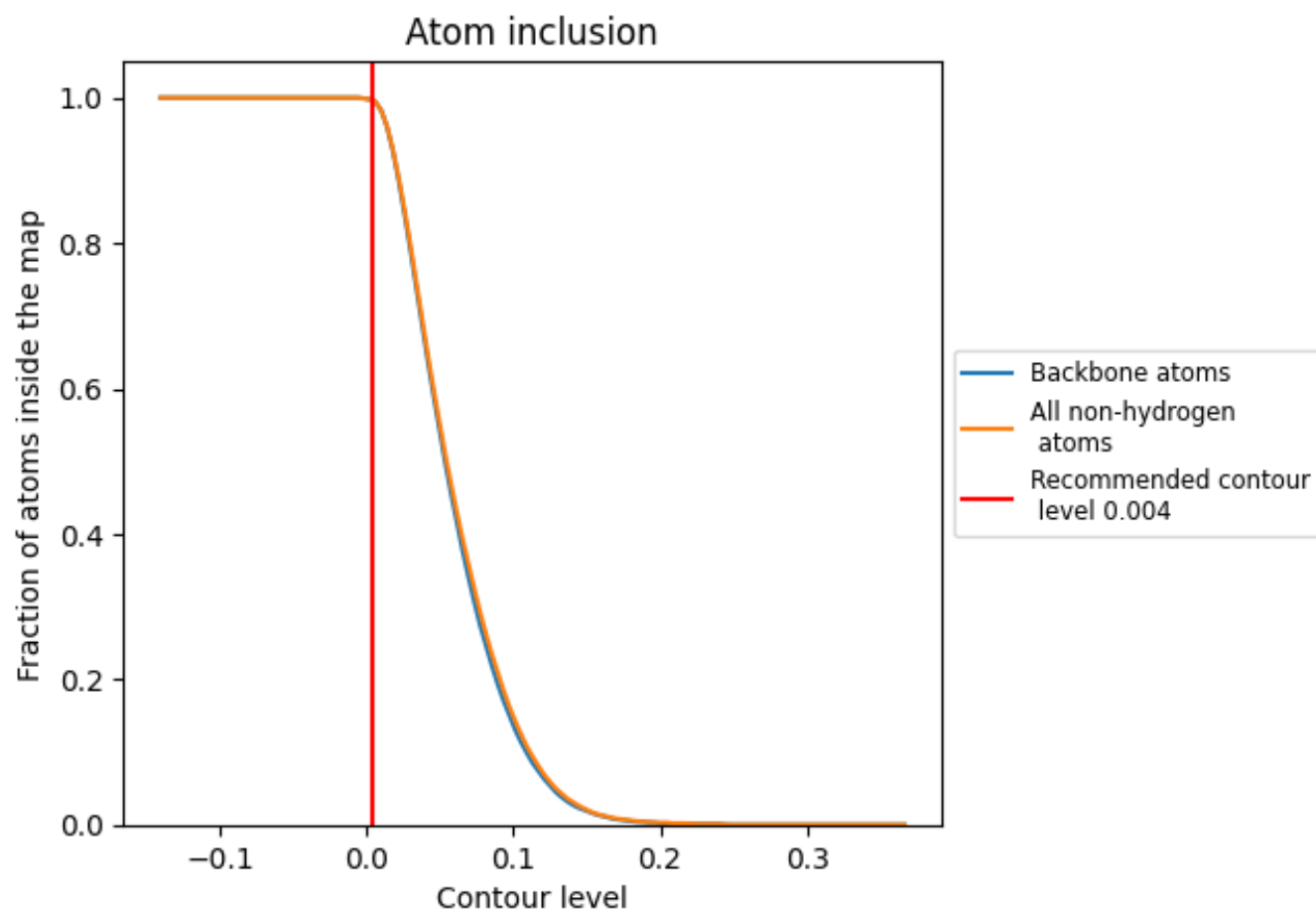
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9970	 0.6530
1	 0.9990	 0.6610
2	 0.9980	 0.6570
3	 0.9960	 0.6410
4	 0.9980	 0.6440
5	 0.9990	 0.6550
6	 0.9980	 0.6150
7	 1.0000	 0.6800
8	 0.9990	 0.6120
A	 1.0000	 0.7100
B	 0.9990	 0.6990
C	 0.9990	 0.6740
D	 0.9980	 0.5280
E	 0.9990	 0.5910
F	 0.9980	 0.6430
G	 0.9970	 0.6500
H	 0.9990	 0.6910
I	 0.9980	 0.6740
J	 0.9990	 0.6930
K	 0.9990	 0.6320
L	 0.9990	 0.7010
M	 0.9990	 0.7190
O	 1.0000	 0.6070
P	 0.9990	 0.6960
Q	 0.9980	 0.6590
R	 0.9970	 0.6680
S	 1.0000	 0.6660
S1	 0.9960	 0.6450
S4	 0.9950	 0.5650
SA	 0.9950	 0.6520
SB	 0.9890	 0.5470
SC	 1.0000	 0.6260
SD	 0.9850	 0.6420
SE	 0.9940	 0.6700
SF	 0.9910	 0.6410

















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Chain	Atom inclusion	Q-score
SG	 0.9940	 0.6410
SH	 0.9980	 0.6630
SI	 0.9920	 0.6410
SJ	 0.9980	 0.6960
SK	 0.9940	 0.6700
SL	 0.9980	 0.6680
SM	 0.9970	 0.6400
SN	 0.9990	 0.6230
SO	 0.9930	 0.6650
SP	 0.9910	 0.6780
SQ	 0.9940	 0.5380
SR	 0.9990	 0.6660
SS	 0.9950	 0.6510
ST	 0.9930	 0.6780
SU	 0.9970	 0.6860
SV	 0.9640	 0.5630
SW	 1.0000	 0.6660
SX	 0.9990	 0.6700
SY	 0.9730	 0.5840
SZ	 0.9950	 0.6460
Sa	 0.9920	 0.6290
Sb	 1.0000	 0.6550
Sc	 0.9790	 0.5890
Sd	 0.9960	 0.6170
Se	 0.9800	 0.6070
Sg	 0.9950	 0.6100
Sh	 0.9560	 0.4460
T	 0.9990	 0.7110
U	 1.0000	 0.5860
V	 0.9980	 0.6810
W	 0.9990	 0.6710
X	 1.0000	 0.6860
Y	 0.9980	 0.6370
Z	 0.9990	 0.6500
a	 1.0000	 0.6700
b	 1.0000	 0.6880
c	 1.0000	 0.6850
d	 1.0000	 0.6370
e	 0.9940	 0.6450
f	 0.9990	 0.7060
g	 0.9990	 0.6780
h	 0.9990	 0.6630

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Chain	Atom inclusion	Q-score
i	 0.9970	 0.6380
j	 0.9980	 0.7250
k	 0.9960	 0.6300
l	 1.0000	 0.7140
n	 0.9880	 0.6180
o	 0.9960	 0.6780
p	 0.9960	 0.6280