



wwPDB EM Validation Summary Report ⓘ

May 28, 2026 – 11:27 am BST

PDB ID : 9RUA / pdb_00009rua
EMDB ID : EMD-54268
Title : RPS26dC HEK mutant 80S ribosome bound to TISU mRNA (RPS26dC-TISU)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 2.90 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.dev132
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) : 2.49

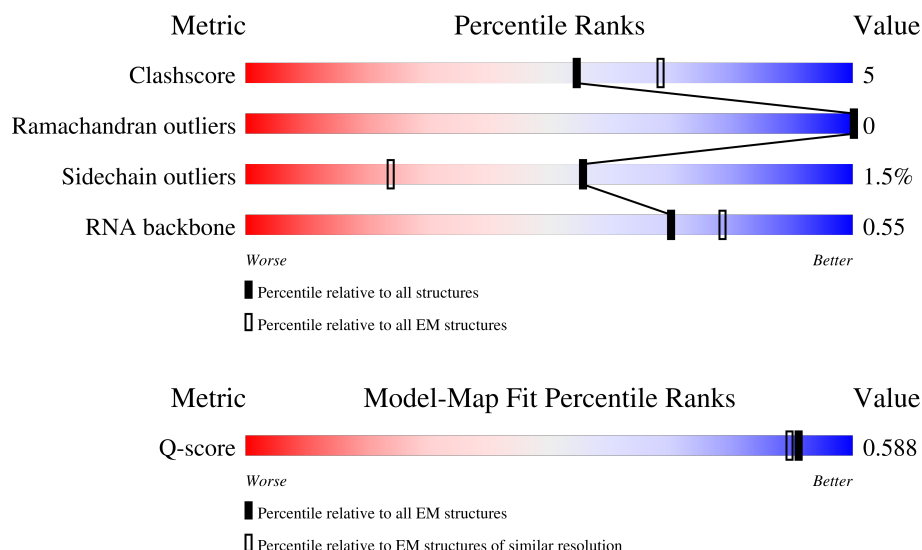
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.















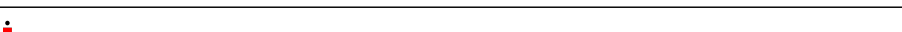

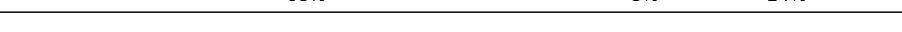

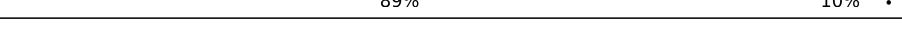








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	Lm	128	
2	Ll	51	
3	Lo	106	









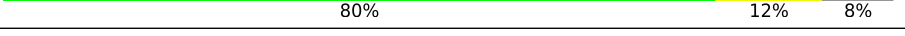

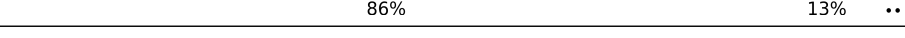
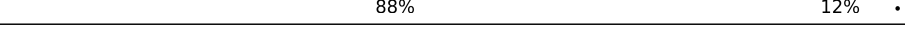

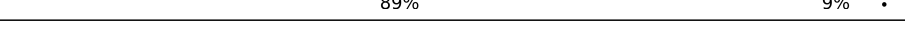


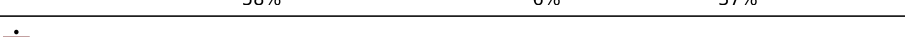

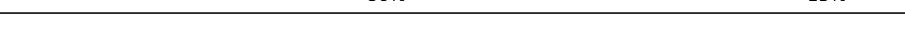






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Mol	Chain	Length	Quality of chain
4	SY	133	
5	SX	143	
6	SW	130	
7	SV	83	
8	SU	119	
9	SR	135	
10	SQ	146	
11	SO	151	
12	SN	151	
13	SL	158	
14	SK	165	
15	SJ	194	
16	SH	194	
17	Sg	317	
18	SF	204	
19	SE	263	
20	Se	133	
21	SD	243	
22	Sd	56	
23	SC	293	
24	Sc	69	
25	SB	264	
26	Sb	84	
27	SA	295	
28	mR	27	

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Mol	Chain	Length	Quality of chain
29	LZ	136	
30	LY	145	
31	LX	156	
32	LW	157	
33	LV	140	
34	LU	128	
35	LT	160	
36	LS	176	
37	LR	196	
38	Lr	138	
39	LQ	188	
40	LP	154	
41	Lp	92	
42	LO	203	
43	LN	204	
44	Ln	25	
45	LM	215	
46	LL	211	
47	Lk	70	
48	LJ	178	
49	Lj	97	
50	LI	214	
51	Li	105	
52	LH	192	
53	Lh	123	

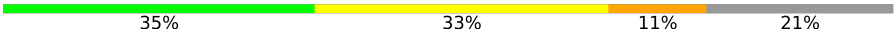

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Mol	Chain	Length	Quality of chain
54	LG	266	
55	Lg	112	
56	LF	248	
57	Lf	111	
58	LE	288	
59	Le	129	
60	LD	297	
61	Ld	125	
62	LC	427	
63	Lc	115	
64	LB	397	
65	Lb	159	
66	LA	257	
67	La	148	
68	L7	120	
69	Pt	77	
70	Sa	115	
71	L8	156	
72	L5	5069	
73	SZ	125	
74	ST	145	
75	SP	145	
76	S2	1869	
77	SG	249	
78	SI	208	

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Mol	Chain	Length	Quality of chain
79	S6	75	 35% 33% 11% 21%
80	SS	152	 78% 12% 9%

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 201456 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 Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Lm	51	Total	C	N	O	S	0	0
			407	251	87	63	6		

- Molecule 2 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ll	50	Total	C	N	O	S	0	0
			434	275	94	64	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ll	34	ILE	LYS	conflict	UNP P62891

- Molecule 3 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Lo	105	Total	C	N	O	S	0	0
			822	516	166	134	6		

- Molecule 4 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SY	123	Total	C	N	O	S	0	0
			894	561	180	150	3		

- Molecule 5 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SX	141	Total	C	N	O	S	0	0
			1060	669	214	174	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SX	62	HIS	PRO	conflict	UNP P62266

- Molecule 6 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SW	129	Total	C	N	O	S	0	0
			1023	653	192	172	6		

- Molecule 7 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SV	83	Total	C	N	O	S	0	0
			623	388	117	113	5		

- Molecule 8 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SU	60	Total	C	N	O	S	0	0
			428	262	90	73	3		

- Molecule 9 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SR	132	Total	C	N	O	S	0	0
			936	591	173	169	3		

- Molecule 10 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SQ	139	Total	C	N	O	S	0	0
			912	567	178	166	1		

- Molecule 11 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SO	134	Total	C	N	O	S	1	0
			981	602	199	174	6		

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SN	150	Total	C	N	O	S	0	0
			1186	761	221	203	1		

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SL	142	Total	C	N	O	S	0	0
			1158	737	218	197	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SK	74	Total	C	N	O	S	0	0
			470	304	86	79	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SK	68	PHE	TYR	conflict	UNP P46783

- Molecule 15 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SJ	178	Total	C	N	O	S	0	0
			1430	915	285	228	2		

- Molecule 16 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SH	189	Total	C	N	O		0	0
			1389	891	263	235			

- Molecule 17 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Sg	241	Total	C	N	O		0	0
			1259	757	255	247			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sg	155	PHE	ARG	conflict	UNP P63244

- Molecule 18 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SF	185	Total	C	N	O	S	0	0
			1324	834	250	237	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SF	15	LYS	PRO	conflict	UNP P46782

- Molecule 19 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SE	260	Total	C	N	O	S	0	0
			2037	1304	383	342	8		

- Molecule 20 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Se	51	Total	C	N	O	S	0	0
			395	240	89	65	1		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SD	175	Total	C	N	O	S	0	0
			1082	680	201	198	3		

- Molecule 22 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Sd	55	Total	C	N	O	S	0	0
			430	270	87	68	5		

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SC	220	Total	C	N	O	S	0	0
			1681	1090	291	290	10		

- Molecule 24 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sc	61	Total	C	N	O	S	0	0
			434	264	87	81	2		

- Molecule 25 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SB	212	Total	C	N	O	S	1	0
			1698	1080	306	297	15		

- Molecule 26 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sb	82	Total	C	N	O	S	0	0
			613	383	113	110	7		

- Molecule 27 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SA	215	Total	C	N	O	S	0	0
			1669	1062	296	303	8		

- Molecule 28 is a RNA chain called TISU mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	mR	8	Total	C	N	O	P	0	0
			172	77	33	54	8		

- Molecule 29 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LZ	135	Total	C	N	O	S	0	0
			1095	709	207	176	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LY	133	Total	C	N	O	S	0	0
			1085	680	220	182	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LY	52	LYS	ASP	conflict	UNP P61254

- Molecule 31 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 32 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LW	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 33 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LV	131	Total	C	N	O	S	1	0
			987	623	187	172	5		

- Molecule 34 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LU	99	Total	C	N	O	S	0	0
			800	513	140	145	2		

- Molecule 35 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LT	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

- Molecule 36 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LS	176	Total	C	N	O	S	0	0
			1454	925	283	235	11		

- Molecule 37 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LR	181	Total	C	N	O	S	0	0
			1462	906	313	234	9		

- Molecule 38 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lr	124	Total	C	N	O	S	0	0
			990	614	205	167	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	1	MET	-	initiating methionine	UNP P46779
Lr	2	ACE	-	expression tag	UNP P46779

- Molecule 39 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LQ	187	Total	C	N	O	S	0	0
			1505	940	312	248	5		

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LP	153	Total	C	N	O	S	0	0
			1234	771	240	214	9		

- Molecule 41 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lp	90	Total	C	N	O	S	0	0
			695	439	134	115	7		

- Molecule 42 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LO	199	Total	C	N	O	S	0	0
			1620	1044	318	253	5		

- Molecule 43 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 44 is a protein called Ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ln	24	Total	C	N	O	S	0	0
			235	142	65	25	3		

- Molecule 45 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LM	136	Total	C	N	O	S	0	0
			1116	716	214	179	7		

- Molecule 46 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LL	210	Total	C	N	O	S	0	0
			1693	1059	351	279	4		

- Molecule 47 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lk	69	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 48 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LJ	169	Total	C	N	O	S	0	0
			1329	843	246	234	6		

- Molecule 49 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lj	86	Total	C	N	O	S	0	0
			701	432	154	110	5		

- Molecule 50 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LI	203	Total	C	N	O	S	0	0
			1632	1038	314	267	13		

- Molecule 51 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Li	102	Total	C	N	O	S	0	0
			812	509	171	127	5		

- Molecule 52 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LH	190	Total	C	N	O	S	0	0
			1499	946	281	266	6		

- Molecule 53 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lh	122	Total	C	N	O	S	0	0
			1010	638	204	167	1		

- Molecule 54 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LG	228	Total	C	N	O	S	0	0
			1791	1142	346	299	4		

- Molecule 55 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lg	110	Total	C	N	O	S	1	0
			872	544	182	140	6		

- Molecule 56 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LF	225	Total	C	N	O	S	0	0
			1835	1178	350	298	9		

- Molecule 57 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lf	109	Total	C	N	O	S	0	0
			868	549	173	143	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lf	111	LYS	-	expression tag	UNP P18077

- Molecule 58 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LE	219	Total	C	N	O	S	1	0
			1742	1123	330	285	4		

- Molecule 59 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Le	128	Total	C	N	O	S	0	0
			1053	666	217	165	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Le	129	LYS	-	expression tag	UNP P62910

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LD	292	Total	C	N	O	S	0	0
			2354	1487	429	424	14		

- Molecule 61 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ld	106	Total	C	N	O	S	0	0
			840	534	165	139	2		

- Molecule 62 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LC	359	Total	C	N	O	S	0	0
			2862	1802	572	475	13		

- Molecule 63 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lc	98	Total	C	N	O	S	0	0
			760	482	134	138	6		

- Molecule 64 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LB	396	Total	C	N	O	S	0	0
			3177	2024	597	542	14		

- Molecule 65 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Lb	101	Total	C	N	O	S	0	0
			815	506	178	127	4		

- Molecule 66 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	LA	248	Total	C	N	O	S	1	0
			1905	1193	392	314	6		

- Molecule 67 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 68 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	L7	119	Total	C	N	O	P	0	0
			2542	1132	454	837	119		

- Molecule 69 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	Pt	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

- Molecule 70 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Sa	98	Total	C	N	O	S	0	0
			770	481	158	127	4		

- Molecule 71 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	L8	153	Total	C	N	O	P	0	0
			3256	1453	574	1076	153		

- Molecule 72 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	L5	3453	Total	C	N	O	P	1	0
			74115	33043	13558	24060	3454		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	483	C	G	conflict	GB 86475748

- Molecule 73 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	SZ	63	Total	C	N	O	0	0
			383	245	69	69		

- Molecule 74 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	ST	129	Total	C	N	O	S	0	0
			837	529	163	143	2		

- Molecule 75 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SP	126	Total	C	N	O	S	0	0
			800	498	155	144	3		

- Molecule 76 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	S2	1575	Total	C	N	O	P	0	0
			33681	15059	6058	10989	1575		

- Molecule 77 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SG	220	Total	C	N	O	S	0	0
			1679	1051	337	284	7		

- Molecule 78 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SI	206	Total	C	N	O	S	0	0
			1648	1035	326	282	5		

- Molecule 79 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	S6	59	Total	C	N	O	P	0	0
			1263	565	238	402	58		

- Molecule 80 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
80	SS	138	Total	C	N	O	0	0
			903	565	178	160		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SS	115	ILE	LYS	conflict	UNP P62269
SS	117	ALA	ILE	conflict	UNP P62269
SS	119	PHE	ALA	conflict	UNP P62269

- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Lm	1	Total	Zn	0
			1	1	
81	Lo	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
81	Sd	1	Total 1	Zn 1	0
81	Lp	1	Total 1	Zn 1	0
81	Lg	1	Total 1	Zn 1	0

- Molecule 82 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
82	SQ	1	Total 1	K 1	0
82	Lf	1	Total 1	K 1	0
82	L8	1	Total 1	K 1	0
82	L5	61	Total 61	K 61	0
82	S2	12	Total 12	K 12	0

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	Sd	2	Total 2	Mg 2	0
83	mR	1	Total 1	Mg 1	0
83	LV	1	Total 1	Mg 1	0
83	LS	1	Total 1	Mg 1	0
83	LP	1	Total 1	Mg 1	0
83	LI	1	Total 1	Mg 1	0
83	Le	1	Total 1	Mg 1	0
83	LB	1	Total 1	Mg 1	0
83	L7	5	Total 5	Mg 5	0

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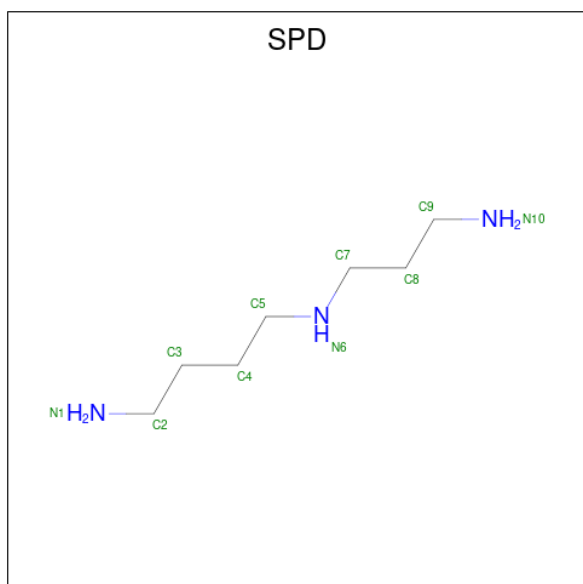
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Mol	Chain	Residues	Atoms		AltConf
83	Pt	1	Total	Mg	0
			1	1	
83	L8	5	Total	Mg	0
			5	5	
83	L5	80	Total	Mg	0
			80	80	
83	S2	19	Total	Mg	0
			19	19	
83	S6	1	Total	Mg	0
			1	1	

- Molecule 84 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
84	LN	1	Total	Na	0
			1	1	
84	L5	47	Total	Na	0
			47	47	
84	S2	11	Total	Na	0
			11	11	

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			10	7	3	

- Molecule 86 is water.

Mol	Chain	Residues	Atoms	AltConf
86	Ll	2	Total O 2 2	0
86	Lo	1	Total O 1 1	0
86	SN	4	Total O 4 4	0
86	SL	1	Total O 1 1	0
86	SF	1	Total O 1 1	0
86	LY	1	Total O 1 1	0
86	LW	1	Total O 1 1	0
86	LV	2	Total O 2 2	0
86	LT	4	Total O 4 4	0
86	LR	5	Total O 5 5	0
86	LQ	2	Total O 2 2	0
86	LP	2	Total O 2 2	0
86	LN	4	Total O 4 4	0
86	Ln	1	Total O 1 1	0
86	LL	5	Total O 5 5	0
86	LJ	1	Total O 1 1	0
86	Lj	1	Total O 1 1	0
86	LI	1	Total O 1 1	0
86	LH	1	Total O 1 1	0
86	Lh	1	Total O 1 1	0
86	LG	1	Total O 1 1	0

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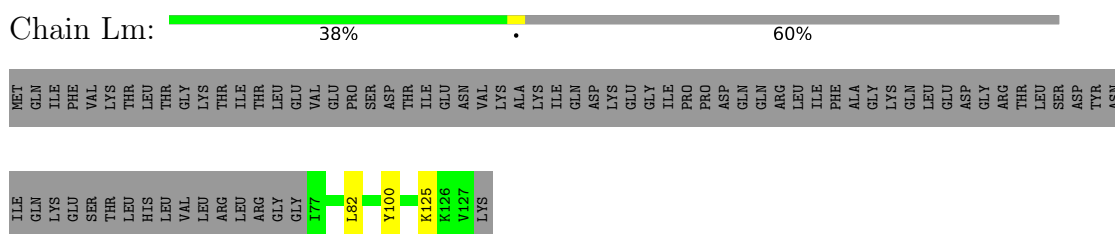
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Mol	Chain	Residues	Atoms		AltConf
86	Lg	4	Total 4	O 4	0
86	LF	2	Total 2	O 2	0
86	Le	2	Total 2	O 2	0
86	LD	1	Total 1	O 1	0
86	LC	3	Total 3	O 3	0
86	Lc	2	Total 2	O 2	0
86	LB	5	Total 5	O 5	0
86	Lb	4	Total 4	O 4	0
86	LA	6	Total 6	O 6	0
86	La	4	Total 4	O 4	0
86	L7	9	Total 9	O 9	0
86	Sa	1	Total 1	O 1	0
86	L8	16	Total 16	O 16	0
86	L5	467	Total 467	O 467	0
86	S2	105	Total 105	O 105	0
86	SI	3	Total 3	O 3	0
86	S6	1	Total 1	O 1	0

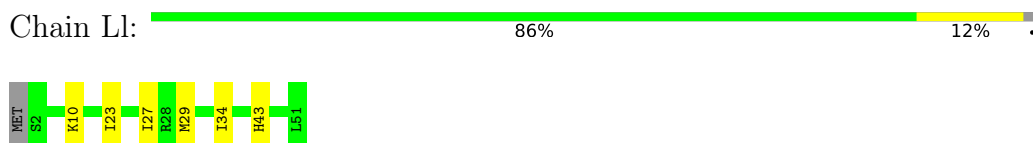
3 Residue-property plots

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.

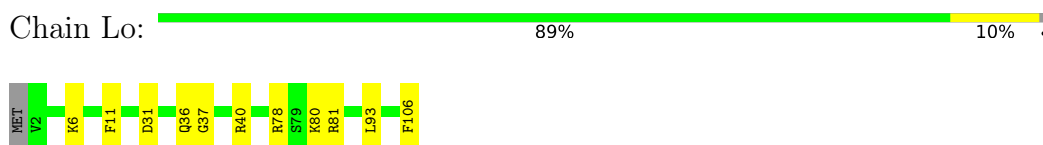
- Molecule 1: Ubiquitin-60S ribosomal protein L40



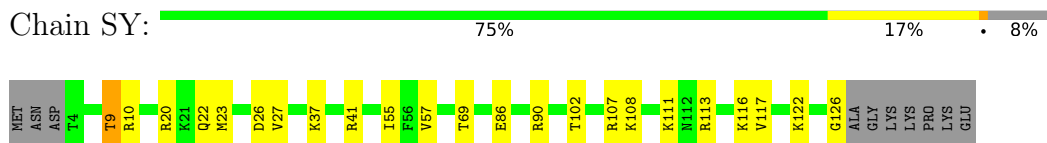
- Molecule 2: Large ribosomal subunit protein eL39



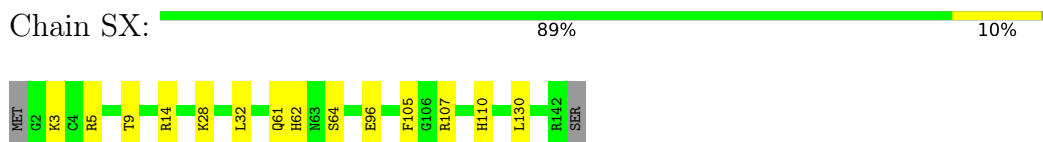
- Molecule 3: Large ribosomal subunit protein eL42



- Molecule 4: 40S ribosomal protein S24



- Molecule 5: Small ribosomal subunit protein uS12




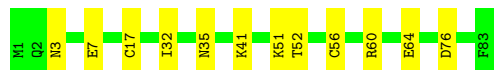
- Molecule 6: 40S ribosomal protein S15a

Chain SW:  88% 10% ..



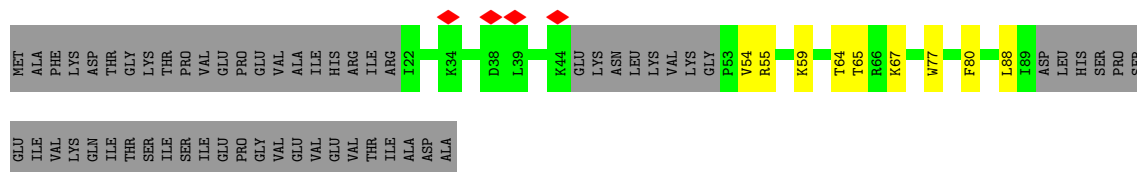
- Molecule 7: 40S ribosomal protein S21

Chain SV:  86% 14%



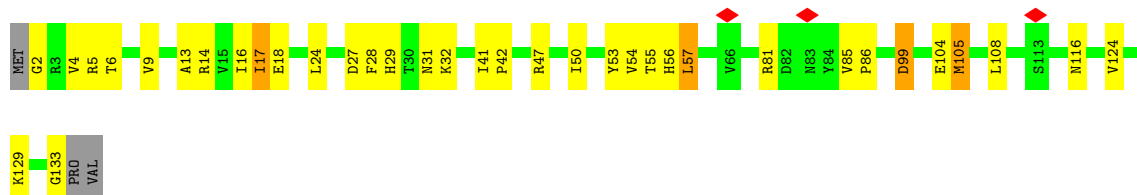
- Molecule 8: 40S ribosomal protein S20

Chain SU:  43% 8% 50%




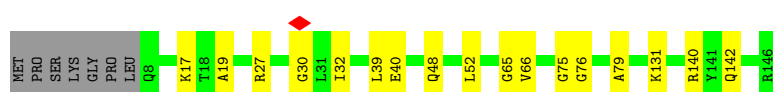
- Molecule 9: 40S ribosomal protein S17

Chain SR:  71% 24% ..




- Molecule 10: 40S ribosomal protein S16

Chain SQ:  84% 12% 5%



- Molecule 11: 40S ribosomal protein S14

Chain SO:  74% 15% 11%




L151

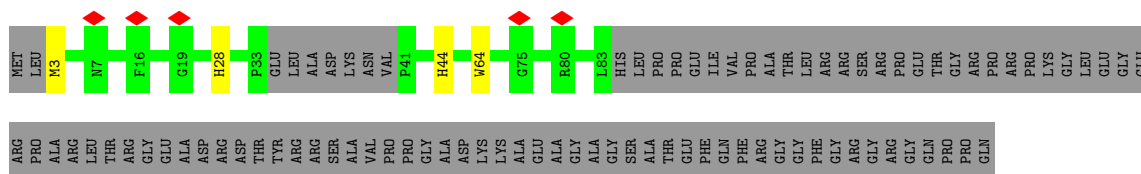
- Molecule 12: 40S ribosomal protein S13

Chain SN:  93% 6% ..


- Molecule 13: 40S ribosomal protein S11

Chain SL:  84% 6% 10%


- Molecule 14: Small ribosomal subunit protein eS10

Chain SK:  42% 55%

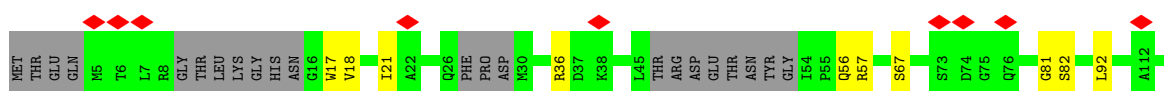
- Molecule 15: 40S ribosomal protein S9

Chain SJ:  81% 11% 8%

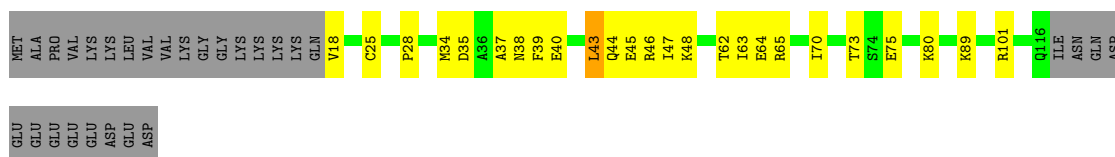
- Molecule 16: 40S ribosomal protein S7

Chain SH:  84% 14% .

- Molecule 17: Small ribosomal subunit protein RACK1

Chain Sg:  7% 68% 8% 24%

Chain LU:  58% 19% • 23%



- Molecule 35: 60S ribosomal protein L21

Chain LT: 88% 11% ..



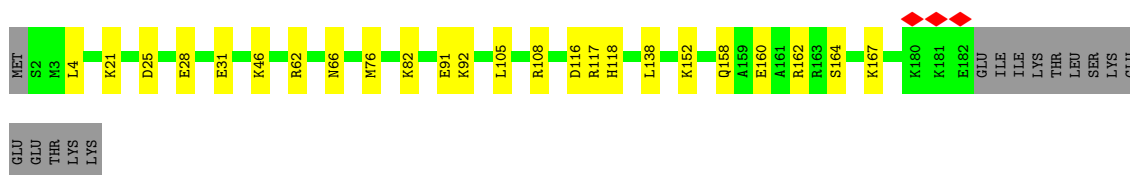
- Molecule 36: 60S ribosomal protein L18a

Chain LS: 86% 14%



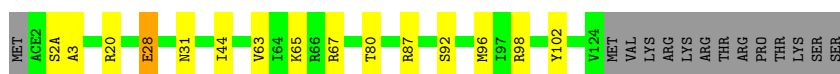
- Molecule 37: 60S ribosomal protein L19

Chain LR: 80% 12% 8%



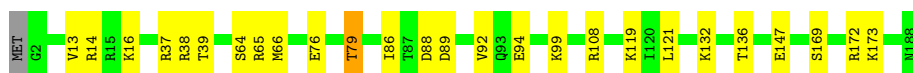
- Molecule 38: Large ribosomal subunit protein eL28

Chain Lr: 79% 10% 10%



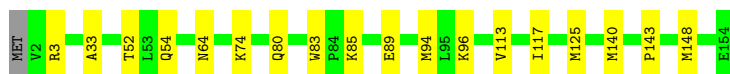
- Molecule 39: 60S ribosomal protein L18

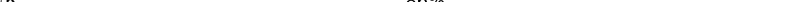
Chain LQ: 86% 13% ..



- Molecule 40: Large ribosomal subunit protein uL22

Chain LP: 88% 12%



- Chain Lk:  86% 13%



- Molecule 48: 60S ribosomal protein L11

Chain LJ: 80% 15% 5%



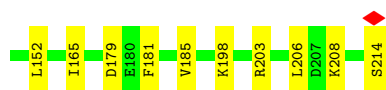
- Molecule 49: Large ribosomal subunit protein eL37

Chain Lj: 77% 11% 11%



- Molecule 50: 60S ribosomal protein L10

Chain LI: 79% 16% 5%



- Molecule 51: 60S ribosomal protein L36

Chain Li: 90% 7% ..



- Molecule 52: 60S ribosomal protein L9

Chain LH: 86% 12% ..



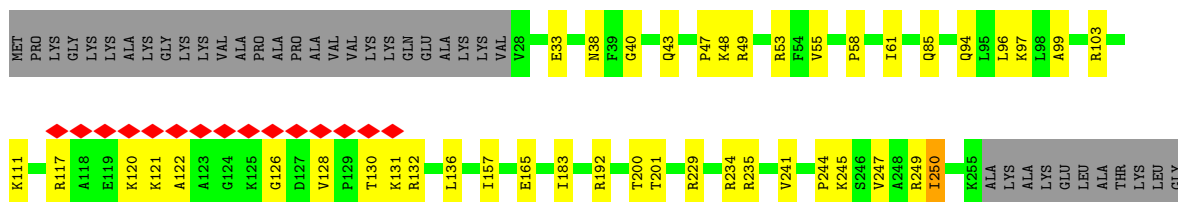
- Molecule 53: 60S ribosomal protein L35

Chain Lh: 84% 15% .




- Molecule 54: 60S ribosomal protein L7a

Chain LG: 




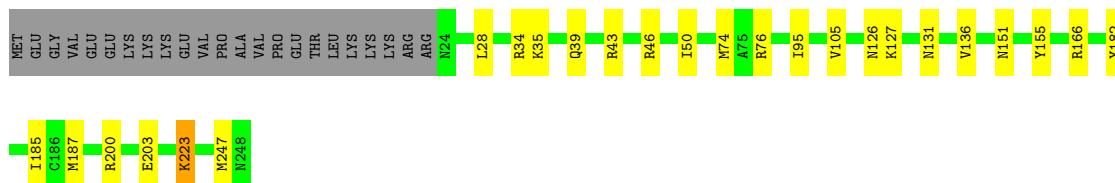
- Molecule 55: Large ribosomal subunit protein eL34

Chain Lg: 




- Molecule 56: Large ribosomal subunit protein uL30

Chain LF: 



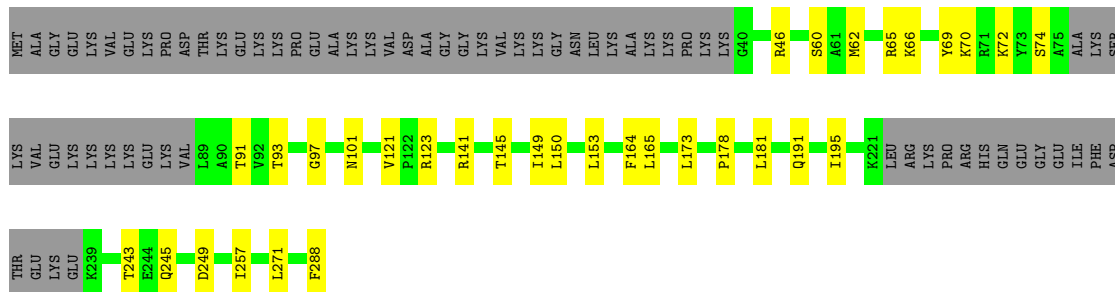
- Molecule 57: Large ribosomal subunit protein eL33

Chain Lf: 




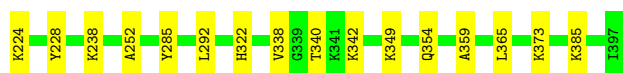
- Molecule 58: Large ribosomal subunit protein eL6

Chain LE: 



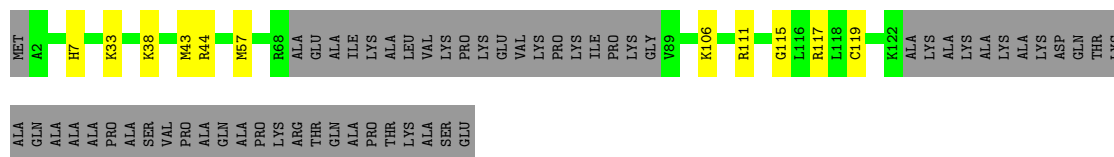
- Molecule 59: Large ribosomal subunit protein eL32

Chain Le: 



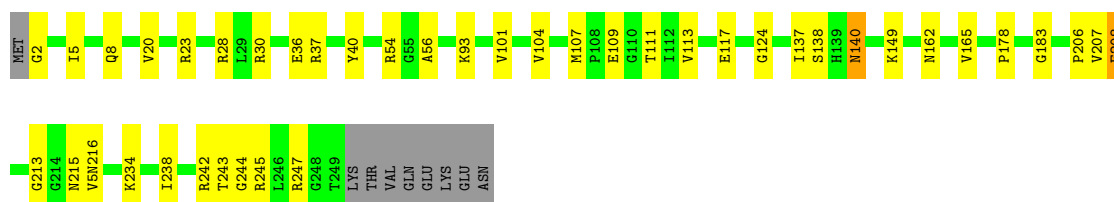
- Molecule 65: Large ribosomal subunit protein eL29

Chain Lb: 57% 7% 36%



- Molecule 66: Large ribosomal subunit protein uL2

Chain LA: 80% 16% . .



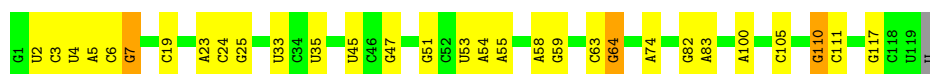
- Molecule 67: Large ribosomal subunit protein uL15

Chain La: 84% 15% .



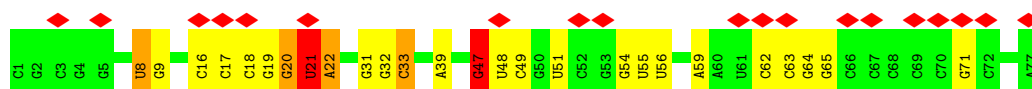
- Molecule 68: 5S rRNA

Chain L7: 74% 22% . .



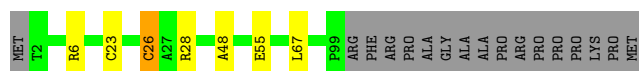
- Molecule 69: P site tRNA

Chain Pt: 25% 66% 26% 5% .

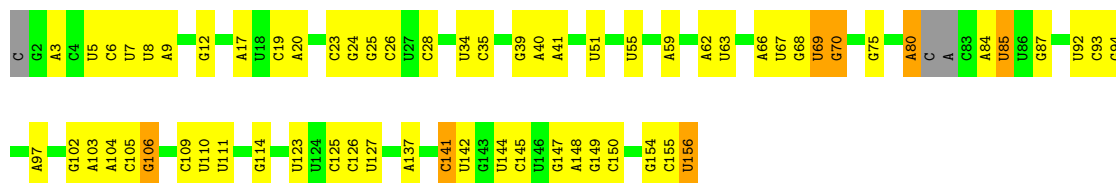


- Molecule 70: 40S ribosomal protein S26

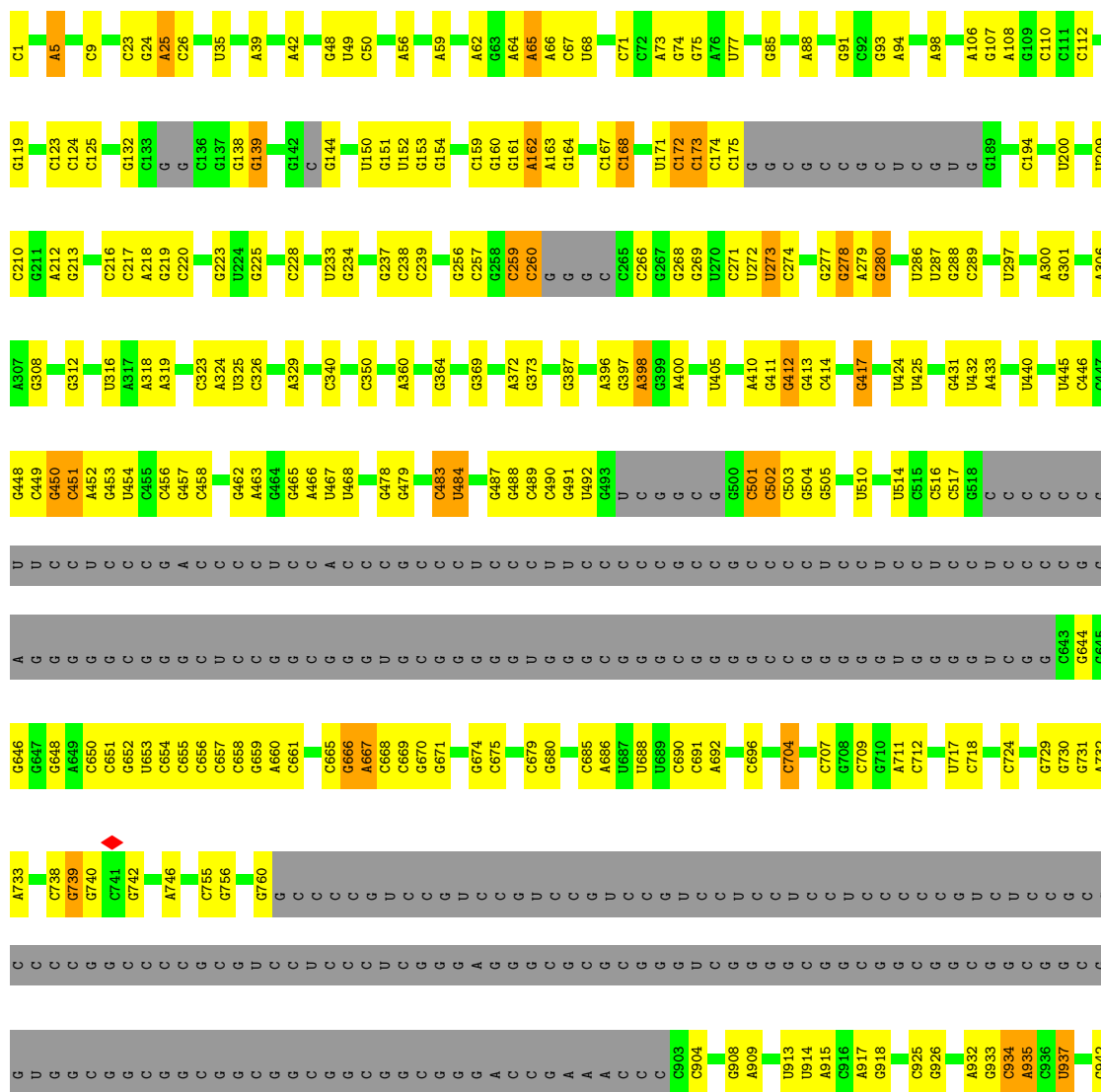
Chain Sa: 79% 5% 15%



• Molecule 71: 5.8S rRNA

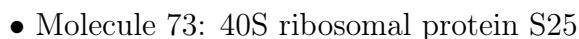
Chain L8:  57% 37%

• Molecule 72: 28S rRNA

Chain L5:  43% 22% 32%



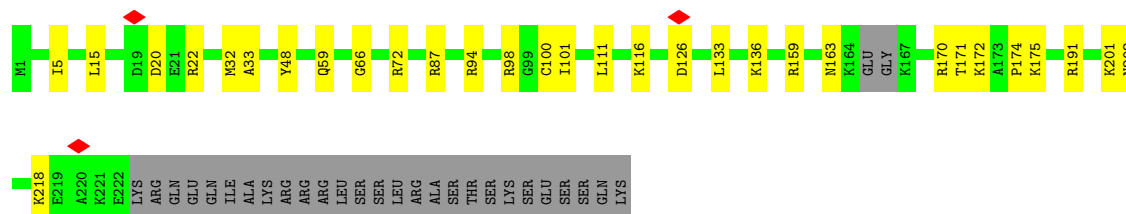
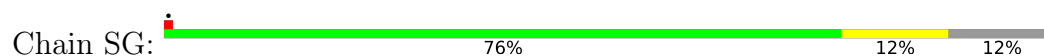




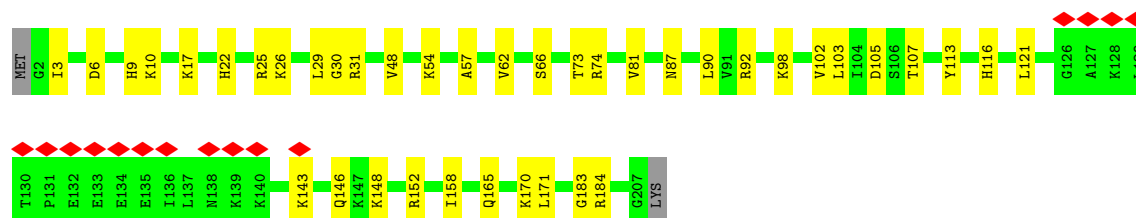
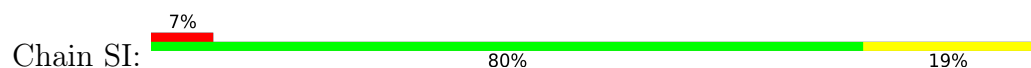




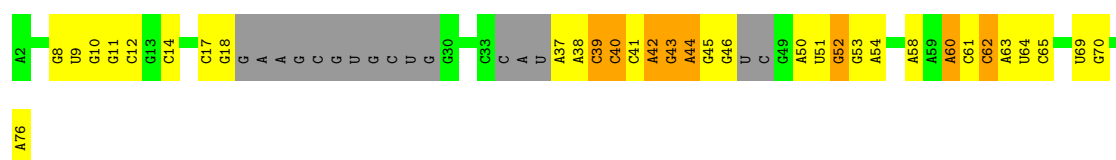
- Molecule 77: 40S ribosomal protein S6



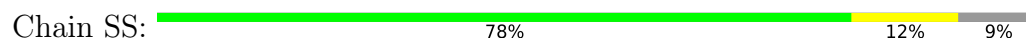
- Molecule 78: 40S ribosomal protein S8



- Molecule 79: E site tRNA



- Molecule 80: Small ribosomal subunit protein uS13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50884	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 ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, V5N, 5MC, OMC, A2M, 4SU, G7M, PSU, NA, ACE, SPD, MG, UR3, 6MZ, OMG, 1MA, ZN, B8N, OMU, K, MLZ, MA6, H2U

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	Lm	0.15	0/413	0.33	0/549
2	Ll	0.16	0/444	0.30	0/588
3	Lo	0.14	0/823	0.26	0/1088
4	SY	0.11	0/911	0.28	0/1227
5	SX	0.12	0/1077	0.30	0/1441
6	SW	0.13	0/1040	0.28	0/1393
7	SV	0.11	0/630	0.26	0/843
8	SU	0.11	0/433	0.27	0/582
9	SR	0.13	0/950	0.36	0/1291
10	SQ	0.09	0/921	0.28	0/1251
11	SO	0.12	0/994	0.28	0/1336
12	SN	0.13	0/1210	0.27	0/1633
13	SL	0.12	0/1178	0.26	0/1578
14	SK	0.08	0/484	0.23	0/667
15	SJ	0.11	0/1455	0.25	0/1954
16	SH	0.12	0/1409	0.30	0/1903
17	Sg	0.11	0/1259	0.37	1/1730 (0.1%)
18	SF	0.09	0/1342	0.25	0/1823
19	SE	0.12	0/2079	0.29	0/2801
20	Se	0.12	0/397	0.35	0/520
21	SD	0.13	0/1090	0.30	0/1487
22	Sd	0.12	0/441	0.32	0/589
23	SC	0.14	0/1718	0.32	0/2326
24	Sc	0.09	0/435	0.22	0/587
25	SB	0.12	0/1725	0.28	0/2309
26	Sb	0.14	0/625	0.30	0/842
27	SA	0.13	0/1706	0.28	0/2322
28	mR	0.15	0/192	0.39	0/297
29	LZ	0.12	0/1118	0.23	0/1494
30	LY	0.13	0/1102	0.27	0/1469
31	LX	0.13	0/993	0.26	0/1334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LW	0.13	0/532	0.27	0/708
33	LV	0.13	0/1004	0.27	0/1346
34	LU	0.17	0/814	0.41	0/1094
35	LT	0.13	0/1325	0.25	0/1770
36	LS	0.14	0/1493	0.27	0/2004
37	LR	0.12	0/1478	0.28	0/1961
38	Lr	0.14	0/1002	0.29	0/1343
39	LQ	0.14	0/1529	0.28	0/2044
40	LP	0.15	0/1260	0.29	0/1692
41	Lp	0.15	0/705	0.34	0/937
42	LO	0.14	0/1652	0.28	0/2211
43	LN	0.14	0/1745	0.26	0/2338
44	Ln	0.12	0/236	0.25	0/300
45	LM	0.13	0/1138	0.25	0/1523
46	LL	0.13	0/1724	0.25	0/2306
47	Lk	0.14	0/563	0.31	0/748
48	LJ	0.14	0/1352	0.34	0/1812
49	Lj	0.14	0/716	0.28	0/947
50	LI	0.14	0/1670	0.29	0/2230
51	Li	0.10	0/823	0.23	0/1092
52	LH	0.13	0/1518	0.25	0/2043
53	Lh	0.13	0/1018	0.30	0/1347
54	LG	0.15	0/1824	0.31	0/2465
55	Lg	0.14	0/885	0.29	0/1180
56	LF	0.15	0/1869	0.29	0/2498
57	Lf	0.15	0/887	0.33	0/1190
58	LE	0.14	0/1779	0.32	0/2388
59	Le	0.15	0/1071	0.28	0/1427
60	LD	0.12	0/2400	0.24	0/3220
61	Ld	0.14	0/854	0.27	0/1153
62	LC	0.14	0/2916	0.28	0/3917
63	Lc	0.13	0/770	0.31	0/1034
64	LB	0.14	0/3245	0.28	0/4346
65	Lb	0.13	0/817	0.29	0/1080
66	LA	0.16	0/1933	0.32	0/2589
67	La	0.15	0/1179	0.29	0/1573
68	L7	0.15	0/2840	0.24	0/4425
69	Pt	0.20	0/1721	0.27	0/2679
70	Sa	0.14	0/783	0.32	0/1052
71	L8	0.16	0/3564	0.29	0/5550
72	L5	0.18	1/79977 (0.0%)	0.29	0/124726
73	SZ	0.11	0/385	0.28	0/530
74	ST	0.09	0/851	0.26	0/1157

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SP	0.14	0/807	0.41	0/1100
76	S2	0.17	0/35874	0.28	0/55878
77	SG	0.13	0/1699	0.31	0/2280
78	SI	0.13	0/1677	0.30	0/2243
79	S6	0.11	0/1411	0.26	0/2192
80	SS	0.11	0/916	0.33	0/1256
All	All	0.16	1/210825 (0.0%)	0.29	1/310178 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	4523	A2M	O3'-P	5.06	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Sg	92	LEU	CB-CA-C	-5.12	110.27	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Lm	407	0	423	3	0
2	Ll	434	0	461	5	0
3	Lo	822	0	856	8	0
4	SY	894	0	815	14	0
5	SX	1060	0	1087	10	0
6	SW	1023	0	1063	11	0
7	SV	623	0	627	7	0
8	SU	428	0	394	8	0
9	SR	936	0	866	22	0
10	SQ	912	0	793	10	0
11	SO	981	0	993	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	SN	1186	0	1247	8	0
13	SL	1158	0	1214	6	0
14	SK	470	0	323	3	0
15	SJ	1430	0	1498	15	0
16	SH	1389	0	1384	18	0
17	Sg	1259	0	646	13	0
18	SF	1324	0	1247	20	0
19	SE	2037	0	2131	17	0
20	Se	395	0	422	3	0
21	SD	1082	0	894	9	0
22	Sd	430	0	397	12	0
23	SC	1681	0	1747	14	0
24	Sc	434	0	419	0	0
25	SB	1698	0	1748	20	0
26	Sb	613	0	614	8	0
27	SA	1669	0	1655	19	0
28	mR	172	0	88	3	0
29	LZ	1095	0	1164	18	0
30	LY	1085	0	1144	16	0
31	LX	976	0	1053	6	0
32	LW	519	0	533	7	0
33	LV	987	0	1052	9	0
34	LU	800	0	816	18	0
35	LT	1297	0	1366	15	0
36	LS	1454	0	1485	16	0
37	LR	1462	0	1566	20	0
38	Lr	990	0	1053	8	0
39	LQ	1505	0	1613	17	0
40	LP	1234	0	1254	14	0
41	Lp	695	0	746	10	0
42	LO	1620	0	1753	14	0
43	LN	1700	0	1749	19	0
44	Ln	235	0	284	4	0
45	LM	1116	0	1176	10	0
46	LL	1693	0	1803	15	0
47	Lk	557	0	611	4	0
48	LJ	1329	0	1346	21	0
49	Lj	701	0	735	10	0
50	LI	1632	0	1675	20	0
51	Li	812	0	870	6	0
52	LH	1499	0	1572	15	0
53	Lh	1010	0	1137	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	LG	1791	0	1883	32	0
55	Lg	872	0	950	7	0
56	LF	1835	0	1926	20	0
57	Lf	868	0	891	5	0
58	LE	1742	0	1878	21	0
59	Le	1053	0	1145	13	0
60	LD	2354	0	2345	22	0
61	Ld	840	0	859	4	0
62	LC	2862	0	3036	24	0
63	Lc	760	0	793	12	0
64	LB	3177	0	3301	29	0
65	Lb	815	0	869	12	0
66	LA	1905	0	1994	34	0
67	La	1163	0	1206	15	0
68	L7	2542	0	1284	21	0
69	Pt	1645	0	843	11	0
70	Sa	770	0	811	7	0
71	L8	3256	0	1652	36	0
72	L5	74115	0	37553	617	0
73	SZ	383	0	313	5	0
74	ST	837	0	694	12	0
75	SP	800	0	645	11	0
76	S2	33681	0	17055	379	0
77	SG	1679	0	1731	26	0
78	SI	1648	0	1700	26	0
79	S6	1263	0	647	17	0
80	SS	903	0	728	14	0
81	Lg	1	0	0	0	0
81	Lm	1	0	0	0	0
81	Lo	1	0	0	0	0
81	Lp	1	0	0	0	0
81	Sd	1	0	0	0	0
82	L5	61	0	0	0	0
82	L8	1	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	12	0	0	0	0
82	SQ	1	0	0	0	0
83	L5	80	0	0	0	0
83	L7	5	0	0	0	0
83	L8	5	0	0	0	0
83	LB	1	0	0	0	0
83	LI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	LP	1	0	0	0	0
83	LS	1	0	0	0	0
83	LV	1	0	0	0	0
83	Le	1	0	0	0	0
83	Pt	1	0	0	0	0
83	S2	19	0	0	0	0
83	S6	1	0	0	0	0
83	Sd	2	0	0	0	0
83	mR	1	0	0	0	0
84	L5	47	0	0	0	0
84	LN	1	0	0	0	0
84	S2	11	0	0	0	0
85	L5	10	0	19	0	0
86	L5	467	0	0	1	0
86	L7	9	0	0	0	0
86	L8	16	0	0	0	0
86	LA	6	0	0	0	0
86	LB	5	0	0	0	0
86	LC	3	0	0	0	0
86	LD	1	0	0	0	0
86	LF	2	0	0	1	0
86	LG	1	0	0	0	0
86	LH	1	0	0	0	0
86	LI	1	0	0	0	0
86	LJ	1	0	0	0	0
86	LL	5	0	0	0	0
86	LN	4	0	0	0	0
86	LP	2	0	0	0	0
86	LQ	2	0	0	0	0
86	LR	5	0	0	1	0
86	LT	4	0	0	0	0
86	LV	2	0	0	0	0
86	LW	1	0	0	0	0
86	LY	1	0	0	0	0
86	La	4	0	0	0	0
86	Lb	4	0	0	0	0
86	Lc	2	0	0	0	0
86	Le	2	0	0	0	0
86	Lg	4	0	0	0	0
86	Lh	1	0	0	0	0
86	Lj	1	0	0	0	0
86	Ll	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Ln	1	0	0	0	0
86	Lo	1	0	0	0	0
86	S2	105	0	0	1	0
86	S6	1	0	0	0	0
86	SF	1	0	0	0	0
86	SI	3	0	0	0	0
86	SL	1	0	0	0	0
86	SN	4	0	0	0	0
86	Sa	1	0	0	1	0
All	All	201456	0	144359	1710	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 5.

The worst 5 of 1710 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)
76:S2:880:G:H1	76:S2:906:U:H3	1.26	0.79
72:L5:4095:G:H1	72:L5:4113:U:H3	1.32	0.78
22:Sd:16:GLN:O	22:Sd:27:ARG:NH2	2.18	0.77
72:L5:2611:A:H5'	72:L5:2688:G:H4'	1.66	0.77
72:L5:3717:A:H2'	72:L5:3718:A2M:H8	1.66	0.77

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	
1	Lm	49/128 (38%)	49 (100%)	0	0	100	100
2	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Lo	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
4	SY	121/133 (91%)	117 (97%)	4 (3%)	0	100	100
5	SX	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
6	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
7	SV	81/83 (98%)	81 (100%)	0	0	100	100
8	SU	56/119 (47%)	52 (93%)	4 (7%)	0	100	100
9	SR	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
10	SQ	137/146 (94%)	127 (93%)	10 (7%)	0	100	100
11	SO	133/151 (88%)	125 (94%)	8 (6%)	0	100	100
12	SN	148/151 (98%)	148 (100%)	0	0	100	100
13	SL	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
14	SK	70/165 (42%)	66 (94%)	4 (6%)	0	100	100
15	SJ	176/194 (91%)	174 (99%)	2 (1%)	0	100	100
16	SH	187/194 (96%)	180 (96%)	7 (4%)	0	100	100
17	Sg	221/317 (70%)	181 (82%)	40 (18%)	0	100	100
18	SF	181/204 (89%)	173 (96%)	8 (4%)	0	100	100
19	SE	258/263 (98%)	254 (98%)	4 (2%)	0	100	100
20	Se	47/133 (35%)	46 (98%)	1 (2%)	0	100	100
21	SD	165/243 (68%)	159 (96%)	6 (4%)	0	100	100
22	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
23	SC	218/293 (74%)	213 (98%)	5 (2%)	0	100	100
24	Sc	59/69 (86%)	56 (95%)	3 (5%)	0	100	100
25	SB	211/264 (80%)	209 (99%)	2 (1%)	0	100	100
26	Sb	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
27	SA	213/295 (72%)	208 (98%)	5 (2%)	0	100	100
29	LZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
30	LY	131/145 (90%)	128 (98%)	3 (2%)	0	100	100
31	LX	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
32	LW	60/157 (38%)	60 (100%)	0	0	100	100
33	LV	130/140 (93%)	129 (99%)	1 (1%)	0	100	100
34	LU	97/128 (76%)	93 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
36	LS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
37	LR	179/196 (91%)	178 (99%)	1 (1%)	0	100	100
38	Lr	120/138 (87%)	118 (98%)	2 (2%)	0	100	100
39	LQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
40	LP	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
41	Lp	88/92 (96%)	84 (96%)	4 (4%)	0	100	100
42	LO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
43	LN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
44	Ln	22/25 (88%)	22 (100%)	0	0	100	100
45	LM	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
46	LL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
47	Lk	67/70 (96%)	67 (100%)	0	0	100	100
48	LJ	167/178 (94%)	164 (98%)	3 (2%)	0	100	100
49	Lj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
50	LI	199/214 (93%)	196 (98%)	3 (2%)	0	100	100
51	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
52	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
53	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
54	LG	226/266 (85%)	219 (97%)	7 (3%)	0	100	100
55	Lg	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
56	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
57	Lf	107/111 (96%)	106 (99%)	1 (1%)	0	100	100
58	LE	214/288 (74%)	201 (94%)	13 (6%)	0	100	100
59	Le	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
60	LD	290/297 (98%)	284 (98%)	6 (2%)	0	100	100
61	Ld	104/125 (83%)	101 (97%)	3 (3%)	0	100	100
62	LC	357/427 (84%)	348 (98%)	9 (2%)	0	100	100
63	Lc	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
64	LB	394/397 (99%)	391 (99%)	3 (1%)	0	100	100
65	Lb	96/159 (60%)	91 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	LA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
67	La	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
70	Sa	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
73	SZ	61/125 (49%)	59 (97%)	2 (3%)	0	100	100
74	ST	125/145 (86%)	122 (98%)	3 (2%)	0	100	100
75	SP	124/145 (86%)	120 (97%)	4 (3%)	0	100	100
77	SG	216/249 (87%)	209 (97%)	7 (3%)	0	100	100
78	SI	204/208 (98%)	202 (99%)	2 (1%)	0	100	100
80	SS	136/152 (90%)	128 (94%)	8 (6%)	0	100	100
All	All	10651/12429 (86%)	10356 (97%)	295 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Lm	43/116 (37%)	43 (100%)	0	100	100
2	Ll	45/48 (94%)	45 (100%)	0	100	100
3	Lo	82/93 (88%)	82 (100%)	0	100	100
4	SY	73/115 (64%)	72 (99%)	1 (1%)	59	85
5	SX	101/115 (88%)	100 (99%)	1 (1%)	68	89
6	SW	109/113 (96%)	107 (98%)	2 (2%)	51	80
7	SV	63/67 (94%)	63 (100%)	0	100	100
8	SU	37/107 (35%)	37 (100%)	0	100	100
9	SR	83/122 (68%)	75 (90%)	8 (10%)	8	26
10	SQ	65/121 (54%)	65 (100%)	0	100	100
11	SO	96/119 (81%)	89 (93%)	7 (7%)	13	38
12	SN	125/131 (95%)	124 (99%)	1 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	SL	127/142 (89%)	127 (100%)	0	100	100
14	SK	25/136 (18%)	25 (100%)	0	100	100
15	SJ	145/168 (86%)	145 (100%)	0	100	100
16	SH	131/174 (75%)	130 (99%)	1 (1%)	73	90
17	Sg	17/275 (6%)	17 (100%)	0	100	100
18	SF	116/170 (68%)	115 (99%)	1 (1%)	70	90
19	SE	215/225 (96%)	214 (100%)	1 (0%)	81	93
20	Se	38/104 (36%)	38 (100%)	0	100	100
21	SD	71/202 (35%)	70 (99%)	1 (1%)	59	85
22	Sd	41/49 (84%)	41 (100%)	0	100	100
23	SC	178/225 (79%)	176 (99%)	2 (1%)	65	88
24	Sc	42/62 (68%)	39 (93%)	3 (7%)	13	40
25	SB	184/231 (80%)	179 (97%)	5 (3%)	39	73
26	Sb	68/76 (90%)	67 (98%)	1 (2%)	57	84
27	SA	172/243 (71%)	168 (98%)	4 (2%)	44	76
29	LZ	113/118 (96%)	111 (98%)	2 (2%)	51	80
30	LY	117/135 (87%)	115 (98%)	2 (2%)	53	82
31	LX	107/133 (80%)	106 (99%)	1 (1%)	70	90
32	LW	54/126 (43%)	54 (100%)	0	100	100
33	LV	102/107 (95%)	101 (99%)	1 (1%)	68	89
34	LU	87/115 (76%)	85 (98%)	2 (2%)	44	76
35	LT	139/140 (99%)	137 (99%)	2 (1%)	59	85
36	LS	155/157 (99%)	151 (97%)	4 (3%)	40	73
37	LR	148/175 (85%)	148 (100%)	0	100	100
38	Lr	107/121 (88%)	103 (96%)	4 (4%)	30	64
39	LQ	162/165 (98%)	158 (98%)	4 (2%)	42	74
40	LP	132/135 (98%)	130 (98%)	2 (2%)	57	84
41	Lp	72/75 (96%)	70 (97%)	2 (3%)	38	72
42	LO	167/174 (96%)	165 (99%)	2 (1%)	63	86
43	LN	171/172 (99%)	170 (99%)	1 (1%)	78	93
44	Ln	23/24 (96%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	LM	115/161 (71%)	114 (99%)	1 (1%)	70	90
46	LL	174/177 (98%)	170 (98%)	4 (2%)	44	76
47	Lk	61/65 (94%)	59 (97%)	2 (3%)	33	67
48	LJ	136/149 (91%)	134 (98%)	2 (2%)	57	84
49	Lj	72/80 (90%)	72 (100%)	0	100	100
50	LI	170/181 (94%)	165 (97%)	5 (3%)	37	71
51	Li	80/89 (90%)	79 (99%)	1 (1%)	61	86
52	LH	164/171 (96%)	161 (98%)	3 (2%)	51	80
53	Lh	108/110 (98%)	107 (99%)	1 (1%)	70	90
54	LG	184/223 (82%)	180 (98%)	4 (2%)	45	77
55	Lg	92/96 (96%)	89 (97%)	3 (3%)	33	67
56	LF	186/215 (86%)	182 (98%)	4 (2%)	45	77
57	Lf	86/90 (96%)	86 (100%)	0	100	100
58	LE	188/252 (75%)	184 (98%)	4 (2%)	47	77
59	Le	114/115 (99%)	114 (100%)	0	100	100
60	LD	239/250 (96%)	237 (99%)	2 (1%)	73	90
61	Ld	85/110 (77%)	82 (96%)	3 (4%)	32	66
62	LC	299/348 (86%)	296 (99%)	3 (1%)	68	89
63	Lc	82/97 (84%)	78 (95%)	4 (5%)	22	54
64	LB	340/346 (98%)	339 (100%)	1 (0%)	86	96
65	Lb	81/125 (65%)	81 (100%)	0	100	100
66	LA	189/198 (96%)	186 (98%)	3 (2%)	55	83
67	La	119/120 (99%)	118 (99%)	1 (1%)	73	90
70	Sa	82/98 (84%)	80 (98%)	2 (2%)	43	75
73	SZ	22/103 (21%)	20 (91%)	2 (9%)	9	28
74	ST	52/115 (45%)	52 (100%)	0	100	100
75	SP	50/130 (38%)	50 (100%)	0	100	100
77	SG	166/218 (76%)	165 (99%)	1 (1%)	78	93
78	SI	168/180 (93%)	166 (99%)	2 (1%)	63	86
80	SS	59/132 (45%)	56 (95%)	3 (5%)	21	53
All	All	8311/10565 (79%)	8182 (98%)	129 (2%)	55	83

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	LA	28	ARG
70	Sa	26	CYS
35	LT	154	ILE
35	LT	68	THR
73	SZ	72	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
62	LC	38	ASN
74	ST	11	GLN
62	LC	329	ASN
65	Lb	61	ASN
23	SC	120	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	mR	7/27 (25%)	2 (28%)	0
68	L7	118/120 (98%)	7 (5%)	0
69	Pt	76/77 (98%)	14 (18%)	0
71	L8	151/156 (96%)	30 (19%)	0
72	L5	3424/5069 (67%)	553 (16%)	15 (0%)
76	S2	1556/1869 (83%)	291 (18%)	6 (0%)
79	S6	55/75 (73%)	18 (32%)	1 (1%)
All	All	5387/7393 (72%)	915 (16%)	22 (0%)

5 of 915 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	mR	33	C
28	mR	37	A
68	L7	7	G
68	L7	33	U
68	L7	53	U

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
72	L5	4741	C
76	S2	1244	PSU
76	S2	169	U
76	S2	1508	A
72	L5	1563	A

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

210 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
76	PSU	S2	1347	76	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
72	A2M	L5	2401	72	22,25,26	3.93	10 (45%)	31,36,39	3.71	15 (48%)
76	OMU	S2	116	76	19,22,23	3.00	8 (42%)	26,31,34	1.66	4 (15%)
72	OMG	L5	4637	72	23,26,27	0.52	0	33,38,41	0.49	0
76	PSU	S2	609	76	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
76	OMU	S2	627	76	19,22,23	3.03	8 (42%)	26,31,34	1.69	5 (19%)
72	PSU	L5	3853	72,84	18,21,22	1.04	1 (5%)	22,30,33	1.61	4 (18%)
72	PSU	L5	2843	72	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
72	OMC	L5	1340	72	19,22,23	0.57	0	26,31,34	0.81	1 (3%)
72	PSU	L5	3734	72	18,21,22	1.00	1 (5%)	22,30,33	1.66	4 (18%)
72	OMC	L5	3841	72	19,22,23	0.53	0	26,31,34	0.68	0
76	A2M	S2	576	76	22,25,26	3.94	11 (50%)	31,36,39	3.72	16 (51%)
76	OMG	S2	1328	76	23,26,27	0.47	0	33,38,41	0.48	0
76	OMG	S2	1490	76	23,26,27	0.50	0	33,38,41	0.48	0
72	OMG	L5	4196	69,72	23,26,27	0.52	0	33,38,41	0.46	0
76	PSU	S2	815	76	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
72	OMG	L5	4228	72	23,26,27	0.51	0	33,38,41	0.57	0
76	PSU	S2	801	76	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
72	OMG	L5	1316	72	23,26,27	0.54	0	33,38,41	0.55	0
72	PSU	L5	4403	72	18,21,22	1.02	1 (5%)	22,30,33	1.78	4 (18%)
72	PSU	L5	3762	72	18,21,22	1.12	1 (5%)	22,30,33	1.71	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	PSU	L5	4972	72	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
72	PSU	L5	4552	72	18,21,22	1.10	1 (5%)	22,30,33	1.76	4 (18%)
76	A2M	S2	1383	76	22,25,26	3.92	10 (45%)	31,36,39	3.69	14 (45%)
69	PSU	Pt	56	69	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)
76	OMG	S2	509	76	23,26,27	0.51	0	33,38,41	0.50	0
76	PSU	S2	1445	76	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
76	A2M	S2	484	76	22,25,26	3.86	11 (50%)	31,36,39	3.68	14 (45%)
72	OMC	L5	2422	72,84	19,22,23	0.57	0	26,31,34	0.75	1 (3%)
72	PSU	L5	3770	72	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
76	OMG	S2	1447	76	23,26,27	0.48	0	33,38,41	0.55	0
72	6MZ	L5	4220	72	22,25,26	2.49	5 (22%)	30,36,39	2.18	10 (33%)
72	A2M	L5	398	72	22,25,26	3.90	10 (45%)	31,36,39	3.68	13 (41%)
72	A2M	L5	3867	72	22,25,26	3.95	10 (45%)	31,36,39	3.76	15 (48%)
72	A2M	L5	1871	72	22,25,26	3.92	10 (45%)	31,36,39	3.67	14 (45%)
72	PSU	L5	4353	72	18,21,22	1.04	1 (5%)	22,30,33	1.77	3 (13%)
72	OMC	L5	4536	72	19,22,23	0.58	0	26,31,34	0.72	0
76	PSU	S2	573	76	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
76	OMG	S2	436	76	23,26,27	0.51	0	33,38,41	0.50	0
76	PSU	S2	649	76	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
72	OMG	L5	2364	72	23,26,27	0.51	0	33,38,41	0.47	0
72	OMC	L5	2351	72	19,22,23	0.60	0	26,31,34	0.94	1 (3%)
72	OMU	L5	4227	72	19,22,23	2.99	8 (42%)	26,31,34	1.76	5 (19%)
69	H2U	Pt	21	69	18,21,22	0.54	0	21,30,33	1.14	1 (4%)
72	PSU	L5	4442	72	18,21,22	1.06	1 (5%)	22,30,33	1.79	5 (22%)
72	OMG	L5	3627	72	23,26,27	0.51	0	33,38,41	0.64	0
76	OMC	S2	517	76	19,22,23	0.56	0	26,31,34	0.75	0
72	OMG	L5	3899	72,83	23,26,27	0.56	0	33,38,41	0.55	0
76	A2M	S2	468	76	22,25,26	3.93	10 (45%)	31,36,39	3.67	14 (45%)
76	PSU	S2	572	76	18,21,22	1.04	1 (5%)	22,30,33	1.70	5 (22%)
72	OMU	L5	2837	72	19,22,23	3.00	8 (42%)	26,31,34	1.74	5 (19%)
72	A2M	L5	1326	72	22,25,26	3.93	10 (45%)	31,36,39	3.66	13 (41%)
76	A2M	S2	1678	76	22,25,26	3.94	10 (45%)	31,36,39	3.81	14 (45%)
72	A2M	L5	3785	72	22,25,26	3.93	11 (50%)	31,36,39	3.78	14 (45%)
76	PSU	S2	218	76	18,21,22	1.02	1 (5%)	22,30,33	1.64	5 (22%)
72	5MC	L5	4447	72	18,22,23	0.72	0	26,32,35	0.72	0
72	A2M	L5	3830	72	22,25,26	3.92	10 (45%)	31,36,39	3.70	14 (45%)
72	OMG	L5	4392	72	23,26,27	0.49	0	33,38,41	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	PSU	S2	1367	76	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
72	PSU	L5	3884	72	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
72	PSU	L5	4296	72	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
72	PSU	L5	1779	72	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
76	A2M	S2	512	76	22,25,26	3.94	10 (45%)	31,36,39	3.68	12 (38%)
76	PSU	S2	918	76	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
65	MLZ	Lb	5	65	8,9,10	0.78	0	4,9,11	0.63	0
72	A2M	L5	4590	72	22,25,26	3.95	10 (45%)	31,36,39	3.75	16 (51%)
76	PSU	S2	1232	76	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)
72	OMC	L5	3887	72	19,22,23	0.59	0	26,31,34	0.72	0
72	OMG	L5	1522	72	23,26,27	0.52	0	33,38,41	0.58	0
72	PSU	L5	4312	72	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
76	OMC	S2	1703	76	19,22,23	0.54	0	26,31,34	0.66	0
66	V5N	LA	216	66	9,11,12	2.67	2 (22%)	9,14,16	1.22	0
72	PSU	L5	4521	72,83	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
72	OMG	L5	4623	72	23,26,27	0.52	0	33,38,41	0.54	0
76	PSU	S2	1136	76	18,21,22	1.06	1 (5%)	22,30,33	1.80	5 (22%)
76	PSU	S2	109	76	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
72	PSU	L5	1792	72	18,21,22	1.05	1 (5%)	22,30,33	1.64	4 (18%)
76	B8N	S2	1248	76	24,29,30	3.03	6 (25%)	29,42,45	1.79	6 (20%)
76	PSU	S2	119	76	18,21,22	1.01	1 (5%)	22,30,33	1.59	4 (18%)
76	PSU	S2	406	76	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
72	PSU	L5	1683	72	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
72	OMC	L5	2824	72	19,22,23	0.57	0	26,31,34	0.77	1 (3%)
72	OMU	L5	3925	72	19,22,23	2.99	8 (42%)	26,31,34	1.76	5 (19%)
72	PSU	L5	4299	72	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
76	OMG	S2	683	76	23,26,27	0.54	0	33,38,41	0.48	0
72	OMC	L5	3701	82,72,84	19,22,23	0.55	0	26,31,34	0.56	0
71	PSU	L8	69	71	18,21,22	1.05	1 (5%)	22,30,33	1.69	5 (22%)
72	A2M	L5	4523	72,83	22,25,26	3.90	11 (50%)	31,36,39	3.65	14 (45%)
76	PSU	S2	36	76	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
76	PSU	S2	1625	76	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
72	PSU	L5	4576	72	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
72	A2M	L5	2363	72,83,84	22,25,26	3.92	10 (45%)	31,36,39	3.72	13 (41%)
72	PSU	L5	3639	72	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
72	PSU	L5	4293	72	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	OMU	S2	1804	76	19,22,23	3.03	8 (42%)	26,31,34	1.72	5 (19%)
72	5MC	L5	3782	72,83	18,22,23	0.59	0	26,32,35	0.65	0
72	PSU	L5	3844	72	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
72	A2M	L5	1534	72,83	22,25,26	3.93	9 (40%)	31,36,39	3.83	15 (48%)
76	PSU	S2	1238	76	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
69	OMC	Pt	33	69	19,22,23	0.55	0	26,31,34	0.89	2 (7%)
72	PSU	L5	3758	72	18,21,22	1.06	1 (5%)	22,30,33	1.82	4 (18%)
72	OMU	L5	4498	72	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
72	PSU	L5	4579	72	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
72	PSU	L5	4500	72	18,21,22	1.07	1 (5%)	22,30,33	1.83	5 (22%)
72	PSU	L5	4493	72	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
72	PSU	L5	3637	72	18,21,22	1.05	1 (5%)	22,30,33	1.78	3 (13%)
72	PSU	L5	4673	72	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
72	1MA	L5	1322	72,84	21,25,26	0.53	0	31,37,40	0.76	1 (3%)
76	PSU	S2	1081	76	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
72	PSU	L5	4532	72	18,21,22	1.06	1 (5%)	22,30,33	1.72	4 (18%)
76	G7M	S2	1639	76,69	23,26,27	2.77	8 (34%)	35,39,42	2.32	10 (28%)
72	PSU	L5	4689	72	18,21,22	1.03	1 (5%)	22,30,33	1.83	4 (18%)
72	OMC	L5	4456	72	19,22,23	0.59	0	26,31,34	0.83	1 (3%)
72	PSU	L5	2508	72	18,21,22	1.06	1 (5%)	22,30,33	1.63	4 (18%)
72	PSU	L5	1860	72	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
76	PSU	S2	34	76	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
76	OMC	S2	1391	76	19,22,23	0.52	0	26,31,34	0.65	0
76	PSU	S2	1243	76	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
71	PSU	L8	55	71	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
72	A2M	L5	3760	72	22,25,26	3.95	10 (45%)	31,36,39	3.95	13 (41%)
76	PSU	S2	681	76	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
72	UR3	L5	4530	72	19,22,23	2.75	8 (42%)	26,32,35	1.30	2 (7%)
72	OMG	L5	4499	72	23,26,27	0.52	0	33,38,41	0.47	0
72	PSU	L5	4628	72	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
72	PSU	L5	3729	72	18,21,22	1.10	1 (5%)	22,30,33	1.69	4 (18%)
76	PSU	S2	93	76	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
76	PSU	S2	1643	76,83	18,21,22	1.08	1 (5%)	22,30,33	1.76	5 (22%)
72	PSU	L5	4423	72	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
76	MA6	S2	1851	76	23,26,27	1.45	3 (13%)	34,38,41	3.34	11 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	PSU	L5	4420	72	18,21,22	1.05	1 (5%)	22,30,33	1.63	5 (22%)
71	OMG	L8	75	71	23,26,27	0.50	0	33,38,41	0.51	0
72	PSU	L5	2839	72	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
67	V5N	La	39	67	9,11,12	2.65	2 (22%)	9,14,16	1.22	1 (11%)
72	OMG	L5	3792	72	23,26,27	0.51	0	33,38,41	0.52	0
72	PSU	L5	1744	72	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
72	A2M	L5	3724	72	22,25,26	3.92	10 (45%)	31,36,39	3.73	14 (45%)
72	PSU	L5	3764	72	18,21,22	1.00	1 (5%)	22,30,33	1.65	5 (22%)
76	PSU	S2	866	76	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
72	OMU	L5	4620	72	19,22,23	2.93	8 (42%)	26,31,34	1.59	4 (15%)
72	PSU	L5	1582	72	18,21,22	1.05	1 (5%)	22,30,33	1.60	4 (18%)
76	PSU	S2	686	76	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
76	PSU	S2	1692	76	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
76	A2M	S2	590	76	22,25,26	3.97	9 (40%)	31,36,39	3.97	14 (45%)
72	OMG	L5	2876	72	23,26,27	0.52	0	33,38,41	0.53	0
72	OMC	L5	2861	72	19,22,23	0.58	0	26,31,34	0.77	1 (3%)
3	MLZ	Lo	53	3	8,9,10	0.76	0	4,9,11	0.59	0
72	OMC	L5	1881	82,72	19,22,23	0.58	0	26,31,34	0.64	0
72	PSU	L5	2632	72	18,21,22	1.03	1 (5%)	22,30,33	1.65	4 (18%)
76	A2M	S2	99	76	22,25,26	3.92	10 (45%)	31,36,39	3.69	14 (45%)
72	A2M	L5	2815	72,84	22,25,26	3.93	11 (50%)	31,36,39	3.80	16 (51%)
76	PSU	S2	651	76	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
72	PSU	L5	3920	72,83	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
72	PSU	L5	3715	72	18,21,22	1.07	1 (5%)	22,30,33	1.77	5 (22%)
72	OMG	L5	3744	72	23,26,27	0.51	0	33,38,41	0.48	0
76	PSU	S2	296	76	18,21,22	1.03	1 (5%)	22,30,33	1.74	4 (18%)
72	OMC	L5	3869	72	19,22,23	0.56	0	26,31,34	0.68	0
72	A2M	L5	3825	72	22,25,26	3.92	10 (45%)	31,36,39	3.75	14 (45%)
72	PSU	L5	3851	72	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
72	A2M	L5	400	72	22,25,26	3.92	10 (45%)	31,36,39	3.71	14 (45%)
72	OMG	L5	2424	72	23,26,27	0.51	0	33,38,41	0.44	0
72	A2M	L5	3718	72	22,25,26	3.91	10 (45%)	31,36,39	3.70	15 (48%)
72	PSU	L5	5010	72	18,21,22	1.03	1 (5%)	22,30,33	1.74	4 (18%)
72	OMC	L5	2365	72,83	19,22,23	0.55	0	26,31,34	0.63	0
72	OMC	L5	2804	72	19,22,23	0.55	0	26,31,34	0.68	0
72	PSU	L5	4361	72	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
76	OMG	S2	867	76	23,26,27	0.50	0	33,38,41	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	PSU	S2	814	76	18,21,22	1.02	1 (5%)	22,30,33	1.69	4 (18%)
76	PSU	S2	1174	76	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
72	A2M	L5	1524	72	22,25,26	3.97	10 (45%)	31,36,39	3.95	13 (41%)
76	A2M	S2	1031	76	22,25,26	3.93	10 (45%)	31,36,39	3.67	14 (45%)
69	G7M	Pt	47	69	23,26,27	2.74	10 (43%)	35,39,42	2.13	11 (31%)
76	PSU	S2	863	76	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
72	OMG	L5	4618	72	23,26,27	0.50	0	33,38,41	0.52	0
76	A2M	S2	668	76,83	22,25,26	3.89	11 (50%)	31,36,39	3.62	15 (48%)
72	OMG	L5	4494	72	23,26,27	0.52	0	33,38,41	0.52	0
72	A2M	L5	4571	72	22,25,26	3.94	10 (45%)	31,36,39	3.75	15 (48%)
72	PSU	L5	1677	72	18,21,22	1.05	1 (5%)	22,30,33	1.78	5 (22%)
72	PSU	L5	5001	72	18,21,22	1.05	1 (5%)	22,30,33	1.68	4 (18%)
76	PSU	S2	1004	76	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
72	PSU	L5	4471	72	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
76	OMG	S2	644	76	23,26,27	0.49	0	33,38,41	0.51	0
69	4SU	Pt	8	69	18,21,22	3.80	8 (44%)	26,30,33	2.22	5 (19%)
76	PSU	S2	966	76	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
72	PSU	L5	1781	72	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
72	PSU	L5	3768	72	18,21,22	1.07	1 (5%)	22,30,33	1.69	4 (18%)
72	PSU	L5	4569	72	18,21,22	1.09	1 (5%)	22,30,33	1.67	4 (18%)
76	PSU	S2	1239	76	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
76	4AC	S2	1337	76	21,24,25	3.52	10 (47%)	29,34,37	1.08	3 (10%)
72	PSU	L5	4457	72	18,21,22	1.05	1 (5%)	22,30,33	1.75	5 (22%)
72	OMC	L5	3808	72	19,22,23	0.61	0	26,31,34	0.91	2 (7%)
72	PSU	L5	1536	72	18,21,22	1.08	1 (5%)	22,30,33	1.80	4 (18%)
76	6MZ	S2	1832	76,83	22,25,26	2.63	3 (13%)	30,36,39	2.50	12 (40%)
72	PSU	L5	1862	72	18,21,22	1.03	1 (5%)	22,30,33	1.76	4 (18%)
76	4AC	S2	1842	76	21,24,25	3.43	10 (47%)	29,34,37	1.09	3 (10%)
76	OMU	S2	428	76	19,22,23	3.02	8 (42%)	26,31,34	1.74	5 (19%)
76	PSU	S2	105	76	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
76	PSU	S2	822	76	18,21,22	1.11	2 (11%)	22,30,33	1.83	5 (22%)
76	PSU	S2	1244	76	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
72	OMG	L5	1625	72	23,26,27	0.51	0	33,38,41	0.50	0
72	PSU	L5	3695	72	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
72	OMG	L5	4370	72	23,26,27	0.51	0	33,38,41	0.49	0
72	PSU	L5	1782	72	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	MA6	S2	1850	76	23,26,27	1.47	4 (17%)	34,38,41	3.31	12 (35%)
72	PSU	L5	4431	72	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
76	PSU	S2	1056	76	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
76	PSU	S2	1177	76	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
72	PSU	L5	4531	72	18,21,22	1.07	1 (5%)	22,30,33	1.80	5 (22%)
76	OMC	S2	462	76	19,22,23	0.54	0	26,31,34	0.71	0
72	PSU	L5	4636	72	18,21,22	1.07	1 (5%)	22,30,33	1.89	6 (27%)
76	A2M	S2	27	76,83	22,25,26	3.92	10 (45%)	31,36,39	3.68	13 (41%)

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
76	PSU	S2	1347	76	-	0/7/25/26	0/2/2/2
72	A2M	L5	2401	72	-	0/9/27/28	0/3/3/3
76	OMU	S2	116	76	-	1/9/27/28	0/2/2/2
72	OMG	L5	4637	72	-	3/9/27/28	0/3/3/3
76	PSU	S2	609	76	-	0/7/25/26	0/2/2/2
76	OMU	S2	627	76	-	4/9/27/28	0/2/2/2
72	PSU	L5	3853	72,84	-	0/7/25/26	0/2/2/2
72	PSU	L5	2843	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	1340	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	3734	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	3841	72	-	0/9/27/28	0/2/2/2
76	A2M	S2	576	76	-	3/9/27/28	0/3/3/3
76	OMG	S2	1328	76	-	0/9/27/28	0/3/3/3
76	OMG	S2	1490	76	-	1/9/27/28	0/3/3/3
72	OMG	L5	4196	69,72	-	1/9/27/28	0/3/3/3
76	PSU	S2	815	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	4228	72	-	0/9/27/28	0/3/3/3
76	PSU	S2	801	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	1316	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	4403	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	3762	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4972	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4552	72	-	0/7/25/26	0/2/2/2
76	A2M	S2	1383	76	-	1/9/27/28	0/3/3/3
69	PSU	Pt	56	69	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	OMG	S2	509	76	-	1/9/27/28	0/3/3/3
76	PSU	S2	1445	76	-	0/7/25/26	0/2/2/2
76	A2M	S2	484	76	-	1/9/27/28	0/3/3/3
72	OMC	L5	2422	72,84	-	2/9/27/28	0/2/2/2
72	PSU	L5	3770	72	-	0/7/25/26	0/2/2/2
76	OMG	S2	1447	76	-	3/9/27/28	0/3/3/3
72	6MZ	L5	4220	72	-	0/9/27/28	0/3/3/3
72	A2M	L5	398	72	-	3/9/27/28	0/3/3/3
72	A2M	L5	3867	72	-	3/9/27/28	0/3/3/3
72	A2M	L5	1871	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	4353	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	4536	72	-	0/9/27/28	0/2/2/2
76	PSU	S2	573	76	-	0/7/25/26	0/2/2/2
76	OMG	S2	436	76	-	0/9/27/28	0/3/3/3
76	PSU	S2	649	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	2364	72	-	2/9/27/28	0/3/3/3
72	OMC	L5	2351	72	-	2/9/27/28	0/2/2/2
72	OMU	L5	4227	72	-	0/9/27/28	0/2/2/2
69	H2U	Pt	21	69	-	4/7/38/39	0/2/2/2
72	PSU	L5	4442	72	-	0/7/25/26	0/2/2/2
72	OMG	L5	3627	72	-	0/9/27/28	0/3/3/3
76	OMC	S2	517	76	-	0/9/27/28	0/2/2/2
72	OMG	L5	3899	72,83	-	0/9/27/28	0/3/3/3
76	A2M	S2	468	76	-	2/9/27/28	0/3/3/3
76	PSU	S2	572	76	-	0/7/25/26	0/2/2/2
72	OMU	L5	2837	72	-	0/9/27/28	0/2/2/2
72	A2M	L5	1326	72	-	1/9/27/28	0/3/3/3
76	A2M	S2	1678	76	-	1/9/27/28	0/3/3/3
72	A2M	L5	3785	72	-	3/9/27/28	0/3/3/3
76	PSU	S2	218	76	-	0/7/25/26	0/2/2/2
72	5MC	L5	4447	72	-	4/7/25/26	0/2/2/2
72	A2M	L5	3830	72	-	0/9/27/28	0/3/3/3
72	OMG	L5	4392	72	-	0/9/27/28	0/3/3/3
76	PSU	S2	1367	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	3884	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4296	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	1779	72	-	0/7/25/26	0/2/2/2
76	A2M	S2	512	76	-	2/9/27/28	0/3/3/3
76	PSU	S2	918	76	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	MLZ	Lb	5	65	-	3/7/8/10	-
72	A2M	L5	4590	72	-	1/9/27/28	0/3/3/3
76	PSU	S2	1232	76	-	2/7/25/26	0/2/2/2
72	OMC	L5	3887	72	-	1/9/27/28	0/2/2/2
72	OMG	L5	1522	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	4312	72	-	0/7/25/26	0/2/2/2
76	OMC	S2	1703	76	-	0/9/27/28	0/2/2/2
66	V5N	LA	216	66	-	1/9/10/12	0/1/1/1
72	PSU	L5	4521	72,83	-	0/7/25/26	0/2/2/2
72	OMG	L5	4623	72	-	0/9/27/28	0/3/3/3
76	PSU	S2	1136	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	109	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	1792	72	-	0/7/25/26	0/2/2/2
76	B8N	S2	1248	76	-	4/16/34/35	0/2/2/2
76	PSU	S2	119	76	-	2/7/25/26	0/2/2/2
76	PSU	S2	406	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	1683	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	2824	72	-	1/9/27/28	0/2/2/2
72	OMU	L5	3925	72	-	1/9/27/28	0/2/2/2
72	PSU	L5	4299	72	-	0/7/25/26	0/2/2/2
76	OMG	S2	683	76	-	2/9/27/28	0/3/3/3
72	OMC	L5	3701	82,72,84	-	4/9/27/28	0/2/2/2
71	PSU	L8	69	71	-	2/7/25/26	0/2/2/2
72	A2M	L5	4523	72,83	-	1/9/27/28	0/3/3/3
76	PSU	S2	36	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1625	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	4576	72	-	0/7/25/26	0/2/2/2
72	A2M	L5	2363	72,83,84	-	0/9/27/28	0/3/3/3
72	PSU	L5	3639	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4293	72	-	0/7/25/26	0/2/2/2
76	OMU	S2	1804	76	-	0/9/27/28	0/2/2/2
72	5MC	L5	3782	72,83	-	0/7/25/26	0/2/2/2
72	PSU	L5	3844	72	-	3/7/25/26	0/2/2/2
72	A2M	L5	1534	72,83	-	2/9/27/28	0/3/3/3
76	PSU	S2	1238	76	-	1/7/25/26	0/2/2/2
69	OMC	Pt	33	69	-	1/9/27/28	0/2/2/2
72	PSU	L5	3758	72	-	2/7/25/26	0/2/2/2
72	OMU	L5	4498	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	4579	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4500	72	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	PSU	L5	4493	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	3637	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4673	72	-	0/7/25/26	0/2/2/2
72	1MA	L5	1322	72,84	-	2/7/25/26	0/3/3/3
76	PSU	S2	1081	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	4532	72	-	0/7/25/26	0/2/2/2
76	G7M	S2	1639	76,69	-	2/7/25/26	0/3/3/3
72	PSU	L5	4689	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	4456	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	2508	72	-	2/7/25/26	0/2/2/2
72	PSU	L5	1860	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	34	76	-	0/7/25/26	0/2/2/2
76	OMC	S2	1391	76	-	0/9/27/28	0/2/2/2
76	PSU	S2	1243	76	-	2/7/25/26	0/2/2/2
71	PSU	L8	55	71	-	0/7/25/26	0/2/2/2
72	A2M	L5	3760	72	-	4/9/27/28	0/3/3/3
76	PSU	S2	681	76	-	0/7/25/26	0/2/2/2
72	UR3	L5	4530	72	-	0/7/25/26	0/2/2/2
72	OMG	L5	4499	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	4628	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	3729	72	-	2/7/25/26	0/2/2/2
76	PSU	S2	93	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1643	76,83	-	0/7/25/26	0/2/2/2
72	PSU	L5	4423	72	-	0/7/25/26	0/2/2/2
76	MA6	S2	1851	76	-	1/11/29/30	0/3/3/3
72	PSU	L5	4420	72	-	3/7/25/26	0/2/2/2
71	OMG	L8	75	71	-	1/9/27/28	0/3/3/3
72	PSU	L5	2839	72	-	0/7/25/26	0/2/2/2
67	V5N	La	39	67	-	0/9/10/12	0/1/1/1
72	OMG	L5	3792	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	1744	72	-	0/7/25/26	0/2/2/2
72	A2M	L5	3724	72	-	1/9/27/28	0/3/3/3
72	PSU	L5	3764	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	866	76	-	0/7/25/26	0/2/2/2
72	OMU	L5	4620	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	1582	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	686	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1692	76	-	0/7/25/26	0/2/2/2
76	A2M	S2	590	76	-	6/9/27/28	0/3/3/3
72	OMG	L5	2876	72	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	OMC	L5	2861	72	-	0/9/27/28	0/2/2/2
3	MLZ	Lo	53	3	-	3/7/8/10	-
72	OMC	L5	1881	82,72	-	0/9/27/28	0/2/2/2
72	PSU	L5	2632	72	-	0/7/25/26	0/2/2/2
76	A2M	S2	99	76	-	2/9/27/28	0/3/3/3
72	A2M	L5	2815	72,84	-	1/9/27/28	0/3/3/3
76	PSU	S2	651	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	3920	72,83	-	0/7/25/26	0/2/2/2
72	PSU	L5	3715	72	-	0/7/25/26	0/2/2/2
72	OMG	L5	3744	72	-	0/9/27/28	0/3/3/3
76	PSU	S2	296	76	-	0/7/25/26	0/2/2/2
72	OMC	L5	3869	72	-	0/9/27/28	0/2/2/2
72	A2M	L5	3825	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	3851	72	-	0/7/25/26	0/2/2/2
72	A2M	L5	400	72	-	1/9/27/28	0/3/3/3
72	OMG	L5	2424	72	-	0/9/27/28	0/3/3/3
72	A2M	L5	3718	72	-	1/9/27/28	0/3/3/3
72	PSU	L5	5010	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	2365	72,83	-	0/9/27/28	0/2/2/2
72	OMC	L5	2804	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	4361	72	-	1/7/25/26	0/2/2/2
76	OMG	S2	867	76	-	1/9/27/28	0/3/3/3
76	PSU	S2	814	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1174	76	-	0/7/25/26	0/2/2/2
72	A2M	L5	1524	72	-	0/9/27/28	0/3/3/3
76	A2M	S2	1031	76	-	0/9/27/28	0/3/3/3
69	G7M	Pt	47	69	-	1/7/25/26	0/3/3/3
76	PSU	S2	863	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	4618	72	-	0/9/27/28	0/3/3/3
76	A2M	S2	668	76,83	-	3/9/27/28	0/3/3/3
72	OMG	L5	4494	72	-	0/9/27/28	0/3/3/3
72	A2M	L5	4571	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	1677	72	-	3/7/25/26	0/2/2/2
72	PSU	L5	5001	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	1004	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	4471	72	-	0/7/25/26	0/2/2/2
76	OMG	S2	644	76	-	4/9/27/28	0/3/3/3
69	4SU	Pt	8	69	-	0/7/25/26	0/2/2/2
76	PSU	S2	966	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	1781	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	3768	72	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	PSU	L5	4569	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	1239	76	-	1/7/25/26	0/2/2/2
76	4AC	S2	1337	76	-	0/11/29/30	0/2/2/2
72	PSU	L5	4457	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	3808	72	-	1/9/27/28	0/2/2/2
72	PSU	L5	1536	72	-	0/7/25/26	0/2/2/2
76	6MZ	S2	1832	76,83	-	2/9/27/28	0/3/3/3
72	PSU	L5	1862	72	-	0/7/25/26	0/2/2/2
76	4AC	S2	1842	76	-	0/11/29/30	0/2/2/2
76	OMU	S2	428	76	-	5/9/27/28	0/2/2/2
76	PSU	S2	105	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	822	76	-	1/7/25/26	0/2/2/2
76	PSU	S2	1244	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	1625	72	-	2/9/27/28	0/3/3/3
72	PSU	L5	3695	72	-	0/7/25/26	0/2/2/2
72	OMG	L5	4370	72	-	1/9/27/28	0/3/3/3
72	PSU	L5	1782	72	-	0/7/25/26	0/2/2/2
76	MA6	S2	1850	76	-	1/11/29/30	0/3/3/3
72	PSU	L5	4431	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	1056	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1177	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	4531	72	-	0/7/25/26	0/2/2/2
76	OMC	S2	462	76	-	0/9/27/28	0/2/2/2
72	PSU	L5	4636	72	-	4/7/25/26	0/2/2/2
76	A2M	S2	27	76,83	-	1/9/27/28	0/3/3/3

The worst 5 of 560 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	3867	A2M	C3'-C2'	-12.75	1.24	1.52
72	L5	1534	A2M	C3'-C2'	-12.70	1.24	1.52
72	L5	4590	A2M	C3'-C2'	-12.69	1.24	1.52
76	S2	590	A2M	C3'-C2'	-12.68	1.24	1.52
76	S2	1031	A2M	C3'-C2'	-12.66	1.24	1.52

The worst 5 of 997 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1851	MA6	N1-C6-N6	-13.30	102.54	117.08
76	S2	1850	MA6	N1-C6-N6	-13.06	102.80	117.08
72	L5	1524	A2M	C1'-N9-C8	-12.67	98.53	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	590	A2M	C1'-N9-C8	-12.64	98.59	127.14
72	L5	3760	A2M	C1'-N9-C8	-12.51	98.88	127.14

There are no chirality outliers.

5 of 153 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Lo	53	MLZ	N-CA-CB-CG
3	Lo	53	MLZ	C-CA-CB-CG
65	Lb	5	MLZ	N-CA-CB-CG
65	Lb	5	MLZ	C-CA-CB-CG
72	L5	398	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

60 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	S2	116	OMU	2	0
72	L5	1340	OMC	2	0
76	S2	576	A2M	1	0
76	S2	801	PSU	1	0
72	L5	1316	OMG	1	0
76	S2	1383	A2M	1	0
76	S2	509	OMG	1	0
76	S2	1445	PSU	1	0
76	S2	484	A2M	1	0
72	L5	3770	PSU	1	0
76	S2	1447	OMG	1	0
72	L5	3867	A2M	2	0
72	L5	1871	A2M	1	0
72	L5	4353	PSU	1	0
72	L5	4536	OMC	1	0
76	S2	436	OMG	1	0
76	S2	649	PSU	1	0
72	L5	2351	OMC	2	0
69	Pt	21	H2U	2	0
76	S2	468	A2M	1	0
72	L5	1326	A2M	1	0
76	S2	1678	A2M	1	0
72	L5	3785	A2M	2	0
76	S2	218	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	L5	4447	5MC	1	0
72	L5	4392	OMG	1	0
76	S2	512	A2M	1	0
76	S2	1248	B8N	1	0
72	L5	1683	PSU	1	0
72	L5	2824	OMC	1	0
72	L5	3925	OMU	1	0
72	L5	4299	PSU	1	0
72	L5	4523	A2M	1	0
72	L5	2363	A2M	1	0
69	Pt	33	OMC	1	0
72	L5	4579	PSU	2	0
76	S2	1639	G7M	1	0
76	S2	1391	OMC	1	0
76	S2	681	PSU	1	0
71	L8	75	OMG	2	0
72	L5	3724	A2M	1	0
72	L5	4620	OMU	3	0
76	S2	1692	PSU	1	0
72	L5	3825	A2M	1	0
72	L5	2424	OMG	1	0
72	L5	3718	A2M	3	0
76	S2	867	OMG	1	0
76	S2	1031	A2M	1	0
69	Pt	47	G7M	1	0
76	S2	668	A2M	1	0
72	L5	4571	A2M	1	0
72	L5	1677	PSU	1	0
76	S2	1004	PSU	2	0
76	S2	644	OMG	1	0
72	L5	1781	PSU	1	0
76	S2	1337	4AC	1	0
72	L5	4457	PSU	1	0
72	L5	3808	OMC	1	0
76	S2	1244	PSU	1	0
76	S2	27	A2M	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 261 ligands modelled in this entry, 260 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
85	SPD	L5	5103	-	9,9,9	0.44	0	8,8,8	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	L5	5103	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	L5	5103	SPD	N1-C2-C3-C4
85	L5	5103	SPD	C8-C7-N6-C5
85	L5	5103	SPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
76	S2	2
38	Lr	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lr	2(A):SER	C	3:ALA	N	4.82
1	S2	1832:6MZ	O3'	1833:C	P	4.80
1	S2	1831:A	O3'	1832:6MZ	P	4.40

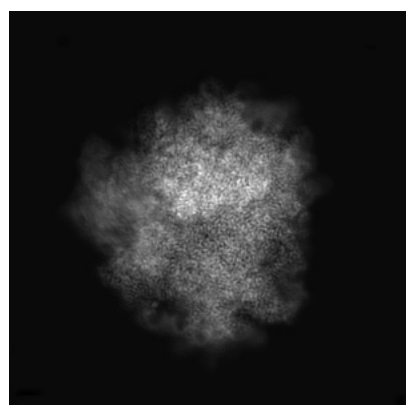
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54268. These allow visual inspection of the internal detail of the map and identification of artifacts.

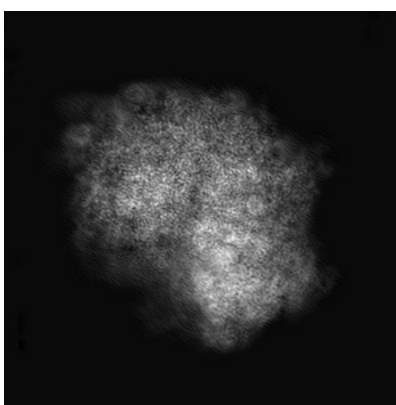
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

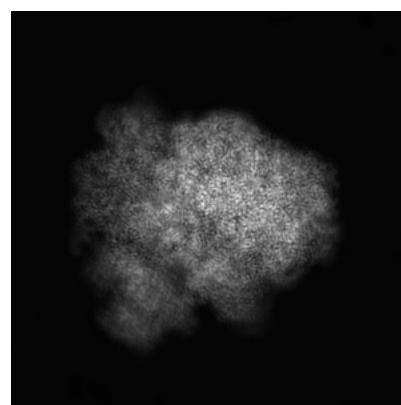
6.1.1 Primary map



X



Y



Z

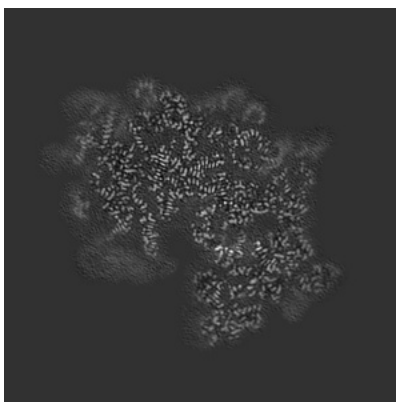
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

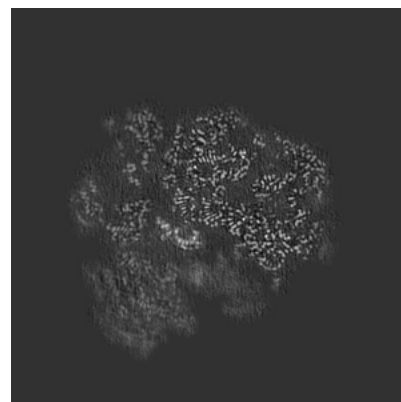
6.2.1 Primary map



X Index: 240



Y Index: 240

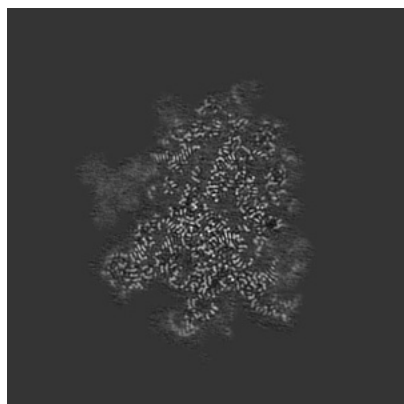


Z Index: 240

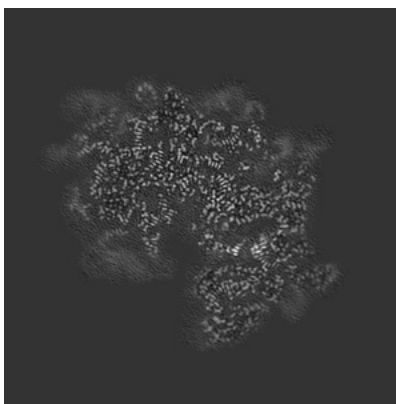
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

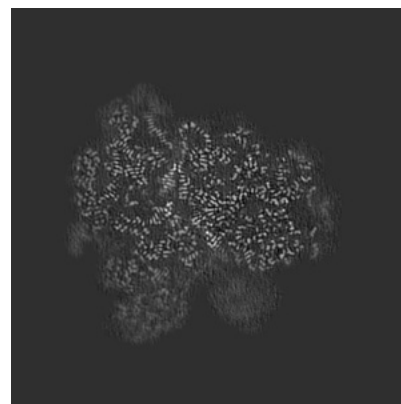
6.3.1 Primary map



X Index: 279



Y Index: 244

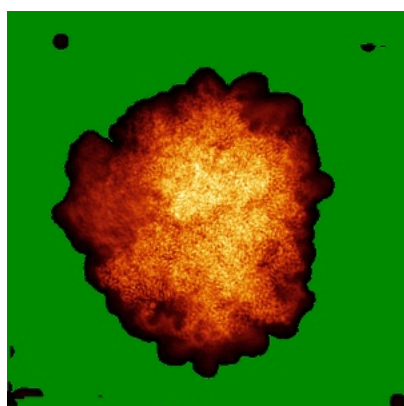


Z Index: 268

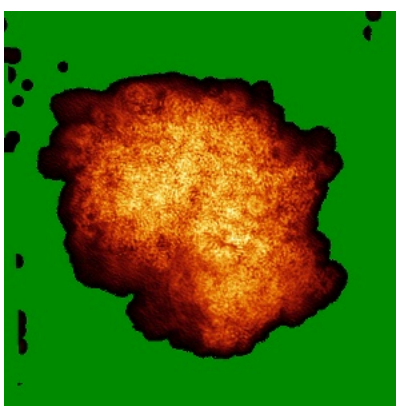
The images above show the largest variance slices of the map in three orthogonal directions.

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

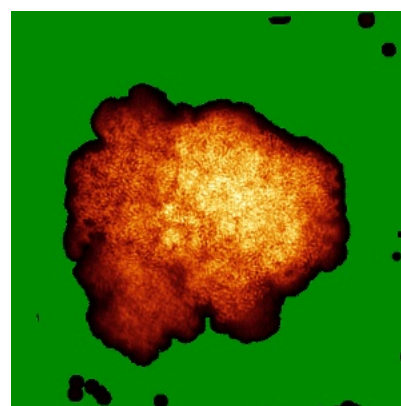
6.4.1 Primary map



X



Y



Z

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 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

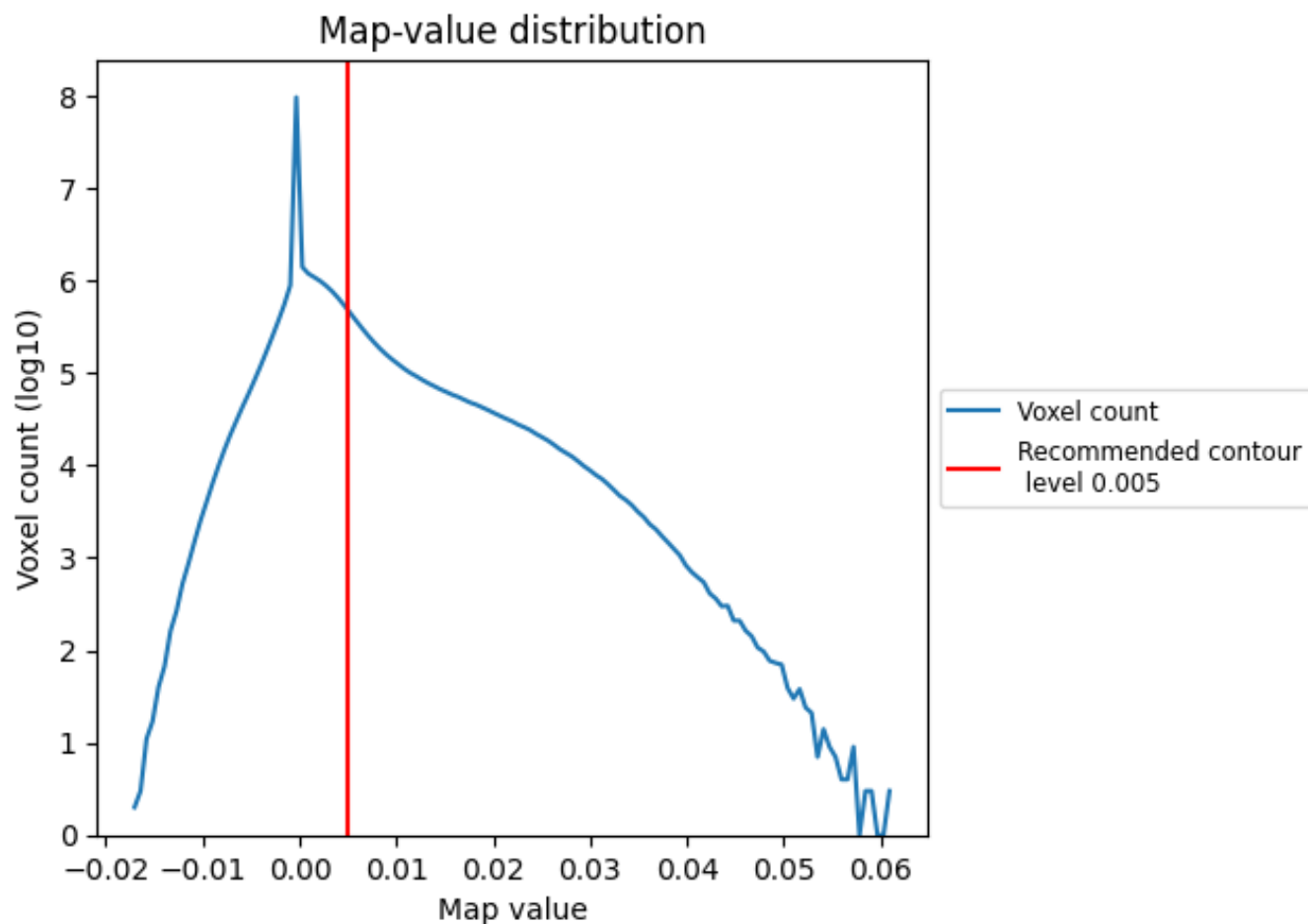
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

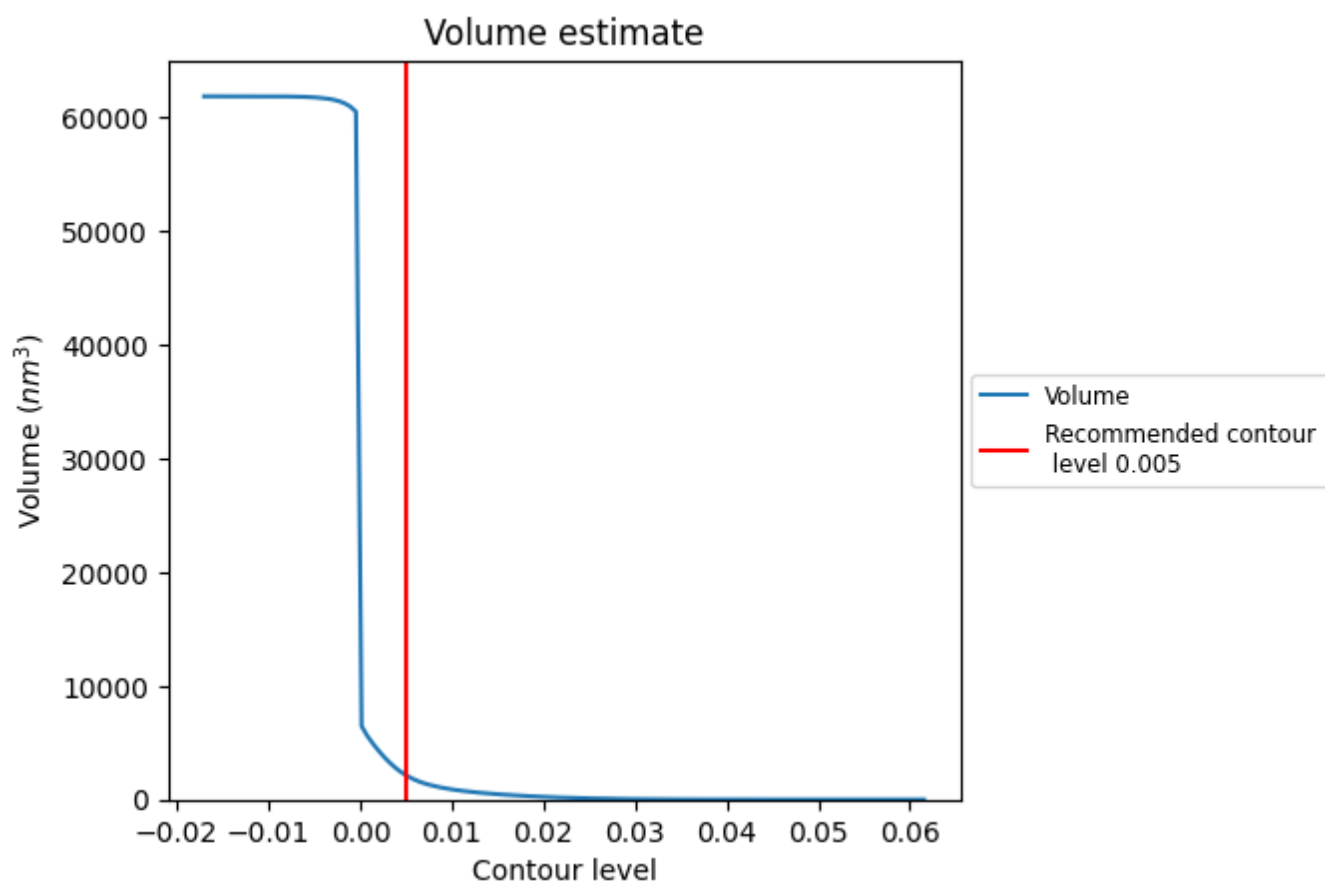
This section contains the results of statistical analysis of the map.

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.

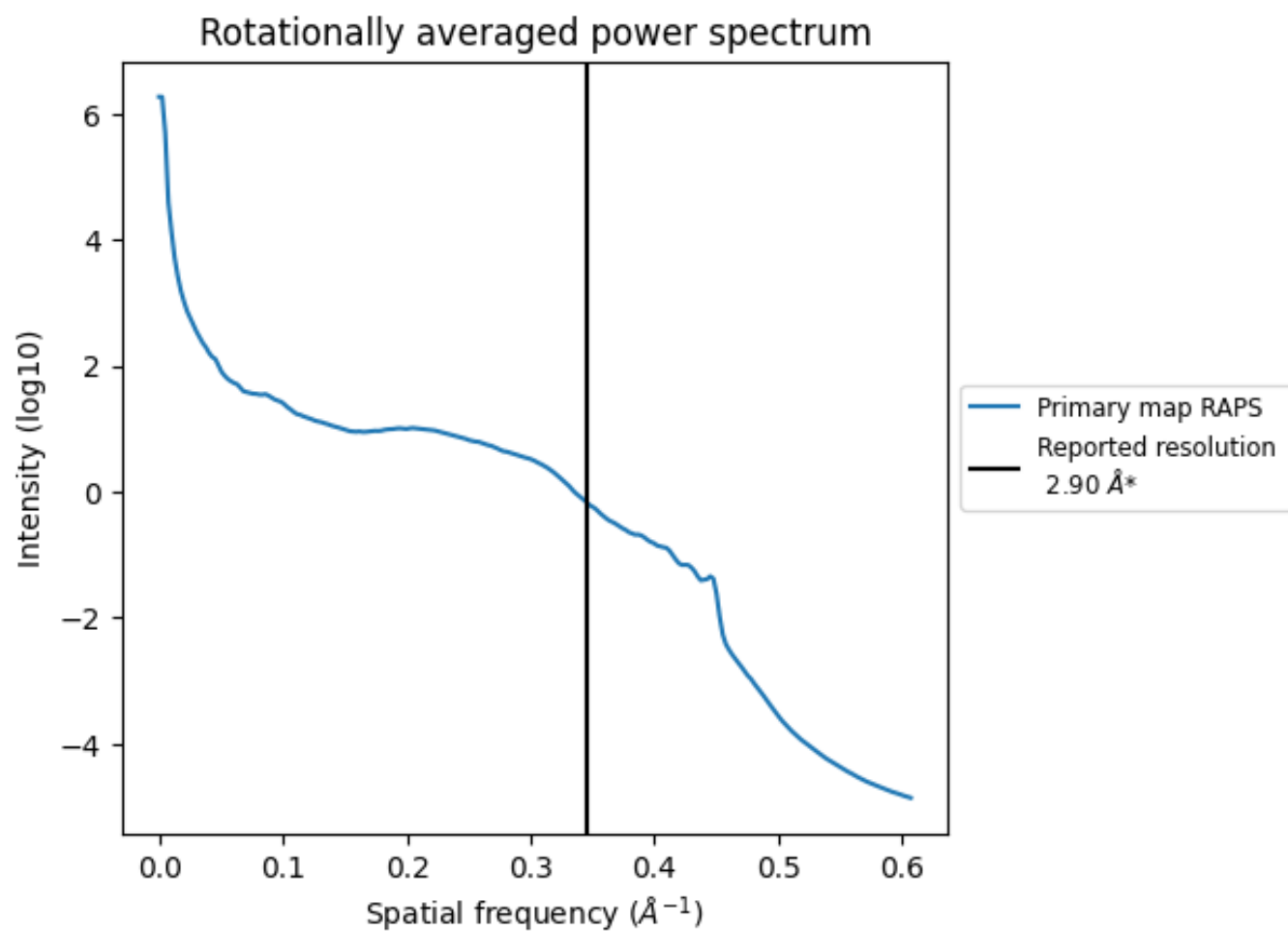
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2149 nm³; this corresponds to an approximate mass of 1941 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 0.345 Å⁻¹

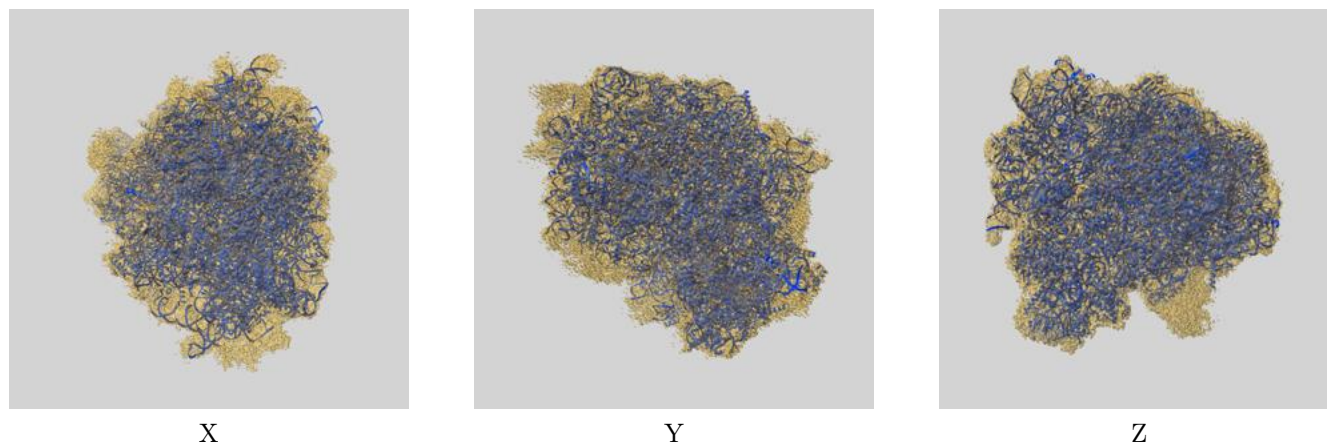
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

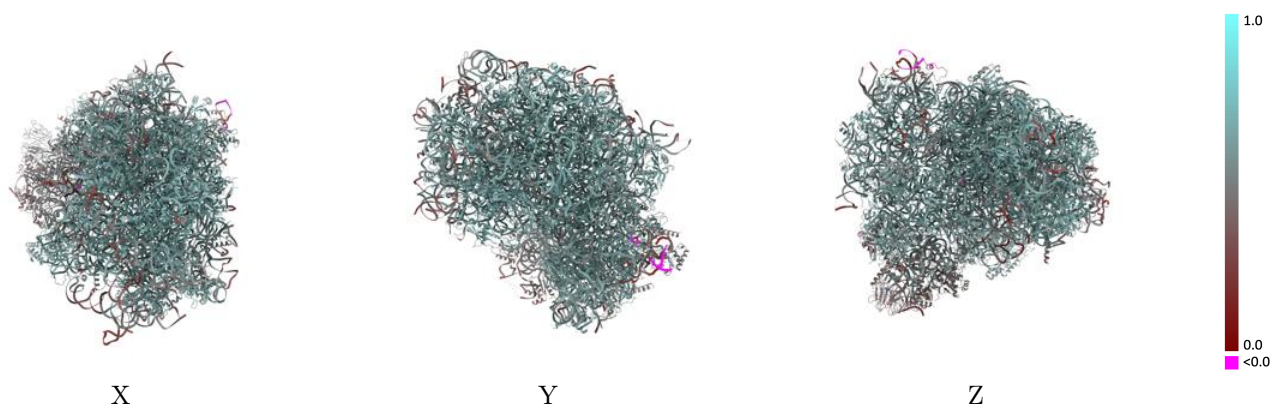
This section contains information regarding the fit between EMDB map EMD-54268 and PDB model 9RUA. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



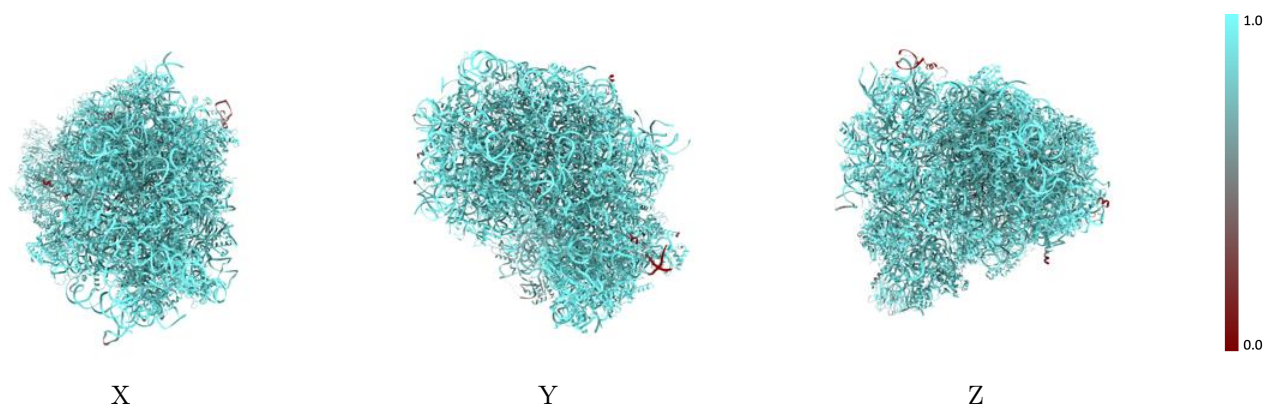
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



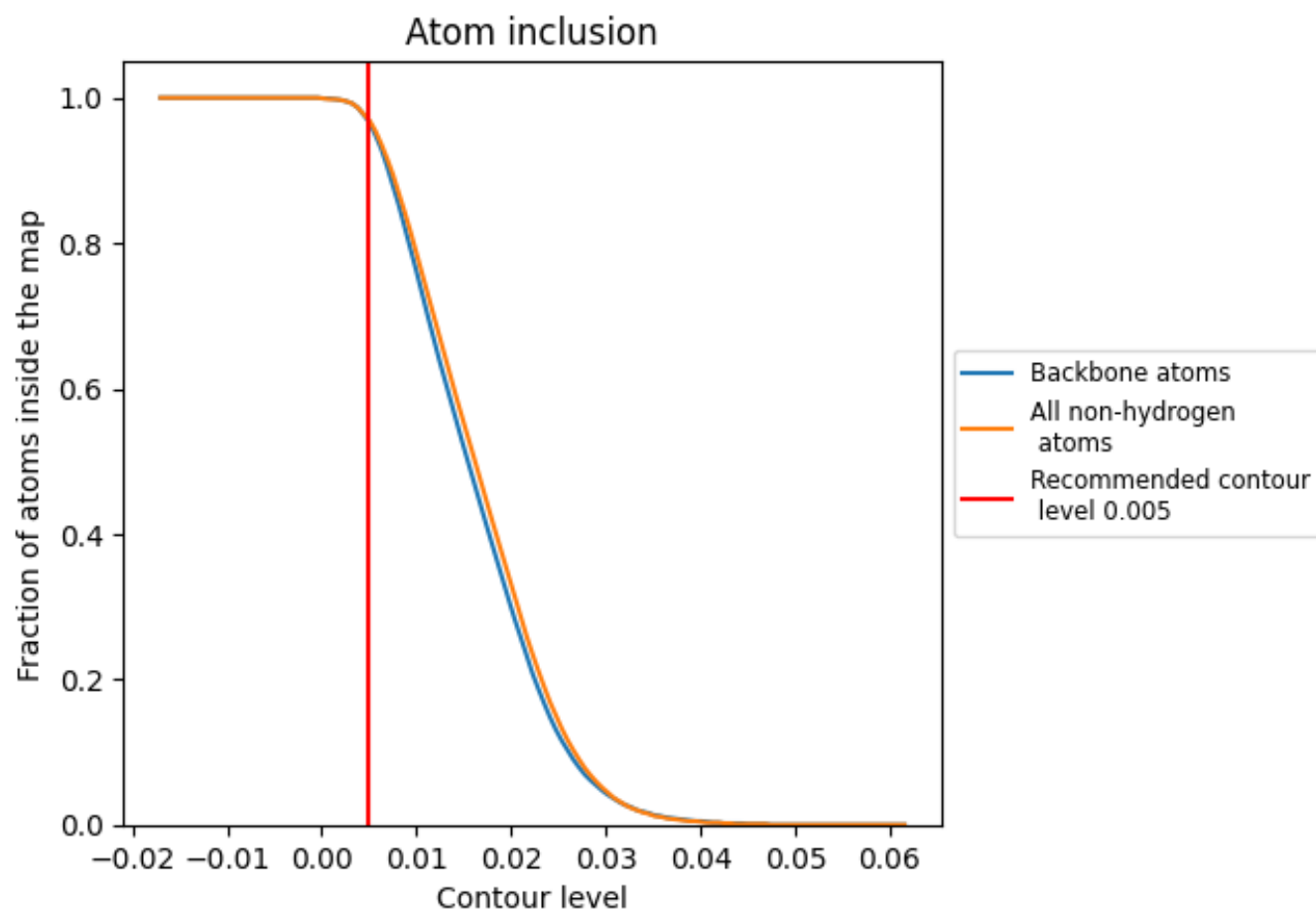
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.5880
L5	 0.9860	 0.5980
L7	 1.0000	 0.6230
L8	 0.9860	 0.6080
LA	 0.9940	 0.6530
LB	 0.9800	 0.6420
LC	 0.9830	 0.6470
LD	 0.9760	 0.6070
LE	 0.9830	 0.6140
LF	 0.9880	 0.6460
LG	 0.9150	 0.5870
LH	 0.9760	 0.6280
LI	 0.9780	 0.6330
LJ	 0.9490	 0.5590
LL	 0.9390	 0.6150
LM	 0.9770	 0.6240
LN	 0.9990	 0.6660
LO	 0.9890	 0.6510
LP	 0.9850	 0.6510
LQ	 0.9950	 0.6560
LR	 0.9730	 0.6070
LS	 0.9890	 0.6480
LT	 0.9760	 0.6330
LU	 0.9590	 0.5590
LV	 0.9890	 0.6450
LW	 0.9940	 0.6380
LX	 0.9760	 0.6310
LY	 0.9860	 0.6390
LZ	 0.9840	 0.6210
La	 0.9900	 0.6580
Lb	 0.9730	 0.5990
Lc	 0.9760	 0.5980
Ld	 0.9890	 0.6370
Le	 0.9890	 0.6590
Lf	 0.9880	 0.6560










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Chain	Atom inclusion	Q-score
Lg	 0.9920	 0.6410
Lh	 0.9530	 0.6170
Li	 0.9740	 0.6150
Lj	 0.9970	 0.6610
Lk	 0.9410	 0.5990
Ll	 0.9860	 0.6340
Lm	 0.9920	 0.6410
Ln	 0.9860	 0.6020
Lo	 0.9890	 0.6420
Lp	 0.9880	 0.6350
Lr	 0.9940	 0.6420
Pt	 0.5970	 0.3410
S2	 0.9680	 0.5530
S6	 0.8700	 0.3220
SA	 0.9450	 0.5880
SB	 0.9490	 0.5950
SC	 0.9660	 0.6040
SD	 0.8770	 0.4980
SE	 0.9720	 0.6030
SF	 0.9240	 0.4950
SG	 0.9500	 0.5620
SH	 0.9180	 0.5460
SI	 0.9170	 0.5690
SJ	 0.9690	 0.5950
SK	 0.8330	 0.4010
SL	 0.9680	 0.6160
SN	 0.9810	 0.6090
SO	 0.9830	 0.5950
SP	 0.8380	 0.4200
SQ	 0.9430	 0.4690
SR	 0.8880	 0.5180
SS	 0.9380	 0.4480
ST	 0.9520	 0.4590
SU	 0.8720	 0.5090
SV	 0.9390	 0.5970
SW	 0.9840	 0.6240
SX	 0.9850	 0.6150
SY	 0.9910	 0.6000
SZ	 0.9290	 0.4260
Sa	 0.9720	 0.6050
Sb	 0.9620	 0.5810
Sc	 0.9210	 0.5260

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Chain	Atom inclusion	Q-score
Sd	 0.9280	 0.4880
Se	 0.9580	 0.5770
Sg	 0.8170	 0.4430
mR	 0.7510	 0.4250