



wwPDB EM Validation Summary Report ⓘ

Jul 6, 2026 – 03:02 pm BST

PDB ID : 9RUC / pdb_00009ruc
EMDB ID : EMD-54269
Title : WT-HEK 80S ribosome bound to H2B mRNA (WT-H2B)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

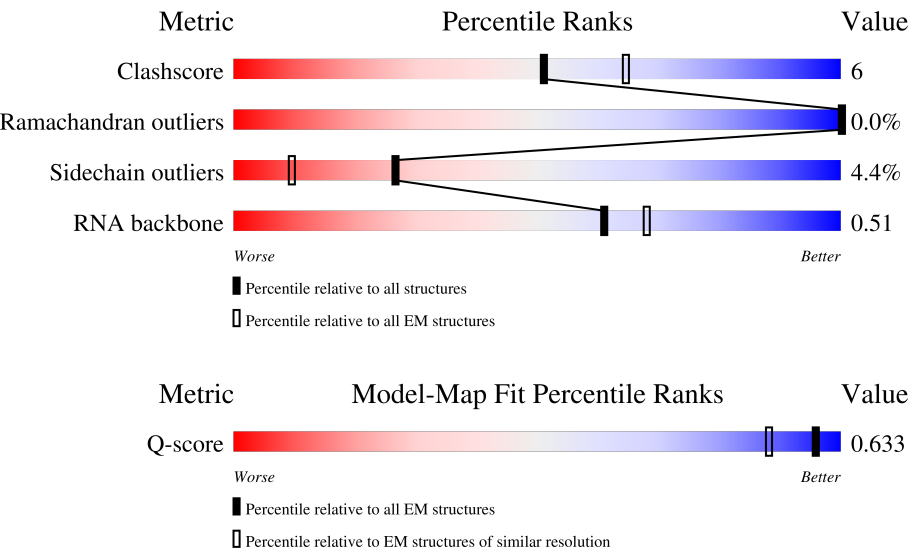
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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.



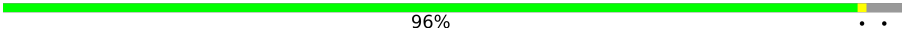
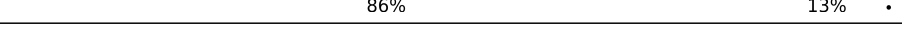
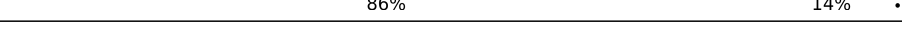
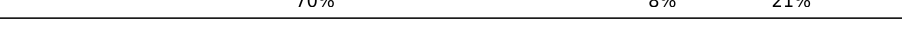
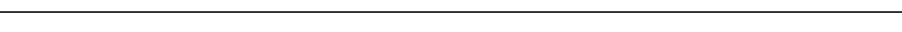
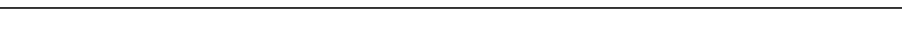
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	L7	120	
2	L8	156	
3	LA	254	

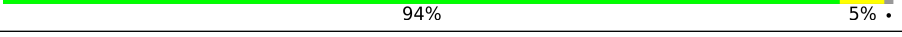
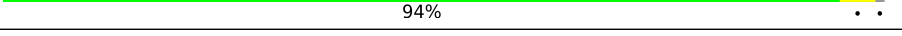
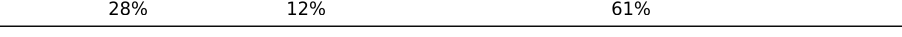
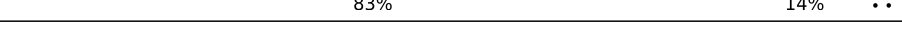
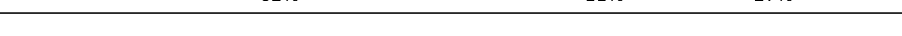
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Mol	Chain	Length	Quality of chain
4	LB	396	 86% 12% ..
5	LC	427	 74% 10% 16%
6	LD	297	 96% ..
7	LE	288	 54% 14% 32%
8	LF	248	 84% 6% 9%
9	LG	266	 70% 9% 21%
10	LH	189	 78% 21% .
11	LI	213	 77% 17% 6%
12	LJ	178	 66% 26% . 6%
13	LL	211	 85% 9% . 5%
14	LM	215	 53% 10% 37%
15	LN	204	 87% 11% .
16	LO	203	 86% 13% .
17	LP	154	 86% 14% .
18	LQ	188	 90% 9% .
19	LR	196	 70% 8% 21%
20	LS	176	 84% 16%
21	LT	160	 86% 13% ..
22	LV	140	 80% 13% 7%
23	LW	157	 38% . 60%
24	LX	156	 64% 12% 24%
25	LY	145	 76% 14% 10%
26	LZ	136	 79% 18% ..
27	La	148	 86% 14% .
28	Lb	159	 53% 8% 39%

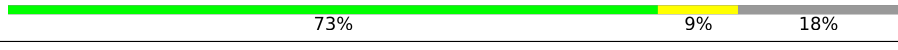
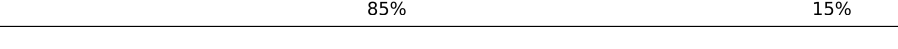
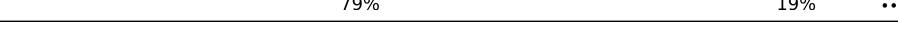
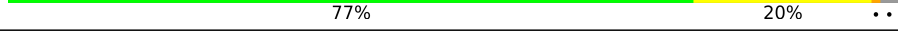
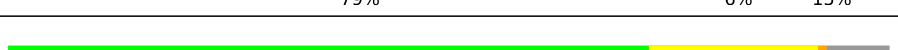
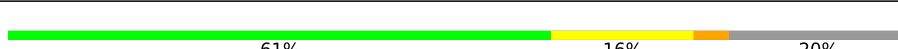
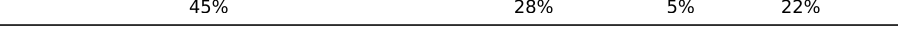
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Mol	Chain	Length	Quality of chain
29	Lc	115	
30	Ld	125	
31	Le	129	
32	Lf	110	
33	Lg	117	
34	Lh	123	
35	Li	105	
36	Lj	87	
37	Lk	70	
38	Ll	51	
39	Lm	127	
40	Ln	25	
41	Lo	105	
42	Lp	92	
43	Lr	137	
44	Pt	77	
45	SA	295	
46	SB	264	
47	SC	293	
48	SF	204	
49	SI	208	
50	mR	27	
51	SD	243	
52	SE	263	
53	SH	194	

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Mol	Chain	Length	Quality of chain
54	SK	165	
55	SL	158	
56	SN	151	
57	SO	151	
58	SP	145	
59	SQ	146	
60	SR	135	
61	SS	152	
62	ST	145	
63	SU	119	
64	SV	84	
65	SW	130	
66	SY	133	
67	SX	143	
68	Sb	84	
69	Sc	69	
70	Sd	56	
71	Se	133	
72	Sg	317	
73	S2	1869	
74	L5	5069	
75	Sa	115	
76	S6	77	
77	SG	249	
78	LU	128	

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Mol	Chain	Length	Quality of chain
79	SZ	125	
80	SJ	194	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 192496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S rRNA.

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

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	150	Total	C	N	O	P	0	0
			3193	1425	565	1053	150		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LA	247	Total	C	N	O	S	0	0
			1888	1182	387	313	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LA	254	LYS	GLU	conflict	UNP P62917

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LB	390	Total	C	N	O	S	0	0
			3091	1968	575	534	14		

- Molecule 5 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LC	357	Total	C	N	O	S	0	0
			2829	1783	563	470	13		

- Molecule 6 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	LD	286	Total	C	N	O		
			1419	846	286	287	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LE	196	Total	C	N	O	S		
			1561	1006	295	256	4	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LF	225	Total	C	N	O	S		
			1845	1187	351	298	9	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LG	211	Total	C	N	O	S		
			1598	1015	308	271	4	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LH	189	Total	C	N	O	S		
			1441	909	269	257	6	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LI	201	Total	C	N	O	S		
			1623	1032	314	265	12	0	0

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LJ	168	Total	C	N	O	S		
			1242	780	234	222	6	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LL	201	Total	C	N	O	S	0	0
			1570	981	327	258	4		

- Molecule 14 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LM	135	Total	C	N	O	S	0	0
			1080	693	207	173	7		

- Molecule 15 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LN	203	Total	C	N	O	S	0	0
			1694	1069	356	265	4		

- Molecule 16 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LO	201	Total	C	N	O	S	0	0
			1634	1055	315	259	5		

- Molecule 17 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 18 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LQ	187	Total	C	N	O	S	0	0
			1497	934	310	248	5		

- Molecule 19 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LR	154	Total	C	N	O	S	0	0
			1251	780	272	190	9		

- Molecule 20 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LS	176	Total	C	N	O	S	0	0
			1456	927	283	235	11		

- Molecule 21 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LT	159	Total	C	N	O	S	0	0
			1293	820	251	216	6		

- Molecule 22 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LV	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

- Molecule 23 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LW	63	Total	C	N	O	S	0	0
			517	329	101	85	2		

- Molecule 24 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LX	118	Total	C	N	O	S	1	0
			977	624	184	168	1		

- Molecule 25 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LY	130	Total	C	N	O	S	0	0
			1084	681	220	180	3		

- Molecule 26 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LZ	135	Total	C	N	O	S	0	0
			1034	668	195	168	3		

- Molecule 27 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	La	147	Total	C	N	O	S	0	0
			1155	730	235	187	3		

- Molecule 28 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Lb	97	Total	C	N	O	S	0	0
			723	450	154	118	1		

- Molecule 29 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lc	98	Total	C	N	O	S	0	0
			738	467	131	134	6		

- Molecule 30 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ld	105	Total	C	N	O	S	0	0
			854	543	167	142	2		

- Molecule 31 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Le	128	Total	C	N	O	S	0	0
			1029	650	209	165	5		

- Molecule 32 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lf	109	Total	C	N	O	S	0	0
			875	555	174	143	3		

- Molecule 33 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lg	106	Total	C	N	O	S	0	0
			825	512	172	135	6		

- Molecule 34 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lh	121	Total	C	N	O	S	1	0
			1012	638	206	167	1		

- Molecule 35 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Li	97	Total	C	N	O	S	0	0
			793	497	167	124	5		

- Molecule 36 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 37 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lk	69	Total	C	N	O	S	0	0
			450	285	85	79	1		

- Molecule 38 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ll	48	Total	C	N	O	S	0	0
			417	266	90	60	1		

- Molecule 39 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lm	50	Total	C	N	O	S	0	0
			400	245	85	64	6		

- Molecule 40 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ln	25	Total	C	N	O	S	0	0
			224	137	58	27	2		

- Molecule 41 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lo	97	Total	C	N	O	S	1	0
			786	494	161	125	6		

- Molecule 42 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 43 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lr	126	Total	C	N	O	S	0	0
			988	611	204	169	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	2	ACE	-	acetylation	UNP P46779

- Molecule 44 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	Pt	75	Total	C	N	O	P	S	0	0
			1605	716	294	519	75	1		

- Molecule 45 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SA	209	Total	C	N	O	S	0	0
			1624	1036	287	293	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	1	ACE	-	acetylation	UNP A0A2J8WY29

- Molecule 46 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SB	219	Total	C	N	O	S	0	0
			1724	1093	313	304	14		

- Molecule 47 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SC	214	Total	C	N	O	S	0	0
			1605	1038	276	282	9		

- Molecule 48 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SF	185	Total	C	N	O	S	0	0
			1362	860	258	237	7		

- Molecule 49 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SI	163	Total	C	N	O	S	0	0
			1123	699	235	187	2		

- Molecule 50 is a RNA chain called Histone H2B mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	mR	8	Total	C	N	O	P	0	0
			172	77	31	56	8		

- Molecule 51 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	202	Total	C	N	O	S	0	0
			1350	852	248	243	7		

- Molecule 52 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE	258	Total	C	N	O	S	0	0
			2029	1296	375	350	8		

- Molecule 53 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	SH	164	Total	C	N	O	0	0
			1133	716	212	205		

- Molecule 54 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SK	47	Total	C	N	O	S	0	0
			339	216	62	57	4		

- Molecule 55 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	130	Total	C	N	O	S	0	0
			1011	646	189	170	6		

- Molecule 56 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SN	150	Total	C	N	O	S	0	0
			1160	745	220	194	1		

- Molecule 57 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SO	129	Total	C	N	O	S	0	0
			956	587	190	173	6		

- Molecule 58 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SP	127	Total	C	N	O	S	0	0
			963	611	178	168	6		

- Molecule 59 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	141	Total	C	N	O	S	0	0
			1099	702	207	187	3		

- Molecule 60 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SR	133	Total	C	N	O	S	0	0
			867	540	172	152	3		

- Molecule 61 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SS	147	Total	C	N	O	S	0	0
			1146	724	230	191	1		

- Molecule 62 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	ST	144	Total	C	N	O	S	0	0
			1043	656	201	183	3		

- Molecule 63 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	SU	75	Total	C	N	O	0	0
			383	230	75	78		

- Molecule 64 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SV	83	Total	C	N	O	S	0	0
			610	376	115	114	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SV	0	ACE	-	acetylation	UNP P63220

- Molecule 65 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SW	129	Total	C	N	O	S	0	0
			1014	649	189	170	6		

- Molecule 66 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SY	121	Total	C	N	O	S	0	0
			952	605	183	159	5		

- Molecule 67 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SX	140	Total	C	N	O	S	0	0
			1082	683	215	181	3		

- Molecule 68 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Sb	71	Total	C	N	O		0	0
			461	285	93	83			

- Molecule 69 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Sc	64	Total	C	N	O	S	0	0
			484	297	93	92	2		

- Molecule 70 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Sd	45	Total	C	N	O	S	0	0
			351	217	71	58	5		

- Molecule 71 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Se	49	Total	C	N	O	S	0	0
			371	226	83	61	1		

- Molecule 72 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sg	261	Total	C	N	O		0	0
			1284	762	261	261			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sg	56	ASN	GLN	conflict	UNP P63244

- Molecule 73 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	S2	1455	Total	C	N	O	P	0	0
			31042	13867	5577	10144	1454		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	140	C	U	conflict	GB 151415227
S2	338	A	G	conflict	GB 151415227
S2	582	C	U	conflict	GB 151415227
S2	583	C	A	conflict	GB 151415227
S2	584	G	A	conflict	GB 151415227
S2	1095	U	C	conflict	GB 151415227

- Molecule 74 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	L5	3192	Total	C	N	O	P	1	0
			68538	30571	12545	22230	3192		

- Molecule 75 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sa	102	Total	C	N	O	S	0	0
			776	484	162	127	3		

- Molecule 76 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	S6	74	Total	C	N	O	P	S	0	0
			1582	705	288	514	74	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SG	214	Total	C	N	O	S	0	0
			1157	700	229	226	2		

- Molecule 78 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	LU	98	Total	C	N	O	S	0	0
			671	423	121	126	1		

- Molecule 79 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
79	SZ	77	Total	C	N	O	0	0
			540	347	101	92		

- Molecule 80 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SJ	178	Total	C	N	O	S	0	0
			1441	922	286	231	2		

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	L7	3	Total	Mg	0
			3	3	
81	L8	4	Total	Mg	0
			4	4	
81	LA	1	Total	Mg	0
			1	1	
81	LB	1	Total	Mg	0
			1	1	
81	LH	2	Total	Mg	0
			2	2	
81	LM	1	Total	Mg	0
			1	1	
81	LN	2	Total	Mg	0
			2	2	
81	LP	1	Total	Mg	0
			1	1	
81	LV	1	Total	Mg	0
			1	1	
81	Lg	1	Total	Mg	0
			1	1	
81	Lj	1	Total	Mg	0
			1	1	
81	S2	14	Total	Mg	0
			14	14	
81	L5	191	Total	Mg	0
			191	191	

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

Mol	Chain	Residues	Atoms	AltConf
82	L8	1	Total K 1 1	0
82	LA	2	Total K 2 2	0
82	LI	1	Total K 1 1	0
82	Lf	1	Total K 1 1	0
82	SL	1	Total K 1 1	0
82	SO	1	Total K 1 1	0
82	S2	2	Total K 2 2	0
82	L5	42	Total K 42 42	0

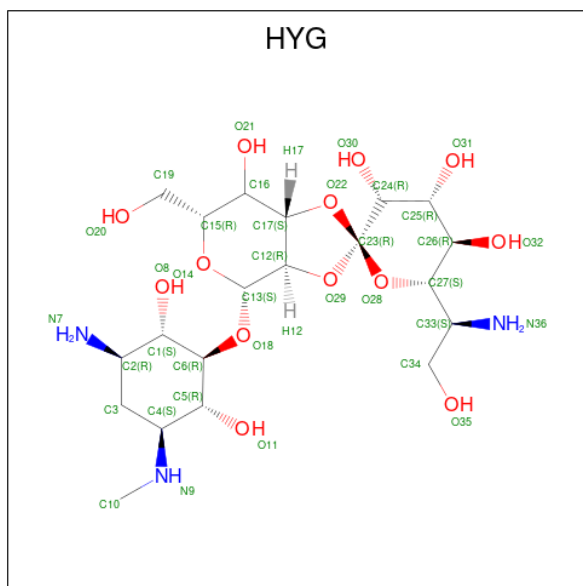
- Molecule 83 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
83	LS	1	Total Na 1 1	0
83	Le	1	Total Na 1 1	0
83	S2	4	Total Na 4 4	0
83	L5	2	Total Na 2 2	0

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

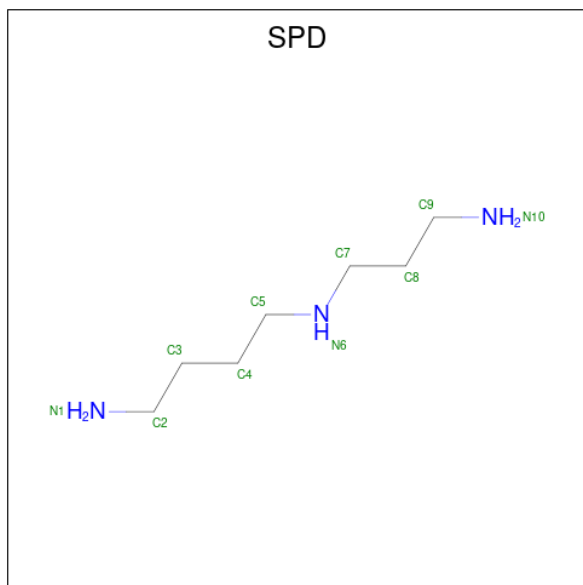
Mol	Chain	Residues	Atoms	AltConf
84	Lg	1	Total Zn 1 1	0
84	Lj	1	Total Zn 1 1	0
84	Lm	1	Total Zn 1 1	0
84	Lo	1	Total Zn 1 1	0
84	Lp	1	Total Zn 1 1	0
84	Sd	1	Total Zn 1 1	0

- Molecule 85 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



Mol	Chain	Residues	Atoms				AltConf
85	S2	1	Total	C	N	O	0
			36	20	3	13	

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

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

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	L7	18	Total	O	0
			18	18	
87	L8	52	Total	O	0
			52	52	
87	LA	41	Total	O	0
			41	41	
87	LB	33	Total	O	0
			33	33	
87	LC	39	Total	O	0
			39	39	
87	LD	5	Total	O	0
			5	5	
87	LE	2	Total	O	0
			2	2	
87	LF	22	Total	O	0
			22	22	
87	LG	2	Total	O	0
			2	2	
87	LH	3	Total	O	0
			3	3	
87	LI	6	Total	O	0
			6	6	
87	LJ	4	Total	O	0
			4	4	
87	LL	21	Total	O	0
			21	21	
87	LM	4	Total	O	0
			4	4	
87	LN	34	Total	O	0
			34	34	
87	LO	6	Total	O	0
			6	6	
87	LP	12	Total	O	0
			12	12	
87	LQ	32	Total	O	0
			32	32	

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Mol	Chain	Residues	Atoms		AltConf
87	LR	31	Total 31	O 31	0
87	LS	8	Total 8	O 8	0
87	LT	14	Total 14	O 14	0
87	LV	8	Total 8	O 8	0
87	LW	1	Total 1	O 1	0
87	LX	1	Total 1	O 1	0
87	LY	6	Total 6	O 6	0
87	La	25	Total 25	O 25	0
87	Lb	11	Total 11	O 11	0
87	Lc	10	Total 10	O 10	0
87	Ld	3	Total 3	O 3	0
87	Le	21	Total 21	O 21	0
87	Lf	11	Total 11	O 11	0
87	Lg	5	Total 5	O 5	0
87	Lh	4	Total 4	O 4	0
87	Lj	19	Total 19	O 19	0
87	Ll	6	Total 6	O 6	0
87	Ln	1	Total 1	O 1	0
87	Lo	9	Total 9	O 9	0
87	Lp	21	Total 21	O 21	0
87	Lr	11	Total 11	O 11	0

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Mol	Chain	Residues	Atoms		AltConf
87	Pt	6	Total 6	O 6	0
87	SB	6	Total 6	O 6	0
87	SC	2	Total 2	O 2	0
87	SF	1	Total 1	O 1	0
87	SI	5	Total 5	O 5	0
87	SE	1	Total 1	O 1	0
87	SL	1	Total 1	O 1	0
87	SN	10	Total 10	O 10	0
87	SO	3	Total 3	O 3	0
87	SS	7	Total 7	O 7	0
87	ST	1	Total 1	O 1	0
87	SW	1	Total 1	O 1	0
87	SX	3	Total 3	O 3	0
87	Sb	1	Total 1	O 1	0
87	S2	237	Total 237	O 237	0
87	L5	1979	Total 1979	O 1979	0
87	Sa	4	Total 4	O 4	0
87	S6	6	Total 6	O 6	0
87	SG	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.

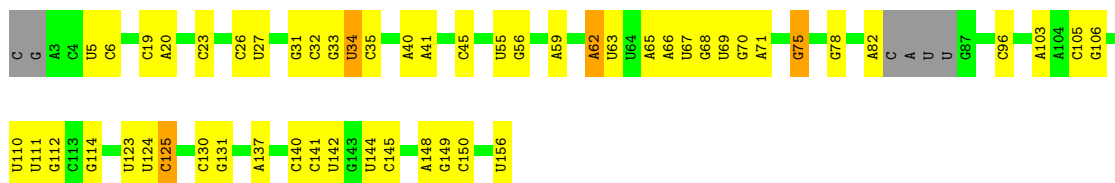
- Molecule 1: 5S rRNA

Chain L7: 



- Molecule 2: 5.8S rRNA

Chain L8: 



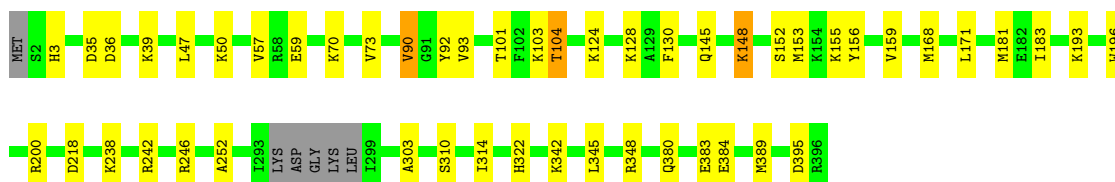
- Molecule 3: Large ribosomal subunit protein uL2

Chain LA: 



- Molecule 4: Large ribosomal subunit protein uL3

Chain LB: 



- Molecule 5: 60S ribosomal protein L4

Chain LC: 

- Molecule 11: Large ribosomal subunit protein uL16

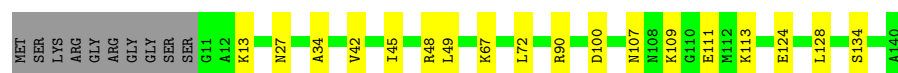
- Molecule 12: 60S ribosomal protein L11

- Molecule 13: Large ribosomal subunit protein eL13

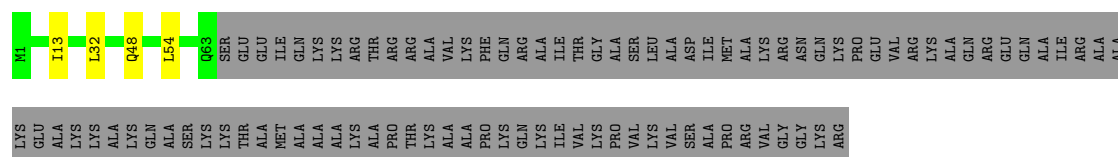
- Molecule 14: 60S ribosomal protein L14

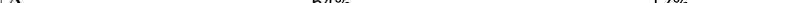
- Molecule 15: 60S ribosomal protein L15

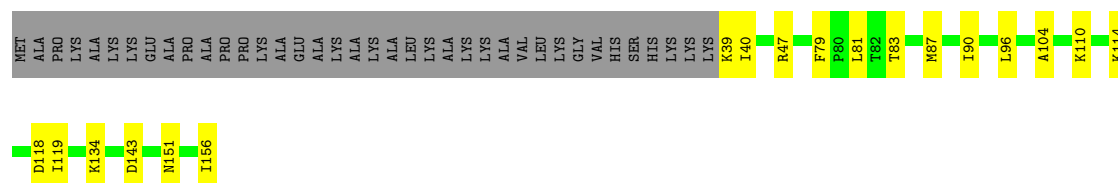
WORLDWIDE
PDB
PROTEIN DATA BANK



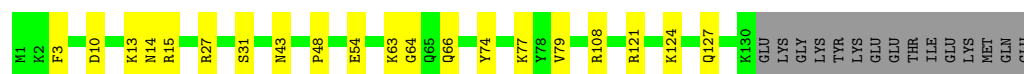
- Chain LW:



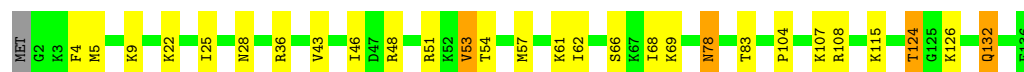
- Chain LX: 

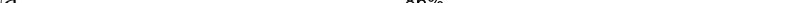


- Chain LY:



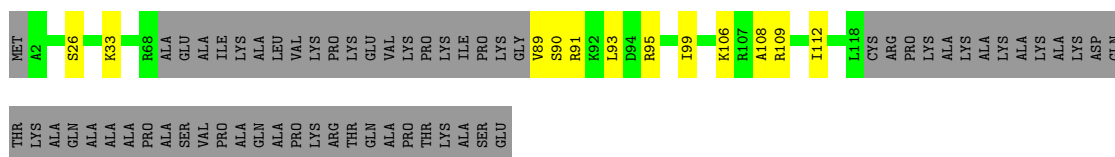
- Chain LZ:  79% 18% 3%



- Chain La:  86% 14%



- Chain Lb:



- Molecule 29: 60S ribosomal protein L30

Chain Lc: 56% 28% 15%



- Molecule 30: 60S ribosomal protein L31

Chain Ld: 72% 11% 16%



- Molecule 31: Large ribosomal subunit protein eL32

Chain Le: 93% 6%



- Molecule 32: Large ribosomal subunit protein eL33

Chain Lf: 87% 12%



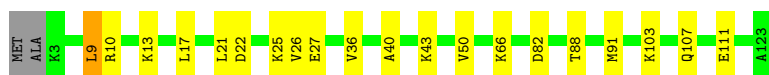
- Molecule 33: 60S ribosomal protein L34

Chain Lg: 80% 10% 9%



- Molecule 34: 60S ribosomal protein L35

Chain Lh: 82% 15% 2%

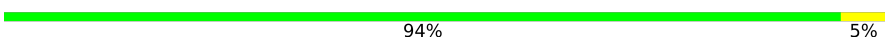


- Molecule 35: 60S ribosomal protein L36

Chain Li:  78% 13% 8%

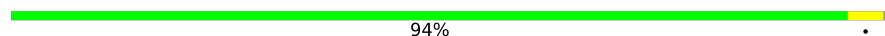


- Molecule 36: Large ribosomal subunit protein eL37

Chain Lj:  94% 5%



- Molecule 37: 60S ribosomal protein L38

Chain Lk:  94%



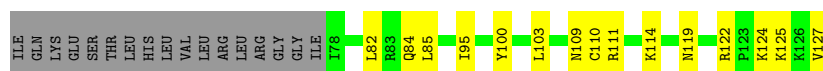
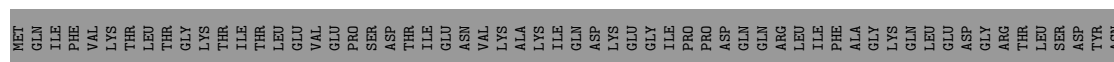
- Molecule 38: 60S ribosomal protein L39

Chain Ll:  76% 18% 6%



- Molecule 39: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  28% 12% 61%



- Molecule 40: 60S ribosomal protein L41

Chain Ln:  88% 12%



- Molecule 41: Large ribosomal subunit protein eL42

Chain Lo:  83% 10% 8%

H272	LEU	M73	ALA	MET
VAL	D104	ASP	ASP	ALA
LYS	L107	ALA	GLY	ALA
HIS	T116	ALA	ALA	ALA
THR	ARG	G119	GLY	GLY
VAL	VAL	Q120	PRO	PRO
VAL	R121	R121	GLY	GLY
GLN	T122	T122	GLY	GLY
ARG	R123	R123	PRO	PRO
THR	GLN	V128	GLY	GLY
GLN	ALA	A129	GLY	GLY
ALA	PRO	I130	PRO	PRO
ALA	ALA	T149	GLY	GLY
VAL	THR	I155	MET	MET
ALA	THR	I155	ASN	ASN
THR	THR	L160	ARG	ARG
		S181	GLY	GLY
		I182	PHE	PHE
		G188	ARG	ARG
		Y169	GLY	GLY
		K173	PHE	PHE
		K176	GLY	GLY
		T179	ILE	ILE
		R187	ARG	GLY
		V191	ARG	GLY
		R194	ARG	GLY
		I195	ARG	GLY
		I196	ARG	ARG
		K212	GLY	GLY
		M216	ARG	GLY
		C222	ARG	GLY
		F236	ALA	GLY
		A237	ALA	ARG
		K238	GLY	GLY
		T247	GLY	GLY
		Y248	LYS	LYS
		D254	ALA	ALA
		T259	GLU	GLU
			ASP	ASP
			LYS	LYS
			F59	F59

E123	D124	S125	G129	ARG	ALA	GLY	THR	V134	R146	R159	K167	A200	K201	R204	MET	THR	GLU	TRP	GLU	THR	ALA	ALA	PRO	ALA	VAL	ALA	GLU	THR	PRO	D16	K22	K23	I30	R31	D32	I33	S34	L35	I39	P50	I68	T73	H78	G84	L87	K88	T89	V90	F97	L103	M107	Q110	V111	L112	V113	M114	A115	I116	I117	R122
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LYS	ARG	SER	LYS	ILE	GLN	LYS	LYS	TYR	ASP	GLU	ARG	LYS	ASN	ALA	LYS	I158	G183	R184	L190	L195	G207	LYS																						
MET	C2	I3	S4	R11	R12	K13	T14	G15	H22	K23	K24	R25	E28	R42	T45	V48	K54	A57	L58	B59	S66	T73	F114	SER	HLI	TYR	ALA	LEU	PRO	LEU	GLY	ARG	LYS	LYS	ALA	THR	PRO	GLU	GLU	GLU	ILE	LEU	ASN	LYS

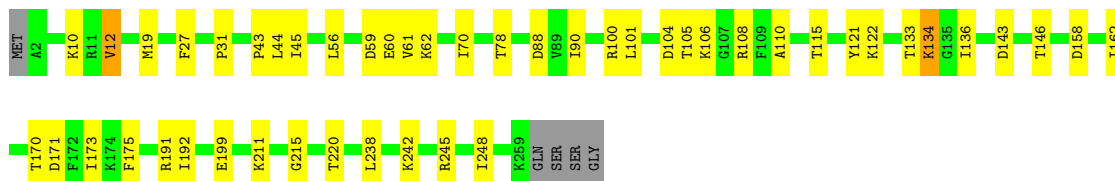
U U U C U G G U G U U U32 U33 A34 A37 U38 G39 C C G G A G U C

V153	V156	V157	V158	G161	D162	P163	Y167	T170	A171	V172	H173	H174	V175	K185	D193	PRO	THR	GLY	LYS	ILE	GLY	PRO	K201	D206	S209	T210	V211	E212	D215	GLU	ILE	LEU	PRO	THR	THR	PRO	ILE	SER	GLN	GLY	GLY	LYS	GLU	GLY	GLU	PRO	PRO	PRO	ALA
V153	V156	V157	V158	G161	D162	P163	Y167	T170	A171	V172	H173	H174	V175	K185	D193	PRO	THR	GLY	LYS	ILE	GLY	PRO	K201	D206	S209	T210	V211	E212	D215	GLU	ILE	LEU	PRO	THR	THR	PRO	ILE	SER	GLN	GLY	GLY	LYS	GLU	GLY	GLU	PRO	PRO	PRO	ALA
Met	V3	S6	A13	I16	F17	K18	T26	R27	A30	E38	V39	I48	L59	GLY	GLU	LVS	ILE	GLY	R64	A71	L86	V91	I99	L105	R106	L109	V115	L123	M127	E128	G133	C134	E135	V136	V137	L342	M150	K151	R152										

PRO
GLN
PRO
VAL
PRO
THR
ALA

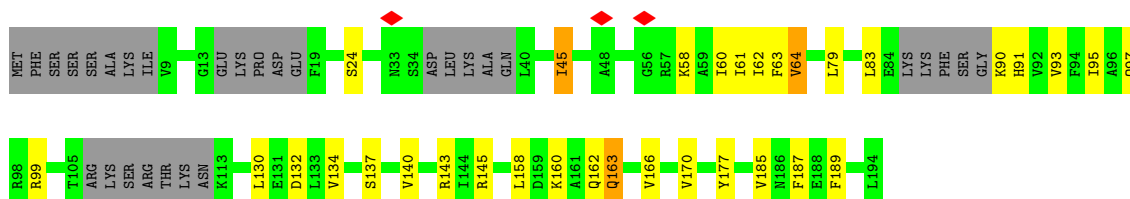
- Molecule 52: Small ribosomal subunit protein eS4, X isoform

Chain SE:  80% 17% ..



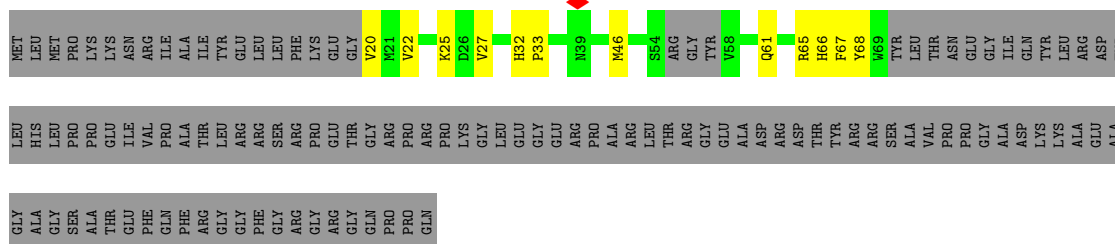
- Molecule 53: 40S ribosomal protein S7

Chain SH:  68% 15% 15%



- Molecule 54: 40S ribosomal protein S10

Chain SK:  21% 7% 72%



- Molecule 55: Small ribosomal subunit protein uS17

Chain SL:  73% 9% 18%



- Molecule 56: 40S ribosomal protein S13

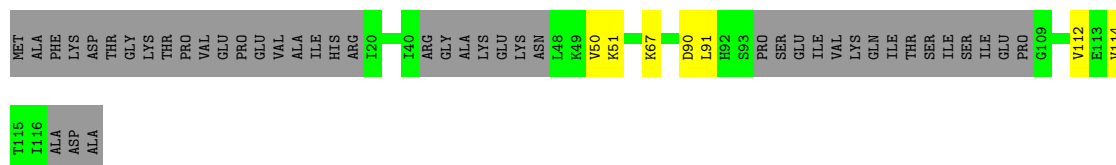
Chain SN:  85% 15%



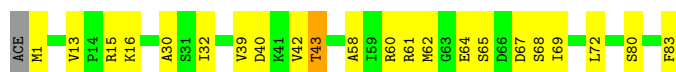
- Chain ST:  79% 19% .



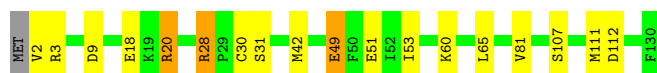
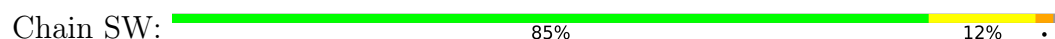
- Molecule 63: 40S ribosomal protein S20



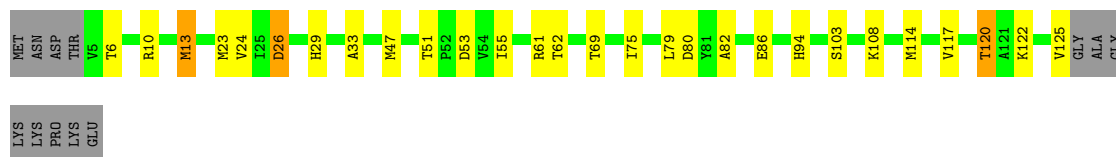
- Molecule 64: Small ribosomal subunit protein eS21



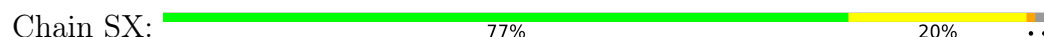
- Molecule 65: 40S ribosomal protein S15a



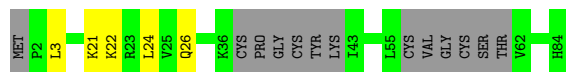
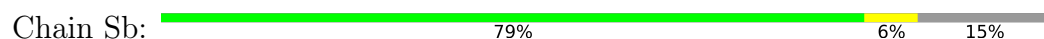
- Molecule 66: 40S ribosomal protein S24



- Molecule 67: 40S ribosomal protein S23

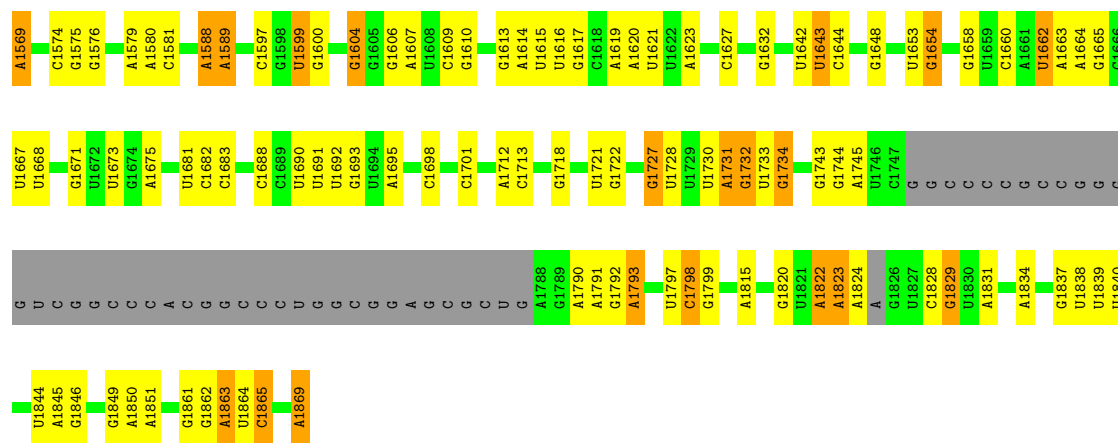


- Molecule 68: 40S ribosomal protein S27

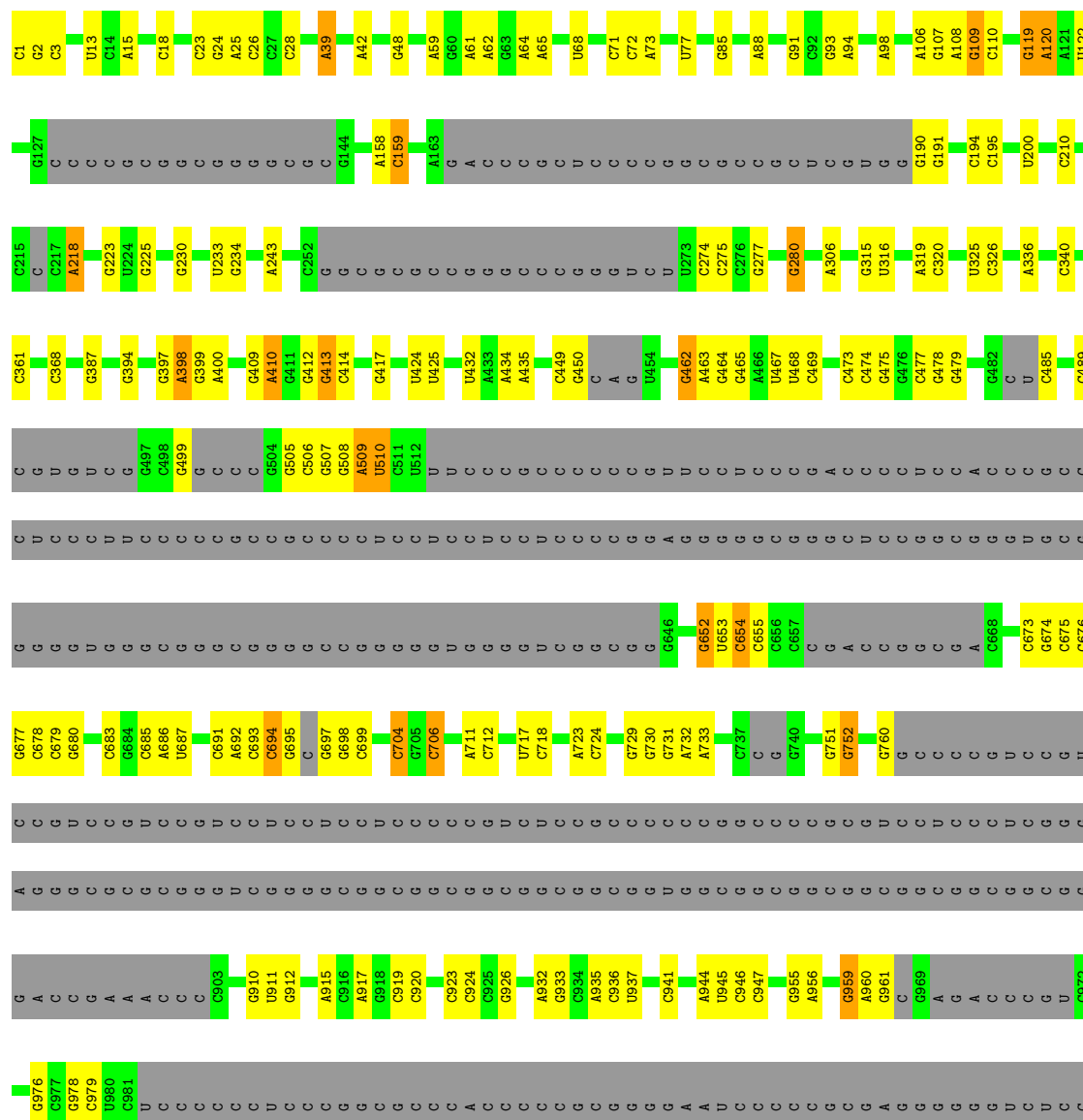


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G1496	G	U1333	C1266	U1178	C1074	C953	U	C504	A670	C552	G507	A398	G312
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U1499	G	G1338	A1181	C1085	C1086	G956	U	U505	G673	G588	G509	C409	C315
U1504	C	U1342	G1270	G1187	G1086	A957	A	A811	C674	G589	A512	C409	G316
U	G	U1343	C1271	A1195	A1087	G958	U	A812	U675	A590	G413	U414	C317
A	U1426	A1344	C1272	U1195	U1088	U959	U	U513	U688	U591	G413	U414	A318
G	C1427	C1273	G1274	U1088	G1089	U960	U	U514	U689	A516	G413	U414	C319
U1508	G1428	U1346	A	C1090	G961	U961	G	A818	G690	C517	A433	G434	G
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G1510	C1430	G1348	C	U1201	A963	U963	G	U522	G	U595	A520	G438	C
U1511	G1431	U1202	A	U1202	A964	U965	G	A825	G	U596	A521	G438	C
C1512	U1432	C1203	G	G1095	G1096	U965	G	A826	A604	A604	A525	C441	C
C1513	C1433	C1204	G	G1097	C1098	U968	U	A827	A605	A605	A526	C441	C
G1514	C1434	C1205	U	C1098	G1099	U968	U	A830	G606	G606	C527	C442	C
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G1516	C1436	G1207	U	A1100	U1101	A972	U	C934	G608	C608	C532	A445	G
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C1521	G	G1212	G	C1109	C1109	U982	G	A	G	U610	G	A449	C
A1522	A	G1212	A	U1114	U1114	A983	A	A	G	G	A	A450	G333
C1527	U	C1215	U	U1115	U1115	U990	C	G	C	G	A	A451	C334
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C1532	C1452	C1218	G	C1117	C1117	A992	U	C	U	C	U	A453	A338
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C1534	A1455	A1220	A	G1119	G1119	A996	G	C942	G617	U455	U	A455	A339
U1535	G1456	G1222	G	U1120	U1120	A997	U	C942	C456	U456	U	A456	C346
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C1544	U1463	A1228	A	U1130	U1130	U1005	U	A	A463	C464	C	A463	C356
A1545	C1464	G1229	G	G1131	G1131	G1006	U	G	A464	C465	C	A464	C356
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C1562	U1408	U1253	U	G1171	G1171	A1027	U	A875	C496	C567	C567	C496	C386
G1563	A1409	G1256	U	U1174	U1174	G1037	U	C876	C500	C568	C568	C496	C387
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C1568	C1415	A1259	G	G1175	G1175	G947	U	C	C501	C570	C570	C501	A389
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Molecule 74: 28S rRNA

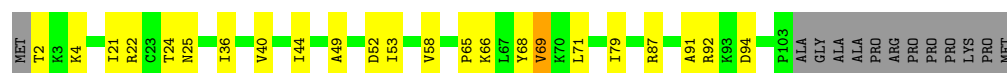




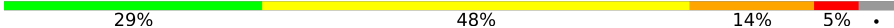


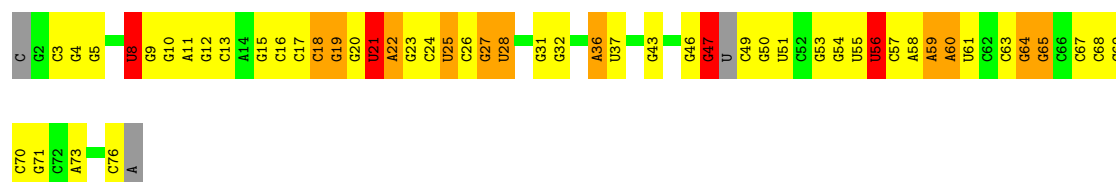
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Chain Sa:  69% 19% 11%



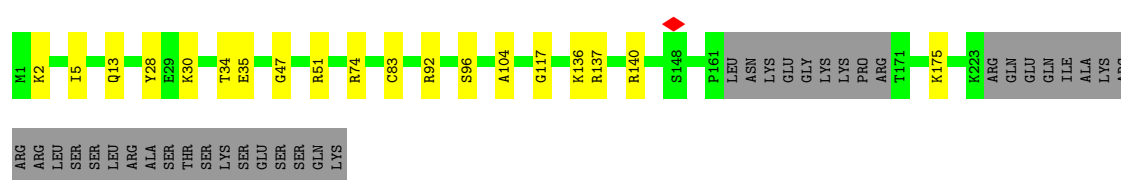
• Molecule 76: E site tRNA

Chain S6:  29% 48% 14% 5%



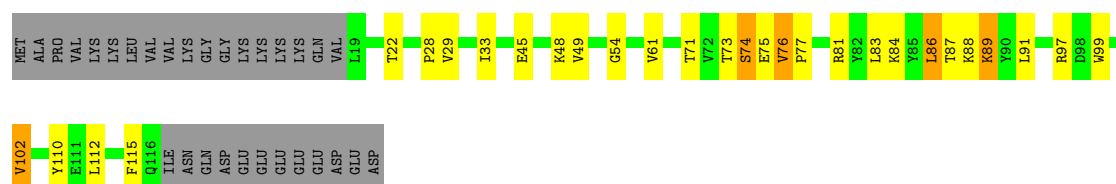
• Molecule 77: 40S ribosomal protein S6

Chain SG:  78% 8% 14%

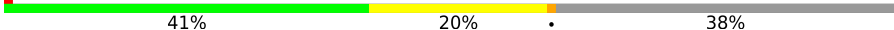


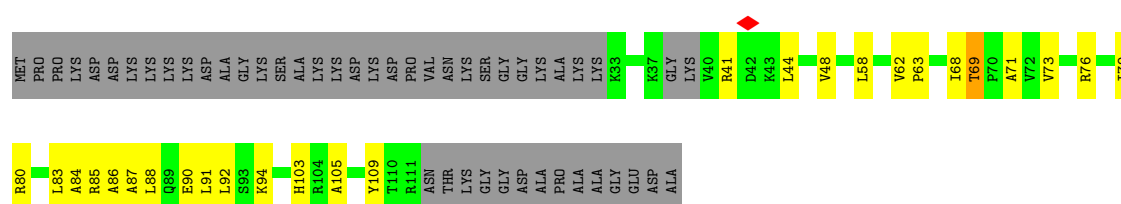
• Molecule 78: 60S ribosomal protein L22

Chain LU:  54% 19% 23%



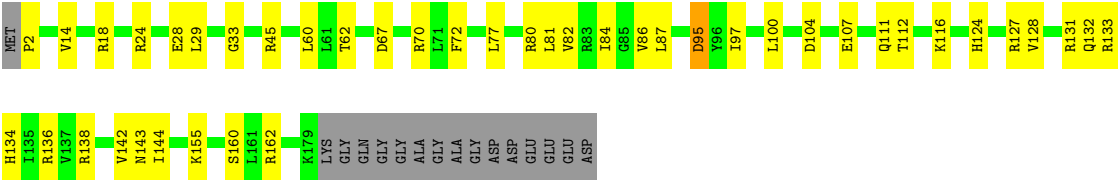
• Molecule 79: Small ribosomal subunit protein eS25

Chain SZ:  41% 20% 38%



• Molecule 80: 40S ribosomal protein S9

Chain SJ:  70% 22% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78814	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	0.153	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	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: MG, 1MA, OMC, PSU, NA, A2M, UR3, OMG, 6MZ, SPD, V5N, HYG, K, ACE, 5MC, G7M, HIC, ZN, MLZ, 4SU, UY1, OMU

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	L7	0.21	0/2840	0.32	0/4425
2	L8	0.24	0/3494	0.33	0/5441
3	LA	0.23	0/1913	0.44	0/2564
4	LB	0.20	0/3145	0.39	0/4220
5	LC	0.21	0/2883	0.38	0/3875
6	LD	0.14	0/1418	0.31	0/1971
7	LE	0.20	0/1591	0.40	0/2138
8	LF	0.21	0/1879	0.39	0/2507
9	LG	0.20	0/1628	0.40	0/2211
10	LH	0.19	0/1460	0.40	0/1974
11	LI	0.19	0/1661	0.35	0/2220
12	LJ	0.18	0/1261	0.43	0/1700
13	LL	0.19	0/1599	0.36	0/2150
14	LM	0.20	0/1102	0.39	0/1479
15	LN	0.23	0/1739	0.39	0/2331
16	LO	0.21	0/1666	0.37	0/2231
17	LP	0.21	0/1260	0.42	0/1692
18	LQ	0.21	0/1521	0.40	0/2036
19	LR	0.24	0/1267	0.38	0/1681
20	LS	0.21	0/1496	0.37	0/2009
21	LT	0.21	0/1321	0.35	0/1766
22	LV	0.20	0/987	0.42	0/1324
23	LW	0.19	0/530	0.40	0/709
24	LX	0.19	0/995	0.38	0/1338
25	LY	0.20	0/1101	0.37	0/1465
26	LZ	0.18	0/1056	0.37	0/1421
27	La	0.20	0/1171	0.37	0/1565
28	Lb	0.20	0/724	0.38	0/969
29	Lc	0.25	0/748	0.43	0/1009
30	Ld	0.24	0/869	0.38	0/1172
31	Le	0.21	0/1047	0.38	0/1403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lf	0.22	0/894	0.39	0/1198
33	Lg	0.20	0/835	0.41	0/1115
34	Lh	0.18	0/1020	0.34	0/1350
35	Li	0.18	0/804	0.39	0/1065
36	Lj	0.21	0/731	0.41	0/967
37	Lk	0.17	0/453	0.32	0/615
38	Ll	0.20	0/427	0.38	0/566
39	Lm	0.17	0/406	0.36	0/541
40	Ln	0.22	0/225	0.33	0/288
41	Lo	0.19	0/803	0.40	0/1063
42	Lp	0.26	0/718	0.41	0/953
43	Lr	0.21	0/1000	0.39	0/1346
44	Pt	0.23	0/1697	0.41	0/2637
45	SA	0.18	0/1660	0.37	0/2259
46	SB	0.19	0/1749	0.35	0/2342
47	SC	0.20	0/1639	0.41	0/2222
48	SF	0.17	0/1382	0.35	0/1873
49	SI	0.19	0/1139	0.39	0/1535
50	mR	0.19	0/192	0.27	0/297
51	SD	0.18	0/1363	0.40	0/1847
52	SE	0.19	0/2071	0.38	0/2793
53	SH	0.17	0/1145	0.39	0/1551
54	SK	0.16	0/349	0.42	0/477
55	SL	0.18	0/1029	0.35	0/1385
56	SN	0.21	0/1184	0.35	0/1600
57	SO	0.21	0/968	0.41	0/1298
58	SP	0.18	0/981	0.38	0/1323
59	SQ	0.18	0/1116	0.36	0/1498
60	SR	0.16	0/876	0.40	0/1189
61	SS	0.19	0/1164	0.42	0/1568
62	ST	0.17	0/1061	0.36	0/1434
63	SU	0.14	0/380	0.36	0/525
64	SV	0.15	0/616	0.27	0/826
65	SW	0.21	0/1031	0.35	0/1382
66	SY	0.17	0/969	0.42	0/1296
67	SX	0.18	0/1098	0.35	0/1464
68	Sb	0.16	0/467	0.31	0/631
69	Sc	0.16	0/486	0.33	0/654
70	Sd	0.16	0/356	0.34	0/472
71	Se	0.16	0/373	0.32	0/493
72	Sg	0.13	0/1278	0.37	0/1766
73	S2	0.24	0/34705	0.37	0/54052
74	L5	0.26	3/73673 (0.0%)	0.37	1/114866 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sa	0.25	0/788	0.53	0/1061
76	S6	0.41	4/1695 (0.2%)	0.45	0/2639
77	SG	0.17	0/1160	0.41	0/1597
78	LU	0.19	0/679	0.48	0/921
79	SZ	0.19	0/546	0.47	0/744
80	SJ	0.20	0/1466	0.40	0/1967
All	All	0.23	7/200219 (0.0%)	0.37	1/294547 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S6	21	U	C5-C6	8.12	1.50	1.34
76	S6	21	U	C2-N3	5.79	1.49	1.37
76	S6	8	4SU	O3'-P	5.46	1.61	1.56
74	L5	3785	A2M	O3'-P	5.22	1.61	1.56
74	L5	1534	A2M	O3'-P	5.18	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	417	G	O4'-C1'-N9	5.57	116.55	108.20

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	L7	2542	0	1285	19	0
2	L8	3193	0	1621	29	0
3	LA	1888	0	1968	16	0
4	LB	3091	0	3148	32	0
5	LC	2829	0	2991	29	0
6	LD	1419	0	665	3	0
7	LE	1561	0	1663	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	LF	1845	0	1959	9	0
9	LG	1598	0	1574	12	0
10	LH	1441	0	1452	20	0
11	LI	1623	0	1665	19	0
12	LJ	1242	0	1190	27	0
13	LL	1570	0	1609	16	0
14	LM	1080	0	1103	18	0
15	LN	1694	0	1738	16	0
16	LO	1634	0	1768	17	0
17	LP	1234	0	1254	13	0
18	LQ	1497	0	1591	12	0
19	LR	1251	0	1351	12	0
20	LS	1456	0	1491	19	0
21	LT	1293	0	1355	11	0
22	LV	973	0	1034	9	0
23	LW	517	0	512	3	0
24	LX	977	0	1046	10	0
25	LY	1084	0	1170	14	0
26	LZ	1034	0	1041	20	0
27	La	1155	0	1184	10	0
28	Lb	723	0	703	9	0
29	Lc	738	0	745	19	0
30	Ld	854	0	897	8	0
31	Le	1029	0	1085	7	0
32	Lf	875	0	912	7	0
33	Lg	825	0	872	8	0
34	Lh	1012	0	1133	14	0
35	Li	793	0	865	10	0
36	Lj	712	0	744	2	0
37	Lk	450	0	385	2	0
38	Ll	417	0	442	8	0
39	Lm	400	0	410	12	0
40	Ln	224	0	260	2	0
41	Lo	786	0	834	6	0
42	Lp	708	0	756	12	0
43	Lr	988	0	1026	10	0
44	Pt	1605	0	824	21	0
45	SA	1624	0	1617	29	0
46	SB	1724	0	1750	36	0
47	SC	1605	0	1637	19	0
48	SF	1362	0	1331	22	0
49	SI	1123	0	989	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	mR	172	0	86	1	0
51	SD	1350	0	1218	22	0
52	SE	2029	0	2103	29	0
53	SH	1133	0	1031	18	0
54	SK	339	0	277	7	0
55	SL	1011	0	1001	9	0
56	SN	1160	0	1195	15	0
57	SO	956	0	979	18	0
58	SP	963	0	938	28	0
59	SQ	1099	0	1150	14	0
60	SR	867	0	729	12	0
61	SS	1146	0	1166	28	0
62	ST	1043	0	1005	18	0
63	SU	383	0	181	3	0
64	SV	610	0	598	16	0
65	SW	1014	0	1050	11	0
66	SY	952	0	973	21	0
67	SX	1082	0	1147	17	0
68	Sb	461	0	360	4	0
69	Sc	484	0	499	8	0
70	Sd	351	0	334	8	0
71	Se	371	0	382	5	0
72	Sg	1284	0	578	9	0
73	S2	31042	0	15693	336	0
74	L5	68538	0	34699	588	0
75	Sa	776	0	805	15	0
76	S6	1582	0	809	23	0
77	SG	1157	0	681	15	0
78	LU	671	0	592	18	0
79	SZ	540	0	507	19	0
80	SJ	1441	0	1520	26	0
81	L5	191	0	0	0	0
81	L7	3	0	0	0	0
81	L8	4	0	0	0	0
81	LA	1	0	0	0	0
81	LB	1	0	0	0	0
81	LH	2	0	0	0	0
81	LM	1	0	0	0	0
81	LN	2	0	0	0	0
81	LP	1	0	0	0	0
81	LV	1	0	0	0	0
81	Lg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	Lj	1	0	0	0	0
81	S2	14	0	0	0	0
82	L5	42	0	0	0	0
82	L8	1	0	0	0	0
82	LA	2	0	0	0	0
82	LI	1	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	2	0	0	0	0
82	SL	1	0	0	0	0
82	SO	1	0	0	0	0
83	L5	2	0	0	0	0
83	LS	1	0	0	0	0
83	Le	1	0	0	0	0
83	S2	4	0	0	0	0
84	Lg	1	0	0	0	0
84	Lj	1	0	0	0	0
84	Lm	1	0	0	0	0
84	Lo	1	0	0	0	0
84	Lp	1	0	0	0	0
84	Sd	1	0	0	0	0
85	S2	36	0	37	0	0
86	L5	30	0	57	0	0
87	L5	1979	0	0	4	0
87	L7	18	0	0	0	0
87	L8	52	0	0	0	0
87	LA	41	0	0	0	0
87	LB	33	0	0	0	0
87	LC	39	0	0	0	0
87	LD	5	0	0	1	0
87	LE	2	0	0	0	0
87	LF	22	0	0	0	0
87	LG	2	0	0	0	0
87	LH	3	0	0	0	0
87	LI	6	0	0	1	0
87	LJ	4	0	0	0	0
87	LL	21	0	0	0	0
87	LM	4	0	0	0	0
87	LN	34	0	0	0	0
87	LO	6	0	0	0	0
87	LP	12	0	0	0	0
87	LQ	32	0	0	0	0
87	LR	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LS	8	0	0	0	0
87	LT	14	0	0	0	0
87	LV	8	0	0	0	0
87	LW	1	0	0	0	0
87	LX	1	0	0	0	0
87	LY	6	0	0	0	0
87	La	25	0	0	0	0
87	Lb	11	0	0	0	0
87	Lc	10	0	0	1	0
87	Ld	3	0	0	0	0
87	Le	21	0	0	0	0
87	Lf	11	0	0	0	0
87	Lg	5	0	0	0	0
87	Lh	4	0	0	0	0
87	Lj	19	0	0	1	0
87	Ll	6	0	0	0	0
87	Ln	1	0	0	0	0
87	Lo	9	0	0	0	0
87	Lp	21	0	0	0	0
87	Lr	11	0	0	0	0
87	Pt	6	0	0	1	0
87	S2	237	0	0	3	0
87	S6	6	0	0	0	0
87	SB	6	0	0	0	0
87	SC	2	0	0	0	0
87	SE	1	0	0	0	0
87	SF	1	0	0	0	0
87	SG	1	0	0	0	0
87	SI	5	0	0	0	0
87	SL	1	0	0	0	0
87	SN	10	0	0	0	0
87	SO	3	0	0	0	0
87	SS	7	0	0	1	0
87	ST	1	0	0	0	0
87	SW	1	0	0	0	0
87	SX	3	0	0	0	0
87	Sa	4	0	0	0	0
87	Sb	1	0	0	0	0
All	All	192496	0	135025	1750	0

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

The worst 5 of 1750 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:S6:21:U:H2'	76:S6:22:A:H4'	1.58	0.86
53:SH:58:LYS:O	53:SH:90:LYS:HA	1.78	0.82
62:ST:43:LYS:NZ	73:S2:1540:G:OP2	2.16	0.79
10:LH:165:THR:HG21	10:LH:179:ILE:H	1.49	0.77
73:S2:1324:G:HO2'	73:S2:1510:G:HO2'	1.26	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	
3	LA	244/254 (96%)	232 (95%)	12 (5%)	0	100	100
4	LB	385/396 (97%)	378 (98%)	7 (2%)	0	100	100
5	LC	355/427 (83%)	347 (98%)	8 (2%)	0	100	100
6	LD	282/297 (95%)	261 (93%)	21 (7%)	0	100	100
7	LE	190/288 (66%)	180 (95%)	10 (5%)	0	100	100
8	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
9	LG	207/266 (78%)	201 (97%)	6 (3%)	0	100	100
10	LH	187/189 (99%)	178 (95%)	9 (5%)	0	100	100
11	LI	197/213 (92%)	191 (97%)	6 (3%)	0	100	100
12	LJ	166/178 (93%)	158 (95%)	8 (5%)	0	100	100
13	LL	199/211 (94%)	193 (97%)	6 (3%)	0	100	100
14	LM	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
15	LN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
16	LO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	LP	151/154 (98%)	147 (97%)	4 (3%)	0	100	100
18	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
19	LR	152/196 (78%)	151 (99%)	1 (1%)	0	100	100
20	LS	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
21	LT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
22	LV	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
23	LW	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
24	LX	117/156 (75%)	115 (98%)	2 (2%)	0	100	100
25	LY	128/145 (88%)	128 (100%)	0	0	100	100
26	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
27	La	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
28	Lb	92/159 (58%)	89 (97%)	3 (3%)	0	100	100
29	Lc	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
30	Ld	103/125 (82%)	102 (99%)	1 (1%)	0	100	100
31	Le	126/129 (98%)	126 (100%)	0	0	100	100
32	Lf	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
33	Lg	104/117 (89%)	102 (98%)	2 (2%)	0	100	100
34	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
35	Li	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
36	Lj	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
37	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
38	Ll	46/51 (90%)	44 (96%)	2 (4%)	0	100	100
39	Lm	48/127 (38%)	46 (96%)	2 (4%)	0	100	100
40	Ln	23/25 (92%)	23 (100%)	0	0	100	100
41	Lo	96/105 (91%)	94 (98%)	2 (2%)	0	100	100
42	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
43	Lr	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
45	SA	207/295 (70%)	196 (95%)	11 (5%)	0	100	100
46	SB	215/264 (81%)	210 (98%)	5 (2%)	0	100	100
47	SC	212/293 (72%)	206 (97%)	6 (3%)	0	100	100
48	SF	181/204 (89%)	169 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	SI	159/208 (76%)	154 (97%)	5 (3%)	0	100	100
51	SD	196/243 (81%)	181 (92%)	15 (8%)	0	100	100
52	SE	256/263 (97%)	240 (94%)	16 (6%)	0	100	100
53	SH	154/194 (79%)	144 (94%)	10 (6%)	0	100	100
54	SK	43/165 (26%)	35 (81%)	8 (19%)	0	100	100
55	SL	126/158 (80%)	121 (96%)	5 (4%)	0	100	100
56	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
57	SO	125/151 (83%)	118 (94%)	7 (6%)	0	100	100
58	SP	125/145 (86%)	120 (96%)	5 (4%)	0	100	100
59	SQ	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
60	SR	131/135 (97%)	122 (93%)	7 (5%)	2 (2%)	8	16
61	SS	145/152 (95%)	133 (92%)	12 (8%)	0	100	100
62	ST	142/145 (98%)	134 (94%)	8 (6%)	0	100	100
63	SU	69/119 (58%)	67 (97%)	2 (3%)	0	100	100
64	SV	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
65	SW	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
66	SY	119/133 (90%)	103 (87%)	15 (13%)	1 (1%)	16	31
67	SX	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
68	Sb	65/84 (77%)	63 (97%)	2 (3%)	0	100	100
69	Sc	62/69 (90%)	59 (95%)	3 (5%)	0	100	100
70	Sd	43/56 (77%)	42 (98%)	1 (2%)	0	100	100
71	Se	45/133 (34%)	42 (93%)	3 (7%)	0	100	100
72	Sg	249/317 (78%)	210 (84%)	39 (16%)	0	100	100
75	Sa	100/115 (87%)	94 (94%)	6 (6%)	0	100	100
77	SG	210/249 (84%)	198 (94%)	12 (6%)	0	100	100
78	LU	96/128 (75%)	81 (84%)	15 (16%)	0	100	100
79	SZ	73/125 (58%)	68 (93%)	5 (7%)	0	100	100
80	SJ	176/194 (91%)	174 (99%)	1 (1%)	1 (1%)	21	38
All	All	10475/12413 (84%)	10040 (96%)	431 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	SR	65	PRO
60	SR	66	VAL
66	SY	103	SER
80	SJ	138	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	LA	187/195 (96%)	185 (99%)	2 (1%)	65	84
4	LB	325/344 (94%)	318 (98%)	7 (2%)	45	73
5	LC	294/348 (84%)	291 (99%)	3 (1%)	68	86
6	LD	1/250 (0%)	1 (100%)	0	100	100
7	LE	168/252 (67%)	159 (95%)	9 (5%)	20	41
8	LF	189/215 (88%)	186 (98%)	3 (2%)	55	79
9	LG	152/223 (68%)	146 (96%)	6 (4%)	28	55
10	LH	150/169 (89%)	136 (91%)	14 (9%)	8	18
11	LI	169/180 (94%)	160 (95%)	9 (5%)	20	42
12	LJ	117/149 (78%)	99 (85%)	18 (15%)	2	5
13	LL	152/177 (86%)	146 (96%)	6 (4%)	28	55
14	LM	106/161 (66%)	102 (96%)	4 (4%)	29	56
15	LN	170/172 (99%)	167 (98%)	3 (2%)	51	77
16	LO	170/174 (98%)	167 (98%)	3 (2%)	51	77
17	LP	132/135 (98%)	128 (97%)	4 (3%)	36	64
18	LQ	160/165 (97%)	159 (99%)	1 (1%)	78	91
19	LR	127/175 (73%)	124 (98%)	3 (2%)	43	70
20	LS	156/157 (99%)	153 (98%)	3 (2%)	50	76
21	LT	138/140 (99%)	129 (94%)	9 (6%)	15	32
22	LV	100/107 (94%)	96 (96%)	4 (4%)	28	54
23	LW	52/126 (41%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	LX	107/133 (80%)	105 (98%)	2 (2%)	50	76
25	LY	121/135 (90%)	118 (98%)	3 (2%)	42	69
26	LZ	98/118 (83%)	93 (95%)	5 (5%)	21	43
27	La	117/120 (98%)	112 (96%)	5 (4%)	26	51
28	Lb	62/125 (50%)	62 (100%)	0	100	100
29	Lc	76/97 (78%)	70 (92%)	6 (8%)	11	24
30	Ld	91/110 (83%)	88 (97%)	3 (3%)	33	61
31	Le	108/115 (94%)	107 (99%)	1 (1%)	70	87
32	Lf	88/89 (99%)	86 (98%)	2 (2%)	44	72
33	Lg	85/100 (85%)	83 (98%)	2 (2%)	43	70
34	Lh	108/110 (98%)	107 (99%)	1 (1%)	70	87
35	Li	83/89 (93%)	80 (96%)	3 (4%)	31	58
36	Lj	74/74 (100%)	73 (99%)	1 (1%)	59	81
37	Lk	31/65 (48%)	30 (97%)	1 (3%)	34	62
38	Ll	43/48 (90%)	43 (100%)	0	100	100
39	Lm	43/115 (37%)	40 (93%)	3 (7%)	14	29
40	Ln	21/24 (88%)	21 (100%)	0	100	100
41	Lo	83/93 (89%)	82 (99%)	1 (1%)	63	83
42	Lp	74/75 (99%)	70 (95%)	4 (5%)	20	41
43	Lr	104/120 (87%)	102 (98%)	2 (2%)	50	76
45	SA	168/242 (69%)	158 (94%)	10 (6%)	17	36
46	SB	183/231 (79%)	173 (94%)	10 (6%)	19	40
47	SC	165/225 (73%)	155 (94%)	10 (6%)	17	35
48	SF	128/170 (75%)	123 (96%)	5 (4%)	28	55
49	SI	79/180 (44%)	76 (96%)	3 (4%)	29	56
51	SD	108/202 (54%)	96 (89%)	12 (11%)	6	12
52	SE	216/225 (96%)	205 (95%)	11 (5%)	21	43
53	SH	97/174 (56%)	89 (92%)	8 (8%)	10	23
54	SK	28/136 (21%)	27 (96%)	1 (4%)	31	58
55	SL	102/142 (72%)	100 (98%)	2 (2%)	48	75
56	SN	116/131 (88%)	115 (99%)	1 (1%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	SO	98/119 (82%)	92 (94%)	6 (6%)	17	35
58	SP	94/130 (72%)	85 (90%)	9 (10%)	8	17
59	SQ	110/121 (91%)	104 (94%)	6 (6%)	19	40
60	SR	59/122 (48%)	56 (95%)	3 (5%)	21	43
61	SS	112/132 (85%)	104 (93%)	8 (7%)	13	29
62	ST	93/115 (81%)	86 (92%)	7 (8%)	12	26
63	SU	5/107 (5%)	3 (60%)	2 (40%)	0	0
64	SV	60/67 (90%)	55 (92%)	5 (8%)	10	22
65	SW	107/113 (95%)	101 (94%)	6 (6%)	19	39
66	SY	95/115 (83%)	87 (92%)	8 (8%)	10	22
67	SX	111/115 (96%)	103 (93%)	8 (7%)	13	28
68	Sb	30/76 (40%)	30 (100%)	0	100	100
69	Sc	53/62 (86%)	49 (92%)	4 (8%)	12	26
70	Sd	35/49 (71%)	31 (89%)	4 (11%)	5	12
71	Se	34/104 (33%)	28 (82%)	6 (18%)	2	3
72	Sg	1/275 (0%)	0	1 (100%)	0	0
75	Sa	78/98 (80%)	73 (94%)	5 (6%)	16	33
77	SG	28/218 (13%)	28 (100%)	0	100	100
78	LU	55/115 (48%)	45 (82%)	10 (18%)	2	3
79	SZ	45/103 (44%)	42 (93%)	3 (7%)	15	31
80	SJ	148/168 (88%)	139 (94%)	9 (6%)	17	35
All	All	7673/10551 (73%)	7334 (96%)	339 (4%)	27	50

5 of 339 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	SO	70	SER
66	SY	80	ASP
58	SP	60	LEU
61	SS	146	VAL
69	Sc	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
56	SN	62	GLN
59	SQ	35	ASN
67	SX	92	ASN
18	LQ	57	ASN
17	LP	133	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L7	118/120 (98%)	13 (11%)	0
2	L8	148/156 (94%)	16 (10%)	0
44	Pt	72/77 (93%)	15 (20%)	0
50	mR	7/27 (25%)	1 (14%)	0
73	S2	1436/1869 (76%)	284 (19%)	8 (0%)
74	L5	3152/5069 (62%)	472 (14%)	9 (0%)
76	S6	72/77 (93%)	36 (50%)	0
All	All	5005/7395 (67%)	837 (16%)	17 (0%)

5 of 837 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L7	7	G
1	L7	24	C
1	L7	33	U
1	L7	41	G
1	L7	49	A

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
74	L5	3876	A
74	L5	4699	U
73	S2	1395	C
74	L5	955	G
74	L5	1590	C

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

140 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
74	PSU	L5	5010	74	18,21,22	1.02	1 (5%)	22,30,33	1.74	4 (18%)
74	OMG	L5	4392	74	23,26,27	2.43	8 (34%)	33,38,41	2.23	10 (30%)
74	PSU	L5	4457	74	18,21,22	1.09	1 (5%)	22,30,33	1.60	4 (18%)
74	PSU	L5	1862	74	18,21,22	1.13	1 (5%)	22,30,33	1.78	2 (9%)
74	OMC	L5	4536	74	19,22,23	2.95	8 (42%)	26,31,34	0.74	0
74	PSU	L5	3729	74	18,21,22	1.10	1 (5%)	22,30,33	1.75	4 (18%)
74	A2M	L5	1326	74	22,25,26	3.93	11 (50%)	31,36,39	3.56	14 (45%)
74	A2M	L5	2815	74	22,25,26	3.92	10 (45%)	31,36,39	3.65	14 (45%)
74	OMG	L5	4499	74	23,26,27	2.43	9 (39%)	33,38,41	2.28	9 (27%)
74	6MZ	L5	4220	74	22,25,26	2.72	3 (13%)	30,36,39	3.50	11 (36%)
74	PSU	L5	4420	74	18,21,22	1.03	1 (5%)	22,30,33	1.61	4 (18%)
74	PSU	L5	3844	74	18,21,22	1.12	1 (5%)	22,30,33	1.74	4 (18%)
74	PSU	L5	4299	74	18,21,22	1.05	1 (5%)	22,30,33	1.72	2 (9%)
74	OMC	L5	4456	74	19,22,23	2.89	8 (42%)	26,31,34	0.77	0
28	MLZ	Lb	5	28	8,9,10	0.80	0	4,9,11	0.58	0
74	PSU	L5	1860	74	18,21,22	1.00	1 (5%)	22,30,33	1.82	4 (18%)
74	PSU	L5	3768	74	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
74	OMG	L5	3792	74	23,26,27	2.40	8 (34%)	33,38,41	2.16	10 (30%)
74	A2M	L5	4571	74	22,25,26	3.97	10 (45%)	31,36,39	3.61	15 (48%)
74	A2M	L5	2363	74,81	22,25,26	3.95	12 (54%)	31,36,39	3.56	13 (41%)
74	PSU	L5	1782	74	18,21,22	1.01	1 (5%)	22,30,33	1.74	3 (13%)
74	A2M	L5	398	74	22,25,26	3.87	10 (45%)	31,36,39	3.79	15 (48%)
74	PSU	L5	1677	74,81	18,21,22	1.13	1 (5%)	22,30,33	1.81	4 (18%)
74	OMC	L5	3808	74	19,22,23	2.98	8 (42%)	26,31,34	0.81	1 (3%)
74	PSU	L5	4689	74	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
74	PSU	L5	3851	74	18,21,22	1.09	1 (5%)	22,30,33	1.68	3 (13%)
74	OMG	L5	4637	82,74	23,26,27	2.41	7 (30%)	33,38,41	2.22	9 (27%)
74	PSU	L5	1792	74	18,21,22	1.01	1 (5%)	22,30,33	1.71	4 (18%)
74	PSU	L5	2843	74	18,21,22	1.04	1 (5%)	22,30,33	1.70	3 (13%)
74	OMG	L5	3899	74,81	23,26,27	2.41	8 (34%)	33,38,41	2.19	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	PSU	L5	3920	74,81	18,21,22	1.12	1 (5%)	22,30,33	1.85	4 (18%)
74	OMG	L5	1316	74	23,26,27	2.43	8 (34%)	33,38,41	2.25	10 (30%)
74	PSU	L5	3884	74	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
74	OMC	L5	2365	74	19,22,23	2.98	8 (42%)	26,31,34	0.83	0
74	A2M	L5	3867	74	22,25,26	3.93	11 (50%)	31,36,39	3.64	12 (38%)
74	PSU	L5	4293	74	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
74	PSU	L5	4552	74	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
74	OMG	L5	3627	74	23,26,27	2.42	8 (34%)	33,38,41	2.26	10 (30%)
44	PSU	Pt	56	44	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
74	OMG	L5	4618	74	23,26,27	2.42	8 (34%)	33,38,41	2.30	10 (30%)
74	OMU	L5	4306	74	19,22,23	2.95	8 (42%)	26,31,34	1.68	5 (19%)
2	OMG	L8	75	2	23,26,27	2.43	8 (34%)	33,38,41	2.18	10 (30%)
74	1MA	L5	1322	74,81	21,25,26	2.78	6 (28%)	31,37,40	1.64	5 (16%)
74	PSU	L5	3639	74	18,21,22	1.08	1 (5%)	22,30,33	1.91	4 (18%)
74	PSU	L5	3695	74	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
74	PSU	L5	4431	74,81	18,21,22	1.08	1 (5%)	22,30,33	1.79	3 (13%)
74	OMG	L5	4228	74	23,26,27	2.43	8 (34%)	33,38,41	2.32	10 (30%)
74	PSU	L5	4972	74	18,21,22	1.00	1 (5%)	22,30,33	1.74	4 (18%)
3	V5N	LA	216	3	9,11,12	2.78	2 (22%)	9,14,16	1.33	1 (11%)
74	A2M	L5	3718	74	22,25,26	3.89	10 (45%)	31,36,39	3.59	14 (45%)
74	OMC	L5	2861	74	19,22,23	2.98	8 (42%)	26,31,34	0.89	1 (3%)
44	G7M	Pt	47	44	23,26,27	2.74	8 (34%)	35,39,42	2.32	10 (28%)
74	OMG	L5	3944	74	23,26,27	2.43	8 (34%)	33,38,41	2.19	9 (27%)
74	PSU	L5	4579	74	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
74	PSU	L5	4353	74	18,21,22	1.03	1 (5%)	22,30,33	1.88	4 (18%)
74	PSU	L5	4442	74	18,21,22	1.08	1 (5%)	22,30,33	1.81	6 (27%)
74	A2M	L5	3723	74	22,25,26	3.96	11 (50%)	31,36,39	3.72	14 (45%)
74	PSU	L5	2632	74	18,21,22	1.06	1 (5%)	22,30,33	1.84	5 (22%)
4	HIC	LB	245	4	10,11,12	0.58	0	8,14,16	0.35	0
74	OMC	L5	3841	74	19,22,23	2.94	8 (42%)	26,31,34	0.68	0
74	PSU	L5	4423	74	18,21,22	1.07	1 (5%)	22,30,33	1.68	4 (18%)
74	PSU	L5	4628	74	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
74	OMC	L5	2824	74	19,22,23	2.96	8 (42%)	26,31,34	0.79	0
74	A2M	L5	3830	74	22,25,26	3.91	11 (50%)	31,36,39	3.66	14 (45%)
76	PSU	S6	56	76	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	5MC	L5	4447	82,74	18,22,23	3.45	7 (38%)	26,32,35	1.11	1 (3%)
74	PSU	L5	3764	74	18,21,22	0.96	1 (5%)	22,30,33	1.80	4 (18%)
74	OMU	L5	4498	74	19,22,23	2.93	8 (42%)	26,31,34	1.71	5 (19%)
74	OMG	L5	2424	74	23,26,27	2.42	8 (34%)	33,38,41	2.21	9 (27%)
74	A2M	L5	3724	74	22,25,26	3.95	10 (45%)	31,36,39	3.67	15 (48%)
74	OMC	L5	1340	74	19,22,23	2.86	8 (42%)	26,31,34	0.66	0
74	PSU	L5	4569	74	18,21,22	1.17	1 (5%)	22,30,33	1.68	3 (13%)
74	OMU	L5	4620	74	19,22,23	2.83	8 (42%)	26,31,34	1.56	5 (19%)
74	A2M	L5	1871	82,74	22,25,26	3.87	12 (54%)	31,36,39	3.63	15 (48%)
74	PSU	L5	5001	74	18,21,22	1.03	1 (5%)	22,30,33	1.71	3 (13%)
74	PSU	L5	4531	74	18,21,22	1.11	1 (5%)	22,30,33	1.86	5 (22%)
74	PSU	L5	1781	74	18,21,22	1.02	1 (5%)	22,30,33	1.69	4 (18%)
74	PSU	L5	4532	74	18,21,22	1.12	1 (5%)	22,30,33	1.66	4 (18%)
74	A2M	L5	400	74	22,25,26	3.94	11 (50%)	31,36,39	3.67	13 (41%)
76	G7M	S6	47	76	23,26,27	2.78	8 (34%)	35,39,42	2.24	10 (28%)
74	PSU	L5	2839	74	18,21,22	1.15	1 (5%)	22,30,33	1.76	4 (18%)
74	PSU	L5	3770	74	18,21,22	1.01	1 (5%)	22,30,33	1.70	4 (18%)
74	OMG	L5	2364	74	23,26,27	2.37	8 (34%)	33,38,41	2.15	8 (24%)
74	PSU	L5	4471	74	18,21,22	1.08	1 (5%)	22,30,33	1.73	4 (18%)
74	UR3	L5	4530	74	19,22,23	2.72	8 (42%)	26,32,35	1.36	3 (11%)
74	PSU	L5	4500	74	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
74	OMG	L5	4196	74	23,26,27	2.44	8 (34%)	33,38,41	2.27	10 (30%)
74	A2M	L5	4523	74,81	22,25,26	3.88	10 (45%)	31,36,39	3.52	15 (48%)
74	OMG	L5	1625	82,74	23,26,27	2.44	8 (34%)	33,38,41	2.18	10 (30%)
74	PSU	L5	3734	74	18,21,22	0.94	1 (5%)	22,30,33	1.79	4 (18%)
74	A2M	L5	1534	74,81	22,25,26	3.91	11 (50%)	31,36,39	3.69	16 (51%)
74	PSU	L5	2508	74	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
74	A2M	L5	3825	74	22,25,26	3.88	10 (45%)	31,36,39	3.47	14 (45%)
74	A2M	L5	2401	74	22,25,26	3.90	11 (50%)	31,36,39	3.67	15 (48%)
74	5MC	L5	3782	74,81	18,22,23	3.42	7 (38%)	26,32,35	1.10	2 (7%)
74	PSU	L5	3758	74	18,21,22	1.01	1 (5%)	22,30,33	1.65	3 (13%)
74	OMU	L5	4227	74	19,22,23	3.02	8 (42%)	26,31,34	1.75	4 (15%)
74	PSU	L5	4403	74	18,21,22	1.02	1 (5%)	22,30,33	1.77	5 (22%)
74	PSU	L5	3853	74,81	18,21,22	1.03	1 (5%)	22,30,33	1.66	3 (13%)
44	4SU	Pt	8	44	18,21,22	3.77	8 (44%)	26,30,33	2.18	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OMC	L5	2351	74	19,22,23	2.96	8 (42%)	26,31,34	0.80	1 (3%)
74	OMG	L5	1522	74	23,26,27	2.44	8 (34%)	33,38,41	2.29	11 (33%)
74	OMU	L5	3925	74	19,22,23	2.96	8 (42%)	26,31,34	1.76	5 (19%)
74	OMC	L5	1881	74,81	19,22,23	2.87	8 (42%)	26,31,34	0.79	0
2	PSU	L8	55	2	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
74	OMC	L5	3869	74	19,22,23	2.96	8 (42%)	26,31,34	0.76	0
74	OMC	L5	2804	74	19,22,23	2.94	8 (42%)	26,31,34	0.65	0
74	OMC	L5	3887	74	19,22,23	2.94	8 (42%)	26,31,34	0.76	0
74	PSU	L5	4312	74	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
74	PSU	L5	4673	74,81	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
74	OMC	L5	2422	74,81	19,22,23	2.87	8 (42%)	26,31,34	0.68	0
74	A2M	L5	3785	74	22,25,26	3.91	11 (50%)	31,36,39	3.66	15 (48%)
74	UY1	L5	3818	82,74,81	19,22,23	4.12	9 (47%)	22,31,34	2.09	5 (22%)
74	A2M	L5	1524	74	22,25,26	3.95	9 (40%)	31,36,39	3.81	12 (38%)
74	PSU	L5	4636	74	18,21,22	1.17	1 (5%)	22,30,33	1.70	4 (18%)
2	PSU	L8	69	2	18,21,22	1.03	1 (5%)	22,30,33	1.68	5 (22%)
74	PSU	L5	1683	82,74	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
74	PSU	L5	3715	74,81	18,21,22	0.99	1 (5%)	22,30,33	1.57	3 (13%)
76	4SU	S6	8	76	18,21,22	3.81	8 (44%)	26,30,33	2.33	6 (23%)
74	PSU	L5	4361	74	18,21,22	1.03	1 (5%)	22,30,33	1.74	3 (13%)
74	PSU	L5	3762	74	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)
27	V5N	La	39	27	9,11,12	2.77	2 (22%)	9,14,16	1.40	2 (22%)
74	PSU	L5	1536	74	18,21,22	1.09	1 (5%)	22,30,33	1.99	5 (22%)
74	OMC	L5	3701	82,74	19,22,23	2.90	8 (42%)	26,31,34	0.90	0
74	OMU	L5	2837	74	19,22,23	2.95	8 (42%)	26,31,34	1.78	5 (19%)
44	OMC	Pt	33	44	19,22,23	3.01	8 (42%)	26,31,34	1.00	1 (3%)
74	PSU	L5	3637	74,81	18,21,22	1.08	1 (5%)	22,30,33	1.75	2 (9%)
74	PSU	L5	1779	74	18,21,22	1.11	1 (5%)	22,30,33	1.80	5 (22%)
74	PSU	L5	4493	82,74	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
74	PSU	L5	4521	82,74,81	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
74	PSU	L5	4296	74	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
74	PSU	L5	1744	82,74	18,21,22	1.12	1 (5%)	22,30,33	1.83	4 (18%)
74	PSU	L5	4576	74	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
74	A2M	L5	4590	74	22,25,26	3.94	11 (50%)	31,36,39	3.69	15 (48%)
74	OMG	L5	4370	74	23,26,27	2.41	8 (34%)	33,38,41	2.23	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OMG	L5	4623	74	23,26,27	2.44	8 (34%)	33,38,41	2.28	10 (30%)
74	OMU	L5	2415	74	19,22,23	2.99	8 (42%)	26,31,34	1.74	4 (15%)
74	OMG	L5	3744	74	23,26,27	2.44	7 (30%)	33,38,41	2.25	10 (30%)
74	OMG	L5	4494	74	23,26,27	2.41	8 (34%)	33,38,41	2.23	10 (30%)
74	PSU	L5	1582	74	18,21,22	1.06	1 (5%)	22,30,33	1.63	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	PSU	L5	5010	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	4392	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4457	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	1862	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	4536	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	3729	74	-	1/7/25/26	0/2/2/2
74	A2M	L5	1326	74	-	1/9/27/28	0/3/3/3
74	A2M	L5	2815	74	-	2/9/27/28	0/3/3/3
74	OMG	L5	4499	74	-	0/9/27/28	0/3/3/3
74	6MZ	L5	4220	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4420	74	-	1/7/25/26	0/2/2/2
74	PSU	L5	3844	74	-	1/7/25/26	0/2/2/2
74	PSU	L5	4299	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	4456	74	-	0/9/27/28	0/2/2/2
28	MLZ	Lb	5	28	-	1/7/8/10	-
74	PSU	L5	1860	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3768	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	3792	74	-	2/9/27/28	0/3/3/3
74	A2M	L5	4571	74	-	2/9/27/28	0/3/3/3
74	A2M	L5	2363	74,81	-	0/9/27/28	0/3/3/3
74	PSU	L5	1782	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	398	74	-	3/9/27/28	0/3/3/3
74	PSU	L5	1677	74,81	-	1/7/25/26	0/2/2/2
74	OMC	L5	3808	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	4689	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3851	74	-	1/7/25/26	0/2/2/2
74	OMG	L5	4637	82,74	-	1/9/27/28	0/3/3/3
74	PSU	L5	1792	74	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	PSU	L5	2843	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	3899	74,81	-	0/9/27/28	0/3/3/3
74	PSU	L5	3920	74,81	-	0/7/25/26	0/2/2/2
74	OMG	L5	1316	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	3884	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	2365	74	-	0/9/27/28	0/2/2/2
74	A2M	L5	3867	74	-	2/9/27/28	0/3/3/3
74	PSU	L5	4293	74	-	1/7/25/26	0/2/2/2
74	PSU	L5	4552	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	3627	74	-	0/9/27/28	0/3/3/3
44	PSU	Pt	56	44	-	1/7/25/26	0/2/2/2
74	OMG	L5	4618	74	-	0/9/27/28	0/3/3/3
74	OMU	L5	4306	74	-	0/9/27/28	0/2/2/2
2	OMG	L8	75	2	-	1/9/27/28	0/3/3/3
74	1MA	L5	1322	74,81	-	2/7/25/26	0/3/3/3
74	PSU	L5	3639	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3695	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4431	74,81	-	0/7/25/26	0/2/2/2
74	OMG	L5	4228	74	-	2/9/27/28	0/3/3/3
74	PSU	L5	4972	74	-	0/7/25/26	0/2/2/2
3	V5N	LA	216	3	-	1/9/10/12	0/1/1/1
74	A2M	L5	3718	74	-	1/9/27/28	0/3/3/3
74	OMC	L5	2861	74	-	0/9/27/28	0/2/2/2
44	G7M	Pt	47	44	-	0/7/25/26	0/3/3/3
74	OMG	L5	3944	74	-	3/9/27/28	0/3/3/3
74	PSU	L5	4579	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4353	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4442	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	3723	74	-	3/9/27/28	0/3/3/3
74	PSU	L5	2632	74	-	0/7/25/26	0/2/2/2
4	HIC	LB	245	4	-	1/5/6/8	0/1/1/1
74	OMC	L5	3841	74	-	1/9/27/28	0/2/2/2
74	PSU	L5	4423	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4628	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	2824	74	-	0/9/27/28	0/2/2/2
74	A2M	L5	3830	74	-	0/9/27/28	0/3/3/3
76	PSU	S6	56	76	-	2/7/25/26	0/2/2/2
74	5MC	L5	4447	82,74	-	4/7/25/26	0/2/2/2
74	PSU	L5	3764	74	-	0/7/25/26	0/2/2/2
74	OMU	L5	4498	74	-	0/9/27/28	0/2/2/2
74	OMG	L5	2424	74	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	A2M	L5	3724	74	-	1/9/27/28	0/3/3/3
74	OMC	L5	1340	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	4569	74	-	0/7/25/26	0/2/2/2
74	OMU	L5	4620	74	-	0/9/27/28	0/2/2/2
74	A2M	L5	1871	82,74	-	0/9/27/28	0/3/3/3
74	PSU	L5	5001	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4531	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	1781	74	-	2/7/25/26	0/2/2/2
74	PSU	L5	4532	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	400	74	-	0/9/27/28	0/3/3/3
76	G7M	S6	47	76	-	2/7/25/26	0/3/3/3
74	PSU	L5	2839	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3770	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	2364	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4471	74	-	0/7/25/26	0/2/2/2
74	UR3	L5	4530	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4500	74	-	1/7/25/26	0/2/2/2
74	OMG	L5	4196	74	-	0/9/27/28	0/3/3/3
74	A2M	L5	4523	74,81	-	1/9/27/28	0/3/3/3
74	OMG	L5	1625	82,74	-	1/9/27/28	0/3/3/3
74	PSU	L5	3734	74	-	1/7/25/26	0/2/2/2
74	A2M	L5	1534	74,81	-	2/9/27/28	0/3/3/3
74	PSU	L5	2508	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	3825	74	-	0/9/27/28	0/3/3/3
74	A2M	L5	2401	74	-	0/9/27/28	0/3/3/3
74	5MC	L5	3782	74,81	-	0/7/25/26	0/2/2/2
74	PSU	L5	3758	74	-	2/7/25/26	0/2/2/2
74	OMU	L5	4227	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	4403	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3853	74,81	-	0/7/25/26	0/2/2/2
44	4SU	Pt	8	44	-	0/7/25/26	0/2/2/2
74	OMC	L5	2351	74	-	2/9/27/28	0/2/2/2
74	OMG	L5	1522	74	-	0/9/27/28	0/3/3/3
74	OMU	L5	3925	74	-	1/9/27/28	0/2/2/2
74	OMC	L5	1881	74,81	-	0/9/27/28	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
74	OMC	L5	3869	74	-	0/9/27/28	0/2/2/2
74	OMC	L5	2804	74	-	0/9/27/28	0/2/2/2
74	OMC	L5	3887	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	4312	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4673	74,81	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OMC	L5	2422	74,81	-	2/9/27/28	0/2/2/2
74	A2M	L5	3785	74	-	2/9/27/28	0/3/3/3
74	UY1	L5	3818	82,74,81	-	3/9/27/28	0/2/2/2
74	A2M	L5	1524	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4636	74	-	2/7/25/26	0/2/2/2
2	PSU	L8	69	2	-	0/7/25/26	0/2/2/2
74	PSU	L5	1683	82,74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3715	74,81	-	0/7/25/26	0/2/2/2
76	4SU	S6	8	76	-	3/7/25/26	0/2/2/2
74	PSU	L5	4361	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3762	74	-	0/7/25/26	0/2/2/2
27	V5N	La	39	27	-	1/9/10/12	0/1/1/1
74	PSU	L5	1536	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	3701	82,74	-	4/9/27/28	0/2/2/2
74	OMU	L5	2837	74	-	0/9/27/28	0/2/2/2
44	OMC	Pt	33	44	-	0/9/27/28	0/2/2/2
74	PSU	L5	3637	74,81	-	0/7/25/26	0/2/2/2
74	PSU	L5	1779	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4493	82,74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4521	82,74,81	-	0/7/25/26	0/2/2/2
74	PSU	L5	4296	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	1744	82,74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4576	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	4590	74	-	2/9/27/28	0/3/3/3
74	OMG	L5	4370	74	-	0/9/27/28	0/3/3/3
74	OMG	L5	4623	74	-	0/9/27/28	0/3/3/3
74	OMU	L5	2415	74	-	1/9/27/28	0/2/2/2
74	OMG	L5	3744	74	-	0/9/27/28	0/3/3/3
74	OMG	L5	4494	74	-	1/9/27/28	0/3/3/3
74	PSU	L5	1582	74	-	0/7/25/26	0/2/2/2

The worst 5 of 685 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	3867	A2M	C3'-C2'	-12.77	1.24	1.52
74	L5	2363	A2M	C3'-C2'	-12.73	1.24	1.52
74	L5	400	A2M	C3'-C2'	-12.73	1.24	1.52
74	L5	1326	A2M	C3'-C2'	-12.71	1.24	1.52
74	L5	3723	A2M	C3'-C2'	-12.70	1.24	1.52

The worst 5 of 808 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	1524	A2M	C1'-N9-C8	-12.20	99.58	127.14
74	L5	3723	A2M	C1'-N9-C8	-11.06	102.16	127.14
74	L5	3867	A2M	C1'-N9-C8	-11.04	102.20	127.14
74	L5	400	A2M	C1'-N9-C8	-11.00	102.29	127.14
74	L5	398	A2M	C1'-N9-C8	-10.80	102.75	127.14

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	LA	216	V5N	O-C-CA-CB
4	LB	245	HIC	O-C-CA-CB
76	S6	8	4SU	C3'-C4'-C5'-O5'
76	S6	47	G7M	O4'-C4'-C5'-O5'
76	S6	47	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

47 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	L5	5010	PSU	2	0
74	L5	4392	OMG	2	0
74	L5	4457	PSU	1	0
74	L5	4536	OMC	1	0
74	L5	1326	A2M	1	0
74	L5	2815	A2M	1	0
74	L5	4571	A2M	1	0
74	L5	2363	A2M	1	0
74	L5	398	A2M	1	0
74	L5	3808	OMC	1	0
74	L5	4637	OMG	2	0
74	L5	3920	PSU	1	0
2	L8	75	OMG	2	0
74	L5	3718	A2M	3	0
74	L5	3944	OMG	2	0
74	L5	3723	A2M	1	0
76	S6	56	PSU	1	0
74	L5	4447	5MC	1	0
74	L5	4498	OMU	1	0
74	L5	2424	OMG	1	0
74	L5	3724	A2M	2	0
74	L5	1340	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	L5	4620	OMU	2	0
74	L5	1871	A2M	1	0
74	L5	5001	PSU	1	0
74	L5	4531	PSU	1	0
76	S6	47	G7M	1	0
74	L5	3770	PSU	3	0
74	L5	4530	UR3	1	0
74	L5	4196	OMG	2	0
74	L5	1534	A2M	2	0
74	L5	4227	OMU	1	0
44	Pt	8	4SU	1	0
74	L5	2351	OMC	2	0
74	L5	3925	OMU	1	0
74	L5	1881	OMC	1	0
74	L5	2804	OMC	1	0
74	L5	3785	A2M	1	0
74	L5	3715	PSU	1	0
76	S6	8	4SU	1	0
74	L5	3762	PSU	1	0
74	L5	1536	PSU	1	0
74	L5	3701	OMC	1	0
44	Pt	33	OMC	1	0
74	L5	1779	PSU	1	0
74	L5	4370	OMG	1	0
74	L5	2415	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 292 ligands modelled in this entry, 288 are monoatomic - leaving 4 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
86	SPD	L5	5101	-	9,9,9	0.28	0	8,8,8	0.42	0
85	HYG	S2	1901	-	35,39,39	3.07	11 (31%)	43,60,60	1.59	10 (23%)
86	SPD	L5	5103	-	9,9,9	0.28	0	8,8,8	0.27	0
86	SPD	L5	5102	-	9,9,9	0.28	0	8,8,8	0.35	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
86	SPD	L5	5101	-	-	0/7/7/7	-
85	HYG	S2	1901	-	-	6/12/87/87	0/4/4/4
86	SPD	L5	5103	-	-	1/7/7/7	-
86	SPD	L5	5102	-	-	3/7/7/7	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	S2	1901	HYG	O29-C12	10.97	1.61	1.43
85	S2	1901	HYG	O22-C17	6.54	1.53	1.43
85	S2	1901	HYG	O14-C13	6.47	1.58	1.41
85	S2	1901	HYG	O28-C23	5.90	1.47	1.40
85	S2	1901	HYG	C16-C15	4.34	1.62	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	1901	HYG	O29-C12-C13	5.06	124.13	110.86
85	S2	1901	HYG	O22-C17-C16	4.38	121.87	111.22
85	S2	1901	HYG	O22-C17-C12	2.88	108.18	103.58
85	S2	1901	HYG	O28-C27-C26	2.48	112.05	108.52
85	S2	1901	HYG	C13-O18-C6	-2.29	112.29	117.96

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	S2	1901	HYG	C26-C27-C33-C34
85	S2	1901	HYG	O28-C27-C33-C34
85	S2	1901	HYG	C27-C33-C34-O35

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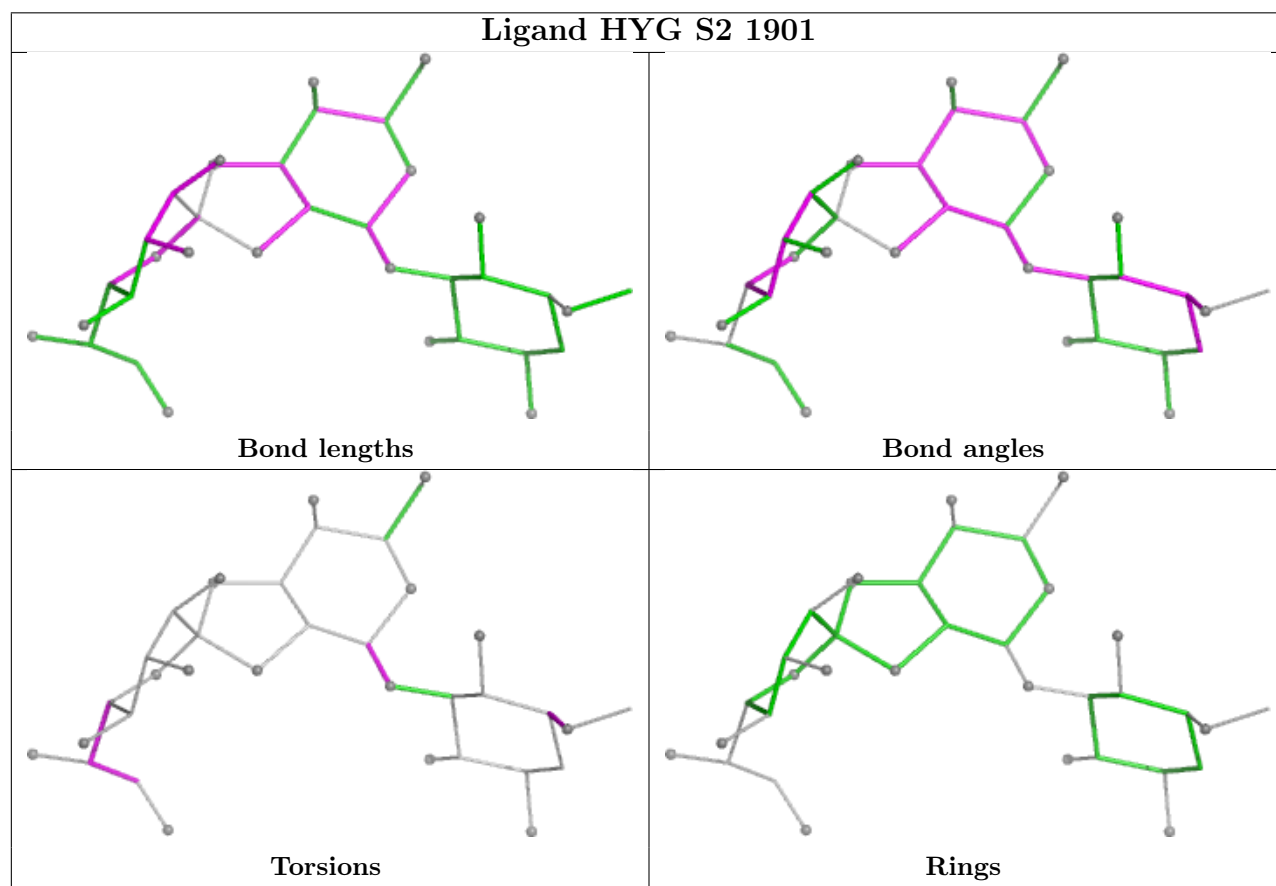
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Mol	Chain	Res	Type	Atoms
85	S2	1901	HYG	N36-C33-C34-O35
85	S2	1901	HYG	O14-C13-O18-C6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
74	L5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	1268:G	O3'	1274:A	P	24.24

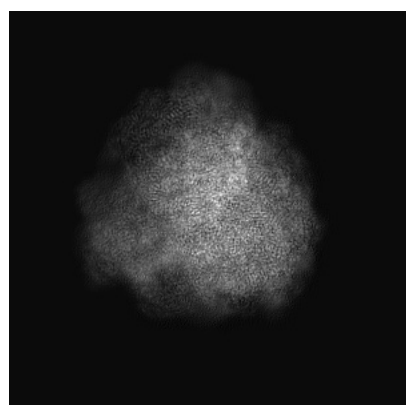
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54269. These allow visual inspection of the internal detail of the map and identification of artifacts.

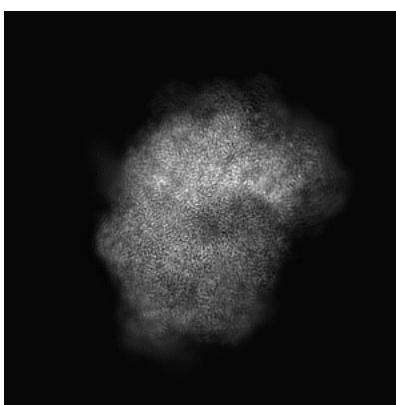
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

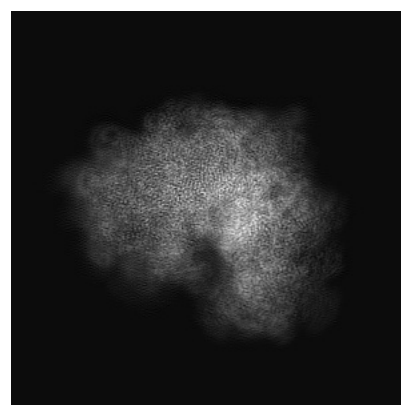
6.1.1 Primary map



X



Y

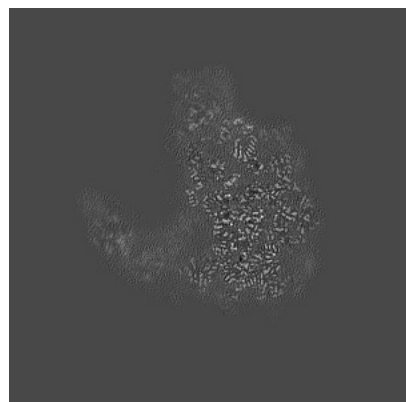


Z

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

6.2 Central slices [i](#)

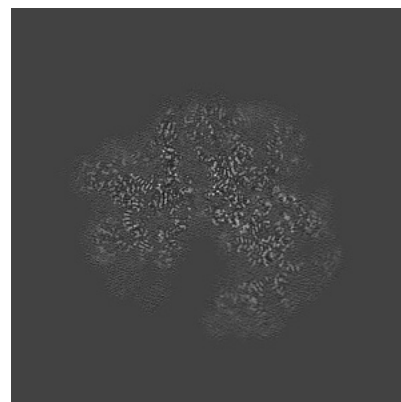
6.2.1 Primary map



X Index: 240



Y Index: 240

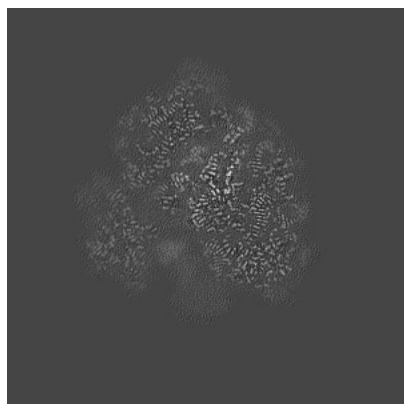


Z Index: 240

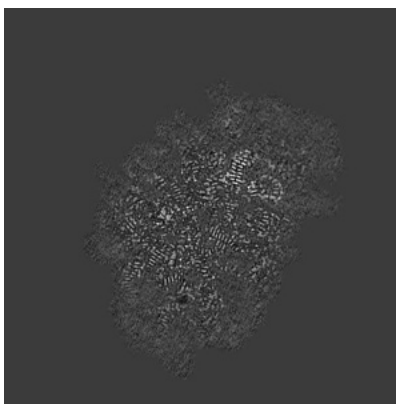
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

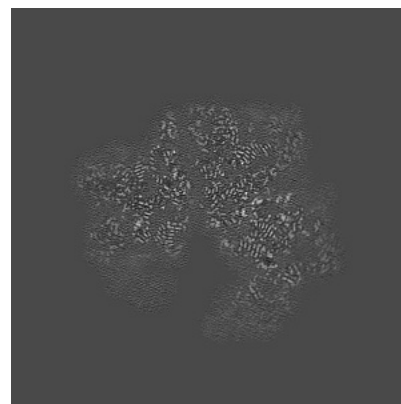
6.3.1 Primary map



X Index: 273



Y Index: 266

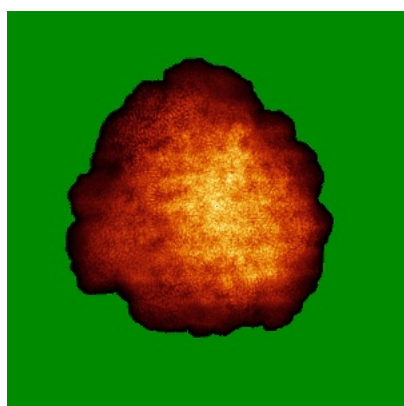


Z Index: 248

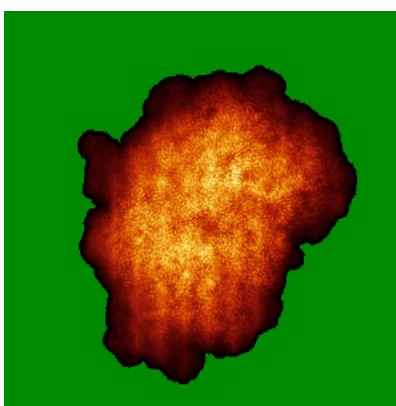
The images above show the largest variance slices of the map in three orthogonal directions.

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

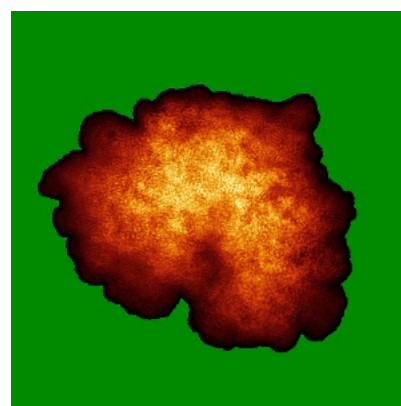
6.4.1 Primary map



X



Y

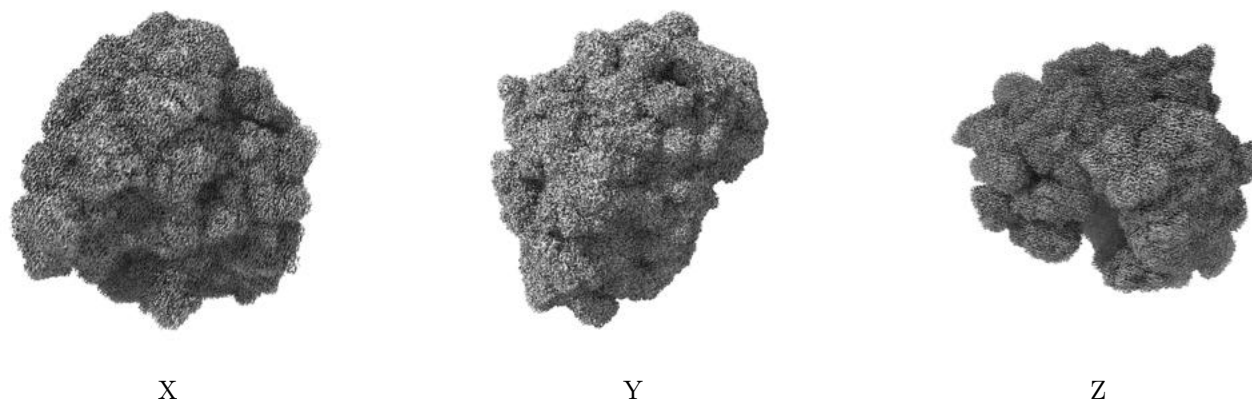


Z

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.

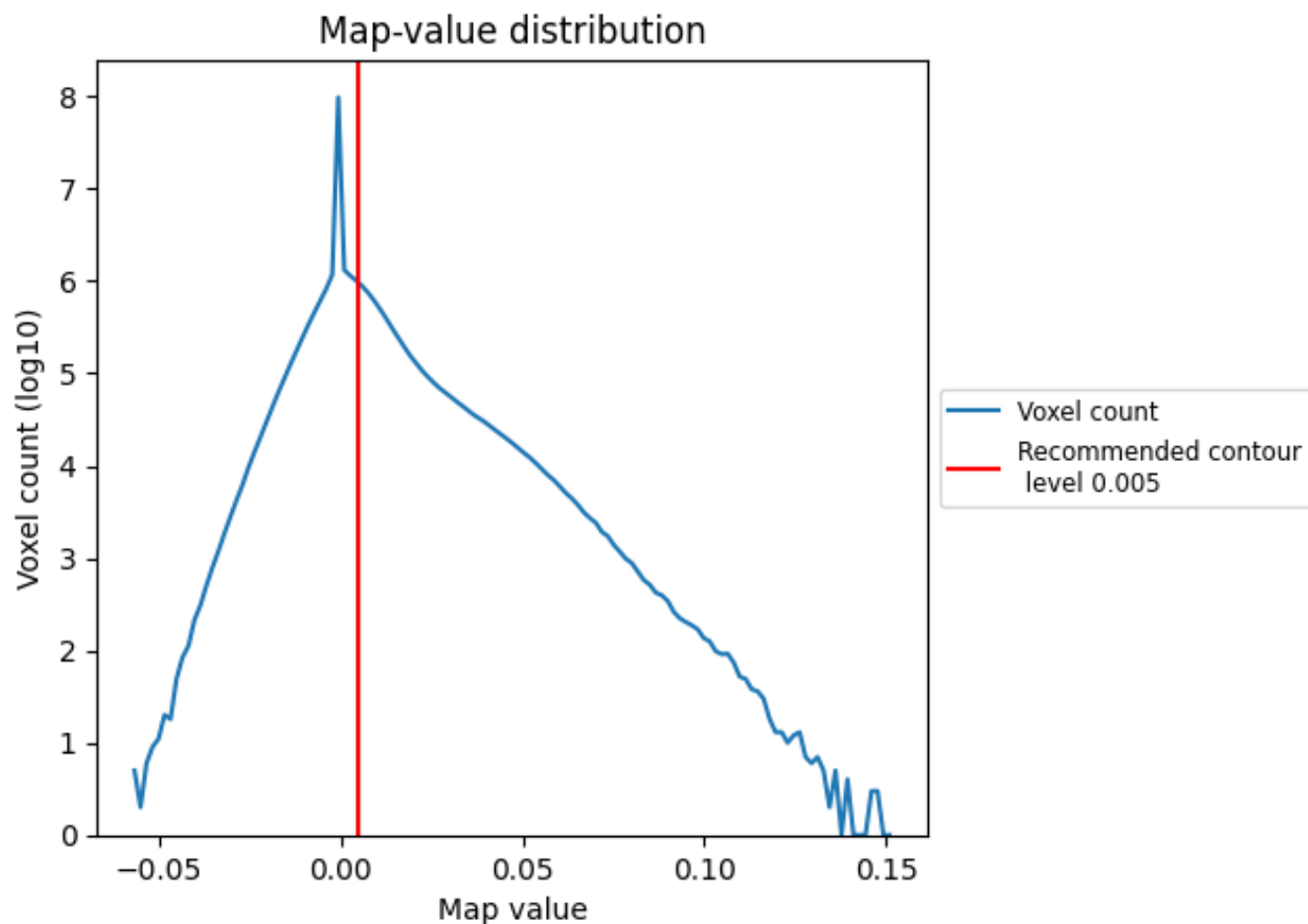
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

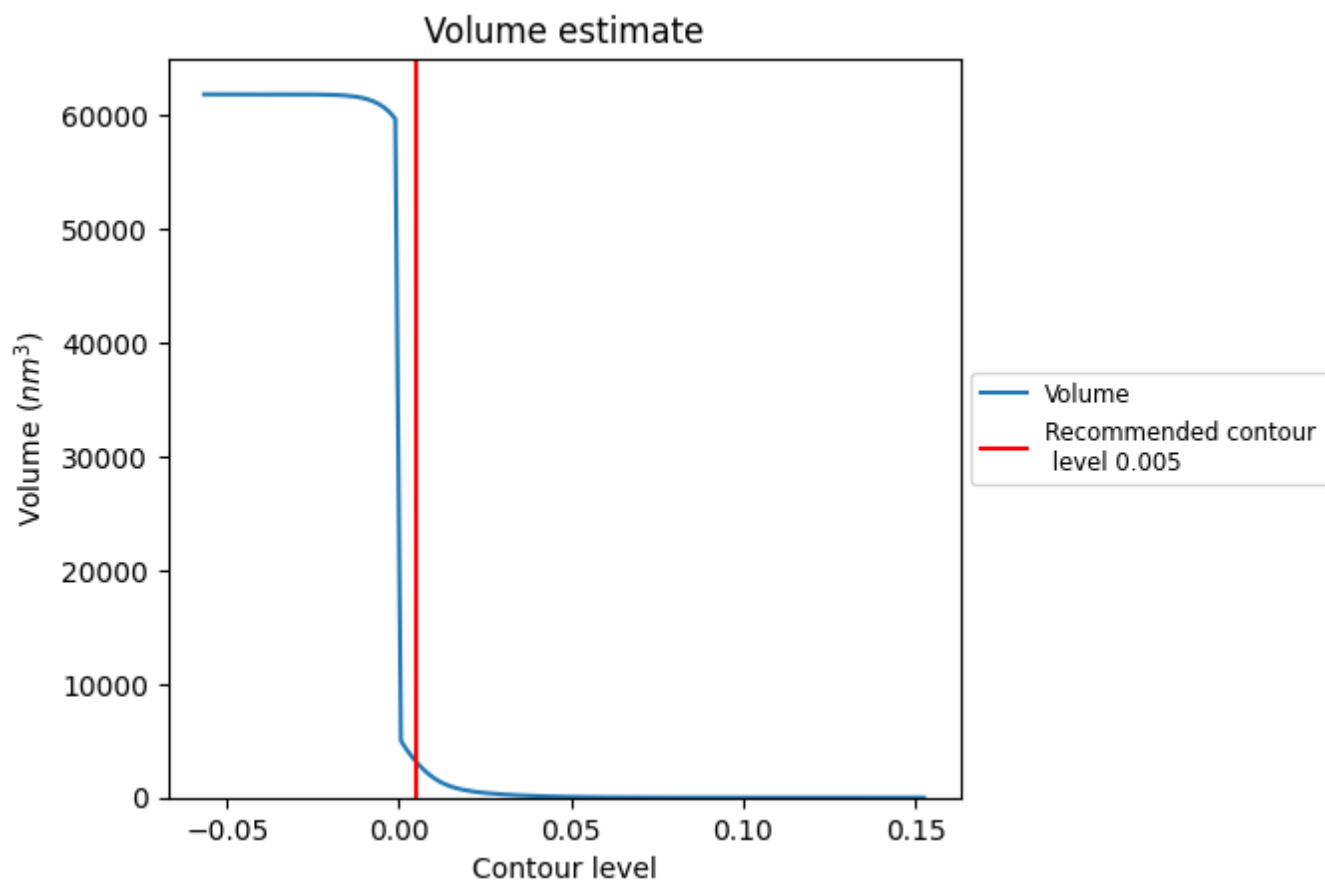
This section contains the results of statistical analysis of the map.

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.

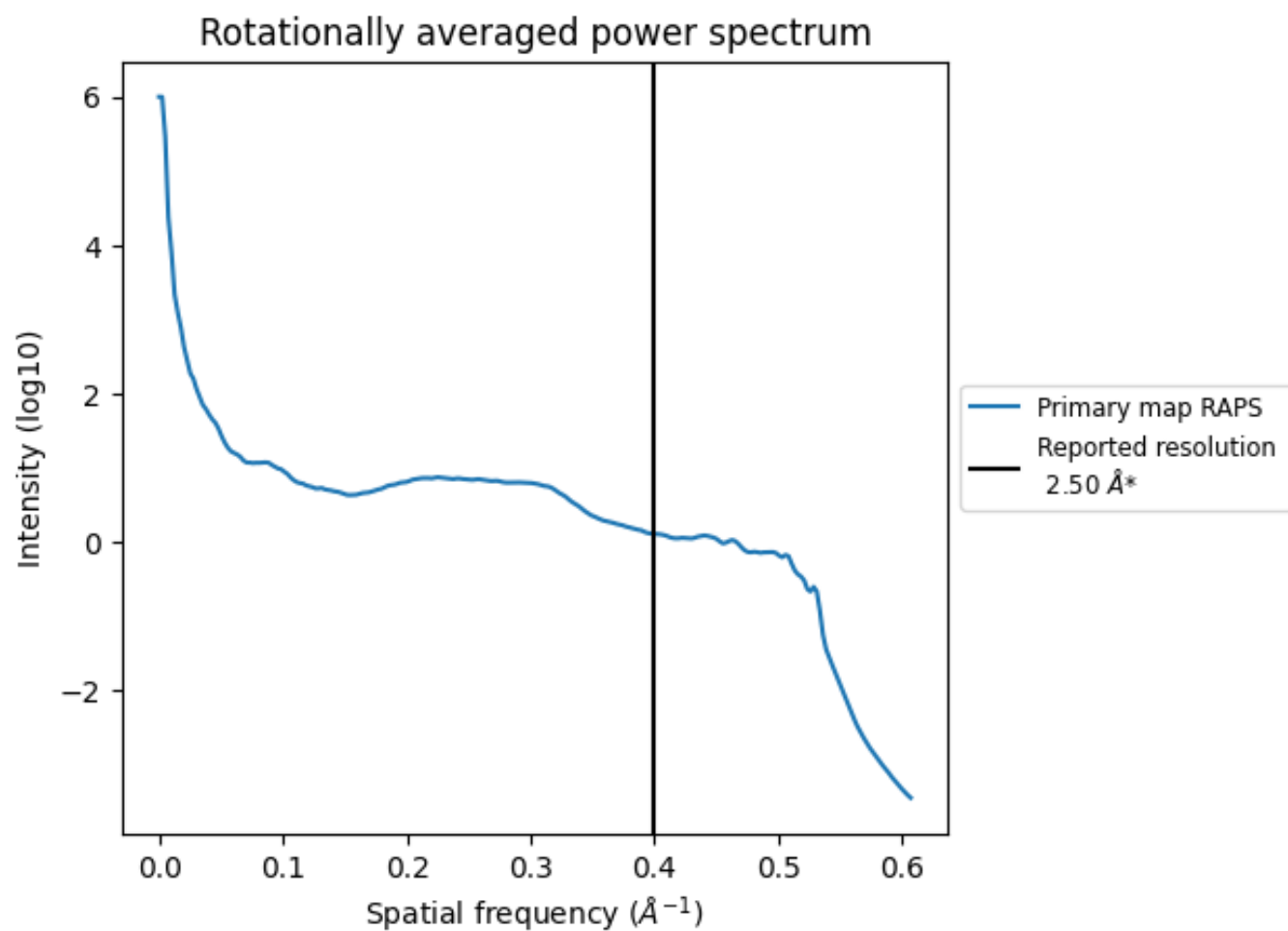
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3149 nm³; this corresponds to an approximate mass of 2845 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 0.400 Å⁻¹

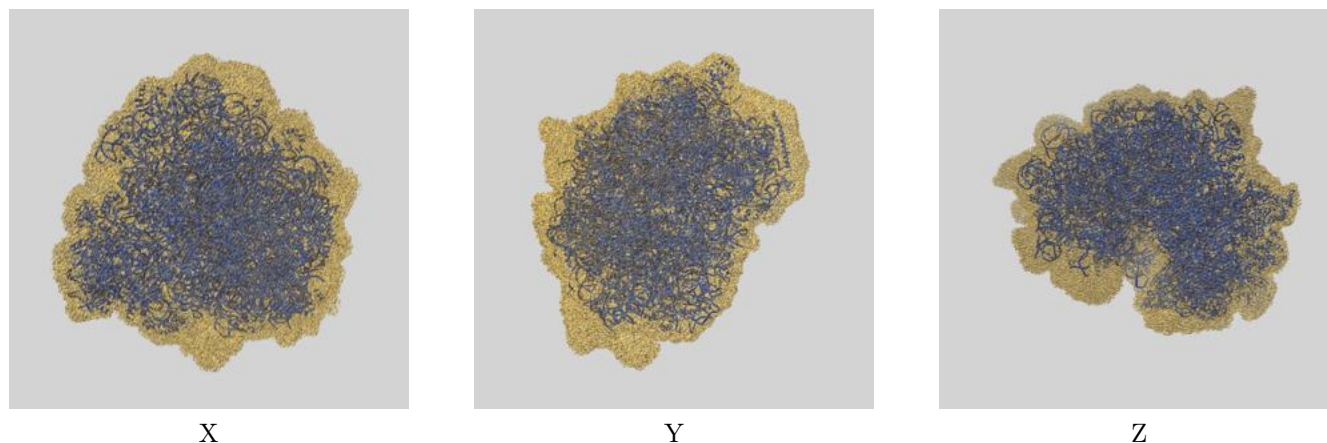
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

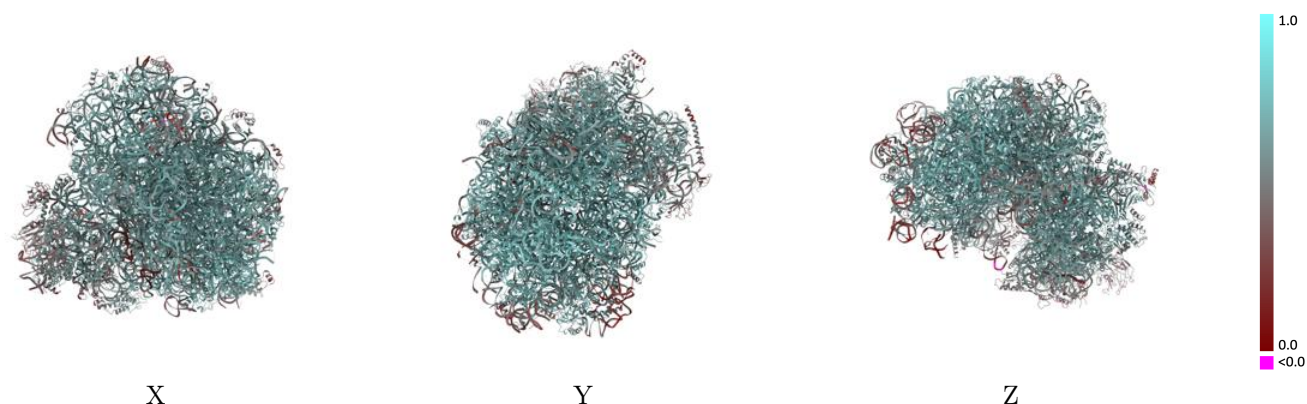
This section contains information regarding the fit between EMDB map EMD-54269 and PDB model 9RUC. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



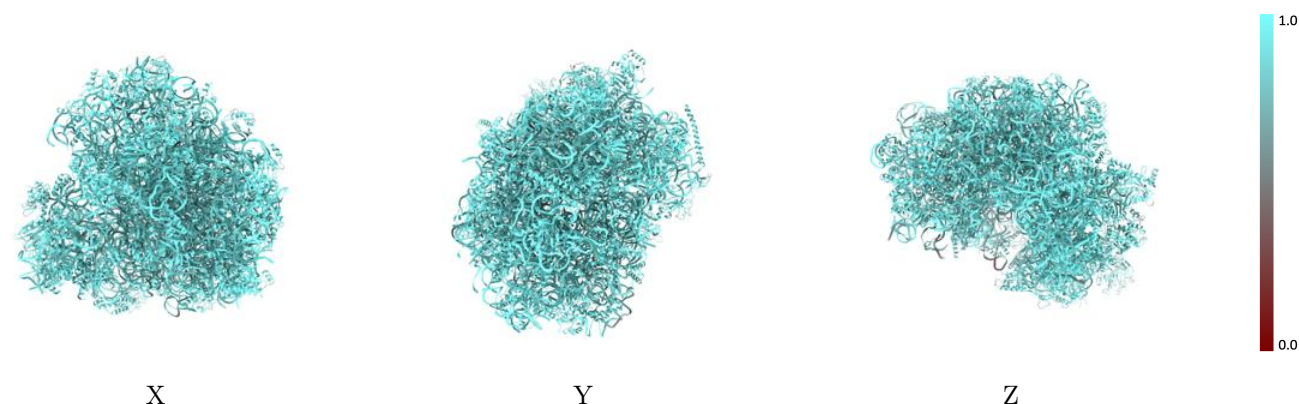
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



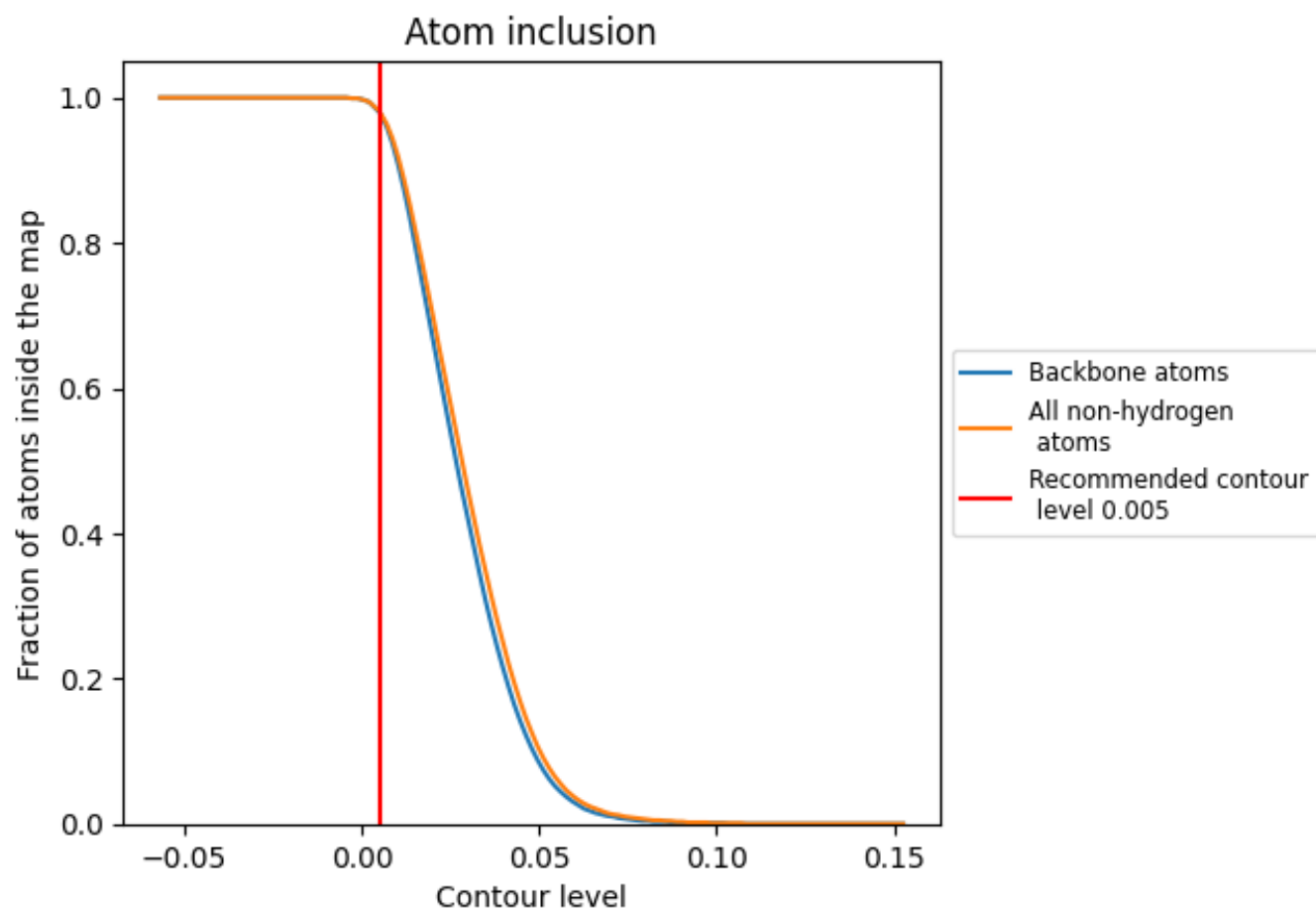
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 98% of all backbone atoms, 98% 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	 0.9820	 0.6330
L5	 0.9800	 0.6440
L7	 0.9950	 0.6230
L8	 0.9940	 0.6690
LA	 1.0000	 0.7360
LB	 0.9970	 0.7120
LC	 0.9970	 0.7210
LD	 0.9840	 0.5580
LE	 0.9930	 0.6320
LF	 0.9960	 0.7200
LG	 0.9880	 0.6360
LH	 0.9860	 0.6000
LI	 0.9920	 0.6610
LJ	 0.9600	 0.4630
LL	 0.9920	 0.6860
LM	 0.9940	 0.6480
LN	 1.0000	 0.7480
LO	 0.9940	 0.7070
LP	 0.9980	 0.7290
LQ	 0.9990	 0.7370
LR	 0.9980	 0.6850
LS	 0.9940	 0.6980
LT	 0.9950	 0.6850
LU	 0.9380	 0.4800
LV	 0.9980	 0.7140
LW	 0.9940	 0.6820
LX	 0.9950	 0.6820
LY	 0.9950	 0.6970
LZ	 0.9870	 0.6030
La	 0.9950	 0.7220
Lb	 0.9890	 0.6340
Lc	 0.9960	 0.6350
Ld	 0.9890	 0.6710
Le	 0.9990	 0.7330
Lf	 0.9980	 0.7370



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Chain	Atom inclusion	Q-score
Lg	 0.9960	 0.6920
Lh	 0.9930	 0.6760
Li	 0.9880	 0.6430
Lj	 0.9990	 0.7400
Lk	 0.9620	 0.5490
Ll	 0.9980	 0.7080
Lm	 0.9690	 0.6060
Ln	 1.0000	 0.6670
Lo	 0.9960	 0.6950
Lp	 0.9990	 0.6980
Lr	 0.9970	 0.7050
Pt	 0.9030	 0.3980
S2	 0.9870	 0.6170
S6	 0.9050	 0.2730
SA	 0.9790	 0.6050
SB	 0.9940	 0.6290
SC	 0.9860	 0.6490
SD	 0.9520	 0.5300
SE	 0.9850	 0.6300
SF	 0.9930	 0.6000
SG	 0.9410	 0.4700
SH	 0.9240	 0.5100
SI	 0.9940	 0.6360
SJ	 0.9850	 0.6050
SK	 0.8650	 0.3870
SL	 0.9980	 0.6700
SN	 0.9980	 0.6600
SO	 0.9960	 0.6630
SP	 0.9330	 0.4810
SQ	 0.9850	 0.5900
SR	 0.9150	 0.5160
SS	 0.9710	 0.5250
ST	 0.9740	 0.5690
SU	 0.9450	 0.5190
SV	 0.9650	 0.6150
SW	 1.0000	 0.6880
SX	 0.9920	 0.6530
SY	 0.9820	 0.5770
SZ	 0.9370	 0.4510
Sa	 0.9920	 0.6450
Sb	 0.9910	 0.6290
Sc	 0.9600	 0.5800

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Chain	Atom inclusion	Q-score
Sd	 0.9850	 0.6020
Se	 0.9640	 0.5600
Sg	 0.8540	 0.4230
mR	 0.9590	 0.5440