



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 02:05 am BST

PDB ID : 9SPF / pdb_00009spf
EMDB ID : EMD-55083
Title : CRYO-EM STRUCTURE OF HUMAN 80S RIBOSOME WITH A/P/E-SITE
TRNA AND MRNA CONTAINING N1-METHYLPSEUDOURIDINE
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2025-09-17
Resolution : 2.40 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:

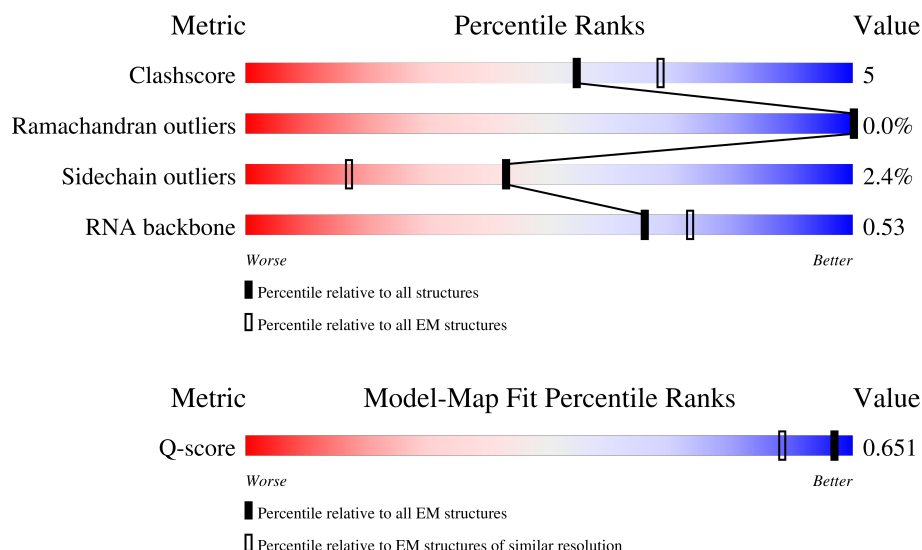
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 2.40 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.











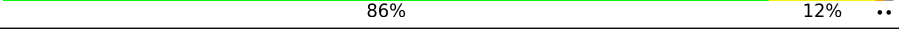

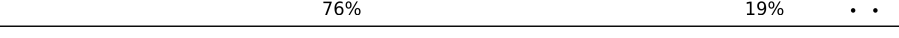
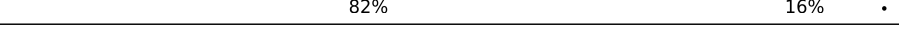

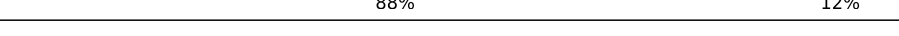


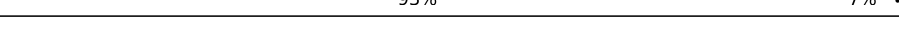

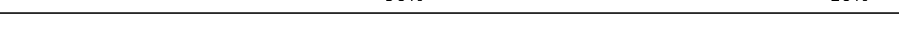






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	At	77	
2	Et	75	
3	L5	5069	







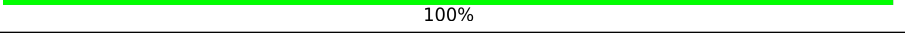

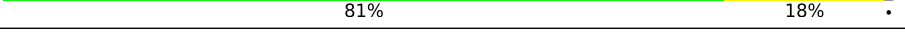

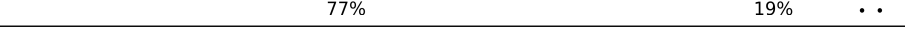
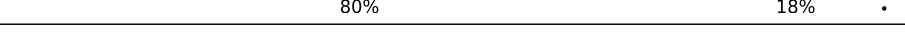

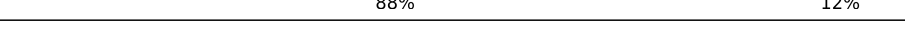


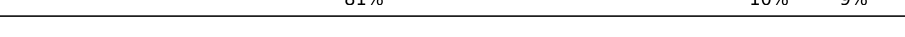

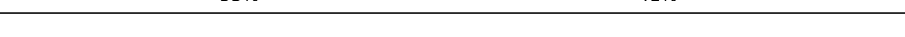






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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LB	403	
7	LC	427	
8	LD	297	
9	LE	288	
10	LF	248	
11	LG	266	
12	LH	192	
13	LI	214	
14	LJ	178	
15	LL	211	
16	LM	215	
17	LN	204	
18	LO	203	
19	LP	184	
20	LQ	188	
21	LR	196	
22	LS	176	
23	LT	160	
24	LU	128	
25	LV	140	
26	LW	157	
27	LX	156	
28	LY	145	

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Mol	Chain	Length	Quality of chain
29	LZ	136	
30	La	148	
31	Lb	159	
32	Lc	115	
33	Ld	125	
34	Le	135	
35	Lf	110	
36	Lg	117	
37	Lh	123	
38	Li	105	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	Mr	7	
47	Pt	76	
48	S2	1869	
49	SB	264	
50	SC	293	
51	SD	243	
52	SE	263	
53	SF	204	



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Mol	Chain	Length	Quality of chain
54	SG	249	
55	SH	194	
56	SI	208	
57	SJ	194	
58	SK	165	
59	SL	158	
60	SM	132	
61	SN	151	
62	SO	151	
63	SP	145	
64	SQ	146	
65	SR	135	
66	SS	152	
67	ST	145	
68	SU	119	
69	SV	83	
70	SW	130	
71	SY	133	
72	SZ	125	
73	Sa	115	
74	Sb	84	
75	Sc	69	
76	Sd	56	
77	Se	133	
78	Sf	156	

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Mol	Chain	Length	Quality of chain
79	Sg	317	
80	LA	257	
81	SA	295	
82	SX	143	
83	Lj	97	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	ZN	Sd	102	-	-	X	-
90	HYG	S2	2021	X	-	-	-

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 211463 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 A-site-tRNA-Ile-AAT-9-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	At	73	Total	C	N	O	P	0	0
			1559	697	280	510	72		

- Molecule 2 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Et	54	Total	C	N	O	P	0	0
			1155	516	214	372	53		

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3466	Total	C	N	O	P	1	0
			74397	33170	13604	24157	3466		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LB	399	Total	C	N	O	S	0	0
			3221	2051	605	551	14		

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD	294	Total	C	N	O	S	0	0
			2385	1507	436	428	14		

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	223	Total	C	N	O	S	0	0
			1782	1147	338	293	4		

- Molecule 10 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LF	225	Total	C	N	O	S	0	0
			1856	1193	357	297	9		

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	232	Total	C	N	O	S	0	0
			1846	1175	356	311	4		

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 13 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	207	Total	C	N	O	S	0	0
			1672	1062	322	275	13		

- Molecule 14 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LL	206	Total	C	N	O	S	1	0
			1672	1046	348	274	4		

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 17 is a protein called 60S ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LO	200	Total	C	N	O	S	0	0
			1640	1058	320	257	5		

- Molecule 19 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LP	153	Total	C	N	O	S	1	0
			1249	781	243	216	9		

- Molecule 20 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 21 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LR	180	Total	C	N	O	S	0	0
			1449	898	311	231	9		

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	159	Total	C	N	O	S	1	0
			1303	828	253	216	6		

- Molecule 24 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 25 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LV	133	Total	C	N	O	S	0	0
			988	623	186	174	5		

- Molecule 26 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LW	105	Total	C	N	O	S	0	0
			847	532	171	140	4		

- Molecule 27 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LX	118	Total	C	N	O	S	0	0
			966	618	181	166	1		

- Molecule 28 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LY	132	Total	C	N	O	S	0	0
			1098	689	222	184	3		

- 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
			1107	714	208	182	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lb	105	Total	C	N	O	S	0	0
			846	526	185	131	4		

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lc	99	Total	C	N	O	S	0	0
			766	485	135	140	6		

- Molecule 33 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Le	128	Total	C	N	O	S	1	0
			1061	672	219	165	5		

- Molecule 35 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lf	110	Total	C	N	O	S	0	0
			880	558	175	144	3		

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lg	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 37 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lk	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 41 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	1	0
			432	269	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	2	0
			875	548	181	140	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lp	90	Total	C	N	O	S	0	0
			698	440	134	117	7		

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 46 is a RNA chain called synthetic mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Mr	7	Total	C	N	O	P	0	0
			147	67	23	50	7		

- Molecule 47 is a RNA chain called P-site tRNA-Arg-ACG.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Pt	74	Total	C	N	O	P	0	0
			1587	710	285	518	74		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1619	Total	C	N	O	P	0	0
			34624	15485	6221	11300	1618		

- Molecule 49 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	221	Total	C	N	O	S	0	0
			1793	1138	323	318	14		

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SC	219	Total	C	N	O	S	0	0
			1700	1100	292	298	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	225	Total	C	N	O	S	0	0
			1742	1112	312	311	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE	259	Total	C	N	O	S	0	0
			2059	1316	383	352	8		

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	183	Total	C	N	O	S	0	0
			1443	905	269	262	7		

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SG	216	Total	C	N	O	S	0	0
			1721	1078	341	295	7		

- Molecule 55 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SH	186	Total	C	N	O	S	0	0
			1486	947	271	267	1		

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 57 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SJ	175	Total	C	N	O	S	0	0
			1424	905	284	233	2		

- Molecule 58 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SK	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 59 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SL	143	Total	C	N	O	S	0	0
			1171	746	221	198	6		

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SM	109	Total	C	N	O	S	0	0
			754	469	135	144	6		

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SN	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SO	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SP	130	Total	C	N	O	S	0	0
			1071	680	203	181	7		

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SQ	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 65 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SR	133	Total	C	N	O	S	0	0
			1075	675	200	196	4		

- Molecule 66 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 67 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ST	142	Total	C	N	O	S	1	0
			1121	707	212	199	3		

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 70 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SY	121	Total	C	N	O	S	0	0
			995	631	195	164	5		

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SZ	87	Total	C	N	O	S	0	0
			693	445	130	117	1		

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 75 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sc	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 76 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 77 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Se	49	Total	C	N	O	S	0	0
			390	239	87	63	1		

- Molecule 78 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	61	Total	C	N	O	S	0	0
			480	300	91	83	6		

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sg	312	Total	C	N	O	S	0	0
			2427	1531	423	463	10		

- Molecule 80 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	LA	250	Total	C	N	O	S	1	0
			1923	1204	395	318	6		

- Molecule 81 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SA	220	Total	C	N	O	S	0	0
			1730	1099	303	321	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	ACE	-	acetylation	UNP P08865

- Molecule 82 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	SX	140	Total	C	N	O	S	0	0
			1088	687	215	183	3		

- Molecule 83 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
84	L5	86	Total	K	0
			86	86	
84	L7	2	Total	K	0
			2	2	
84	L8	1	Total	K	0
			1	1	
84	LH	1	Total	K	0
			1	1	
84	LI	1	Total	K	0
			1	1	
84	Lb	1	Total	K	0
			1	1	
84	Le	1	Total	K	0
			1	1	
84	Lf	1	Total	K	0
			1	1	
84	Lg	1	Total	K	0
			1	1	
84	Pt	1	Total	K	0
			1	1	
84	S2	48	Total	K	0
			48	48	
84	SF	1	Total	K	0
			1	1	
84	SL	1	Total	K	0
			1	1	
84	SO	1	Total	K	0
			1	1	
84	SS	1	Total	K	0
			1	1	
84	Sd	1	Total	K	0
			1	1	
84	LA	2	Total	K	0
			2	2	

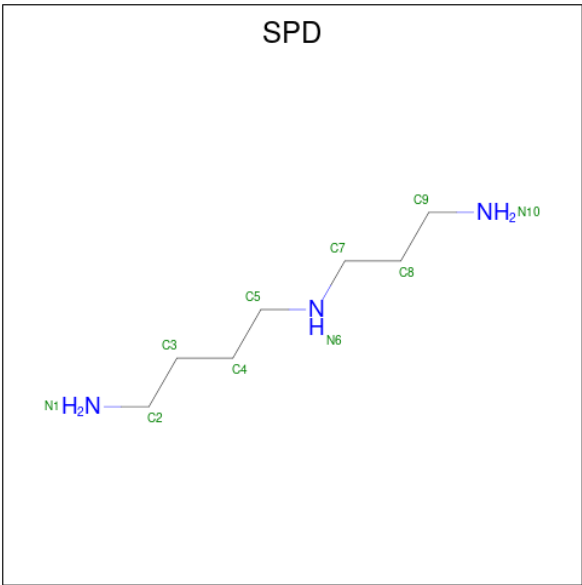
- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	L5	160	Total 160	Mg 160	0
85	L7	3	Total 3	Mg 3	0
85	L8	2	Total 2	Mg 2	0
85	LI	1	Total 1	Mg 1	0
85	LP	1	Total 1	Mg 1	0
85	LV	1	Total 1	Mg 1	0
85	Ln	2	Total 2	Mg 2	0
85	Pt	1	Total 1	Mg 1	0
85	S2	54	Total 54	Mg 54	0

- Molecule 86 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
86	L5	22	Total 22	Na 22	0
86	L8	1	Total 1	Na 1	0
86	La	1	Total 1	Na 1	0
86	S2	11	Total 11	Na 11	0

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



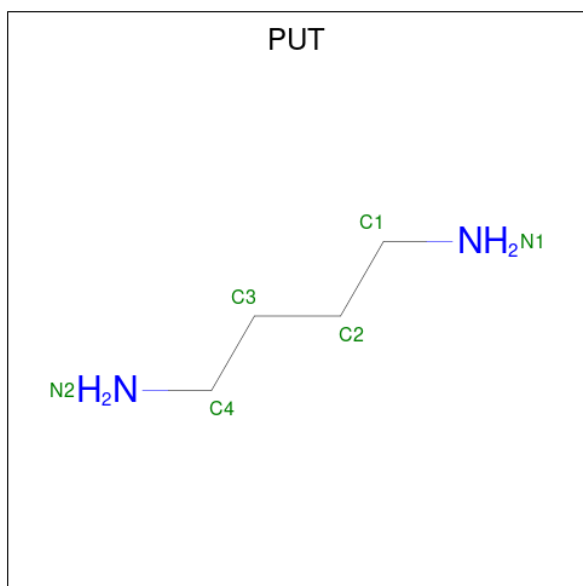
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L8	1	Total	C	N	0
			10	7	3	
87	LN	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
87	S2	1	Total	C	N	0
			10	7	3	
87	S2	1	Total	C	N	0
			10	7	3	
87	S2	1	Total	C	N	0
			10	7	3	
87	S2	1	Total	C	N	0
			10	7	3	
87	S2	1	Total	C	N	0
			10	7	3	

- Molecule 88 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	

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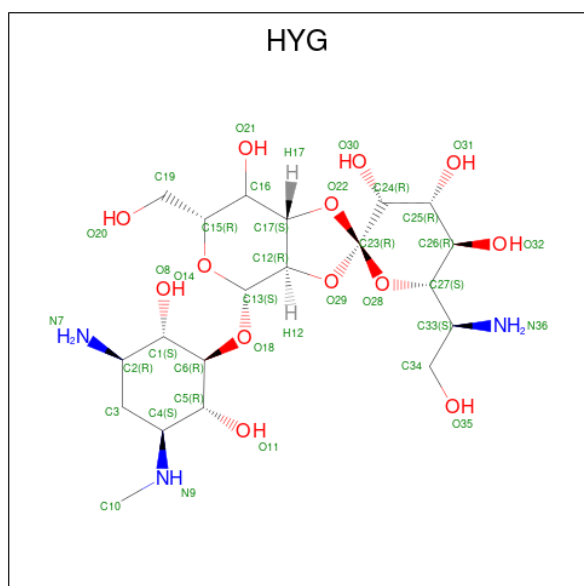
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Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			6	4	2	
88	S2	1	Total	C	N	0
			6	4	2	
88	S2	1	Total	C	N	0
			6	4	2	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 90 is HYGROMYCIN B (CCD ID: HYG) (formula: C₂₀H₃₇N₃O₁₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
91	At	1	Total	O	0
			1	1	
91	Et	1	Total	O	0
			1	1	
91	L5	281	Total	O	0
			281	281	
91	L7	1	Total	O	0
			1	1	
91	L8	6	Total	O	0
			6	6	
91	LC	1	Total	O	0
			1	1	
91	LI	1	Total	O	0
			1	1	
91	LN	1	Total	O	0
			1	1	
91	LP	1	Total	O	0
			1	1	
91	LQ	1	Total	O	0
			1	1	
91	LY	1	Total	O	0
			1	1	
91	La	3	Total	O	0
			3	3	
91	Ld	1	Total	O	0
			1	1	
91	Le	3	Total	O	0
			3	3	
91	Ln	7	Total	O	0
			7	7	
91	Lo	4	Total	O	0
			4	4	
91	Lp	1	Total	O	0
			1	1	
91	Mr	11	Total	O	0
			11	11	
91	Pt	11	Total	O	0
			11	11	

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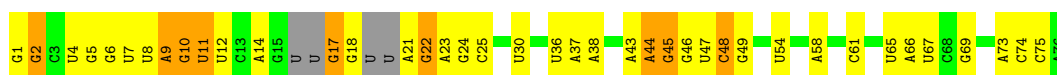
Mol	Chain	Residues	Atoms		AltConf
91	S2	171	Total 171	O 171	0
91	SN	1	Total 1	O 1	0
91	SO	1	Total 1	O 1	0
91	SQ	1	Total 1	O 1	0
91	SW	1	Total 1	O 1	0
91	LA	4	Total 4	O 4	0
91	SX	1	Total 1	O 1	0

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.

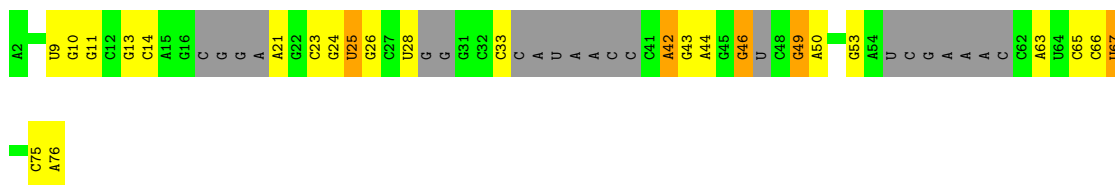
• Molecule 1: A-site-tRNA-Ile-AAT-9-1

Chain At: 



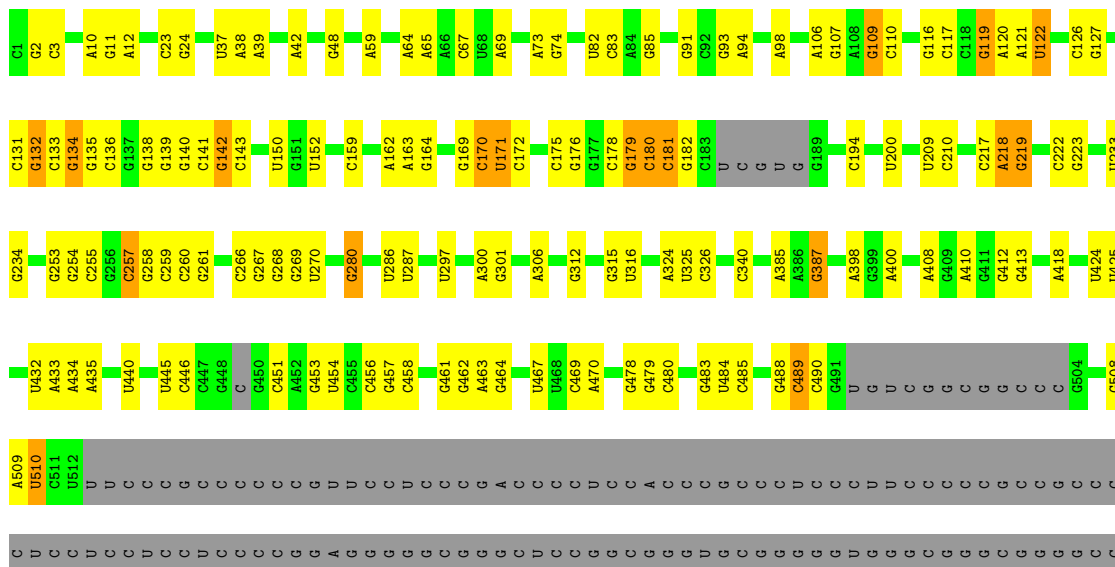
• Molecule 2: E site tRNA

Chain Et: 



• Molecule 3: 28S rRNA

Chain L5: 



WORLDWIDE
PDB
PROTEIN DATA BANK







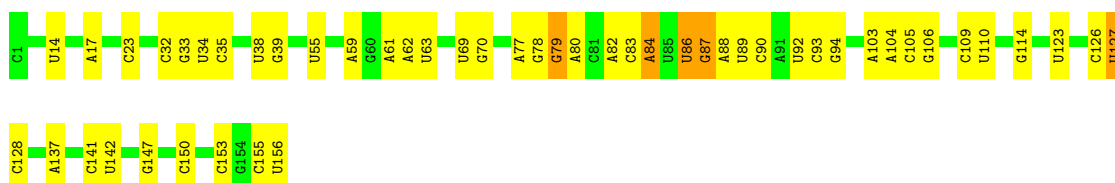
- Molecule 4: 5S rRNA

Chain L7: 78% 21% ..



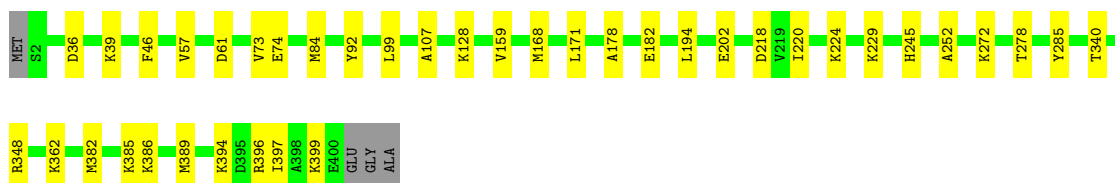
- Molecule 5: 5.8S rRNA

Chain L8: 68% 29% .



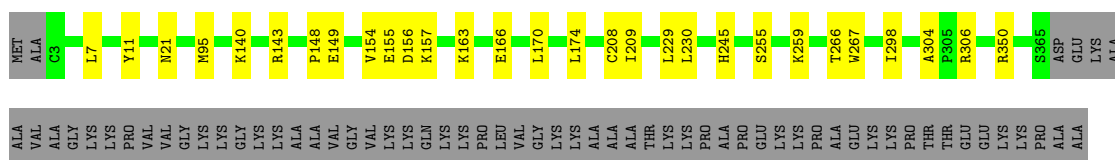
- Molecule 6: Large ribosomal subunit protein uL3

Chain LB: 89% 10% .



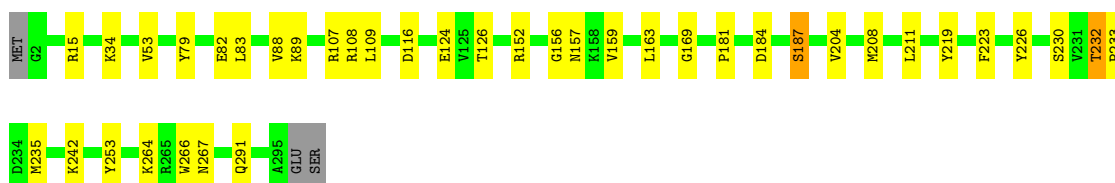
- Molecule 7: 60S ribosomal protein L4

Chain LC: 78% 7% 15%

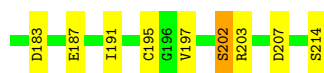


- Molecule 8: 60S ribosomal protein L5

Chain LD: 86% 12% ..



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|
| MET | G2 | R7 | R32 | I33 | L36 | K39 | L48 | S54 | S61 | S62 | S63 | A64 | L65 | R69 | K74 | V77 | G81 | K82 | I87 | P93 | L103 | SER | CYS | ALA | GLY | ALA | ASP | R110 | T113 | T125 | I135 | R139 | K145 | E146 | I149 | L152 | I156 |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|



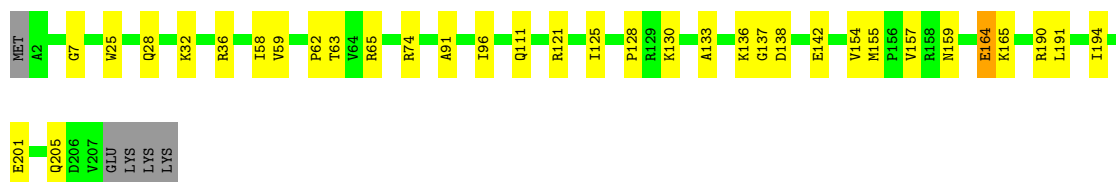
- Molecule 14: 60S ribosomal protein L11

Chain LJ: 76% 19% . .



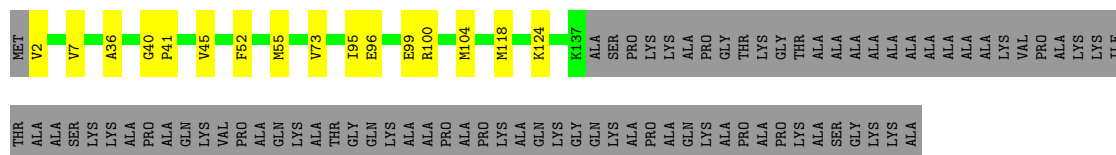
- Molecule 15: Large ribosomal subunit protein eL13

Chain LL: 82% 16% .



- Molecule 16: 60S ribosomal protein L14

Chain LM: 56% 7% 37%



- Molecule 17: 60S ribosomal protein L15

Chain LN: 88% 12%



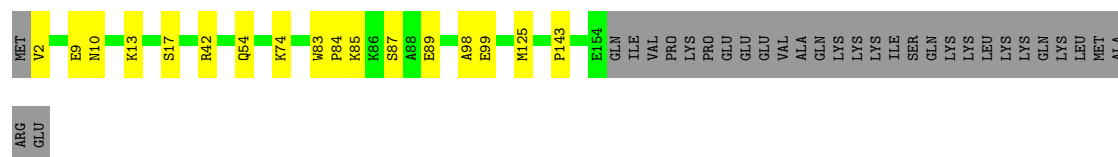
- Molecule 18: 60S ribosomal protein L13a

Chain LO: 91% 7% .



- Molecule 19: 60S ribosomal protein L17

Chain LP: 74% 9% 17%



- Molecule 20: 60S ribosomal protein L18

Chain LQ: 93% 7%



- Molecule 21: 60S ribosomal protein L19

Chain LR: 85% 7% 8%



- Molecule 22: 60S ribosomal protein L18a

Chain LS: 90% 10%



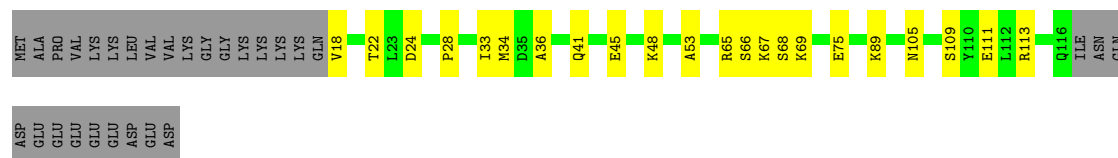
- Molecule 23: 60S ribosomal protein L21

Chain LT: 87% 12%



- Molecule 24: 60S ribosomal protein L22

Chain LU: 60% 17% 23%



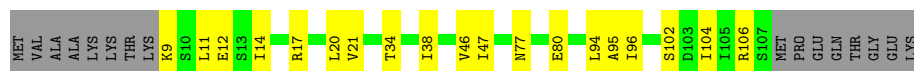
- Molecule 25: 60S ribosomal protein L23

Chain LV: 87% 8% 5%



- Molecule 32: 60S ribosomal protein L30

Chain Lc:  70% 17% 14%




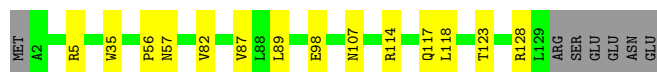
- Molecule 33: 60S ribosomal protein L31

Chain Ld:  73% 12% 14%



- Molecule 34: 60S ribosomal protein L32

Chain Le:  84% 10% 5%




- Molecule 35: 60S ribosomal protein L35a

Chain Lf:  100%


There are no outlier residues recorded for this chain.

- Molecule 36: 60S ribosomal protein L34

Chain Lg:  81% 15%




- Molecule 37: 60S ribosomal protein L35

Chain Lh:  81% 18%




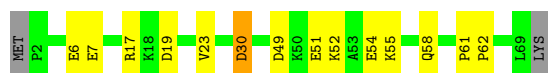
- Molecule 38: 60S ribosomal protein L36

Chain Li:  82% 15%



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  77% 19%



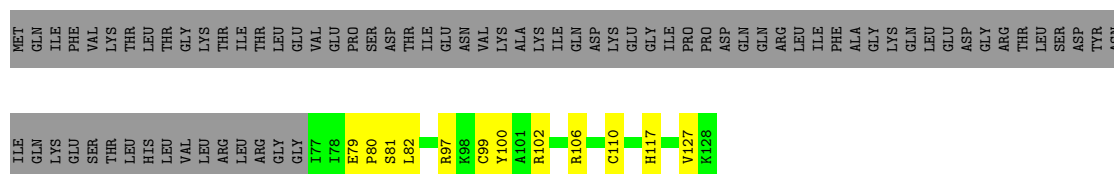
- Molecule 40: 60S ribosomal protein L39

Chain Ll: 80% 18% .



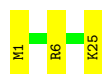
- Molecule 41: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm: 31% 9% 59%



- Molecule 42: 60S ribosomal protein L41

Chain Ln: 88% 12%



- Molecule 43: Large ribosomal subunit protein eL42

Chain Lo: 81% 16% ..



- Molecule 44: 60S ribosomal protein L37a

Chain Lp: 91% 5% ..



- Molecule 45: 60S ribosomal protein L28

Chain Lr: 81% 10% 9%



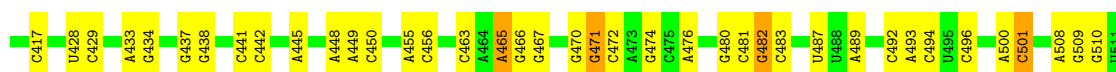
- Molecule 46: synthetic mRNA



Chain Pt: 53% 41% . .




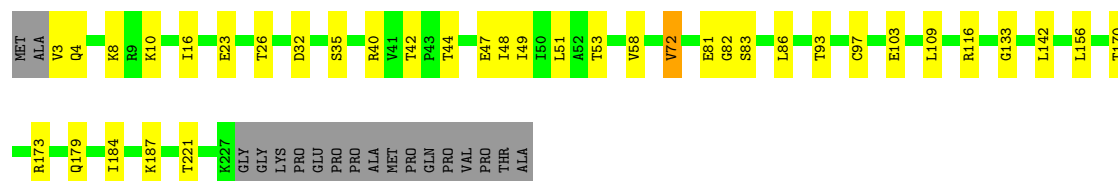
U1	A2	C3	C4		U15	G16	C17		U21	A22	G23		A27		G33	U34	C35	U36		G41		U44	A45	A46		U51	G52		G56		U59	A60	A61		A64	C65	G66	C67	C68	A69	G70	G71	G72	C	C	G	G	U76	A77	C78	A79	G80	U81	G82		A92	U93		A99	
----	----	----	----	--	-----	-----	-----	--	-----	-----	-----	--	-----	--	-----	-----	-----	-----	--	-----	--	-----	-----	-----	--	-----	-----	--	-----	--	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	---	---	---	---	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	--	-----	--





- Molecule 51: 40S ribosomal protein S3

Chain SD: 




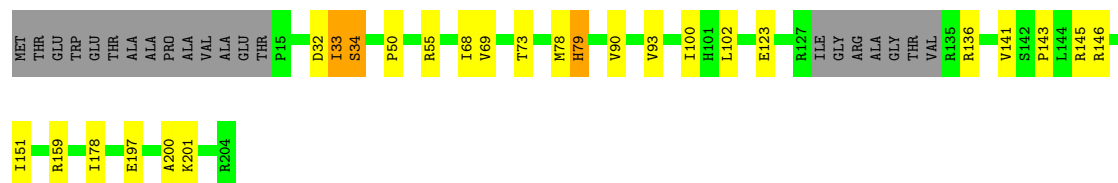
- Molecule 52: Small ribosomal subunit protein eS4, X isoform

Chain SE: 83% 15%



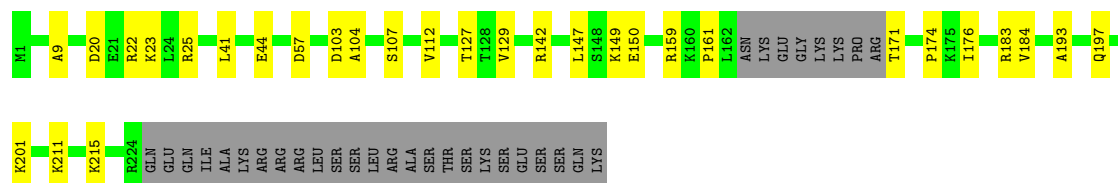
- Molecule 53: 40S ribosomal protein S5

Chain SF:  77% 11% • 10%



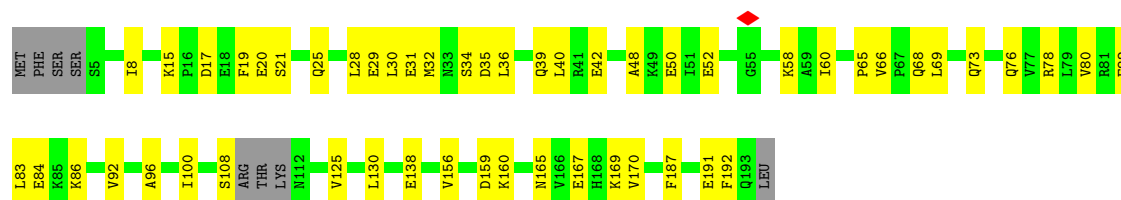
- Molecule 54: 40S ribosomal protein S6

Chain SG: 75% 12% 13%



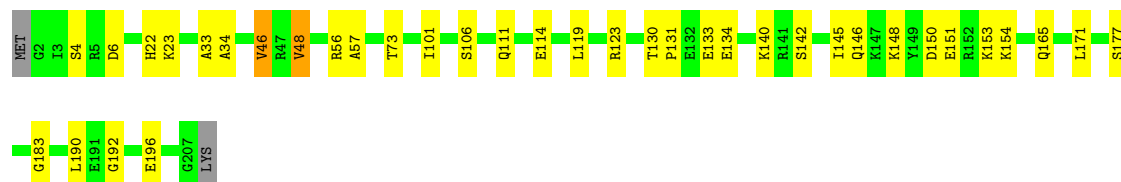
- Molecule 55: 40S ribosomal protein S7

Chain SH:  69% 27%



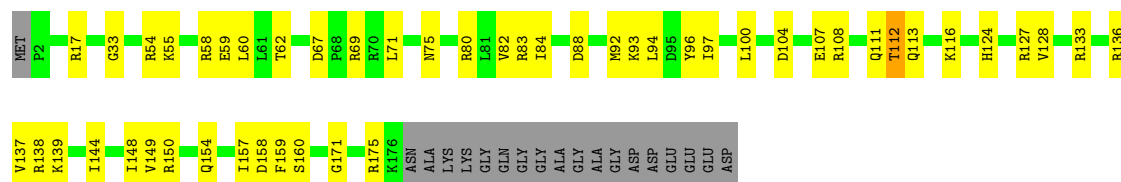
- Molecule 56: 40S ribosomal protein S8

Chain SI: 81% 17% ..



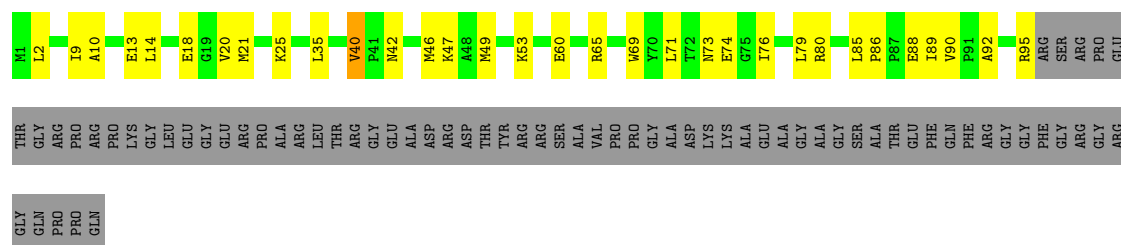
- Molecule 57: 40S ribosomal protein S9

Chain SJ: 65% 25% 10%



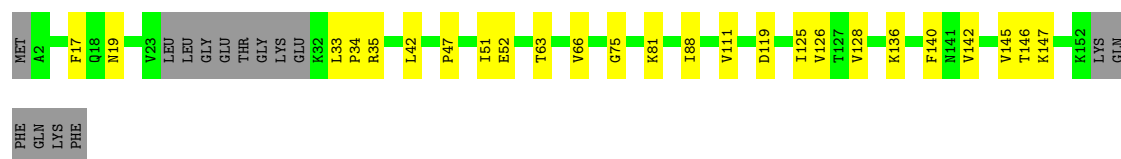
- Molecule 58: 40S ribosomal protein S10

Chain SK: 38% 19% 42%



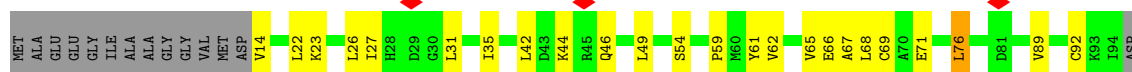
- Molecule 59: 40S ribosomal protein S11

Chain SL: 75% 16% 9%




- Molecule 60: 40S ribosomal protein S12

Chain SM:  60% 22% 17%



- Molecule 61: 40S ribosomal protein S13

Chain SN:  83% 16%




- Molecule 62: 40S ribosomal protein S14

Chain SO:  71% 19% 11%




- Molecule 63: 40S ribosomal protein S15

Chain SP:  81% 6% 10%




- Molecule 64: 40S ribosomal protein S16

Chain SQ:  82% 12%




- Molecule 65: 40S ribosomal protein S17

Chain SR:  76% 21%




- Molecule 66: 40S ribosomal protein S18

Chain SS:  83% 14% ..



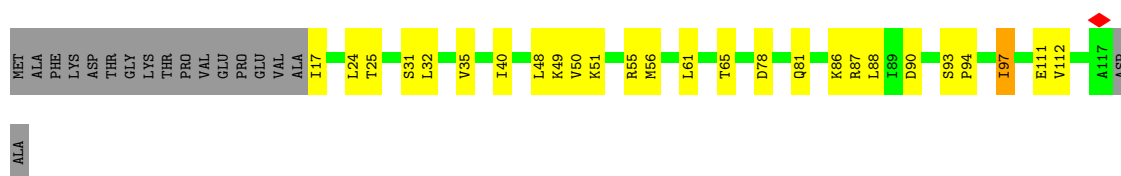
- Molecule 67: 40S ribosomal protein S19

Chain ST:  87% 10% ..




- Molecule 68: 40S ribosomal protein S20

Chain SU:  63% 21% 15%



- Molecule 69: 40S ribosomal protein S21

Chain SV:  83% 14%



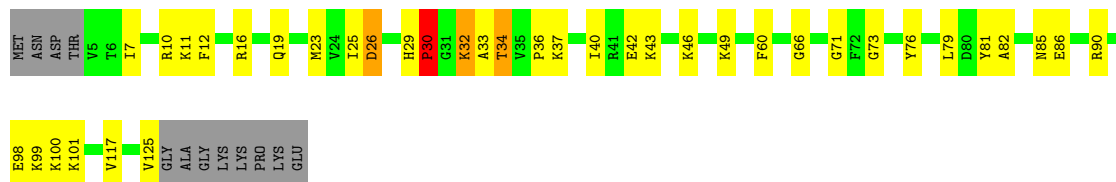
- Molecule 70: 40S ribosomal protein S15a

Chain SW:  86% 12% ..



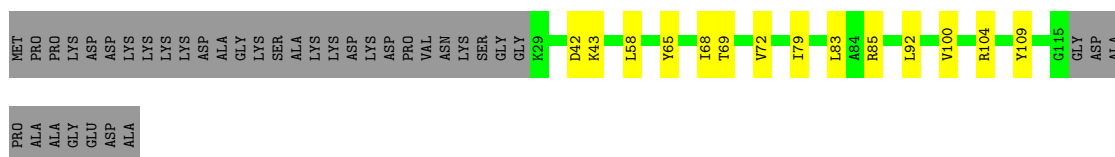
- Molecule 71: 40S ribosomal protein S24

Chain SY:  62% 26% 9%



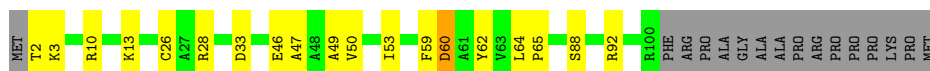
- Molecule 72: 40S ribosomal protein S25

Chain SZ:  58% 11% 30%



- Molecule 73: 40S ribosomal protein S26

Chain Sa: 70% 16% 14%



- Molecule 74: 40S ribosomal protein S27

Chain Sb: 80% 18% ..



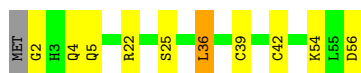
- Molecule 75: 40S ribosomal protein S28

Chain Sc: 65% 26% 9%



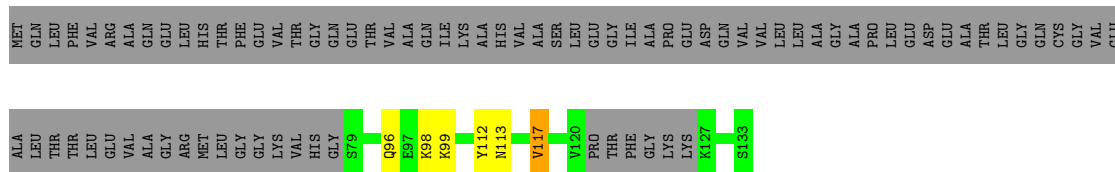
- Molecule 76: 40S ribosomal protein S29

Chain Sd: 80% 16% ..



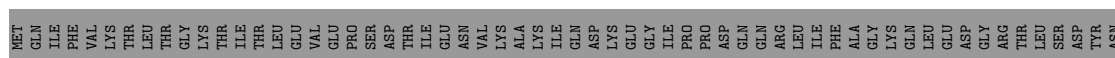
- Molecule 77: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se: 32% 63%



- Molecule 78: Ubiquitin

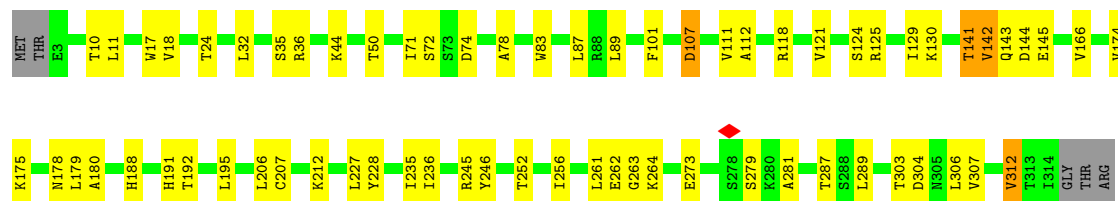
Chain Sf: 29% 10% 61%





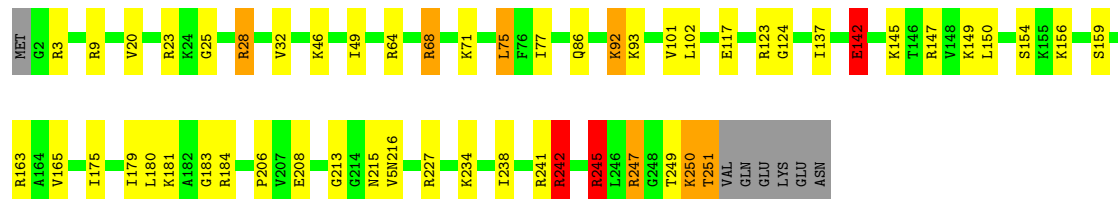
- Molecule 79: Receptor of activated protein C kinase 1

Chain Sg: 77% 20% ..



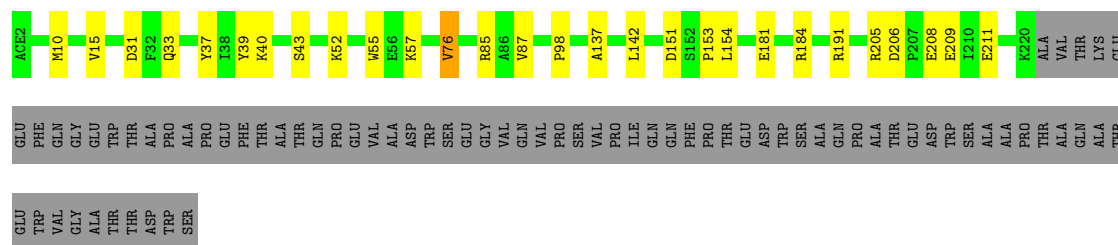
- Molecule 80: Large ribosomal subunit protein uL2

Chain LA: 76% 17% . . .



- Molecule 81: Small ribosomal subunit protein uS2

Chain SA: 65% 9% 25%



- Molecule 82: 40S ribosomal protein S23

Chain SX: 84% 12% ..



- Molecule 83: Large ribosomal subunit protein eL37

Chain Lj: 81% 7% 11%

MET	T2	S7	R20	K36	Y39	P40	W49	K87	ARG	ALA	ALA	VAL	ALA	ALA	SER	SER	SER
-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121901	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 ($e^-/\text{\AA}^2$)	1.077	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, PUT, UR3, A2M, UY1, M3L, ACE, SPD, 6MZ, HIC, MA7, B8H, MG, OMC, M2G, 1MA, K, OMU, NA, OMG, 5MC, V5N, MA6, HY3, 1MG, PSU, B8N, 4AC, HYG, ZN, G7M

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	At	0.70	0/1714	0.99	1/2662 (0.0%)
2	Et	0.20	0/1287	0.28	0/1994
3	L5	0.29	0/80395	0.32	2/125381 (0.0%)
4	L7	0.66	0/2836	0.84	0/4421
5	L8	0.66	0/3609	0.84	0/5623
6	LB	0.22	0/3276	0.31	0/4382
7	LC	0.22	0/2942	0.31	0/3951
8	LD	0.20	0/2430	0.30	0/3254
9	LE	0.19	0/1816	0.28	0/2438
10	LF	0.23	0/1890	0.32	0/2521
11	LG	0.21	0/1877	0.31	0/2532
12	LH	0.21	0/1537	0.33	0/2066
13	LI	0.33	0/1710	0.52	1/2284 (0.0%)
14	LJ	0.19	0/1385	0.39	0/1852
15	LL	0.20	0/1706	0.30	0/2284
16	LM	0.21	0/1142	0.32	0/1527
17	LN	0.25	0/1745	0.33	0/2338
18	LO	0.22	0/1672	0.31	0/2238
19	LP	0.22	0/1279	0.34	0/1716
20	LQ	0.23	0/1536	0.31	0/2052
21	LR	0.20	0/1465	0.31	0/1945
22	LS	0.24	0/1500	0.32	0/2013
23	LT	0.22	0/1334	0.34	0/1781
24	LU	0.18	0/822	0.36	0/1103
25	LV	0.21	0/1002	0.32	0/1345
26	LW	0.21	0/861	0.39	0/1146
27	LX	0.21	0/983	0.33	0/1323
28	LY	0.21	0/1115	0.33	0/1484
29	LZ	0.21	0/1130	0.27	0/1507
30	La	0.24	0/1178	0.32	0/1573
31	Lb	0.20	0/848	0.35	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.20	0/776	0.29	0/1042
33	Ld	0.21	0/903	0.30	0/1216
34	Le	0.22	0/1082	0.29	0/1443
35	Lf	0.23	0/899	0.29	0/1205
36	Lg	0.21	0/898	0.32	0/1197
37	Lh	0.20	0/1022	0.29	0/1351
38	Li	0.19	0/843	0.30	0/1115
39	Lk	0.21	0/565	0.36	0/750
40	Ll	0.23	0/453	0.29	0/599
41	Lm	0.56	0/429	0.73	0/571
42	Ln	0.39	0/240	0.31	0/305
43	Lo	0.29	0/881	0.38	0/1161
44	Lp	0.22	0/708	0.33	0/941
45	Lr	0.22	0/1017	0.31	0/1364
46	Mr	0.60	0/114	0.96	0/170
47	Pt	0.71	0/1663	0.90	1/2585 (0.0%)
48	S2	0.67	0/36806	0.86	5/57350 (0.0%)
49	SB	0.20	0/1819	0.31	0/2432
50	SC	0.22	0/1737	0.33	0/2347
51	SD	0.20	0/1770	0.30	0/2385
52	SE	0.20	0/2101	0.32	0/2828
53	SF	0.23	0/1464	0.35	0/1969
54	SG	0.18	0/1742	0.33	0/2326
55	SH	0.17	0/1508	0.34	0/2022
56	SI	0.22	0/1715	0.37	0/2287
57	SJ	0.23	0/1446	0.40	0/1937
58	SK	0.23	0/823	0.41	0/1111
59	SL	0.23	0/1191	0.35	0/1593
60	SM	0.15	0/758	0.40	0/1028
61	SN	0.20	0/1231	0.29	0/1656
62	SO	0.28	0/1022	0.42	0/1372
63	SP	0.32	0/1093	0.48	1/1460 (0.1%)
64	SQ	0.24	0/1133	0.38	0/1517
65	SR	0.22	0/1090	0.41	1/1464 (0.1%)
66	SS	0.21	0/1232	0.33	0/1651
67	ST	0.21	0/1148	0.32	0/1540
68	SU	0.20	0/813	0.30	0/1092
69	SV	0.19	0/643	0.31	0/860
70	SW	0.23	0/1051	0.36	0/1406
71	SY	0.32	0/1012	0.48	0/1344
72	SZ	0.20	0/701	0.35	0/936
73	Sa	0.38	0/805	0.52	0/1079
74	Sb	0.46	0/665	0.61	1/891 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sc	0.22	0/497	0.34	0/666
76	Sd	0.50	0/469	0.63	0/623
77	Se	0.16	0/392	0.31	0/514
78	Sf	0.13	0/489	0.37	0/650
79	Sg	0.20	0/2484	0.39	0/3382
80	LA	1.03	2/1951 (0.1%)	1.23	8/2613 (0.3%)
81	SA	0.31	0/1765	0.47	0/2398
82	SX	0.35	0/1096	0.45	0/1461
83	Lj	0.41	0/720	0.61	0/952
All	All	0.40	2/220897 (0.0%)	0.52	21/324011 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	LI	0	2
41	Lm	0	2
57	SJ	0	1
63	SP	0	1
74	Sb	0	1
80	LA	0	15
82	SX	0	1
83	Lj	0	1
All	All	0	24

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	LA	245[A]	ARG	C-O	10.29	1.36	1.23
80	LA	245[B]	ARG	C-O	10.29	1.36	1.23

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1581	G	OP1-P-O3'	-24.59	34.24	108.00
80	LA	245[A]	ARG	CA-C-O	11.07	132.03	120.95
80	LA	245[B]	ARG	CA-C-O	11.07	132.03	120.95
80	LA	245[A]	ARG	O-C-N	-7.47	114.74	123.11
80	LA	245[B]	ARG	O-C-N	-7.47	114.74	123.11

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	LI	32	ARG	Sidechain
13	LI	69	ARG	Sidechain
41	Lm	102	ARG	Sidechain
41	Lm	97	ARG	Sidechain
57	SJ	133	ARG	Sidechain

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	At	1559	0	793	13	0
2	Et	1155	0	593	15	0
3	L5	74397	0	37669	646	0
4	L7	2538	0	1284	9	0
5	L8	3316	0	1687	15	0
6	LB	3221	0	3363	24	0
7	LC	2888	0	3064	21	0
8	LD	2385	0	2419	23	0
9	LE	1782	0	1934	17	0
10	LF	1856	0	1981	17	0
11	LG	1846	0	1954	22	0
12	LH	1518	0	1600	15	0
13	LI	1672	0	1717	20	0
14	LJ	1362	0	1399	23	0
15	LL	1672	0	1786	30	0
16	LM	1120	0	1187	13	0
17	LN	1700	0	1749	16	0
18	LO	1640	0	1788	10	0
19	LP	1249	0	1276	10	0
20	LQ	1512	0	1628	13	0
21	LR	1449	0	1549	7	0
22	LS	1460	0	1502	14	0
23	LT	1303	0	1379	17	0
24	LU	808	0	831	12	0
25	LV	988	0	1047	8	0
26	LW	847	0	873	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	LX	966	0	1040	5	0
28	LY	1098	0	1178	11	0
29	LZ	1107	0	1182	14	0
30	La	1162	0	1206	13	0
31	Lb	846	0	914	12	0
32	Lc	766	0	798	9	0
33	Ld	888	0	930	9	0
34	Le	1061	0	1160	8	0
35	Lf	880	0	916	0	0
36	Lg	888	0	977	12	0
37	Lh	1014	0	1148	16	0
38	Li	832	0	917	8	0
39	Lk	559	0	624	9	0
40	Ll	443	0	483	6	0
41	Lm	432	0	465	7	0
42	Ln	239	0	289	4	0
43	Lo	875	0	941	14	0
44	Lp	698	0	748	3	0
45	Lr	1002	0	1068	11	0
46	Mr	147	0	56	0	0
47	Pt	1587	0	810	10	0
48	S2	34624	0	17520	262	0
49	SB	1793	0	1879	21	0
50	SC	1700	0	1784	20	0
51	SD	1742	0	1833	18	0
52	SE	2059	0	2164	28	0
53	SF	1443	0	1483	18	0
54	SG	1721	0	1840	19	0
55	SH	1486	0	1560	35	0
56	SI	1686	0	1772	23	0
57	SJ	1424	0	1499	31	0
58	SK	799	0	823	22	0
59	SL	1171	0	1241	13	0
60	SM	754	0	705	20	0
61	SN	1207	0	1293	15	0
62	SO	1009	0	1034	19	0
63	SP	1071	0	1114	8	0
64	SQ	1116	0	1185	14	0
65	SR	1075	0	1128	21	0
66	SS	1214	0	1275	14	0
67	ST	1121	0	1151	15	0
68	SU	803	0	873	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	SV	636	0	637	13	0
70	SW	1034	0	1080	9	0
71	SY	995	0	1068	31	0
72	SZ	693	0	768	11	0
73	Sa	792	0	841	11	0
74	Sb	651	0	672	16	0
75	Sc	495	0	523	9	0
76	Sd	458	0	449	9	0
77	Se	390	0	431	6	0
78	Sf	480	0	469	10	0
79	Sg	2427	0	2380	37	0
80	LA	1923	0	2019	17	0
81	SA	1730	0	1731	20	0
82	SX	1088	0	1149	8	0
83	Lj	705	0	737	3	0
84	L5	86	0	0	0	0
84	L7	2	0	0	0	0
84	L8	1	0	0	0	0
84	LA	2	0	0	0	0
84	LH	1	0	0	0	0
84	LI	1	0	0	0	0
84	Lb	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lf	1	0	0	0	0
84	Lg	1	0	0	0	0
84	Pt	1	0	0	0	0
84	S2	48	0	0	0	0
84	SF	1	0	0	0	0
84	SL	1	0	0	0	0
84	SO	1	0	0	0	0
84	SS	1	0	0	0	0
84	Sd	1	0	0	0	0
85	L5	160	0	0	0	0
85	L7	3	0	0	0	0
85	L8	2	0	0	0	0
85	LI	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0
85	Ln	2	0	0	0	0
85	Pt	1	0	0	0	0
85	S2	54	0	0	0	0
86	L5	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L8	1	0	0	0	0
86	La	1	0	0	0	0
86	S2	11	0	0	0	0
87	L5	120	0	228	7	0
87	L8	10	0	19	1	0
87	LN	10	0	19	0	0
87	S2	50	0	95	3	0
88	L5	42	0	84	3	0
88	S2	12	0	24	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	1	0	0	2	0
90	S2	36	0	37	1	0
91	At	1	0	0	0	0
91	Et	1	0	0	0	0
91	L5	281	0	0	2	0
91	L7	1	0	0	0	0
91	L8	6	0	0	0	0
91	LA	4	0	0	0	0
91	LC	1	0	0	0	0
91	LI	1	0	0	0	0
91	LN	1	0	0	0	0
91	LP	1	0	0	0	0
91	LQ	1	0	0	0	0
91	LY	1	0	0	0	0
91	La	3	0	0	0	0
91	Ld	1	0	0	0	0
91	Le	3	0	0	0	0
91	Ln	7	0	0	0	0
91	Lo	4	0	0	0	0
91	Lp	1	0	0	0	0
91	Mr	11	0	0	0	0
91	Pt	11	0	0	0	0
91	S2	171	0	0	0	0
91	SN	1	0	0	0	0
91	SO	1	0	0	0	0
91	SQ	1	0	0	0	0
91	SW	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	SX	1	0	0	0	0
All	All	211463	0	156518	1844	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 1844 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)
48:S2:551:U:H2'	48:S2:552:G:C8	1.98	0.98
48:S2:857:U:H2'	48:S2:858:A:C8	2.04	0.91
3:L5:4095:G:H1	3:L5:4113:U:H3	0.89	0.89
50:SC:249:SER:HA	69:SV:23:ILE:HD11	1.56	0.88
48:S2:394:G:H5''	59:SL:81:LYS:HB3	1.57	0.86

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	
6	LB	396/403 (98%)	388 (98%)	8 (2%)	0	100	100
7	LC	361/427 (84%)	355 (98%)	6 (2%)	0	100	100
8	LD	292/297 (98%)	287 (98%)	5 (2%)	0	100	100
9	LE	217/288 (75%)	212 (98%)	5 (2%)	0	100	100
10	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
11	LG	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
12	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
13	LI	203/214 (95%)	201 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	LJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
15	LL	205/211 (97%)	201 (98%)	4 (2%)	0	100	100
16	LM	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
17	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
18	LO	198/203 (98%)	198 (100%)	0	0	100	100
19	LP	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
20	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
21	LR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
22	LS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
23	LT	158/160 (99%)	155 (98%)	3 (2%)	0	100	100
24	LU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
25	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
26	LW	101/157 (64%)	95 (94%)	6 (6%)	0	100	100
27	LX	116/156 (74%)	116 (100%)	0	0	100	100
28	LY	130/145 (90%)	127 (98%)	3 (2%)	0	100	100
29	LZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
30	La	144/148 (97%)	141 (98%)	3 (2%)	0	100	100
31	Lb	100/159 (63%)	99 (99%)	1 (1%)	0	100	100
32	Lc	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
33	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
34	Le	127/135 (94%)	127 (100%)	0	0	100	100
35	Lf	108/110 (98%)	108 (100%)	0	0	100	100
36	Lg	110/117 (94%)	110 (100%)	0	0	100	100
37	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
38	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
39	Lk	66/70 (94%)	66 (100%)	0	0	100	100
40	Ll	48/51 (94%)	48 (100%)	0	0	100	100
41	Lm	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
42	Ln	23/25 (92%)	23 (100%)	0	0	100	100
43	Lo	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
44	Lp	88/92 (96%)	84 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	Lr	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
49	SB	217/264 (82%)	210 (97%)	7 (3%)	0	100	100
50	SC	217/293 (74%)	213 (98%)	4 (2%)	0	100	100
51	SD	223/243 (92%)	214 (96%)	9 (4%)	0	100	100
52	SE	257/263 (98%)	249 (97%)	8 (3%)	0	100	100
53	SF	179/204 (88%)	174 (97%)	4 (2%)	1 (1%)	21	32
54	SG	212/249 (85%)	206 (97%)	6 (3%)	0	100	100
55	SH	182/194 (94%)	174 (96%)	8 (4%)	0	100	100
56	SI	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
57	SJ	173/194 (89%)	166 (96%)	7 (4%)	0	100	100
58	SK	93/165 (56%)	90 (97%)	3 (3%)	0	100	100
59	SL	139/158 (88%)	133 (96%)	6 (4%)	0	100	100
60	SM	105/132 (80%)	96 (91%)	9 (9%)	0	100	100
61	SN	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
62	SO	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
63	SP	128/145 (88%)	125 (98%)	3 (2%)	0	100	100
64	SQ	138/146 (94%)	132 (96%)	6 (4%)	0	100	100
65	SR	131/135 (97%)	128 (98%)	3 (2%)	0	100	100
66	SS	146/152 (96%)	139 (95%)	7 (5%)	0	100	100
67	ST	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
68	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
69	SV	81/83 (98%)	81 (100%)	0	0	100	100
70	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
71	SY	119/133 (90%)	111 (93%)	6 (5%)	2 (2%)	7	10
72	SZ	85/125 (68%)	79 (93%)	6 (7%)	0	100	100
73	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
74	Sb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
75	Sc	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
76	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
77	Se	45/133 (34%)	45 (100%)	0	0	100	100
78	Sf	59/156 (38%)	50 (85%)	9 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	Sg	310/317 (98%)	297 (96%)	13 (4%)	0	100	100
80	LA	248/257 (96%)	230 (93%)	18 (7%)	0	100	100
81	SA	218/295 (74%)	209 (96%)	9 (4%)	0	100	100
82	SX	137/143 (96%)	132 (96%)	4 (3%)	1 (1%)	18	28
83	Lj	84/97 (87%)	84 (100%)	0	0	100	100
All	All	11153/12762 (87%)	10863 (97%)	286 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
71	SY	30	PRO
71	SY	34	THR
82	SX	124	LYS
53	SF	79	HIS

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	
6	LB	346/348 (99%)	342 (99%)	4 (1%)	63	81
7	LC	302/348 (87%)	301 (100%)	1 (0%)	86	93
8	LD	246/250 (98%)	238 (97%)	8 (3%)	33	55
9	LE	195/252 (77%)	189 (97%)	6 (3%)	35	57
10	LF	191/215 (89%)	190 (100%)	1 (0%)	81	91
11	LG	192/223 (86%)	187 (97%)	5 (3%)	40	63
12	LH	169/171 (99%)	167 (99%)	2 (1%)	63	81
13	LI	175/181 (97%)	168 (96%)	7 (4%)	28	47
14	LJ	143/149 (96%)	139 (97%)	4 (3%)	38	60
15	LL	173/177 (98%)	170 (98%)	3 (2%)	53	74
16	LM	116/161 (72%)	115 (99%)	1 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	LN	171/172 (99%)	169 (99%)	2 (1%)	63	81
18	LO	172/174 (99%)	170 (99%)	2 (1%)	63	81
19	LP	135/163 (83%)	134 (99%)	1 (1%)	76	88
20	LQ	164/165 (99%)	163 (99%)	1 (1%)	78	89
21	LR	146/175 (83%)	144 (99%)	2 (1%)	59	79
22	LS	157/157 (100%)	156 (99%)	1 (1%)	78	89
23	LT	140/140 (100%)	138 (99%)	2 (1%)	59	79
24	LU	89/115 (77%)	86 (97%)	3 (3%)	32	54
25	LV	102/107 (95%)	102 (100%)	0	100	100
26	LW	84/126 (67%)	80 (95%)	4 (5%)	23	40
27	LX	106/133 (80%)	105 (99%)	1 (1%)	70	85
28	LY	122/135 (90%)	121 (99%)	1 (1%)	73	86
29	LZ	117/118 (99%)	115 (98%)	2 (2%)	53	74
30	La	119/120 (99%)	117 (98%)	2 (2%)	53	74
31	Lb	84/125 (67%)	84 (100%)	0	100	100
32	Lc	83/97 (86%)	82 (99%)	1 (1%)	63	81
33	Ld	98/110 (89%)	97 (99%)	1 (1%)	68	84
34	Le	115/121 (95%)	113 (98%)	2 (2%)	53	74
35	Lf	88/89 (99%)	88 (100%)	0	100	100
36	Lg	96/100 (96%)	95 (99%)	1 (1%)	68	84
37	Lh	109/110 (99%)	107 (98%)	2 (2%)	51	73
38	Li	86/89 (97%)	82 (95%)	4 (5%)	23	41
39	Lk	63/65 (97%)	61 (97%)	2 (3%)	34	56
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/115 (41%)	46 (98%)	1 (2%)	47	69
42	Ln	24/24 (100%)	24 (100%)	0	100	100
43	Lo	93/93 (100%)	90 (97%)	3 (3%)	34	56
44	Lp	73/75 (97%)	72 (99%)	1 (1%)	59	79
45	Lr	109/121 (90%)	107 (98%)	2 (2%)	51	73
49	SB	201/231 (87%)	197 (98%)	4 (2%)	48	70
50	SC	185/225 (82%)	179 (97%)	6 (3%)	34	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	SD	187/202 (93%)	177 (95%)	10 (5%)	20	36
52	SE	222/225 (99%)	221 (100%)	1 (0%)	81	91
53	SF	154/170 (91%)	152 (99%)	2 (1%)	61	80
54	SG	182/218 (84%)	178 (98%)	4 (2%)	45	67
55	SH	164/174 (94%)	161 (98%)	3 (2%)	51	73
56	SI	178/180 (99%)	175 (98%)	3 (2%)	53	74
57	SJ	147/168 (88%)	144 (98%)	3 (2%)	48	70
58	SK	86/136 (63%)	84 (98%)	2 (2%)	44	66
59	SL	129/142 (91%)	127 (98%)	2 (2%)	55	76
60	SM	69/108 (64%)	63 (91%)	6 (9%)	9	16
61	SN	130/131 (99%)	125 (96%)	5 (4%)	29	49
62	SO	105/119 (88%)	101 (96%)	4 (4%)	29	49
63	SP	116/130 (89%)	113 (97%)	3 (3%)	40	63
64	SQ	116/121 (96%)	112 (97%)	4 (3%)	32	54
65	SR	120/122 (98%)	115 (96%)	5 (4%)	26	45
66	SS	128/132 (97%)	125 (98%)	3 (2%)	44	66
67	ST	114/115 (99%)	113 (99%)	1 (1%)	70	85
68	SU	93/107 (87%)	89 (96%)	4 (4%)	26	44
69	SV	67/67 (100%)	65 (97%)	2 (3%)	36	58
70	SW	112/113 (99%)	107 (96%)	5 (4%)	24	42
71	SY	106/115 (92%)	102 (96%)	4 (4%)	29	49
72	SZ	75/103 (73%)	74 (99%)	1 (1%)	61	80
73	Sa	86/98 (88%)	84 (98%)	2 (2%)	44	66
74	Sb	75/76 (99%)	72 (96%)	3 (4%)	28	47
75	Sc	56/62 (90%)	54 (96%)	2 (4%)	31	52
76	Sd	48/49 (98%)	46 (96%)	2 (4%)	26	45
77	Se	40/104 (38%)	39 (98%)	1 (2%)	42	64
78	Sf	50/140 (36%)	48 (96%)	2 (4%)	28	47
79	Sg	269/275 (98%)	258 (96%)	11 (4%)	27	46
80	LA	192/198 (97%)	167 (87%)	25 (13%)	4	5
81	SA	181/242 (75%)	176 (97%)	5 (3%)	38	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	SX	111/114 (97%)	105 (95%)	6 (5%)	20	35
83	Lj	73/80 (91%)	72 (99%)	1 (1%)	59	79
All	All	9654/10849 (89%)	9421 (98%)	233 (2%)	43	65

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	SH	83	LEU
81	SA	31	ASP
63	SP	133	ILE
80	LA	250	LYS
80	LA	68	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
54	SG	70	HIS
67	ST	63	HIS
54	SG	177	GLN
58	SK	66	HIS
67	ST	117	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	At	66/77 (85%)	25 (37%)	0
2	Et	48/75 (64%)	13 (27%)	0
3	L5	3437/5069 (67%)	425 (12%)	8 (0%)
4	L7	118/120 (98%)	11 (9%)	1 (0%)
46	Mr	6/7 (85%)	2 (33%)	0
47	Pt	70/76 (92%)	19 (27%)	0
48	S2	1607/1869 (85%)	350 (21%)	28 (1%)
5	L8	155/156 (99%)	27 (17%)	2 (1%)
All	All	5507/7449 (73%)	872 (15%)	39 (0%)

5 of 872 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	At	2	G

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Mol	Chain	Res	Type
1	At	5	G
1	At	7	U
1	At	8	U
1	At	9	A

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	S2	1312	G
48	S2	1700	C
48	S2	1344	A
48	S2	1586	U
48	S2	1835	A

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

216 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	$\# Z > 2$
3	PSU	L5	4442	3	18,21,22	4.41	7 (38%)	22,30,33	1.93	6 (27%)
48	A2M	S2	576	48	22,25,26	0.18	0	31,36,39	0.43	0
47	M2G	Pt	26	47	24,27,28	0.41	0	35,40,43	0.48	0
3	OMG	L5	4228	3	23,26,27	2.38	9 (39%)	33,38,41	2.04	10 (30%)
48	PSU	S2	1445	48	18,21,22	0.87	1 (5%)	22,30,33	0.57	0
3	OMU	L5	4227	3	19,22,23	2.97	8 (42%)	26,31,34	1.76	5 (19%)
3	PSU	L5	1536	3	18,21,22	4.39	7 (38%)	22,30,33	1.78	5 (22%)
3	OMC	L5	3869	3	19,22,23	2.90	8 (42%)	26,31,34	0.71	0
3	PSU	L5	3770	3	18,21,22	4.26	8 (44%)	22,30,33	1.83	5 (22%)
48	OMU	S2	172	48	19,22,23	0.22	0	26,31,34	0.58	0
3	OMU	L5	4306	3	19,22,23	2.95	8 (42%)	26,31,34	1.69	5 (19%)
5	OMG	L8	75	5	23,26,27	0.30	0	33,38,41	0.41	0
3	A2M	L5	400	3	22,25,26	3.44	10 (45%)	31,36,39	2.35	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UY1	L5	3818	85,3,84	19,22,23	4.01	8 (42%)	22,31,34	1.95	5 (22%)
48	PSU	S2	1625	48	18,21,22	0.85	1 (5%)	22,30,33	0.56	0
48	OMC	S2	1703	48	19,22,23	0.30	0	26,31,34	0.49	0
3	A2M	L5	1871	3,85	22,25,26	3.46	10 (45%)	31,36,39	2.41	10 (32%)
3	A2M	L5	3785	3	22,25,26	3.42	10 (45%)	31,36,39	2.51	11 (35%)
3	OMU	L5	2415	3	19,22,23	2.98	8 (42%)	26,31,34	1.71	4 (15%)
3	OMG	L5	2364	3	23,26,27	2.38	7 (30%)	33,38,41	2.03	10 (30%)
3	UR3	L5	4530	3	19,22,23	2.53	6 (31%)	26,32,35	1.27	1 (3%)
3	OMC	L5	3841	3	19,22,23	2.91	8 (42%)	26,31,34	0.75	0
3	PSU	L5	4689	3	18,21,22	4.38	7 (38%)	22,30,33	1.83	5 (22%)
3	OMC	L5	3808	3	19,22,23	2.88	8 (42%)	26,31,34	0.71	0
3	PSU	L5	5001	3	18,21,22	4.45	7 (38%)	22,30,33	1.70	4 (18%)
48	OMG	S2	644	48	23,26,27	0.28	0	33,38,41	0.47	0
3	PSU	L5	4628	3	18,21,22	4.33	7 (38%)	22,30,33	1.76	5 (22%)
3	OMG	L5	4623	3	23,26,27	2.39	9 (39%)	33,38,41	2.07	10 (30%)
3	OMC	L5	3701	3,84	19,22,23	2.86	8 (42%)	26,31,34	0.81	0
48	PSU	S2	1081	48	18,21,22	0.88	1 (5%)	22,30,33	0.84	1 (4%)
3	PSU	L5	4500	3,84	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
3	OMC	L5	4536	3	19,22,23	2.88	8 (42%)	26,31,34	0.75	0
47	1MG	Pt	9	47	22,26,27	0.58	0	33,39,42	0.61	0
3	OMU	L5	4620	3	19,22,23	2.86	8 (42%)	26,31,34	1.66	5 (19%)
48	A2M	S2	468	48	22,25,26	0.17	0	31,36,39	0.59	0
48	B8N	S2	1248	48	24,29,30	0.41	0	29,42,45	0.50	0
48	OMU	S2	1804	48	19,22,23	0.22	0	26,31,34	0.54	0
48	4AC	S2	1842	48	21,24,25	0.42	0	29,34,37	0.38	0
3	OMG	L5	3627	3	23,26,27	2.38	9 (39%)	33,38,41	2.09	9 (27%)
3	PSU	L5	4420	3	18,21,22	4.48	9 (50%)	22,30,33	1.69	4 (18%)
3	PSU	L5	3695	3,84	18,21,22	4.39	7 (38%)	22,30,33	1.82	5 (22%)
3	PSU	L5	4431	3	18,21,22	4.41	7 (38%)	22,30,33	1.85	5 (22%)
48	PSU	S2	918	48	18,21,22	0.86	1 (5%)	22,30,33	0.90	1 (4%)
3	A2M	L5	1524	3	22,25,26	3.44	10 (45%)	31,36,39	2.47	12 (38%)
3	PSU	L5	3758	3	18,21,22	4.32	7 (38%)	22,30,33	1.78	5 (22%)
3	A2M	L5	3830	3	22,25,26	3.44	10 (45%)	31,36,39	2.38	11 (35%)
3	PSU	L5	4569	3,84	18,21,22	4.43	8 (44%)	22,30,33	1.76	5 (22%)
3	PSU	L5	4353	3,84	18,21,22	4.42	7 (38%)	22,30,33	1.83	5 (22%)
48	PSU	S2	1174	86,84,48	18,21,22	0.88	1 (5%)	22,30,33	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	398	3	22,25,26	3.44	9 (40%)	31,36,39	2.46	11 (35%)
48	OMU	S2	627	48	19,22,23	0.22	0	26,31,34	0.42	0
3	OMC	L5	2351	3	19,22,23	2.87	8 (42%)	26,31,34	0.81	0
48	PSU	S2	1004	48	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
3	A2M	L5	2363	3,85	22,25,26	3.47	10 (45%)	31,36,39	2.37	10 (32%)
3	OMC	L5	1340	3	19,22,23	2.82	8 (42%)	26,31,34	0.68	0
3	A2M	L5	4590	3	22,25,26	3.47	9 (40%)	31,36,39	2.45	10 (32%)
3	5MC	L5	4447	3,84	18,22,23	3.40	7 (38%)	26,32,35	1.18	1 (3%)
3	A2M	L5	2815	3,85	22,25,26	3.44	10 (45%)	31,36,39	2.38	9 (29%)
48	OMG	S2	683	48	23,26,27	0.30	0	33,38,41	0.43	0
3	PSU	L5	3853	3,85	18,21,22	4.35	7 (38%)	22,30,33	1.73	4 (18%)
3	A2M	L5	3825	3	22,25,26	3.47	10 (45%)	31,36,39	2.36	10 (32%)
48	PSU	S2	866	48	18,21,22	0.86	1 (5%)	22,30,33	0.67	0
48	PSU	S2	1692	48	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
3	OMC	L5	2804	3	19,22,23	2.86	8 (42%)	26,31,34	0.74	0
48	OMG	S2	1447	48	23,26,27	0.30	0	33,38,41	0.42	0
3	PSU	L5	4299	3	18,21,22	4.37	7 (38%)	22,30,33	1.79	5 (22%)
3	PSU	L5	3734	3,84	18,21,22	4.44	7 (38%)	22,30,33	1.94	5 (22%)
3	OMG	L5	4499	3,1	23,26,27	0.33	0	33,38,41	0.48	0
82	HY3	SX	62	82	6,8,9	1.14	0	5,10,12	1.36	1 (20%)
3	PSU	L5	1779	3	18,21,22	4.43	7 (38%)	22,30,33	1.85	5 (22%)
48	A2M	S2	484	48	22,25,26	0.19	0	31,36,39	0.35	0
48	PSU	S2	1056	48	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
48	PSU	S2	1177	48	18,21,22	0.87	1 (5%)	22,30,33	0.65	0
48	PSU	S2	406	48	18,21,22	0.87	1 (5%)	22,30,33	0.55	0
80	V5N	LA	216	80	9,11,12	0.55	0	9,14,16	0.91	1 (11%)
3	OMC	L5	2365	3	19,22,23	2.85	8 (42%)	26,31,34	0.70	0
41	M3L	Lm	98	41	10,11,12	0.41	0	9,14,16	0.09	0
48	OMU	S2	121	48	19,22,23	0.21	0	26,31,34	0.51	0
48	OMC	S2	174	85,48	19,22,23	0.26	0	26,31,34	0.47	0
1	MA7	At	58	1	20,24,25	0.51	0	24,35,38	0.64	0
3	A2M	L5	3724	3	22,25,26	3.46	10 (45%)	31,36,39	2.39	10 (32%)
48	PSU	S2	34	48	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
48	A2M	S2	1383	48	22,25,26	0.17	0	31,36,39	0.45	0
5	OMU	L8	14	3,5	19,22,23	0.21	0	26,31,34	0.36	0
48	A2M	S2	99	85,48	22,25,26	0.17	0	31,36,39	0.42	0
48	OMU	S2	354	48	19,22,23	0.21	0	26,31,34	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	4618	3	23,26,27	2.40	8 (34%)	33,38,41	2.05	10 (30%)
3	PSU	L5	4423	3	18,21,22	4.45	7 (38%)	22,30,33	1.79	5 (22%)
48	OMG	S2	1328	84,48	23,26,27	0.28	0	33,38,41	0.34	0
48	PSU	S2	1243	48	18,21,22	0.91	1 (5%)	22,30,33	1.01	1 (4%)
3	PSU	L5	1862	3	18,21,22	4.38	7 (38%)	22,30,33	1.87	5 (22%)
48	PSU	S2	686	48	18,21,22	0.86	1 (5%)	22,30,33	0.61	0
3	OMU	L5	4498	3,84	19,22,23	2.95	8 (42%)	26,31,34	1.76	5 (19%)
31	MLZ	Lb	5	84,31	8,9,10	0.78	0	4,9,11	0.72	0
3	OMG	L5	2424	3	23,26,27	2.41	8 (34%)	33,38,41	2.02	9 (27%)
3	OMC	L5	1881	3,85	19,22,23	2.89	8 (42%)	26,31,34	0.85	0
3	A2M	L5	3718	3	22,25,26	3.47	9 (40%)	31,36,39	2.25	9 (29%)
3	OMG	L5	1522	3	23,26,27	2.38	9 (39%)	33,38,41	2.11	10 (30%)
3	A2M	L5	1326	3	22,25,26	3.42	10 (45%)	31,36,39	2.42	9 (29%)
3	OMC	L5	2422	3,85	19,22,23	2.89	8 (42%)	26,31,34	0.73	0
48	OMC	S2	517	48	19,22,23	0.28	0	26,31,34	0.43	0
3	A2M	L5	1534	85,3,84	22,25,26	3.46	10 (45%)	31,36,39	2.37	10 (32%)
3	PSU	L5	1782	3	18,21,22	4.43	7 (38%)	22,30,33	1.83	5 (22%)
3	OMC	L5	2824	3	19,22,23	2.91	8 (42%)	26,31,34	0.70	0
3	PSU	L5	4296	3	18,21,22	4.40	7 (38%)	22,30,33	1.83	5 (22%)
3	OMG	L5	4370	3	23,26,27	2.36	8 (34%)	33,38,41	2.10	10 (30%)
48	PSU	S2	1239	48	18,21,22	0.85	1 (5%)	22,30,33	0.57	0
3	PSU	L5	4673	3,84	18,21,22	4.39	7 (38%)	22,30,33	1.82	5 (22%)
3	OMG	L5	4637	3,84	23,26,27	2.37	7 (30%)	33,38,41	2.01	10 (30%)
3	PSU	L5	4293	3	18,21,22	4.33	7 (38%)	22,30,33	1.67	4 (18%)
3	PSU	L5	3920	3,85	18,21,22	4.34	7 (38%)	22,30,33	1.82	5 (22%)
48	G7M	S2	1639	48,47	23,26,27	0.66	1 (4%)	35,39,42	0.53	0
48	MA6	S2	1850	48	23,26,27	0.29	0	34,38,41	0.68	1 (2%)
3	PSU	L5	3637	3,84	18,21,22	4.36	8 (44%)	22,30,33	1.86	4 (18%)
48	OMG	S2	867	48	23,26,27	0.30	0	33,38,41	0.35	0
48	OMC	S2	1391	48	19,22,23	0.28	0	26,31,34	0.46	0
6	HIC	LB	245	6	10,11,12	1.46	1 (10%)	8,14,16	1.07	1 (12%)
3	PSU	L5	4552	3	18,21,22	4.35	7 (38%)	22,30,33	1.82	5 (22%)
48	A2M	S2	512	48	22,25,26	0.18	0	31,36,39	0.54	0
3	PSU	L5	4457	3	18,21,22	4.35	7 (38%)	22,30,33	1.87	5 (22%)
3	PSU	L5	1781	3	18,21,22	4.40	7 (38%)	22,30,33	1.77	5 (22%)
3	A2M	L5	3760	3	22,25,26	3.48	10 (45%)	31,36,39	2.51	13 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3867	3	22,25,26	3.44	9 (40%)	31,36,39	2.39	9 (29%)
48	A2M	S2	27	85,48	22,25,26	0.17	0	31,36,39	0.44	0
48	A2M	S2	1031	48	22,25,26	0.17	0	31,36,39	0.48	0
48	PSU	S2	573	48	18,21,22	0.83	1 (5%)	22,30,33	0.71	0
46	B8H	Mr	4	47,46	19,22,23	0.23	0	22,32,35	0.31	0
48	OMU	S2	1288	48	19,22,23	0.21	0	26,31,34	0.35	0
48	PSU	S2	822	48	18,21,22	0.88	1 (5%)	22,30,33	0.87	1 (4%)
3	PSU	L5	4521	85,3,84	18,21,22	4.35	7 (38%)	22,30,33	1.85	5 (22%)
47	1MG	Pt	37	84,47	22,26,27	0.47	0	33,39,42	0.95	2 (6%)
43	MLZ	Lo	53	43	8,9,10	0.79	0	4,9,11	0.47	0
3	PSU	L5	4972	3	18,21,22	4.40	7 (38%)	22,30,33	1.80	5 (22%)
3	OMU	L5	3925	3	19,22,23	2.95	8 (42%)	26,31,34	1.79	5 (19%)
48	OMG	S2	436	48	23,26,27	0.29	0	33,38,41	0.42	0
3	OMG	L5	4494	3	23,26,27	2.38	8 (34%)	33,38,41	2.02	10 (30%)
3	PSU	L5	4579	3	18,21,22	4.37	7 (38%)	22,30,33	1.79	5 (22%)
3	OMG	L5	3744	3	23,26,27	2.39	8 (34%)	33,38,41	2.03	10 (30%)
3	OMG	L5	4392	3	23,26,27	2.39	7 (30%)	33,38,41	2.07	10 (30%)
3	PSU	L5	2632	3	18,21,22	4.43	7 (38%)	22,30,33	1.73	4 (18%)
48	OMG	S2	601	48	23,26,27	0.29	0	33,38,41	0.36	0
48	PSU	S2	1232	48	18,21,22	0.88	1 (5%)	22,30,33	0.72	0
48	PSU	S2	649	48	18,21,22	0.86	1 (5%)	22,30,33	0.69	0
48	PSU	S2	1244	48	18,21,22	0.89	1 (5%)	22,30,33	0.71	0
48	PSU	S2	119	48	18,21,22	0.86	1 (5%)	22,30,33	0.57	0
3	PSU	L5	3851	3	18,21,22	4.35	7 (38%)	22,30,33	1.82	5 (22%)
3	PSU	L5	4532	3	18,21,22	4.36	7 (38%)	22,30,33	1.79	5 (22%)
3	PSU	L5	4576	3	18,21,22	4.39	7 (38%)	22,30,33	1.87	5 (22%)
48	OMU	S2	116	48	19,22,23	0.23	0	26,31,34	0.43	0
48	OMC	S2	462	48	19,22,23	0.26	0	26,31,34	0.39	0
48	PSU	S2	651	48	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
3	OMG	L5	3899	3	23,26,27	2.41	9 (39%)	33,38,41	2.11	10 (30%)
3	PSU	L5	1744	3,84	18,21,22	4.37	7 (38%)	22,30,33	1.81	5 (22%)
3	OMG	L5	1316	3,84	23,26,27	2.39	7 (30%)	33,38,41	2.07	10 (30%)
3	PSU	L5	1792	85,3,84	18,21,22	4.35	7 (38%)	22,30,33	1.73	5 (22%)
3	OMG	L5	2876	3	23,26,27	2.42	8 (34%)	33,38,41	2.07	10 (30%)
3	PSU	L5	4403	3	18,21,22	4.34	7 (38%)	22,30,33	1.84	6 (27%)
48	OMU	S2	1442	85,48	19,22,23	0.23	0	26,31,34	0.32	0
48	PSU	S2	814	48	18,21,22	0.88	1 (5%)	22,30,33	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1677	3	18,21,22	4.50	8 (44%)	22,30,33	1.90	6 (27%)
48	PSU	S2	966	48	18,21,22	0.87	1 (5%)	22,30,33	0.63	0
3	OMG	L5	3792	3	23,26,27	2.40	8 (34%)	33,38,41	1.96	9 (27%)
48	MA6	S2	1851	48	23,26,27	0.27	0	34,38,41	0.75	1 (2%)
3	1MA	L5	1322	3,85	21,25,26	2.85	6 (28%)	31,37,40	2.86	10 (32%)
3	OMG	L5	4196	3,47	23,26,27	2.35	8 (34%)	33,38,41	2.02	9 (27%)
48	OMG	S2	1490	85,48	23,26,27	0.32	0	33,38,41	0.35	0
48	PSU	S2	36	48	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
3	6MZ	L5	4220	3	22,25,26	2.45	5 (22%)	30,36,39	2.29	11 (36%)
3	OMG	L5	1625	3,84	23,26,27	2.41	8 (34%)	33,38,41	1.99	9 (27%)
3	A2M	L5	4571	3	22,25,26	3.50	10 (45%)	31,36,39	2.36	10 (32%)
5	PSU	L8	69	5	18,21,22	0.85	1 (5%)	22,30,33	0.69	0
48	A2M	S2	668	85,48	22,25,26	0.20	0	31,36,39	0.42	0
48	4AC	S2	1337	48	21,24,25	0.41	0	29,34,37	0.58	0
48	PSU	S2	1367	84,48	18,21,22	0.86	1 (5%)	22,30,33	0.69	0
3	PSU	L5	1860	3	18,21,22	4.39	7 (38%)	22,30,33	1.80	5 (22%)
48	OMG	S2	509	48	23,26,27	0.28	0	33,38,41	0.39	0
3	PSU	L5	4312	3	18,21,22	4.39	7 (38%)	22,30,33	1.88	5 (22%)
3	PSU	L5	4471	3	18,21,22	4.41	7 (38%)	22,30,33	1.81	5 (22%)
48	UY1	S2	1326	85,48	19,22,23	0.19	0	22,31,34	0.34	0
3	OMU	L5	2837	3	19,22,23	2.94	8 (42%)	26,31,34	1.76	4 (15%)
48	PSU	S2	1238	48	18,21,22	0.98	2 (11%)	22,30,33	0.82	0
48	A2M	S2	166	48	22,25,26	0.17	0	31,36,39	0.59	0
48	PSU	S2	109	48	18,21,22	0.86	1 (5%)	22,30,33	0.60	0
3	PSU	L5	3639	3	18,21,22	4.32	7 (38%)	22,30,33	1.81	5 (22%)
3	A2M	L5	2787	3,85	22,25,26	3.42	10 (45%)	31,36,39	2.39	11 (35%)
3	PSU	L5	3844	3	18,21,22	4.43	7 (38%)	22,30,33	1.77	5 (22%)
3	OMC	L5	4456	3	19,22,23	2.84	8 (42%)	26,31,34	0.72	0
3	PSU	L5	4361	3,84	18,21,22	4.35	7 (38%)	22,30,33	1.78	5 (22%)
3	OMC	L5	2861	3	19,22,23	2.90	8 (42%)	26,31,34	0.70	0
3	A2M	L5	2401	3	22,25,26	3.42	10 (45%)	31,36,39	2.39	10 (32%)
48	PSU	S2	681	48	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
3	PSU	L5	1683	3,84	18,21,22	4.34	7 (38%)	22,30,33	1.84	5 (22%)
3	A2M	L5	4523	3,85	22,25,26	3.43	9 (40%)	31,36,39	2.39	10 (32%)
3	OMC	L5	3887	3	19,22,23	2.89	8 (42%)	26,31,34	0.76	0
48	A2M	S2	159	48	22,25,26	0.17	0	31,36,39	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	2508	3	18,21,22	4.37	7 (38%)	22,30,33	1.87	5 (22%)
48	PSU	S2	863	48	18,21,22	0.88	1 (5%)	22,30,33	0.54	0
48	PSU	S2	572	48	18,21,22	0.83	1 (5%)	22,30,33	0.65	0
30	V5N	La	39	30	9,11,12	2.86	2 (22%)	9,14,16	1.30	1 (11%)
48	PSU	S2	105	48	18,21,22	0.88	1 (5%)	22,30,33	0.67	0
3	PSU	L5	2839	3	18,21,22	4.36	7 (38%)	22,30,33	1.94	5 (22%)
48	6MZ	S2	1832	85,84,48	22,25,26	0.19	0	30,36,39	0.38	0
48	A2M	S2	1678	48	22,25,26	0.17	0	31,36,39	0.35	0
46	B8H	Mr	6	1,46	19,22,23	0.23	0	22,32,35	0.39	0
48	PSU	S2	218	48	18,21,22	0.85	1 (5%)	22,30,33	0.63	0
48	PSU	S2	93	48	18,21,22	0.88	1 (5%)	22,30,33	0.68	0
48	PSU	S2	815	48	18,21,22	0.84	1 (5%)	22,30,33	0.66	0
3	PSU	L5	3768	3	18,21,22	0.86	1 (5%)	22,30,33	0.64	0
3	PSU	L5	4493	3,84	18,21,22	4.41	7 (38%)	22,30,33	1.81	5 (22%)
48	OMU	S2	428	48	19,22,23	0.21	0	26,31,34	0.38	0
47	1MA	Pt	58	47	21,25,26	4.24	11 (52%)	31,37,40	1.76	6 (19%)
3	PSU	L5	3884	3	18,21,22	4.39	8 (44%)	22,30,33	1.75	4 (18%)
48	PSU	S2	1347	48	18,21,22	0.86	1 (5%)	22,30,33	0.63	0
48	PSU	S2	1643	85,48	18,21,22	0.85	1 (5%)	22,30,33	0.58	0
5	PSU	L8	55	5	18,21,22	0.84	1 (5%)	22,30,33	0.72	0
3	5MC	L5	3782	3,85	18,22,23	3.46	7 (38%)	26,32,35	1.04	2 (7%)

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
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
48	A2M	S2	576	48	-	2/9/27/28	0/3/3/3
47	M2G	Pt	26	47	-	0/11/29/30	0/3/3/3
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
48	PSU	S2	1445	48	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
48	OMU	S2	172	48	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	UY1	L5	3818	85,3,84	-	1/9/27/28	0/2/2/2
48	PSU	S2	1625	48	-	0/7/25/26	0/2/2/2
48	OMC	S2	1703	48	-	0/9/27/28	0/2/2/2
3	A2M	L5	1871	3,85	-	0/9/27/28	0/3/3/3
3	A2M	L5	3785	3	-	3/9/27/28	0/3/3/3
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	2364	3	-	0/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	644	48	-	4/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3701	3,84	-	4/9/27/28	0/2/2/2
48	PSU	S2	1081	48	-	1/7/25/26	0/2/2/2
3	PSU	L5	4500	3,84	-	3/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
47	1MG	Pt	9	47	-	1/7/25/26	0/3/3/3
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
48	A2M	S2	468	48	-	0/9/27/28	0/3/3/3
48	B8N	S2	1248	48	-	2/16/34/35	0/2/2/2
48	OMU	S2	1804	48	-	1/9/27/28	0/2/2/2
48	4AC	S2	1842	48	-	2/11/29/30	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4420	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3,84	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	918	48	-	1/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4569	3,84	-	2/7/25/26	0/2/2/2
3	PSU	L5	4353	3,84	-	0/7/25/26	0/2/2/2
48	PSU	S2	1174	86,84,48	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMU	S2	627	48	-	2/9/27/28	0/2/2/2
3	OMC	L5	2351	3	-	1/9/27/28	0/2/2/2
48	PSU	S2	1004	48	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	3,85	-	1/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
3	5MC	L5	4447	3,84	-	4/7/25/26	0/2/2/2
3	A2M	L5	2815	3,85	-	3/9/27/28	0/3/3/3
48	OMG	S2	683	48	-	2/9/27/28	0/3/3/3
3	PSU	L5	3853	3,85	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
48	PSU	S2	866	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1692	48	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
48	OMG	S2	1447	48	-	2/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3,1	-	0/9/27/28	0/3/3/3
82	HY3	SX	62	82	-	0/1/12/14	0/1/1/1
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
48	A2M	S2	484	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	1056	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1177	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	406	48	-	0/7/25/26	0/2/2/2
80	V5N	LA	216	80	-	1/9/10/12	0/1/1/1
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
41	M3L	Lm	98	41	-	3/9/10/12	-
48	OMU	S2	121	48	-	0/9/27/28	0/2/2/2
48	OMC	S2	174	85,48	-	0/9/27/28	0/2/2/2
1	MA7	At	58	1	-	3/7/21/22	0/3/3/3
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
48	PSU	S2	34	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	1383	48	-	0/9/27/28	0/3/3/3
5	OMU	L8	14	3,5	-	1/9/27/28	0/2/2/2
48	A2M	S2	99	85,48	-	2/9/27/28	0/3/3/3
48	OMU	S2	354	48	-	0/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	1328	84,48	-	1/9/27/28	0/3/3/3
48	PSU	S2	1243	48	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	686	48	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3,84	-	0/9/27/28	0/2/2/2
31	MLZ	Lb	5	84,31	-	1/7/8/10	-
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1881	3,85	-	0/9/27/28	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2422	3,85	-	2/9/27/28	0/2/2/2
48	OMC	S2	517	48	-	0/9/27/28	0/2/2/2
3	A2M	L5	1534	85,3,84	-	2/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
48	PSU	S2	1239	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3,84	-	1/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	3,85	-	0/7/25/26	0/2/2/2
48	G7M	S2	1639	48,47	-	0/7/25/26	0/3/3/3
48	MA6	S2	1850	48	-	0/11/29/30	0/3/3/3
3	PSU	L5	3637	3,84	-	0/7/25/26	0/2/2/2
48	OMG	S2	867	48	-	1/9/27/28	0/3/3/3
48	OMC	S2	1391	48	-	0/9/27/28	0/2/2/2
6	HIC	LB	245	6	-	0/5/6/8	0/1/1/1
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
48	A2M	S2	512	48	-	2/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	3760	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3867	3	-	0/9/27/28	0/3/3/3
48	A2M	S2	27	85,48	-	1/9/27/28	0/3/3/3
48	A2M	S2	1031	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	573	48	-	2/7/25/26	0/2/2/2
46	B8H	Mr	4	47,46	-	2/7/25/26	0/2/2/2
48	OMU	S2	1288	48	-	1/9/27/28	0/2/2/2
48	PSU	S2	822	48	-	2/7/25/26	0/2/2/2
3	PSU	L5	4521	85,3,84	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	1MG	Pt	37	84,47	-	0/7/25/26	0/3/3/3
43	MLZ	Lo	53	43	-	2/7/8/10	-
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
48	OMG	S2	436	48	-	0/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	601	48	-	1/9/27/28	0/3/3/3
48	PSU	S2	1232	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	649	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1244	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	119	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
48	OMU	S2	116	48	-	0/9/27/28	0/2/2/2
48	OMC	S2	462	48	-	0/9/27/28	0/2/2/2
48	PSU	S2	651	48	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1744	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3,84	-	0/9/27/28	0/3/3/3
3	PSU	L5	1792	85,3,84	-	1/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
48	OMU	S2	1442	85,48	-	3/9/27/28	0/2/2/2
48	PSU	S2	814	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	1/7/25/26	0/2/2/2
48	PSU	S2	966	48	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
48	MA6	S2	1851	48	-	3/11/29/30	0/3/3/3
3	1MA	L5	1322	3,85	-	2/7/25/26	0/3/3/3
3	OMG	L5	4196	3,47	-	3/9/27/28	0/3/3/3
48	OMG	S2	1490	85,48	-	3/9/27/28	0/3/3/3
48	PSU	S2	36	48	-	0/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1625	3,84	-	2/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
48	A2M	S2	668	85,48	-	3/9/27/28	0/3/3/3
48	4AC	S2	1337	48	-	0/11/29/30	0/2/2/2
48	PSU	S2	1367	84,48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	509	48	-	1/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
48	UY1	S2	1326	85,48	-	0/9/27/28	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
48	PSU	S2	1238	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	166	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	109	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3,85	-	3/9/27/28	0/3/3/3
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4361	3,84	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
48	PSU	S2	681	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3,84	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,85	-	1/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
48	A2M	S2	159	48	-	0/9/27/28	0/3/3/3
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	863	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	572	48	-	2/7/25/26	0/2/2/2
30	V5N	La	39	30	-	1/9/10/12	0/1/1/1
48	PSU	S2	105	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
48	6MZ	S2	1832	85,84,48	-	2/9/27/28	0/3/3/3
48	A2M	S2	1678	48	-	1/9/27/28	0/3/3/3
46	B8H	Mr	6	1,46	-	0/7/25/26	0/2/2/2
48	PSU	S2	218	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	93	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	815	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3,84	-	0/7/25/26	0/2/2/2
48	OMU	S2	428	48	-	6/9/27/28	0/2/2/2
47	1MA	Pt	58	47	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	1347	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1643	85,48	-	0/7/25/26	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	3,85	-	0/7/25/26	0/2/2/2

The worst 5 of 962 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1677	PSU	C6-C5	11.61	1.48	1.35
3	L5	4423	PSU	C6-C5	11.57	1.48	1.35
3	L5	3844	PSU	C6-C5	11.55	1.48	1.35
3	L5	3884	PSU	C6-C5	11.53	1.48	1.35
3	L5	2632	PSU	C6-C5	11.48	1.48	1.35

The worst 5 of 702 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1322	1MA	C1'-N9-C8	-8.96	101.19	126.70
3	L5	1322	1MA	C1'-N9-C4	8.45	151.61	126.50
3	L5	2876	OMG	C5-C4-N3	-6.00	118.72	128.46
3	L5	1322	1MA	N1-C2-N3	-5.96	118.92	126.00
3	L5	4590	A2M	N3-C2-N1	-5.88	119.40	128.60

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	LA	216	V5N	O-C-CA-CB
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	C1'-C2'-O2'-CM'
3	L5	2415	OMU	C1'-C2'-O2'-CM2
3	L5	2815	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

61 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S2	576	A2M	1	0
47	Pt	26	M2G	2	0
3	L5	3770	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4306	OMU	1	0
3	L5	3818	UY1	1	0
3	L5	1871	A2M	1	0
3	L5	2415	OMU	4	0
3	L5	2364	OMG	2	0
48	S2	644	OMG	1	0
3	L5	3701	OMC	1	0
3	L5	4536	OMC	1	0
47	Pt	9	1MG	1	0
3	L5	4620	OMU	3	0
3	L5	2351	OMC	2	0
3	L5	2363	A2M	2	0
3	L5	1340	OMC	2	0
3	L5	4447	5MC	2	0
3	L5	2815	A2M	1	0
3	L5	2804	OMC	1	0
3	L5	4299	PSU	3	0
3	L5	4499	OMG	2	0
48	S2	121	OMU	2	0
1	At	58	MA7	1	0
3	L5	3724	A2M	1	0
5	L8	14	OMU	1	0
48	S2	1328	OMG	1	0
3	L5	4498	OMU	1	0
3	L5	3718	A2M	4	0
3	L5	1326	A2M	2	0
3	L5	2422	OMC	1	0
48	S2	1239	PSU	1	0
3	L5	4637	OMG	3	0
48	S2	1639	G7M	1	0
48	S2	867	OMG	1	0
48	S2	1391	OMC	1	0
3	L5	4552	PSU	1	0
3	L5	4457	PSU	1	0
3	L5	3867	A2M	2	0
48	S2	27	A2M	2	0
48	S2	573	PSU	1	0
3	L5	3925	OMU	1	0
3	L5	4579	PSU	1	0
3	L5	3744	OMG	1	0
3	L5	4392	OMG	2	0
3	L5	2632	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S2	601	OMG	1	0
3	L5	4532	PSU	1	0
48	S2	116	OMU	2	0
3	L5	2876	OMG	1	0
48	S2	1442	OMU	2	0
48	S2	1851	MA6	1	0
3	L5	4196	OMG	1	0
48	S2	1490	OMG	1	0
3	L5	4220	6MZ	3	0
3	L5	1625	OMG	2	0
3	L5	4571	A2M	1	0
3	L5	1860	PSU	1	0
48	S2	509	OMG	4	0
3	L5	2861	OMC	2	0
3	L5	4523	A2M	1	0
48	S2	1678	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 447 ligands modelled in this entry, 418 are monoatomic - leaving 29 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	$\# Z > 2$
88	PUT	L5	5379	-	5,5,5	0.22	0	4,4,4	0.19	0
87	SPD	L5	5377	-	9,9,9	0.43	0	8,8,8	0.31	0
90	HYG	S2	2021	84	35,39,39	0.54	1 (2%)	43,60,60	0.88	3 (6%)
88	PUT	L5	5381	-	5,5,5	0.25	0	4,4,4	0.25	0
88	PUT	S2	2018	-	5,5,5	0.15	0	4,4,4	0.20	0
87	SPD	L5	5376	-	9,9,9	0.42	0	8,8,8	0.36	0
87	SPD	L5	5386	-	9,9,9	0.43	0	8,8,8	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	SPD	LN	301	-	9,9,9	0.41	0	8,8,8	0.35	0
87	SPD	L5	5385	-	9,9,9	0.44	0	8,8,8	0.33	0
87	SPD	L8	205	-	9,9,9	0.44	0	8,8,8	0.35	0
87	SPD	S2	2017	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	S2	2016	-	9,9,9	0.17	0	8,8,8	0.20	0
88	PUT	L5	5382	-	5,5,5	0.24	0	4,4,4	0.20	0
88	PUT	L5	5387	-	5,5,5	0.24	0	4,4,4	0.07	0
88	PUT	L5	5384	-	5,5,5	0.23	0	4,4,4	0.17	0
87	SPD	L5	5370	-	9,9,9	0.43	0	8,8,8	0.26	0
88	PUT	L5	5383	-	5,5,5	0.22	0	4,4,4	0.20	0
87	SPD	S2	2014	-	9,9,9	0.43	0	8,8,8	0.19	0
87	SPD	L5	5374	-	9,9,9	0.41	0	8,8,8	0.41	0
88	PUT	L5	5380	-	5,5,5	0.23	0	4,4,4	0.17	0
87	SPD	L5	5369	-	9,9,9	0.42	0	8,8,8	0.41	0
87	SPD	S2	2019	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	L5	5372	-	9,9,9	0.42	0	8,8,8	0.29	0
87	SPD	L5	5373	-	9,9,9	0.44	0	8,8,8	0.27	0
88	PUT	S2	2020	-	5,5,5	0.16	0	4,4,4	0.25	0
87	SPD	L5	5378	-	9,9,9	0.43	0	8,8,8	0.23	0
87	SPD	S2	2015	-	9,9,9	0.18	0	8,8,8	0.21	0
87	SPD	L5	5375	-	9,9,9	0.44	0	8,8,8	0.42	0
87	SPD	L5	5371	-	9,9,9	0.39	0	8,8,8	0.43	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
88	PUT	L5	5379	-	-	0/3/3/3	-
87	SPD	L5	5377	-	-	0/7/7/7	-
90	HYG	S2	2021	84	1/1/16/17	4/12/87/87	0/4/4/4
88	PUT	L5	5381	-	-	0/3/3/3	-
88	PUT	S2	2018	-	-	2/3/3/3	-
87	SPD	L5	5376	-	-	0/7/7/7	-
87	SPD	L5	5386	-	-	0/7/7/7	-
87	SPD	LN	301	-	-	1/7/7/7	-
87	SPD	L5	5385	-	-	0/7/7/7	-
87	SPD	L8	205	-	-	0/7/7/7	-
87	SPD	S2	2017	-	-	5/7/7/7	-
87	SPD	S2	2016	-	-	3/7/7/7	-
88	PUT	L5	5382	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	PUT	L5	5387	-	-	0/3/3/3	-
88	PUT	L5	5384	-	-	0/3/3/3	-
87	SPD	L5	5370	-	-	0/7/7/7	-
88	PUT	L5	5383	-	-	0/3/3/3	-
87	SPD	S2	2014	-	-	0/7/7/7	-
87	SPD	L5	5374	-	-	1/7/7/7	-
88	PUT	L5	5380	-	-	0/3/3/3	-
87	SPD	L5	5369	-	-	0/7/7/7	-
87	SPD	S2	2019	-	-	7/7/7/7	-
87	SPD	L5	5372	-	-	0/7/7/7	-
87	SPD	L5	5373	-	-	0/7/7/7	-
88	PUT	S2	2020	-	-	2/3/3/3	-
87	SPD	L5	5378	-	-	0/7/7/7	-
87	SPD	S2	2015	-	-	6/7/7/7	-
87	SPD	L5	5375	-	-	1/7/7/7	-
87	SPD	L5	5371	-	-	1/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	S2	2021	HYG	O28-C23	2.32	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	S2	2021	HYG	C23-O28-C27	2.12	116.04	112.00
90	S2	2021	HYG	O14-C13-C12	2.06	113.59	109.51
90	S2	2021	HYG	O29-C12-C13	2.01	116.14	110.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
90	S2	2021	HYG	C12

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	S2	2016	SPD	C4-C5-N6-C7
87	S2	2017	SPD	C8-C7-N6-C5
87	S2	2019	SPD	N6-C7-C8-C9
87	S2	2017	SPD	C3-C4-C5-N6

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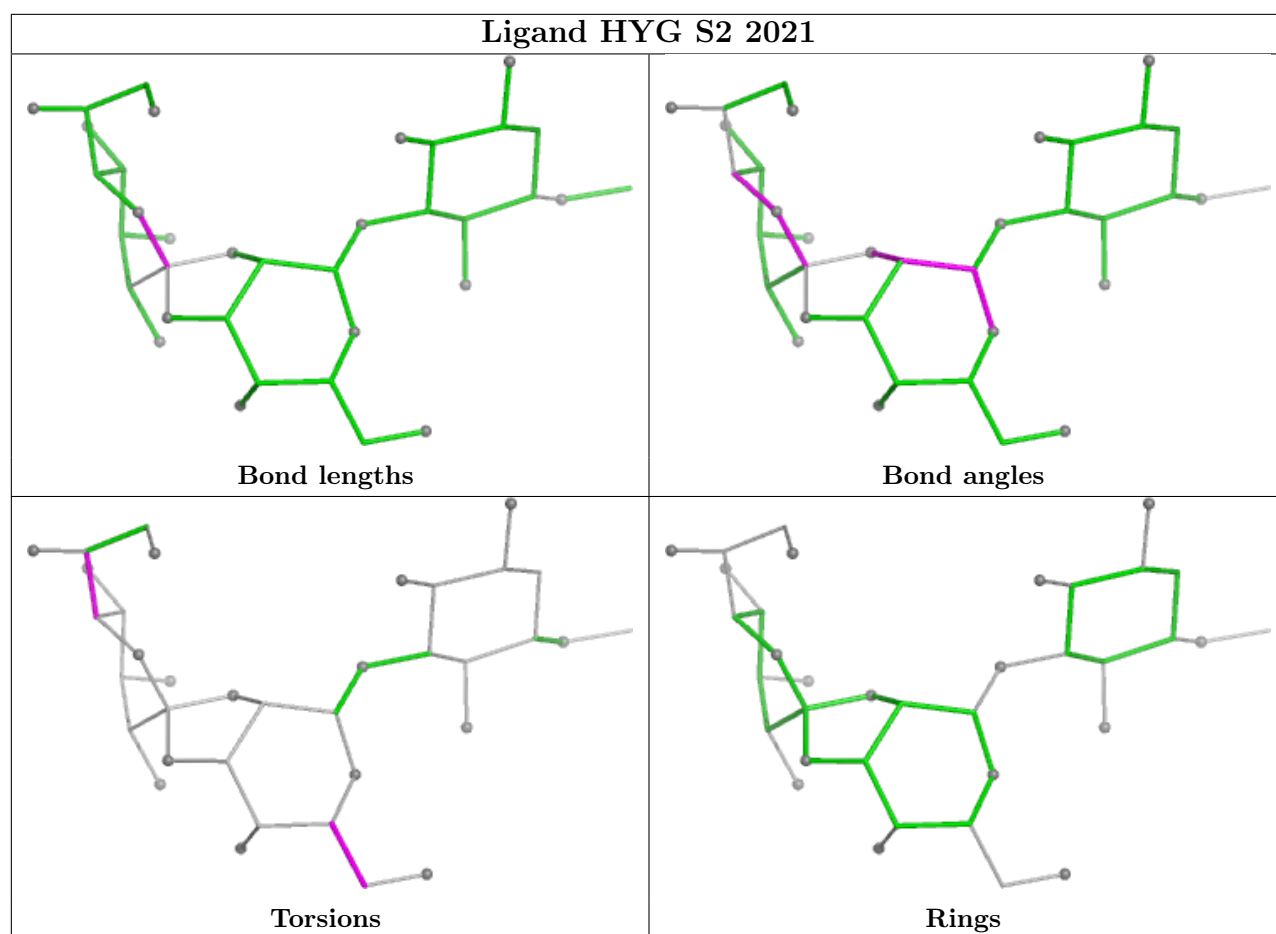
Mol	Chain	Res	Type	Atoms
87	S2	2015	SPD	C3-C4-C5-N6

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	S2	2021	HYG	1	0
88	L5	5381	PUT	1	0
87	L8	205	SPD	1	0
87	S2	2017	SPD	1	0
87	S2	2016	SPD	1	0
88	L5	5387	PUT	1	0
87	L5	5374	SPD	1	0
88	L5	5380	PUT	1	0
87	S2	2019	SPD	1	0
87	L5	5373	SPD	3	0
87	L5	5371	SPD	3	0

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](#)

There are no chain breaks in this entry.

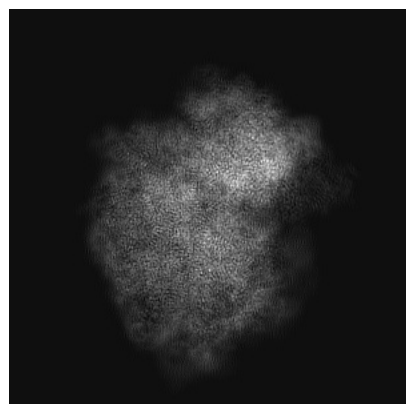
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55083. These allow visual inspection of the internal detail of the map and identification of artifacts.

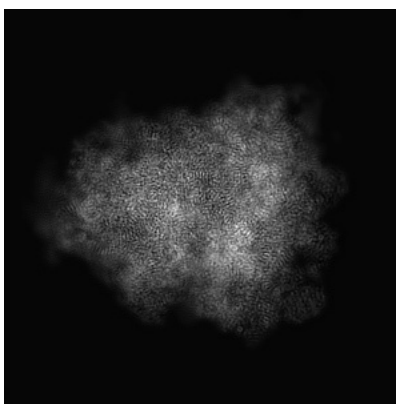
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

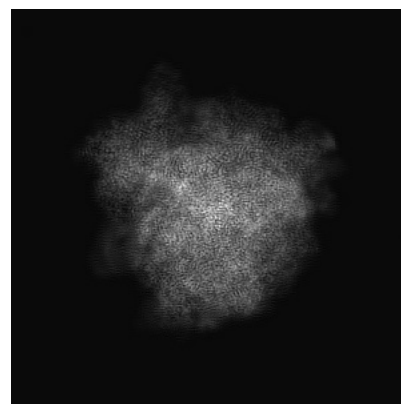
6.1.1 Primary map



X

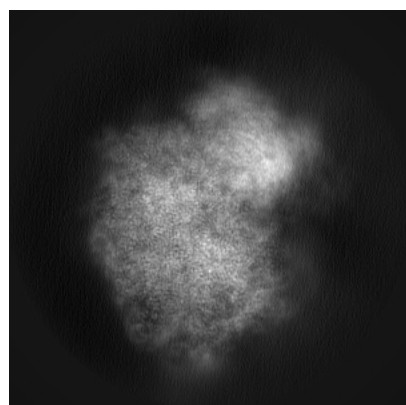


Y

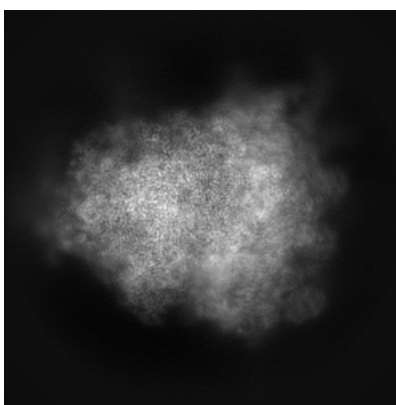


Z

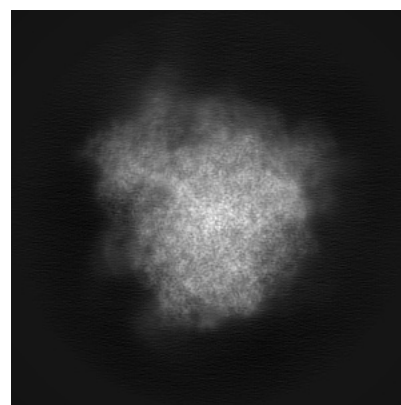
6.1.2 Raw map



X



Y

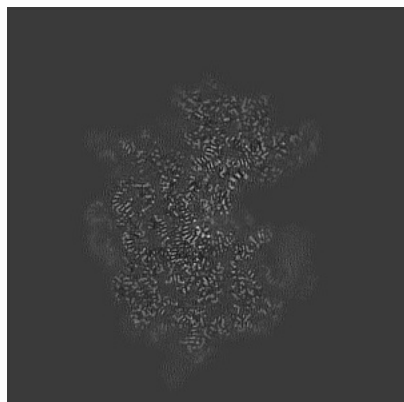


Z

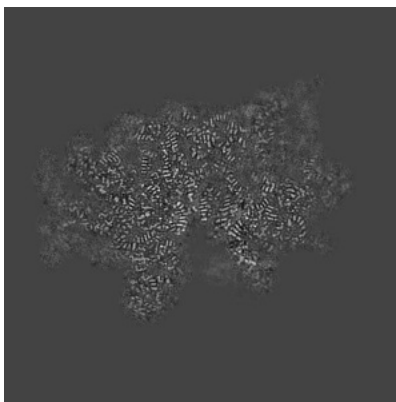
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

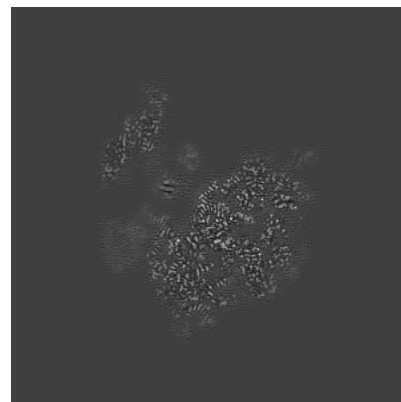
6.2.1 Primary map



X Index: 240

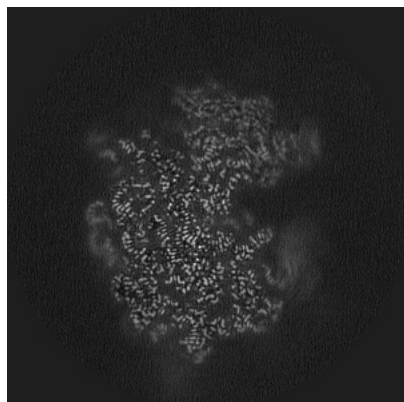


Y Index: 240

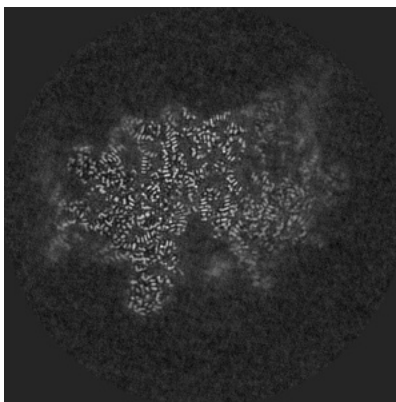


Z Index: 240

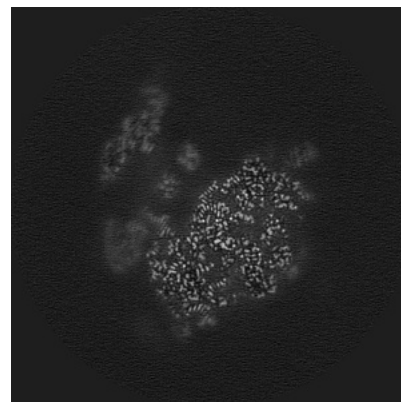
6.2.2 Raw map



X Index: 240



Y Index: 240

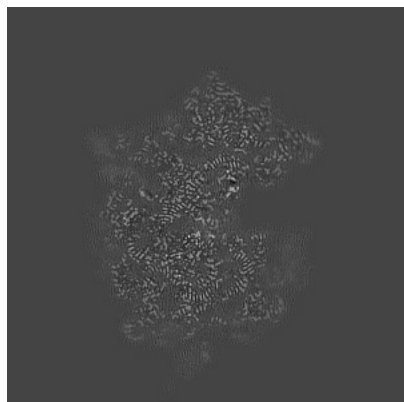


Z Index: 240

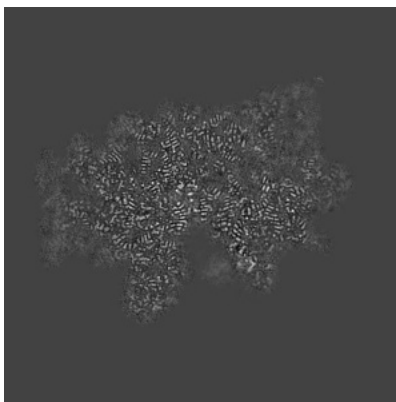
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

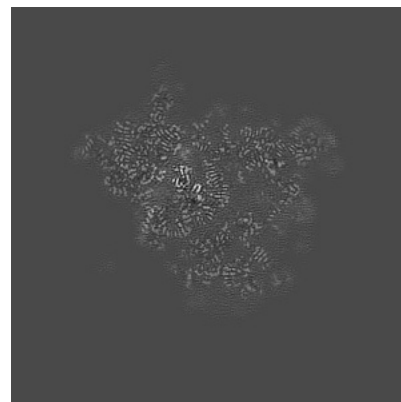
6.3.1 Primary map



X Index: 250

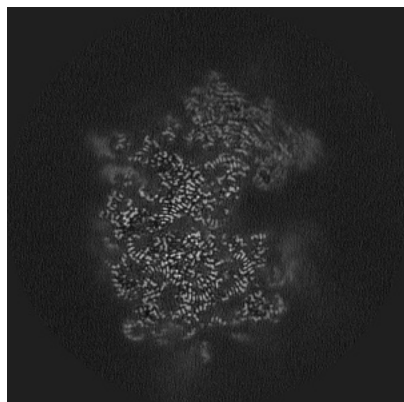


Y Index: 239

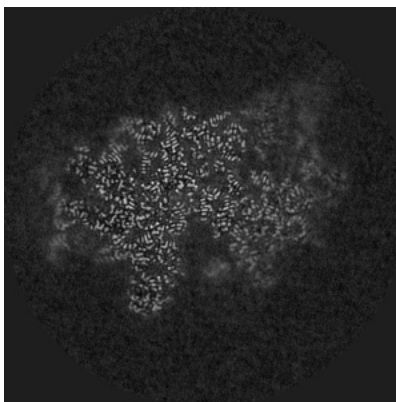


Z Index: 294

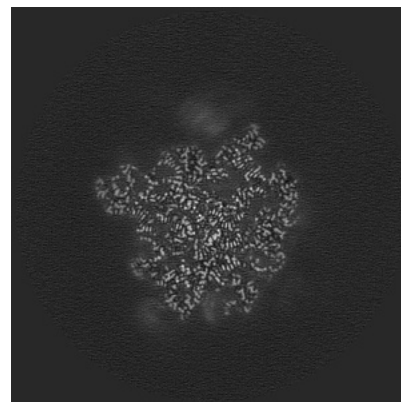
6.3.2 Raw map



X Index: 250



Y Index: 239

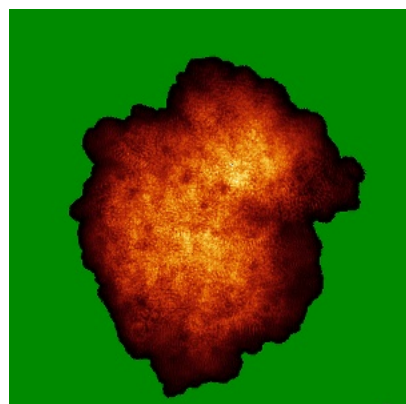


Z Index: 184

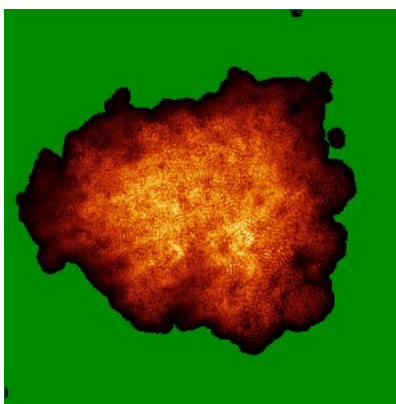
The images above show the largest variance slices of the map in three orthogonal directions.

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

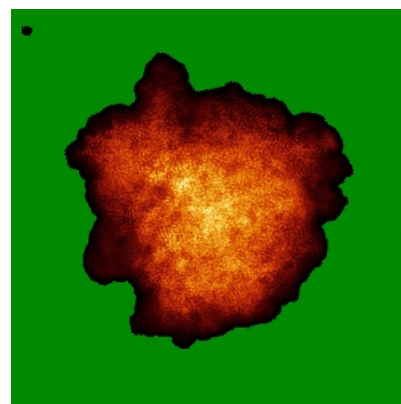
6.4.1 Primary map



X

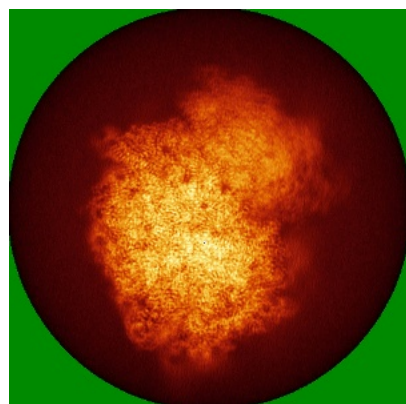


Y

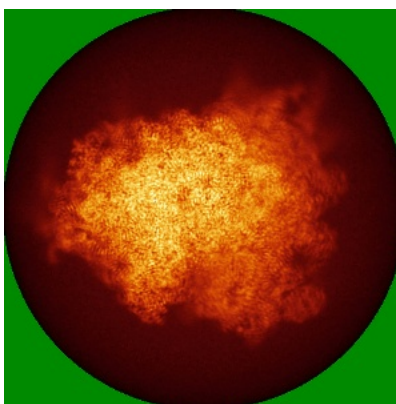


Z

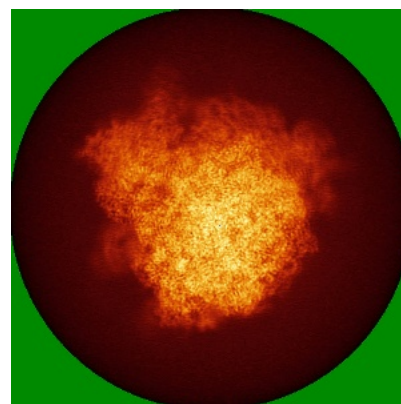
6.4.2 Raw map



X



Y

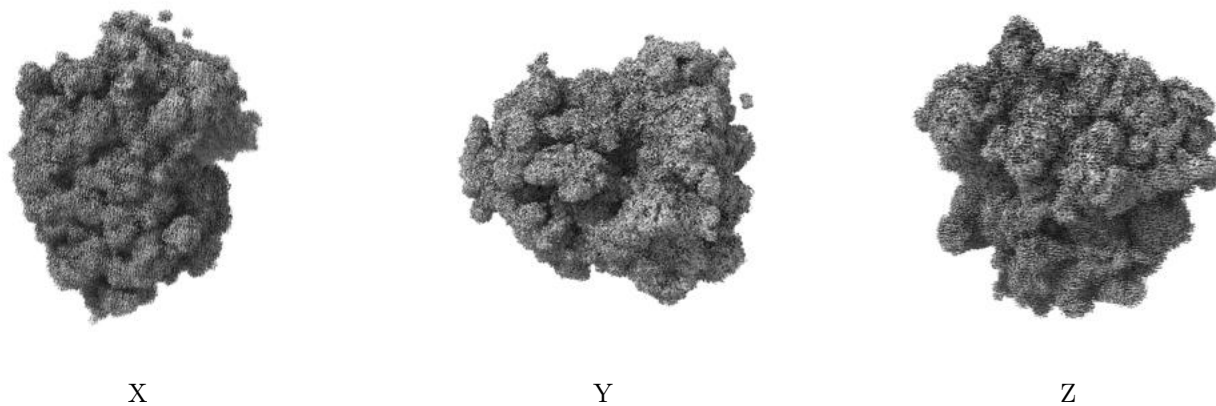


Z

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

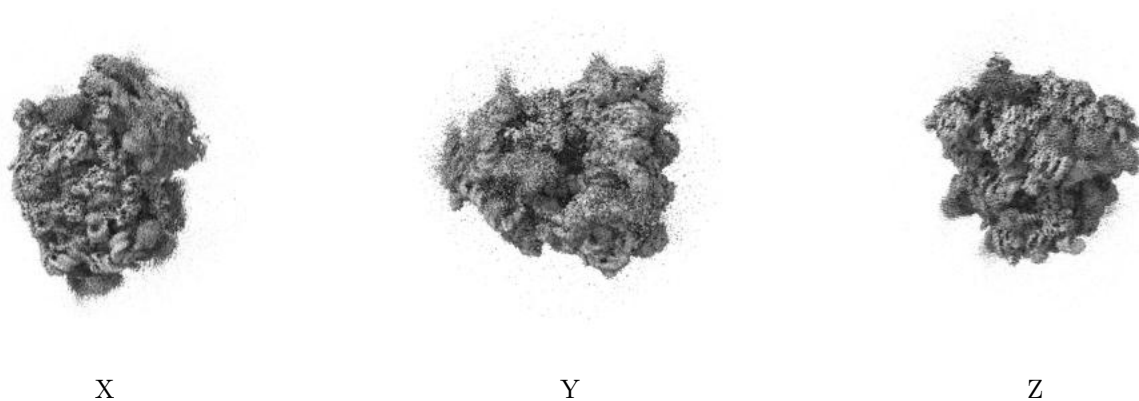
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

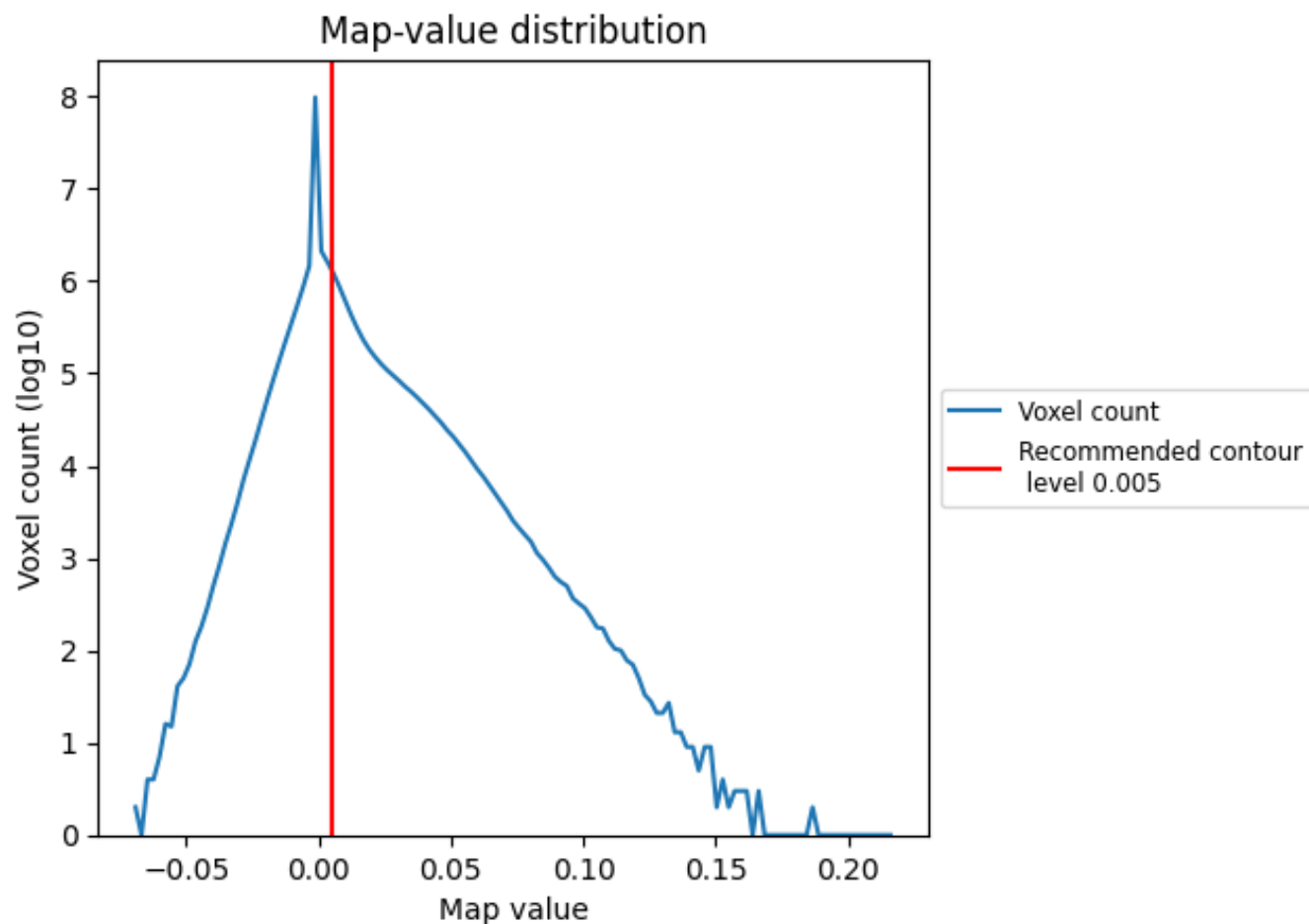
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

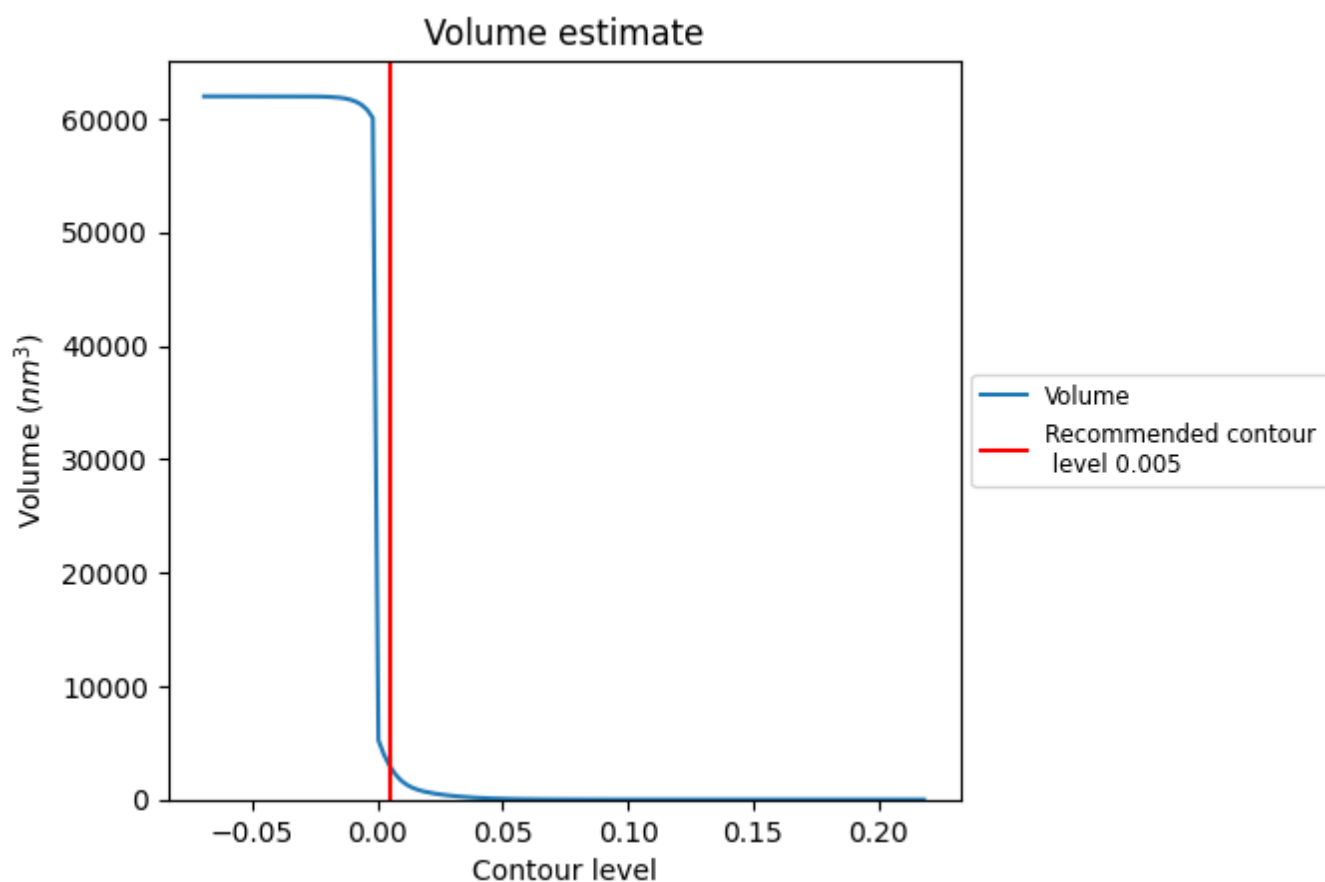
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

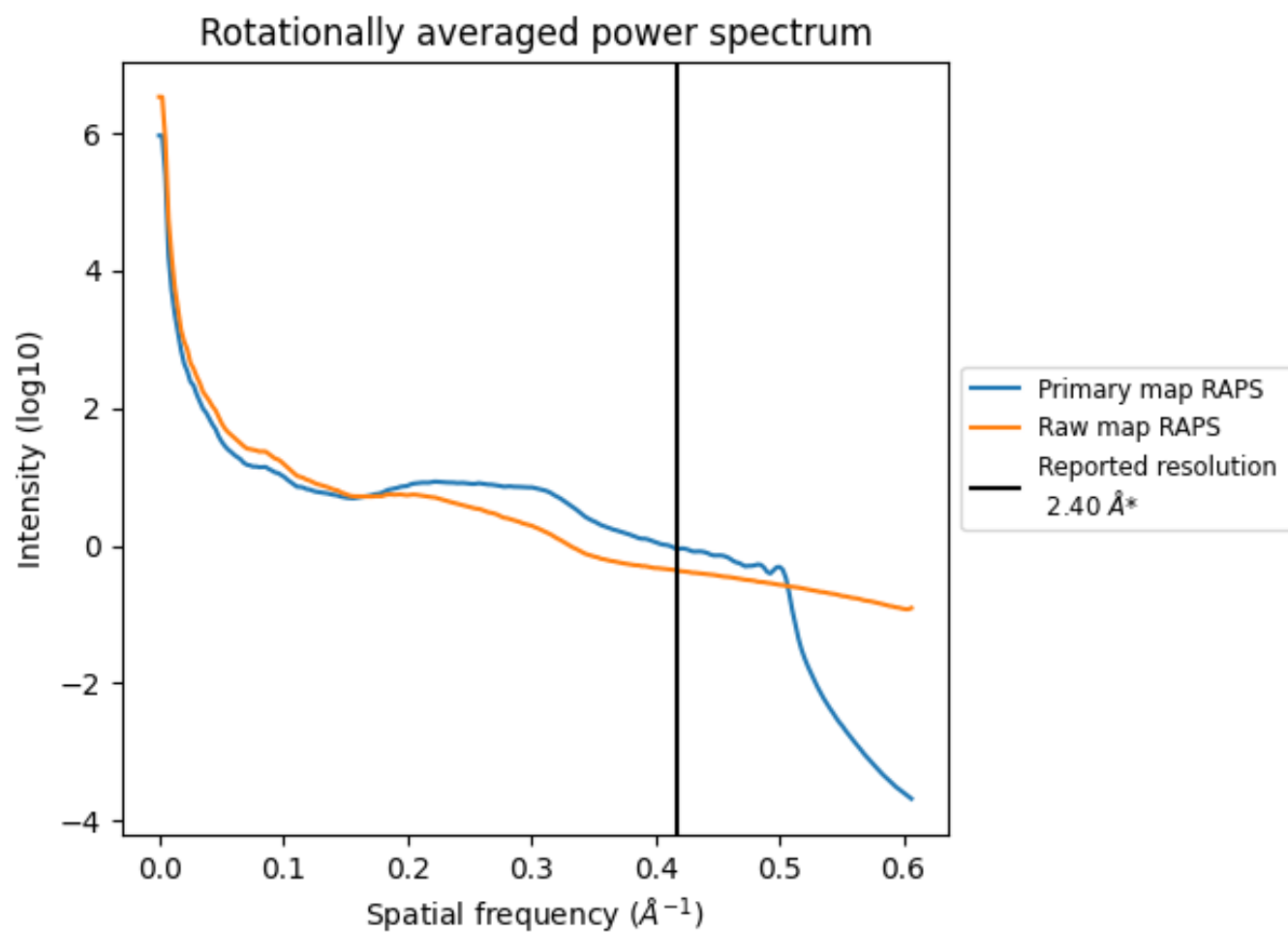
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2960 nm^3 ; this corresponds to an approximate mass of 2674 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 ⓘ

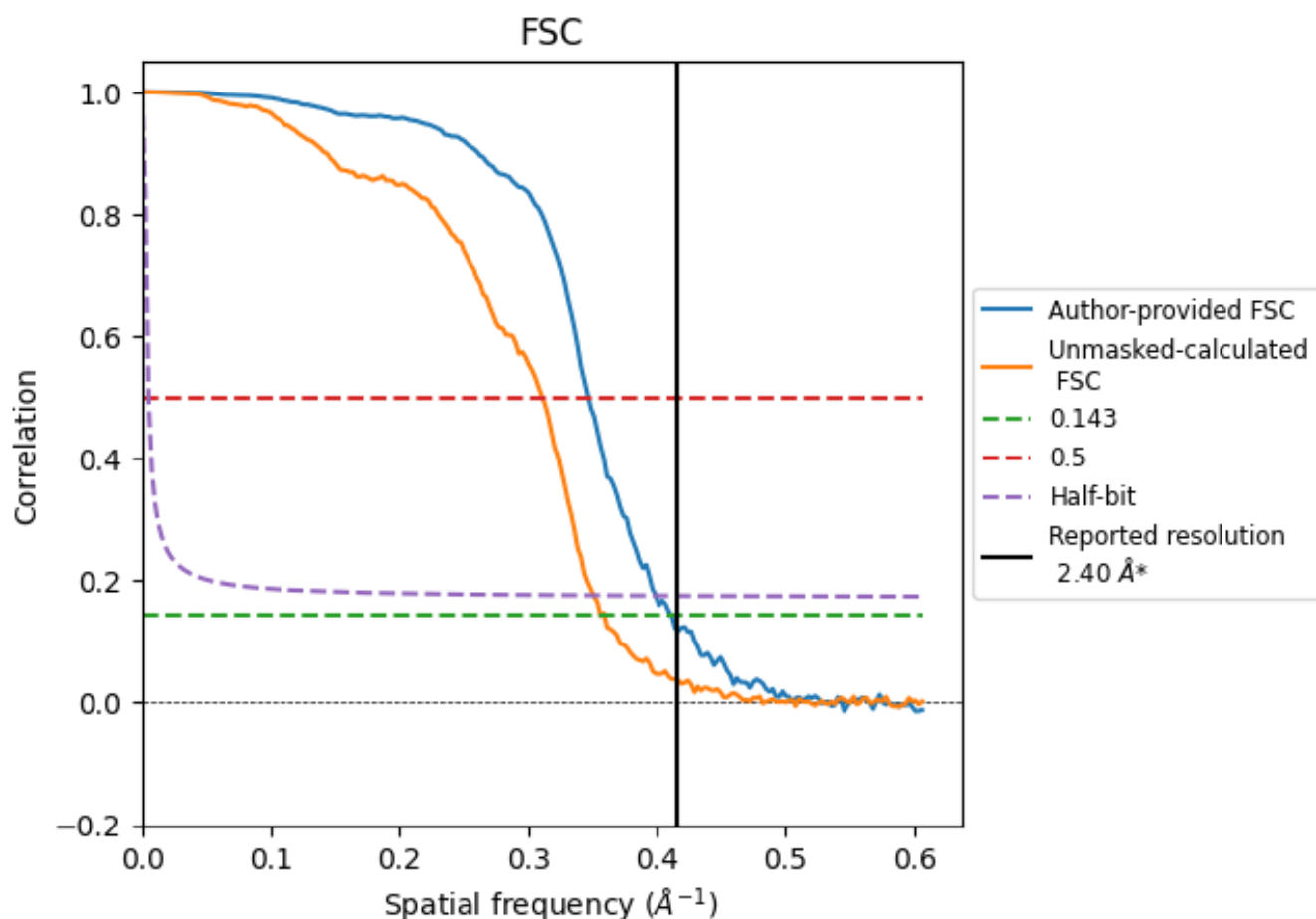


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

8.2 Resolution estimates [i](#)

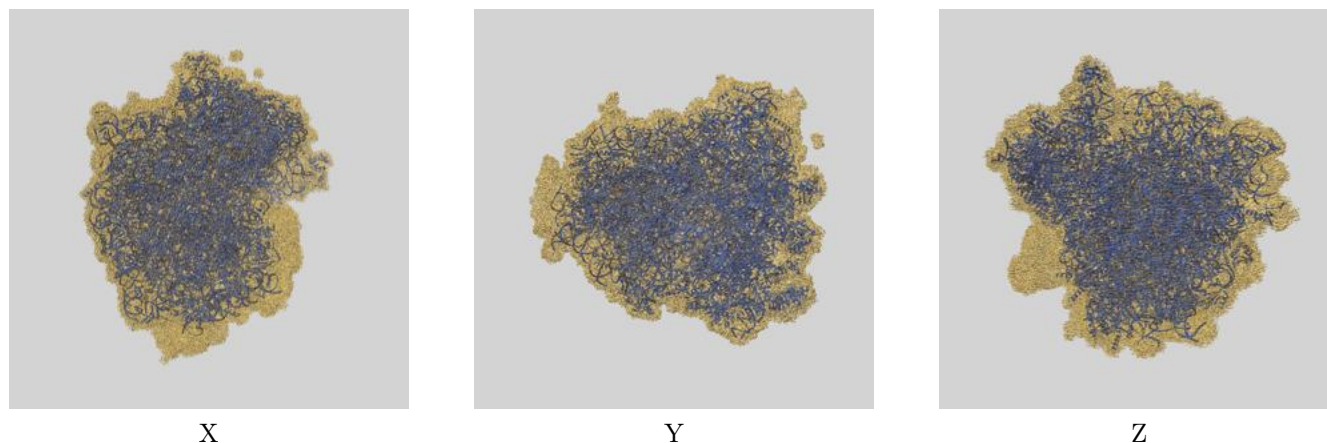
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.43	2.89	2.50
Unmasked-calculated*	2.81	3.21	2.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.81 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

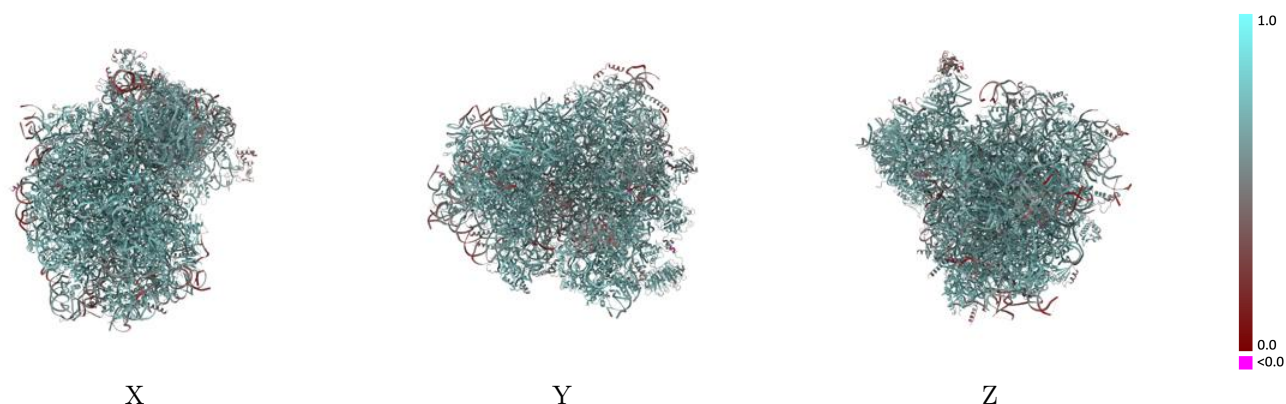
This section contains information regarding the fit between EMDB map EMD-55083 and PDB model 9SPF. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



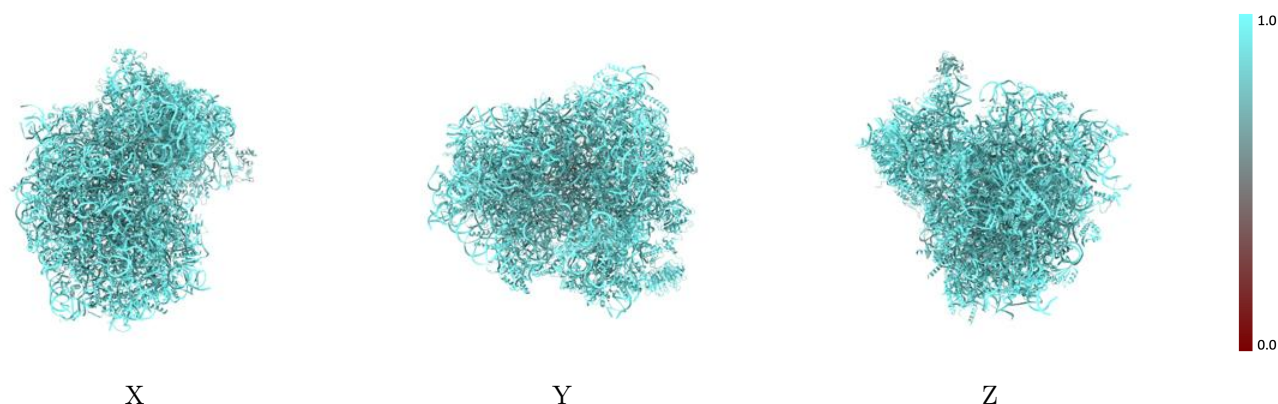
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



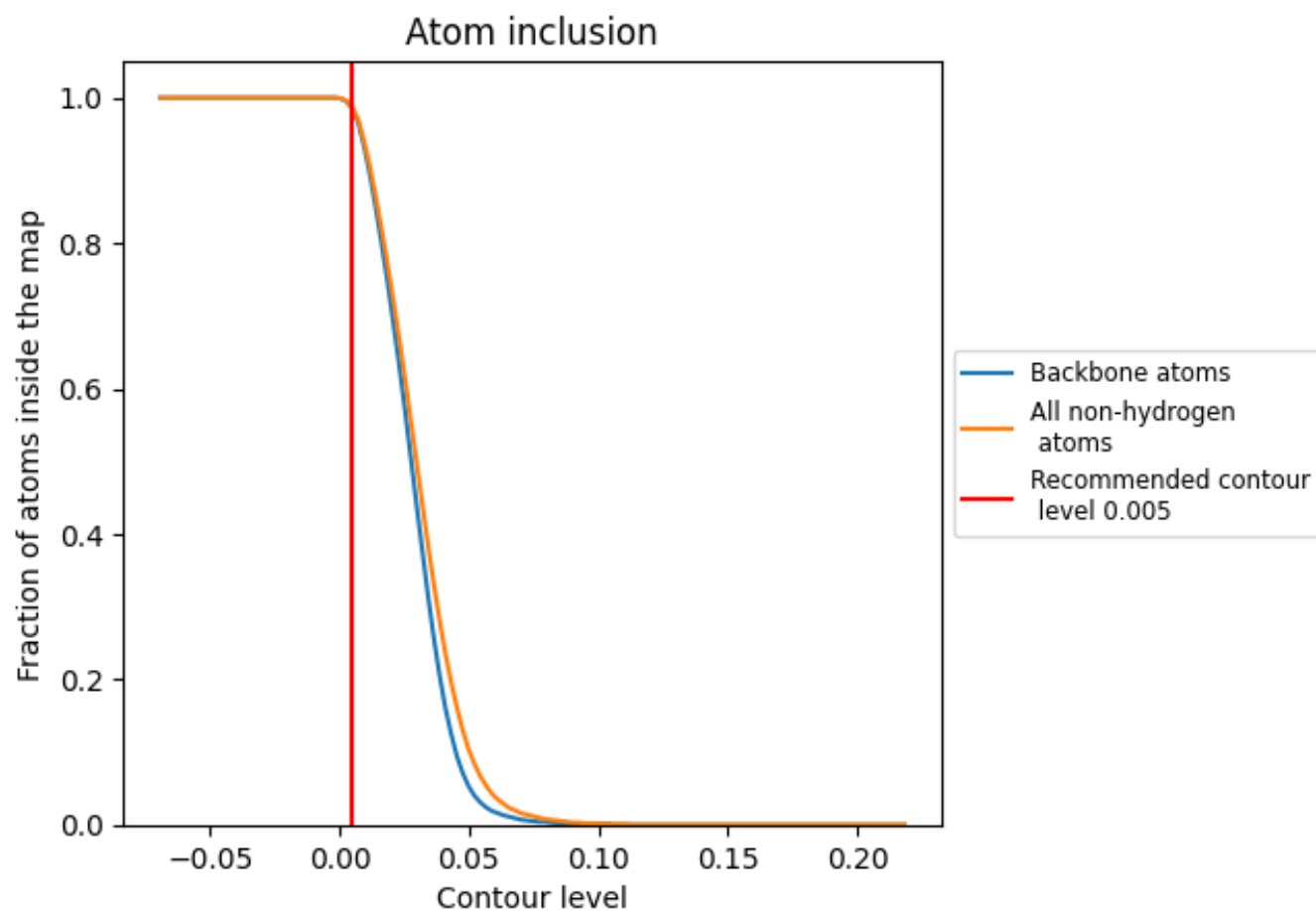
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 99% 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	 0.9870	 0.6510
At	 0.9670	 0.4410
Et	 0.9690	 0.3890
L5	 0.9880	 0.6520
L7	 1.0000	 0.6890
L8	 0.9910	 0.6620
LA	 0.9970	 0.7250
LB	 0.9920	 0.7110
LC	 0.9940	 0.7150
LD	 0.9870	 0.6580
LE	 0.9950	 0.6600
LF	 0.9980	 0.7230
LG	 0.9780	 0.6430
LH	 0.9900	 0.6770
LI	 0.9960	 0.6890
LJ	 0.9750	 0.5940
LL	 0.9900	 0.6870
LM	 0.9900	 0.6850
LN	 1.0000	 0.7400
LO	 0.9960	 0.7160
LP	 0.9950	 0.7200
LQ	 1.0000	 0.7350
LR	 0.9970	 0.6690
LS	 0.9940	 0.7160
LT	 0.9830	 0.6780
LU	 0.9770	 0.5880
LV	 0.9940	 0.7110
LW	 0.9840	 0.5700
LX	 0.9880	 0.6870
LY	 0.9960	 0.6940
LZ	 0.9940	 0.6630
La	 0.9970	 0.7290
Lb	 0.9880	 0.6370
Lc	 0.9880	 0.6640
Ld	 0.9800	 0.6730

















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Chain	Atom inclusion	Q-score
Le	 0.9990	 0.7280
Lf	 0.9950	 0.7350
Lg	 0.9880	 0.6940
Lh	 0.9940	 0.6830
Li	 0.9890	 0.6660
Lj	 1.0000	 0.7350
Lk	 0.9890	 0.6070
Ll	 0.9950	 0.7130
Lm	 0.9930	 0.6970
Ln	 1.0000	 0.6920
Lo	 1.0000	 0.7050
Lp	 0.9960	 0.7110
Lr	 0.9930	 0.7070
Mr	 0.9800	 0.5910
Pt	 0.9880	 0.5690
S2	 0.9920	 0.6400
SA	 0.9830	 0.6460
SB	 0.9890	 0.6300
SC	 0.9910	 0.6480
SD	 0.9710	 0.6210
SE	 0.9910	 0.6340
SF	 0.9940	 0.6850
SG	 0.9750	 0.5890
SH	 0.9300	 0.5380
SI	 0.9660	 0.6220
SJ	 0.9740	 0.5520
SK	 0.9830	 0.6330
SL	 0.9890	 0.6590
SM	 0.7550	 0.3670
SN	 0.9920	 0.6630
SO	 0.9950	 0.6490
SP	 0.9850	 0.6500
SQ	 0.9940	 0.6850
SR	 0.9690	 0.6100
SS	 0.9890	 0.6650
ST	 0.9850	 0.6740
SU	 0.9540	 0.6020
SV	 0.9840	 0.6380
SW	 0.9950	 0.6810
SX	 0.9900	 0.6520
SY	 0.9830	 0.5820
SZ	 0.9560	 0.6040

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Chain	Atom inclusion	Q-score
Sa	 0.9970	 0.6790
Sb	 0.9660	 0.6030
Sc	 0.9830	 0.6330
Sd	 0.9960	 0.6910
Se	 0.9810	 0.5800
Sf	 0.8490	 0.4530
Sg	 0.9690	 0.6070