



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 09:58 PM EDT

PDB ID : 8GLP / pdb_00008glp
EMDB ID : EMD-40205
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria
(Consensus LSU focused refined structure)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Watson, Z.L.;
Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-03-22
Resolution : 1.67 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:

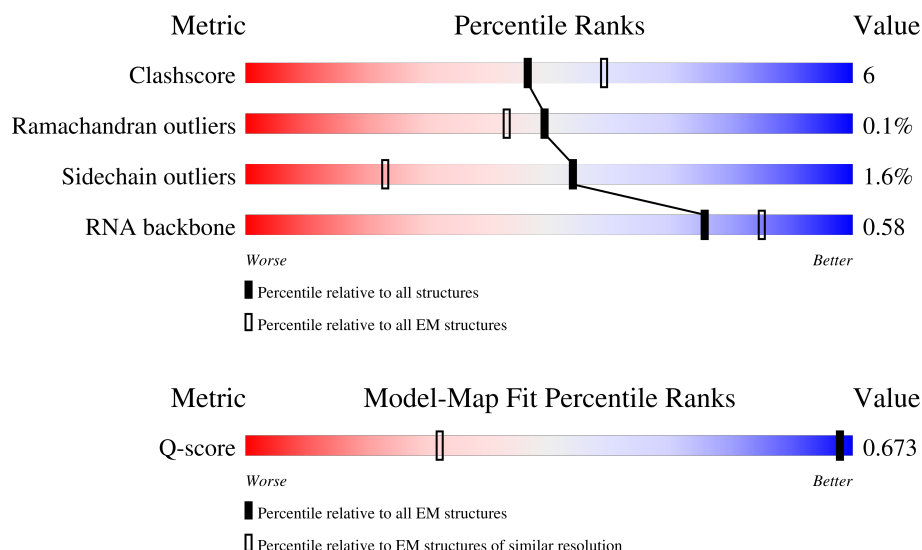
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 1.67 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.



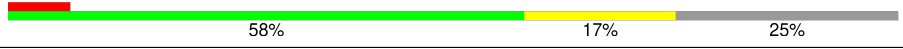
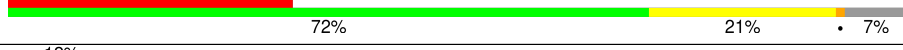
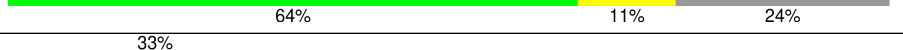
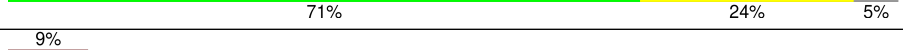
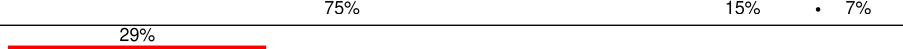
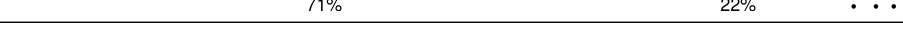
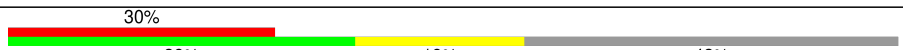
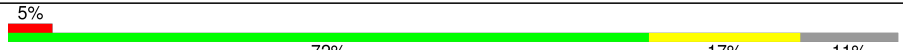
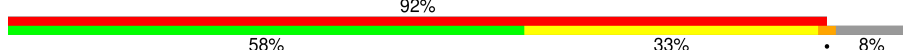
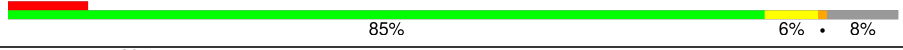
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	465 (1.19 - 2.17)

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	S2	1869	
2	L8	156	
3	L5	5069	

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	SB	264	
6	SA	295	
7	SD	243	
8	SJ	194	
9	SE	263	
10	SC	293	
11	SG	249	
12	SF	204	
13	SH	194	
14	SW	130	
15	SI	208	
16	SQ	146	
17	SU	119	
18	SK	165	
19	SO	151	
20	SX	143	
21	SM	132	
22	SS	152	
23	Sd	56	
24	SN	151	
25	SL	158	
26	SR	135	
27	SP	145	
28	ST	145	

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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	133	
31	SZ	125	
32	Sa	115	
33	Sb	84	
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	LA	257	
39	LB	403	
40	LC	427	
41	LJ	178	
42	LH	192	
43	LE	288	
44	LG	266	
45	LO	203	
46	LL	211	
47	LV	140	
48	LM	215	
49	La	148	
50	LN	204	
51	LI	214	
52	LD	297	
53	LQ	188	

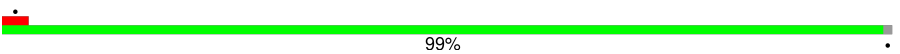
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Mol	Chain	Length	Quality of chain
54	LR	196	
55	LS	176	
56	LT	160	
57	LP	184	
58	LU	128	
59	LX	156	
60	LY	145	
61	LW	157	
62	LZ	136	
63	Lr	137	
64	Lh	123	
65	Lb	159	
66	LF	248	
67	Lc	115	
68	Ld	125	
69	Le	135	
70	Lf	110	
71	Lg	117	
72	Li	105	
73	Lj	97	
74	Lk	70	
75	Ll	51	
76	Lm	128	
77	Ln	25	
78	Lo	106	

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Mol	Chain	Length	Quality of chain
79	Lp	92	 99%
80	mR	60	 87%
81	Pt	77	 71%

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
6	SAC	SA	2	-	X	-	-
82	SPD	L5	5112	-	-	X	-
82	SPD	L5	5114	-	-	X	-

2 Entry composition [i](#)

There are 91 unique types of molecules in this entry. The entry contains 220877 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1672	Total	C	N	O	P	0	0
			35736	15981	6403	11681	1671		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3546	Total	C	N	O	P	1	0
			76116	33935	13923	24712	3546		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	223	Total	C	N	O	S	0	0
			1806	1145	325	322	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SA	222	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		

- Molecule 8 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 9 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 10 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SF	189	Total	C	N	O	S	0	0
			1494	934	284	269	7		

- Molecule 13 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SH	189	Total	C	N	O	S	0	0
			1517	966	279	271	1		

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S8.

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

- Molecule 16 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SQ	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 17 is a protein called 40S ribosomal protein S20.

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

- Molecule 18 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 19 is a protein called 40S ribosomal protein S14.

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

- Molecule 20 is a protein called 40S ribosomal protein S23 (uS12).

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SM	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 22 is a protein called 40S ribosomal protein S18.

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

- Molecule 23 is a protein called 40S ribosomal protein S29.

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

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SL	146	Total	C	N	O	S	0	0
			1200	766	226	202	6		

- Molecule 26 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	131	Total	C	N	O	S	0	0
			1078	684	204	183	7		

- Molecule 28 is a protein called 40S ribosomal protein S19.

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

- Molecule 29 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SV	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	84	Total	C	N	O	S	0	0
			674	433	126	114	1		

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	99	Total	C	N	O	S	1	0
			800	497	168	130	5		

- Molecule 33 is a protein called 40S ribosomal protein S27.

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

- Molecule 34 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sc	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 35 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	50	Total	C	N	O	S	0	0
			394	241	88	64	1		

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 38 is a protein called 60S ribosomal protein L8 (uL2).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LA	251	Total	C	N	O	S	1	0
			1930	1209	396	319	6		

- Molecule 39 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 40 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LC	366	Total	C	N	O	S	0	0
			2914	1832	581	487	14		

- Molecule 41 is a protein called 60S ribosomal protein L11.

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

- Molecule 42 is a protein called 60S ribosomal protein L9.

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

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LE	223	Total	C	N	O	S	0	0
			1786	1150	339	293	4		

- Molecule 44 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LG	241	Total	C	N	O	S	0	0
			1926	1228	371	323	4		

- Molecule 45 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LO	202	Total	C	N	O	S	0	0
			1654	1066	322	261	5		

- Molecule 46 is a protein called 60S ribosomal protein L13.

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

- Molecule 47 is a protein called 60S ribosomal protein L23.

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

- Molecule 48 is a protein called 60S ribosomal protein L14.

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

- Molecule 49 is a protein called 60S ribosomal protein L27a.

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

- Molecule 50 is a protein called 60S ribosomal protein L15.

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

- Molecule 51 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LI	203	Total	C	N	O	S	0	0
			1645	1045	317	270	13		

- Molecule 52 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 53 is a protein called 60S ribosomal protein L18.

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

- Molecule 54 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 55 is a protein called 60S ribosomal protein L18a.

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

- Molecule 56 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LT	159	Total	C	N	O	S	2	0
			1311	833	256	216	6		

- Molecule 57 is a protein called 60S ribosomal protein L17.

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

- Molecule 58 is a protein called 60S ribosomal protein L22.

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

- Molecule 59 is a protein called 60S ribosomal protein L23a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 61 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LW	118	Total	C	N	O	S	0	0
			950	595	192	159	4		

- Molecule 62 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LZ	135	Total	C	N	O	S	1	0
			1115	719	211	182	3		

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lr	125	Total	C	N	O	S	1	0
			1011	629	208	169	5		

- Molecule 64 is a protein called 60S ribosomal protein L35.

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

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Lb	111	Total	C	N	O	S	0	0
			898	560	195	139	4		

- Molecule 66 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	LF	225	Total	C	N	O	S	2	0
			1885	1212	364	300	9		

- Molecule 67 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lc	99	Total	C	N	O	S	0	0
			770	488	136	140	6		

- Molecule 68 is a protein called 60S ribosomal protein L31.

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

- Molecule 69 is a protein called 60S ribosomal protein L32.

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

- Molecule 70 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lf	110	Total	C	N	O	S	0	0
			883	560	175	144	4		

- Molecule 71 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 72 is a protein called 60S ribosomal protein L36.

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

- Molecule 73 is a protein called 60S ribosomal protein L37.

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

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Lk	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

- Molecule 75 is a protein called 60S ribosomal protein L39.

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

- Molecule 76 is a protein called 60S ribosomal protein L40 (eL40).

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lm	52	Total	C	N	O	S	1	0
			436	272	91	67	6		

- Molecule 77 is a protein called 60S ribosomal protein L41.

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

- Molecule 78 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 79 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lp	91	Total	C	N	O	S	1	0
			715	450	139	119	7		

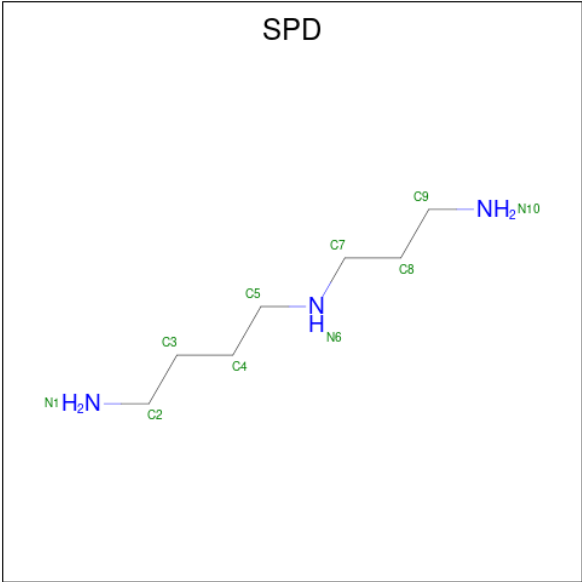
- Molecule 80 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	mR	8	Total	C	N	O	P	0	0
			172	77	32	55	8		

- Molecule 81 is a RNA chain called P-site tRNA.

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

- Molecule 82 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



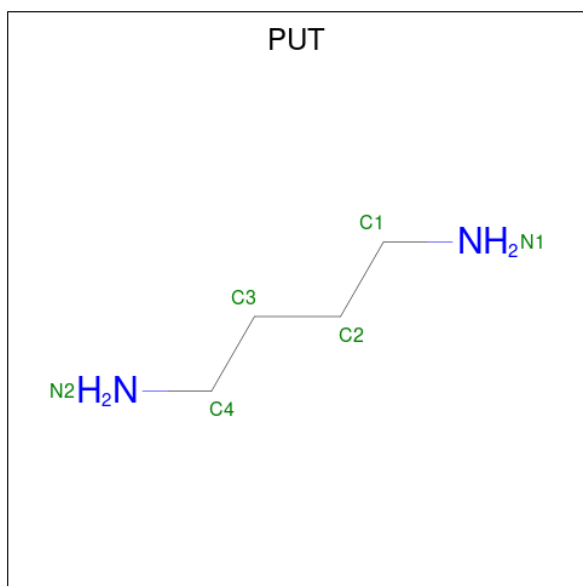
Mol	Chain	Residues	Atoms			AltConf
82	S2	1	Total	C	N	0
			10	7	3	
82	S2	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	
82	L5	1	Total	C	N	0
			10	7	3	

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

- Molecule 83 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



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

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

Mol	Chain	Residues	Atoms		AltConf
84	S2	12	Total 12	K 12	0
84	L8	4	Total 4	K 4	0
84	L5	117	Total 117	K 117	0
84	L7	4	Total 4	K 4	0
84	SO	1	Total 1	K 1	0
84	SL	1	Total 1	K 1	0
84	Sa	1	Total 1	K 1	0
84	LA	3	Total 3	K 3	0
84	LH	1	Total 1	K 1	0
84	LL	1	Total 1	K 1	0
84	LN	1	Total 1	K 1	0
84	LI	1	Total 1	K 1	0
84	LQ	1	Total 1	K 1	0
84	Lb	1	Total 1	K 1	0
84	Le	1	Total 1	K 1	0
84	Lf	1	Total 1	K 1	0
84	Ll	1	Total 1	K 1	0

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

Mol	Chain	Residues	Atoms		AltConf
85	S2	137	Total 137	Mg 137	0
85	L8	16	Total 16	Mg 16	0
85	L5	463	Total 463	Mg 463	0

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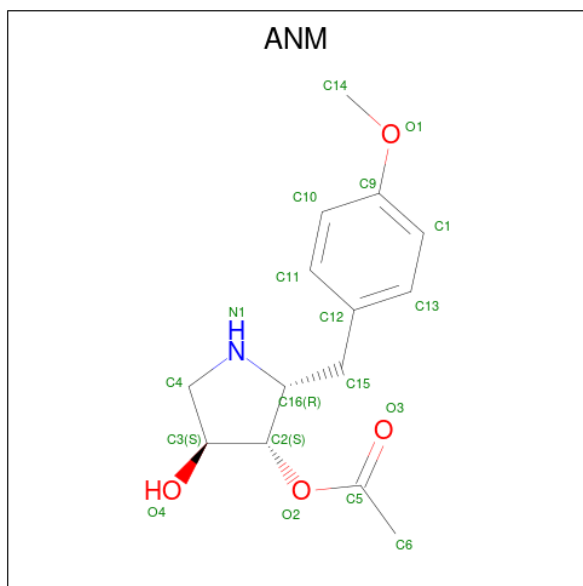
Mol	Chain	Residues	Atoms		AltConf
85	L7	15	Total 15	Mg 15	0
85	SG	1	Total 1	Mg 1	0
85	SX	1	Total 1	Mg 1	0
85	SS	2	Total 2	Mg 2	0
85	Sd	1	Total 1	Mg 1	0
85	SN	1	Total 1	Mg 1	0
85	ST	1	Total 1	Mg 1	0
85	LB	1	Total 1	Mg 1	0
85	LC	1	Total 1	Mg 1	0
85	LH	1	Total 1	Mg 1	0
85	LG	1	Total 1	Mg 1	0
85	LO	2	Total 2	Mg 2	0
85	LL	1	Total 1	Mg 1	0
85	LV	1	Total 1	Mg 1	0
85	La	1	Total 1	Mg 1	0
85	LN	3	Total 3	Mg 3	0
85	LD	1	Total 1	Mg 1	0
85	LQ	2	Total 2	Mg 2	0
85	LR	1	Total 1	Mg 1	0
85	LS	1	Total 1	Mg 1	0
85	LP	2	Total 2	Mg 2	0

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Mol	Chain	Residues	Atoms		AltConf
85	Lr	3	Total	Mg	0
			3	3	
85	LF	1	Total	Mg	0
			1	1	
85	Lc	1	Total	Mg	0
			1	1	
85	Lf	1	Total	Mg	0
			1	1	
85	Lg	1	Total	Mg	0
			1	1	
85	Lj	2	Total	Mg	0
			2	2	
85	Lo	1	Total	Mg	0
			1	1	
85	Lp	2	Total	Mg	0
			2	2	
85	Pt	2	Total	Mg	0
			2	2	

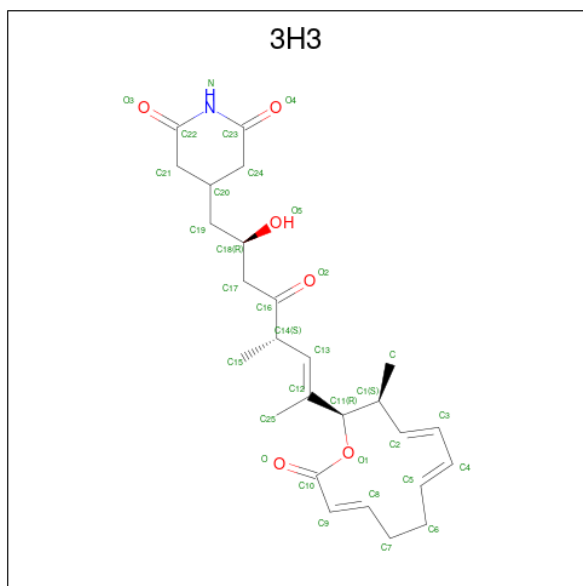
- Molecule 86 is ANISOMYCIN (CCD ID: ANM) (formula: C₁₄H₁₉NO₄).



Mol	Chain	Residues	Atoms				AltConf
86	L5	1	Total	C	N	O	0
			19	14	1	4	

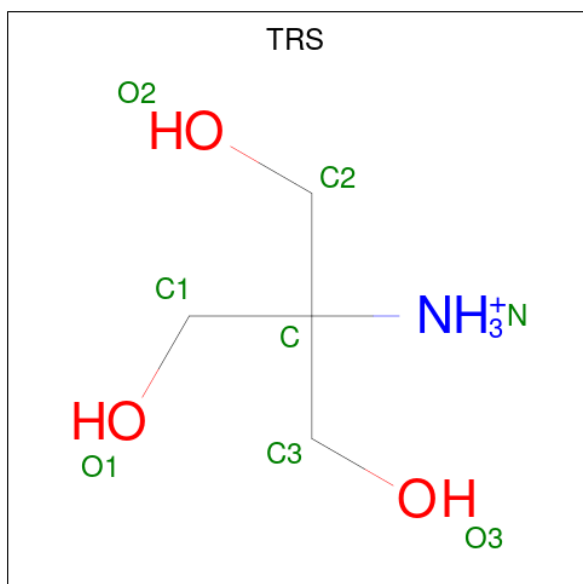
- Molecule 87 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxo-oxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (CCD ID: 3H3)

(formula: $C_{26}H_{35}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
87	L5	1	Total	C	N	O	0
			33	26	1	6	

- Molecule 88 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
88	L5	1	Total	C	N	O	0
			8	4	1	3	

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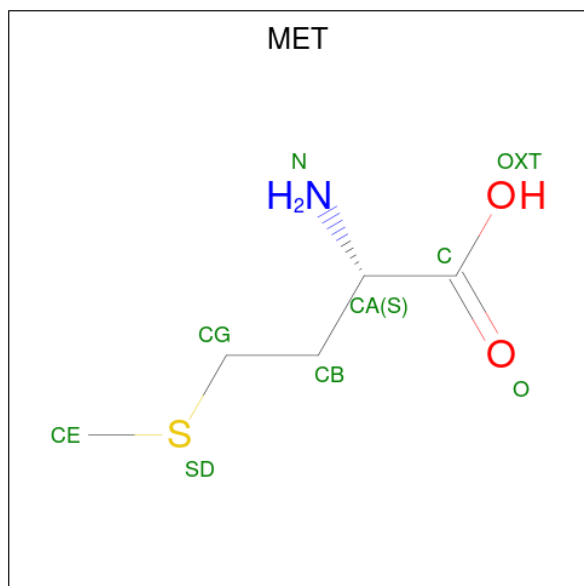
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Mol	Chain	Residues	Atoms				AltConf
88	L5	1	Total	C	N	O	0
			8	4	1	3	

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

Mol	Chain	Residues	Atoms		AltConf
89	Sd	1	Total	Zn	0
			1	1	
89	Sa	1	Total	Zn	0
			1	1	
89	Sf	1	Total	Zn	0
			1	1	
89	Lg	1	Total	Zn	0
			1	1	
89	Lj	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	

- Molecule 90 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
90	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
91	S2	266	Total	O	0
			266	266	
91	L8	189	Total	O	0
			189	189	
91	L5	5661	Total	O	0
			5661	5661	
91	L7	133	Total	O	0
			133	133	
91	SA	1	Total	O	0
			1	1	
91	SE	1	Total	O	0
			1	1	
91	SF	1	Total	O	0
			1	1	
91	SO	3	Total	O	0
			3	3	
91	SN	3	Total	O	0
			3	3	
91	SL	2	Total	O	0
			2	2	
91	Sa	4	Total	O	0
			4	4	
91	Sb	1	Total	O	0
			1	1	
91	LA	93	Total	O	0
			93	93	
91	LB	113	Total	O	0
			113	113	
91	LC	137	Total	O	0
			137	137	
91	LJ	4	Total	O	0
			4	4	
91	LH	14	Total	O	0
			14	14	
91	LE	28	Total	O	0
			28	28	
91	LG	28	Total	O	0
			28	28	

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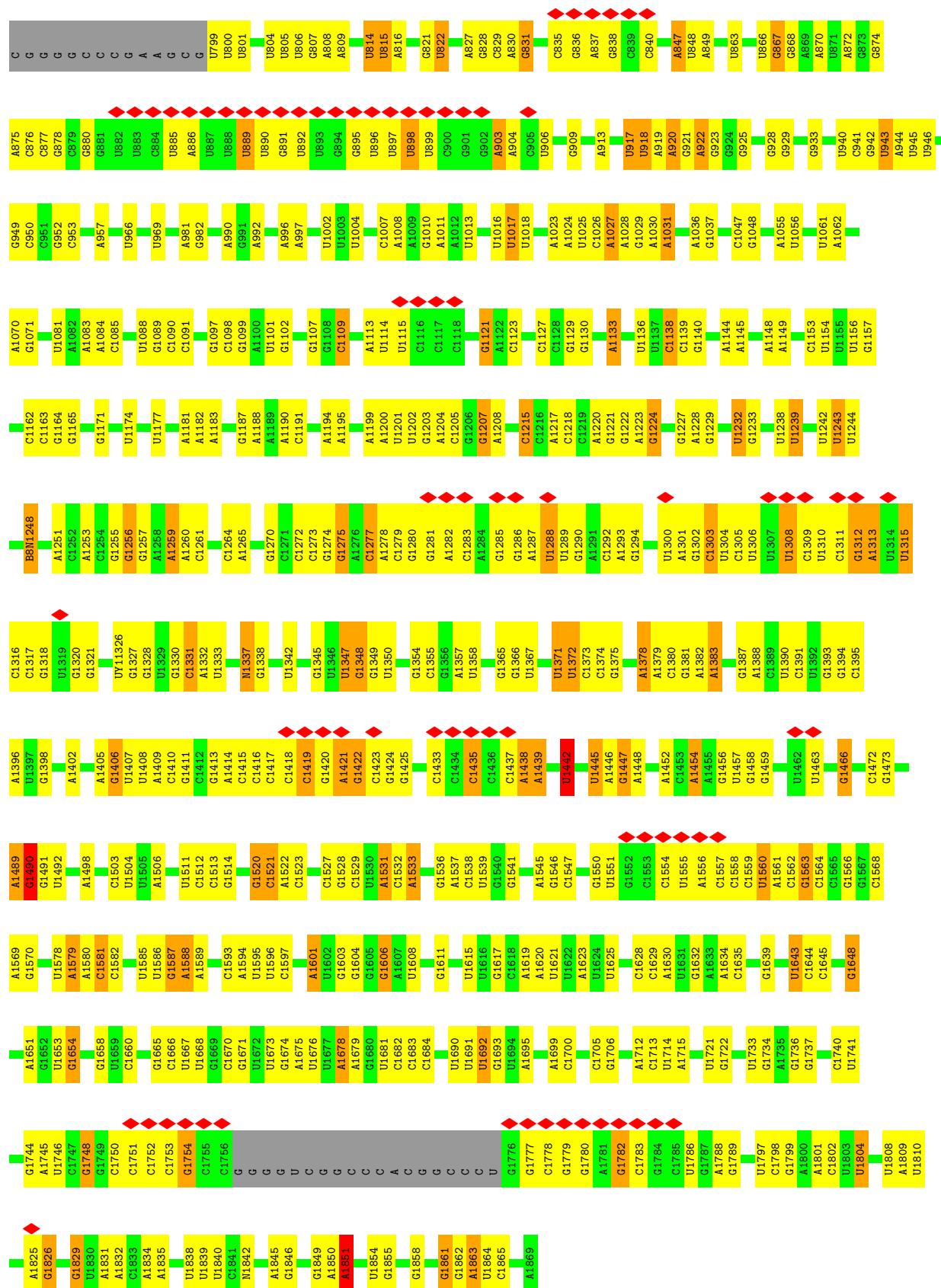
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Mol	Chain	Residues	Atoms		AltConf
91	LO	69	Total 69	O 69	0
91	LL	62	Total 62	O 62	0
91	LV	25	Total 25	O 25	0
91	LM	10	Total 10	O 10	0
91	La	71	Total 71	O 71	0
91	LN	112	Total 112	O 112	0
91	LI	33	Total 33	O 33	0
91	LD	37	Total 37	O 37	0
91	LQ	81	Total 81	O 81	0
91	LR	34	Total 34	O 34	0
91	LS	51	Total 51	O 51	0
91	LT	58	Total 58	O 58	0
91	LP	44	Total 44	O 44	0
91	LU	1	Total 1	O 1	0
91	LX	15	Total 15	O 15	0
91	LY	23	Total 23	O 23	0
91	LW	8	Total 8	O 8	0
91	LZ	7	Total 7	O 7	0
91	Lr	53	Total 53	O 53	0
91	Lh	10	Total 10	O 10	0
91	Lb	21	Total 21	O 21	0

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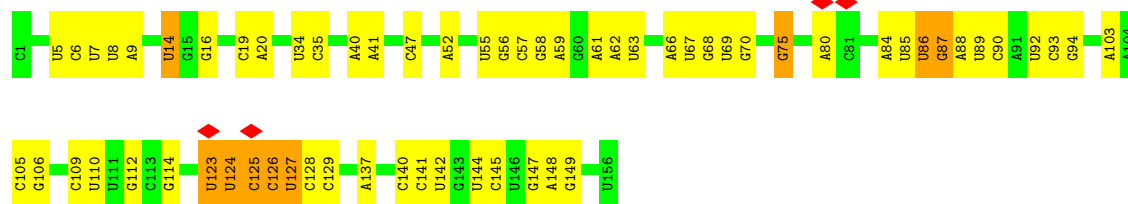
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Mol	Chain	Residues	Atoms		AltConf
91	LF	77	Total 77	O 77	0
91	Lc	5	Total 5	O 5	0
91	Ld	20	Total 20	O 20	0
91	Le	71	Total 71	O 71	0
91	Lf	45	Total 45	O 45	0
91	Lg	39	Total 39	O 39	0
91	Li	15	Total 15	O 15	0
91	Lj	36	Total 36	O 36	0
91	Lk	2	Total 2	O 2	0
91	Ll	14	Total 14	O 14	0
91	Lm	8	Total 8	O 8	0
91	Ln	4	Total 4	O 4	0
91	Lo	37	Total 37	O 37	0
91	Lp	24	Total 24	O 24	0
91	Pt	1	Total 1	O 1	0



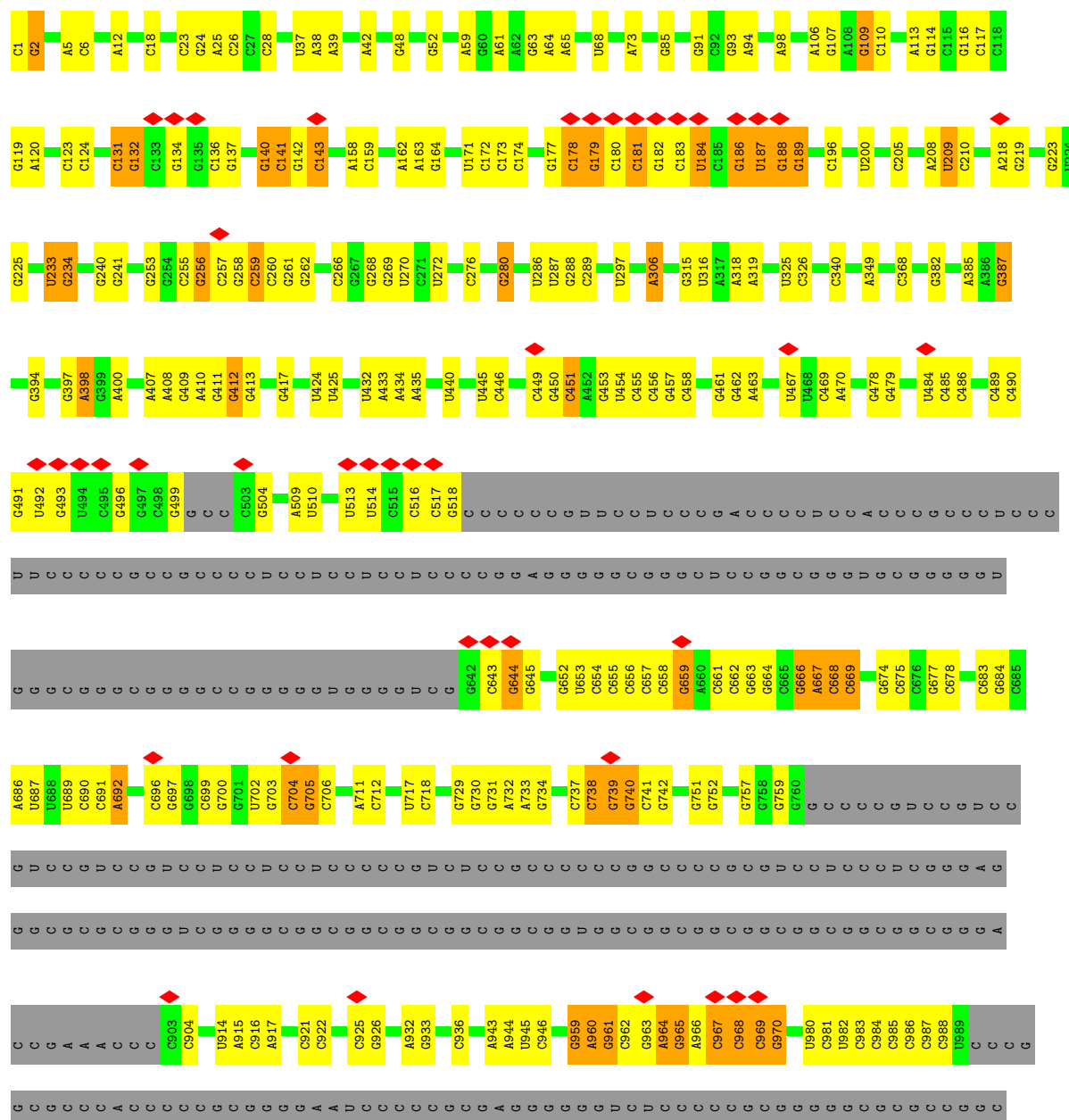
• Molecule 2: 5.8S rRNA

Chain L8: 



• Molecule 3: 28S rRNA

Chain L5: 

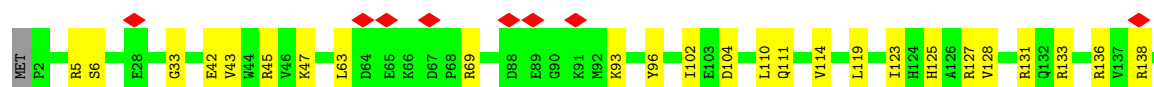


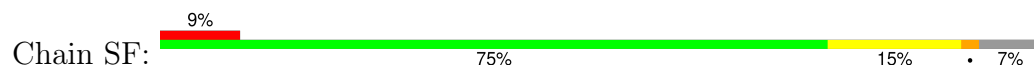


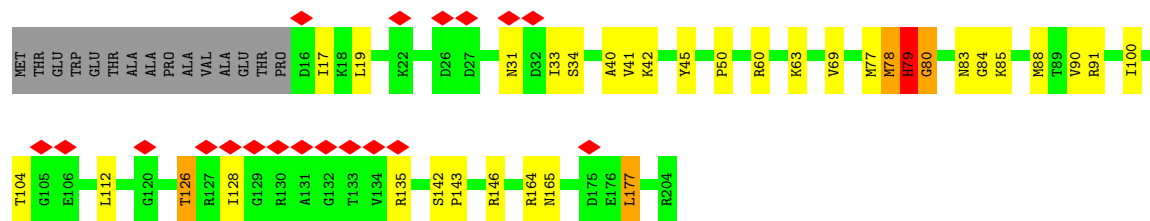




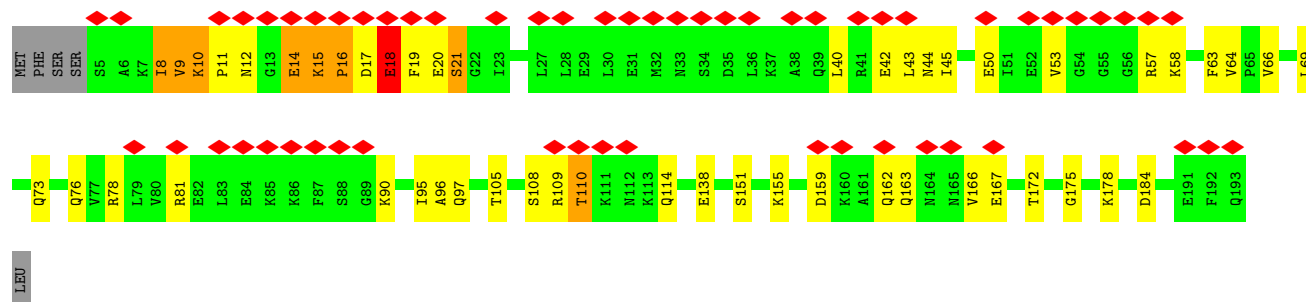
WORLDWIDE
PDB
PROTEIN DATA BANK



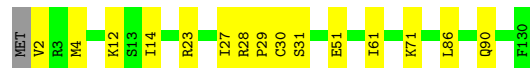
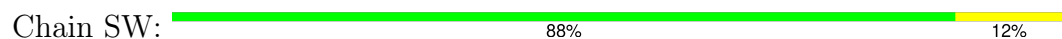




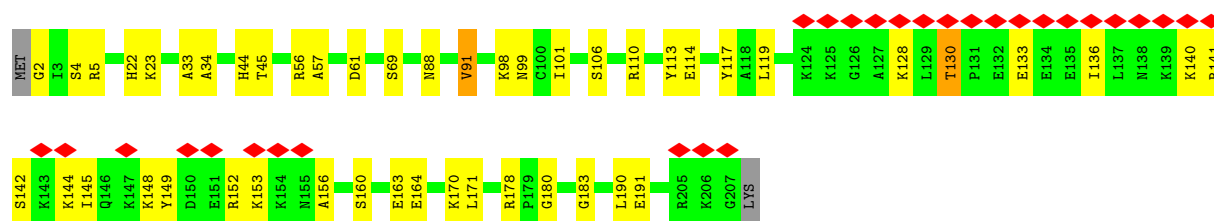
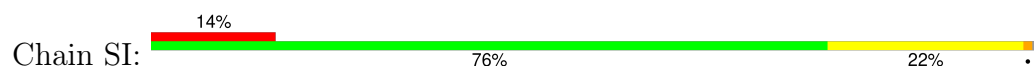
• Molecule 13: 40S ribosomal protein S7



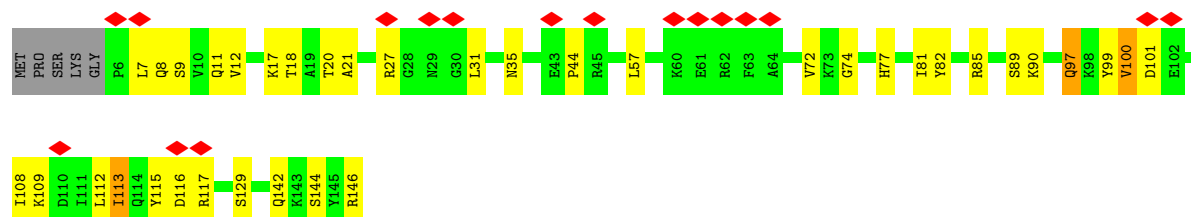
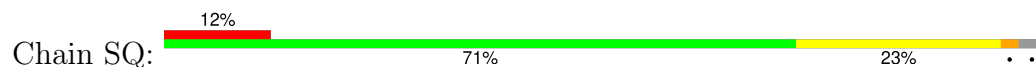
• Molecule 14: 40S ribosomal protein S15a



• Molecule 15: 40S ribosomal protein S8

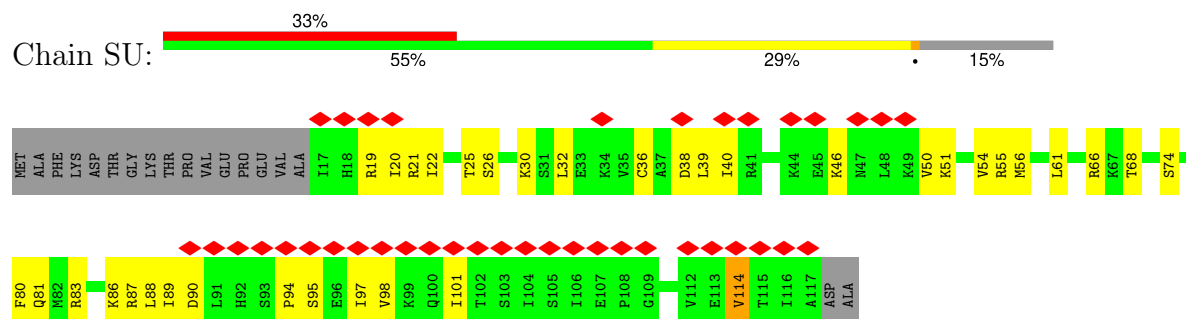


• Molecule 16: 40S ribosomal protein S16



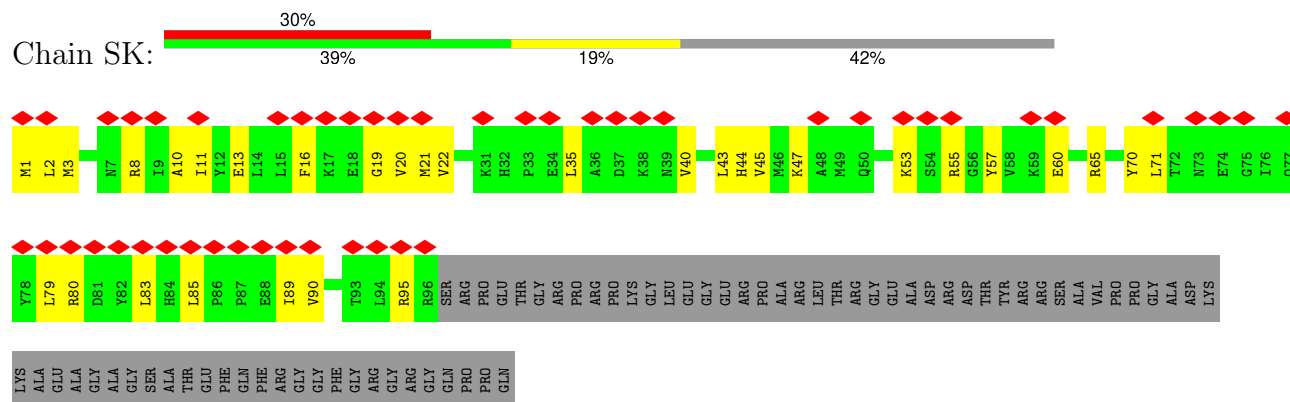
- Molecule 17: 40S ribosomal protein S20

Chain SU:



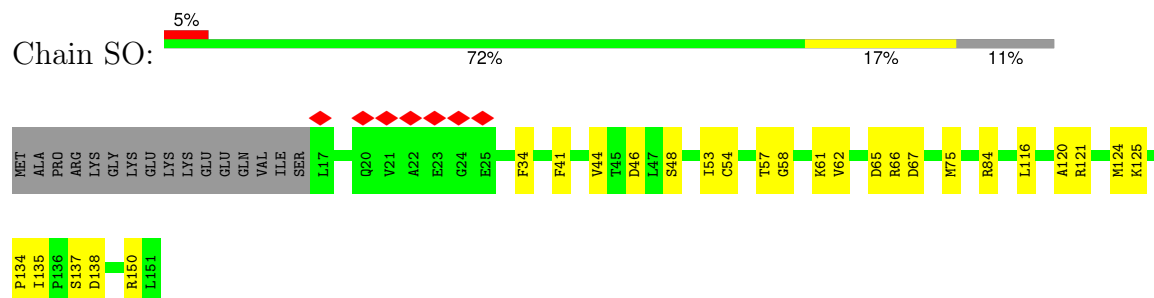
- Molecule 18: 40S ribosomal protein S10

Chain SK:



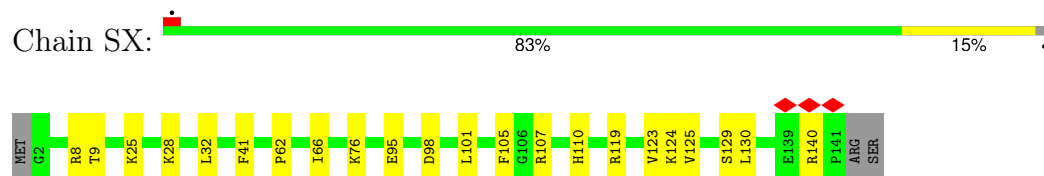
- Molecule 19: 40S ribosomal protein S14

Chain SO:



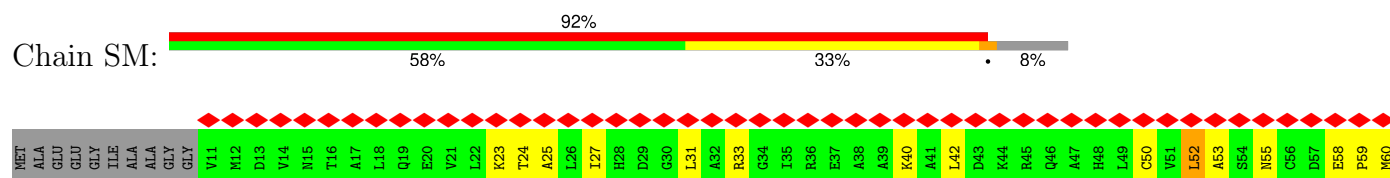
- Molecule 20: 40S ribosomal protein S23 (uS12)

Chain SX:

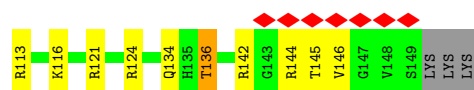
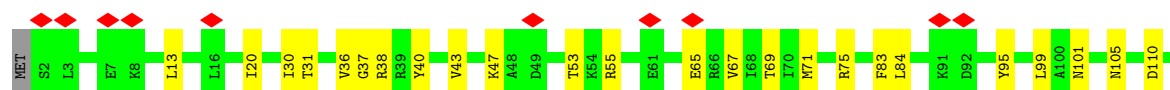
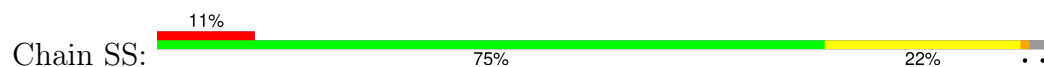


- Molecule 21: 40S ribosomal protein S12

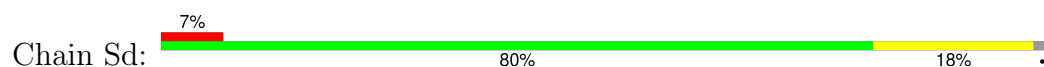
Chain SM:



- Molecule 22: 40S ribosomal protein S18



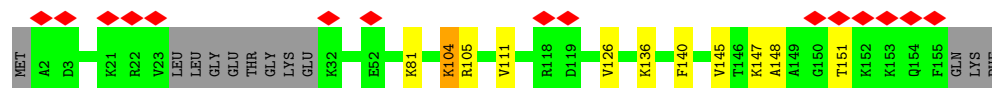
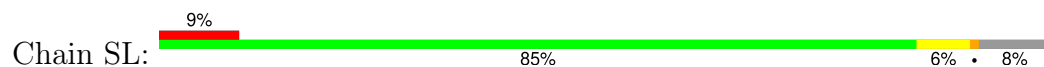
- Molecule 23: 40S ribosomal protein S29



- Molecule 24: 40S ribosomal protein S13



- Molecule 25: 40S ribosomal protein S11

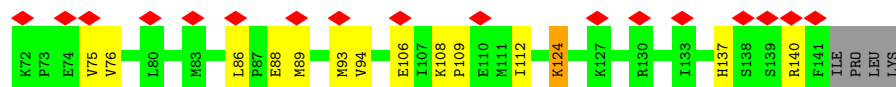
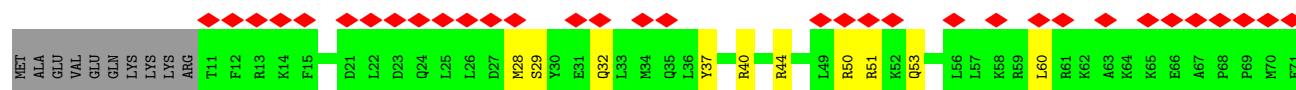
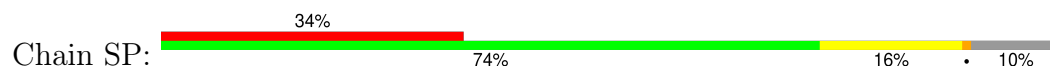


- Molecule 26: 40S ribosomal protein S17

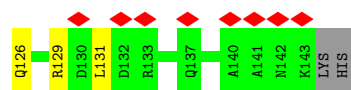
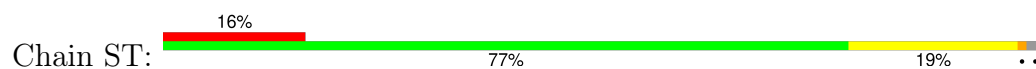




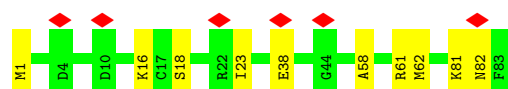
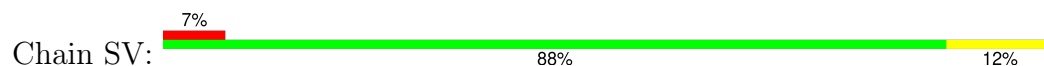
- Molecule 27: 40S ribosomal protein S15



- Molecule 28: 40S ribosomal protein S19



- Molecule 29: 40S ribosomal protein S21



- Molecule 30: 40S ribosomal protein S24

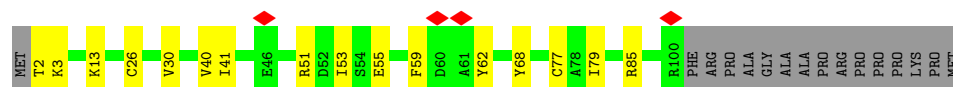


- Molecule 31: 40S ribosomal protein S25

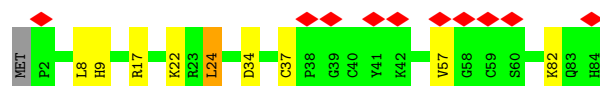
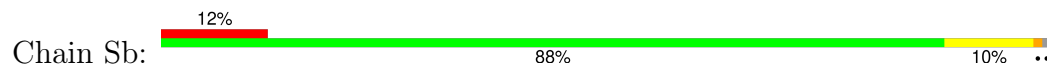




- Molecule 32: 40S ribosomal protein S26



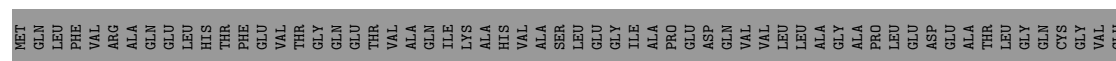
- Molecule 33: 40S ribosomal protein S27



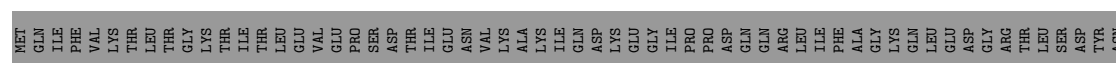
- Molecule 34: 40S ribosomal protein S28



- Molecule 35: FAU ubiquitin-like and ribosomal protein S30

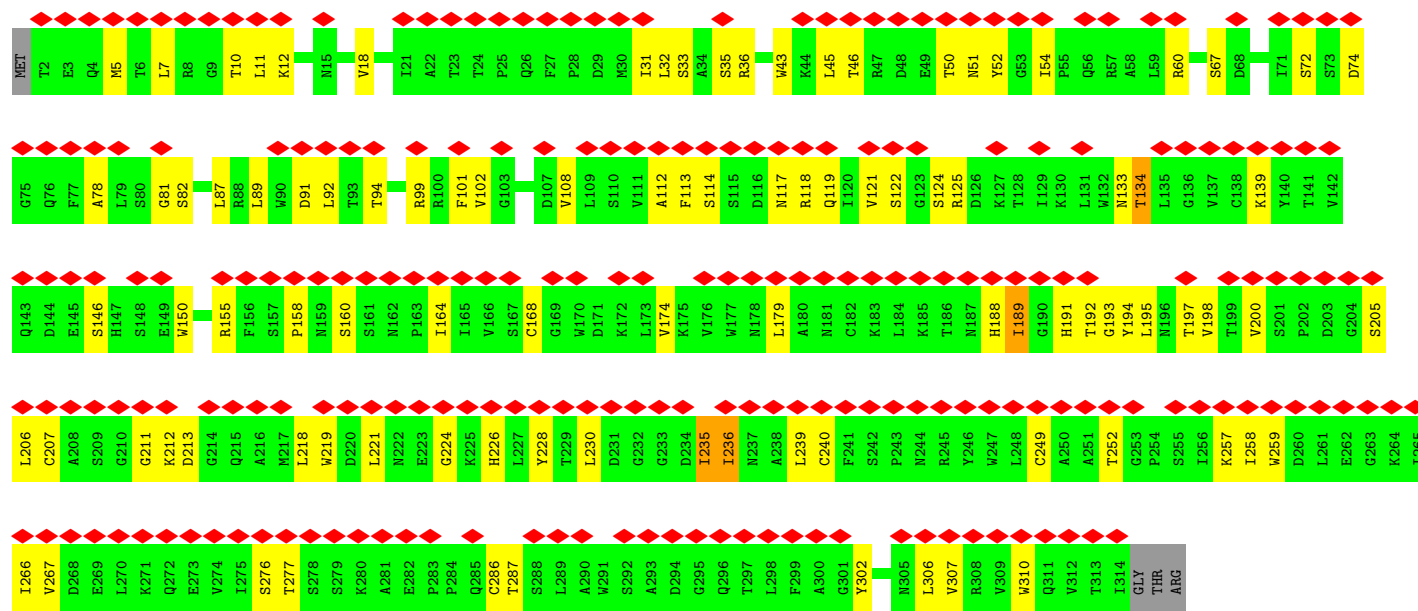
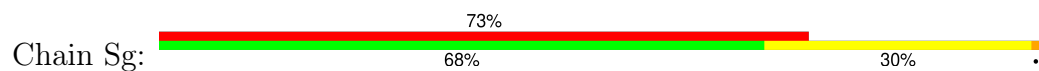


- Molecule 36: Ubiquitin-40S ribosomal protein S27a





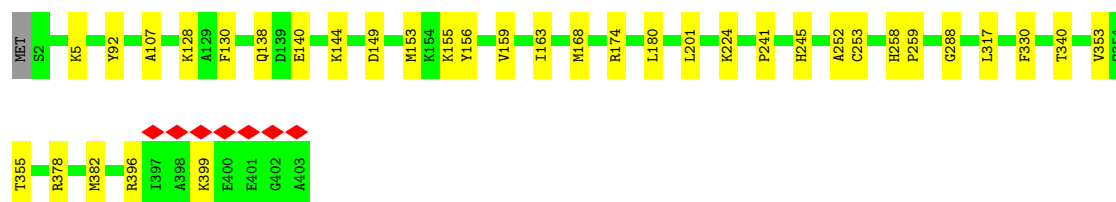
- Molecule 37: Receptor of activated protein C kinase 1



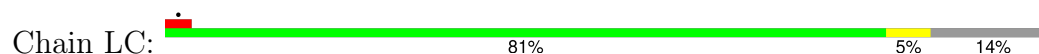
- Molecule 38: 60S ribosomal protein L8 (uL2)

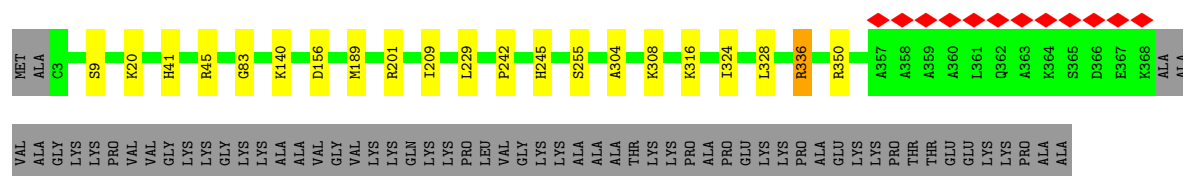


- Molecule 39: 60S ribosomal protein L3



- Molecule 40: 60S ribosomal protein L4

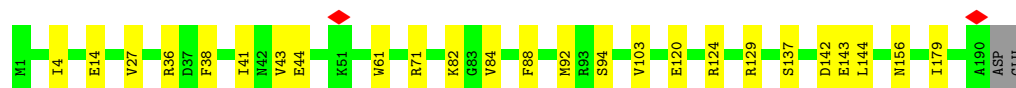
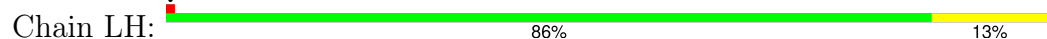




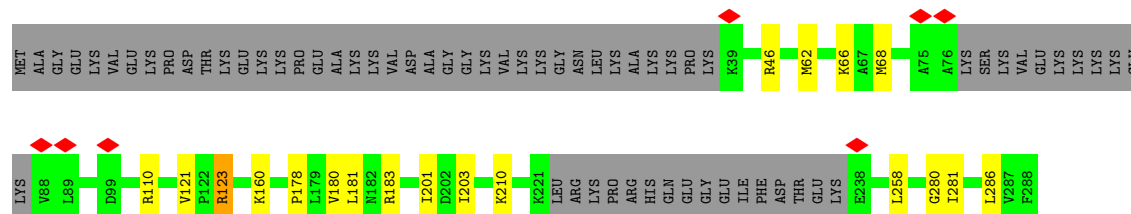
- Molecule 41: 60S ribosomal protein L11



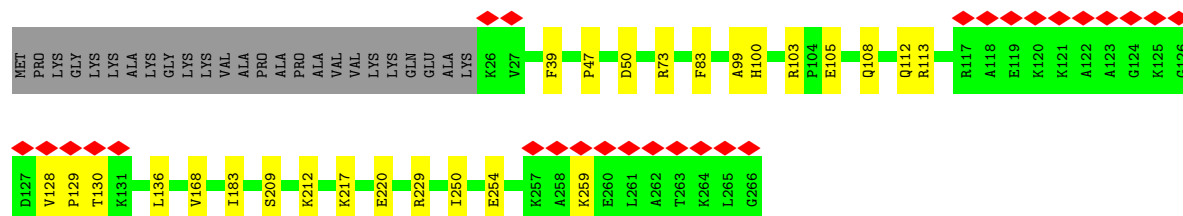
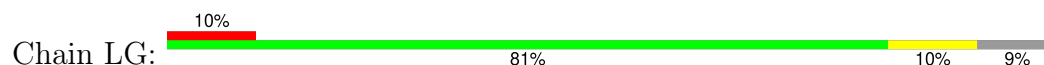
- Molecule 42: 60S ribosomal protein L9



- Molecule 43: 60S ribosomal protein L6



- Molecule 44: 60S ribosomal protein L7a



- Molecule 45: 60S ribosomal protein L13a



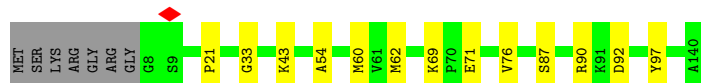
- Molecule 46: 60S ribosomal protein L13

Chain LL:  89% 9%



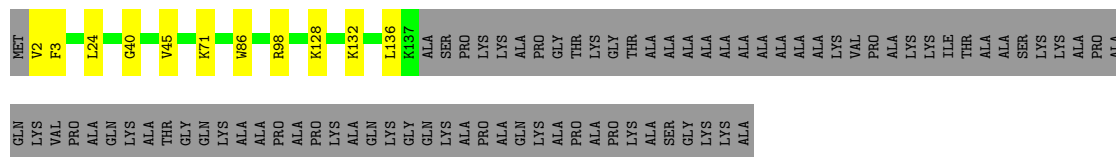
- Molecule 47: 60S ribosomal protein L23

Chain LV:  86% 9% 5%

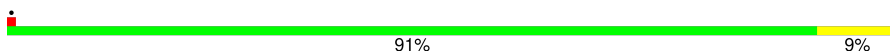


- Molecule 48: 60S ribosomal protein L14

Chain LM:  58% 5% 37%



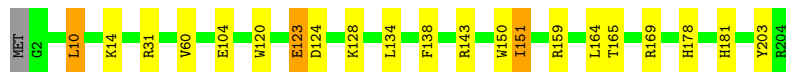
- Molecule 49: 60S ribosomal protein L27a

Chain La:  91% 9%



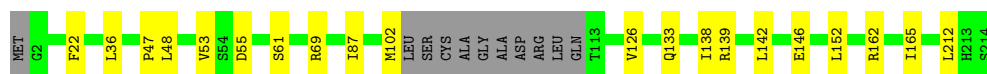
- Molecule 50: 60S ribosomal protein L15

Chain LN:  89% 9%



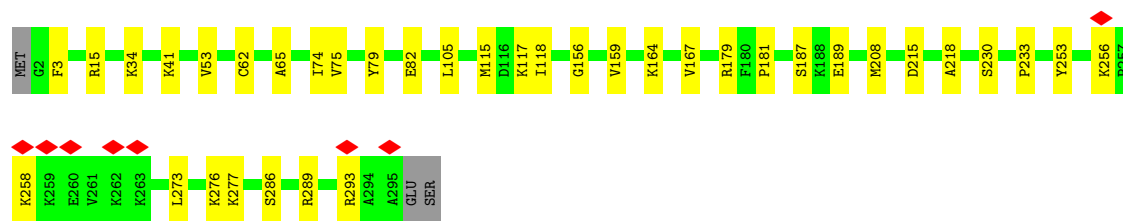
- Molecule 51: 60S ribosomal protein L10

Chain LI:  86% 9% 5%



- Molecule 52: 60S ribosomal protein L5

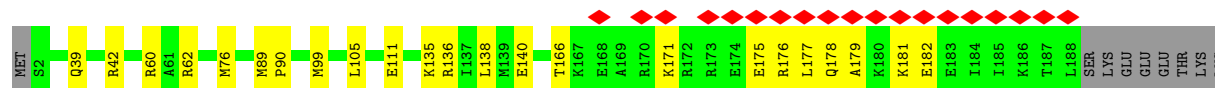
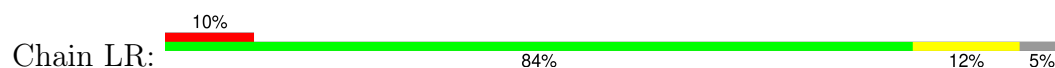
Chain LD:  87% 12%



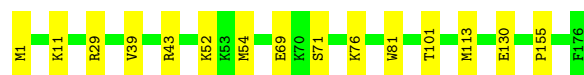
- Molecule 53: 60S ribosomal protein L18



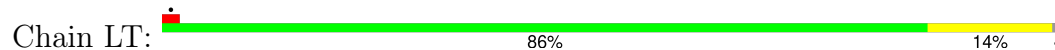
- Molecule 54: 60S ribosomal protein L19



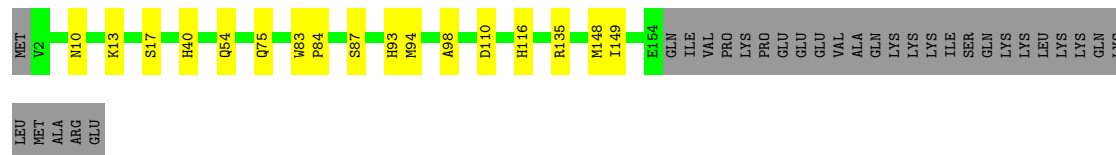
- Molecule 55: 60S ribosomal protein L18a



- Molecule 56: 60S ribosomal protein L21



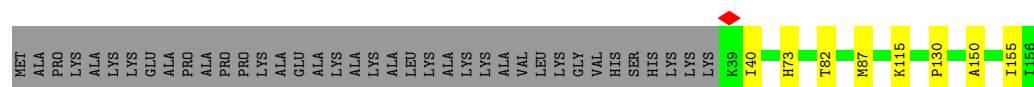
- Molecule 57: 60S ribosomal protein L17



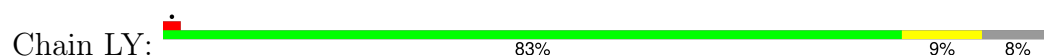
- Molecule 58: 60S ribosomal protein L22



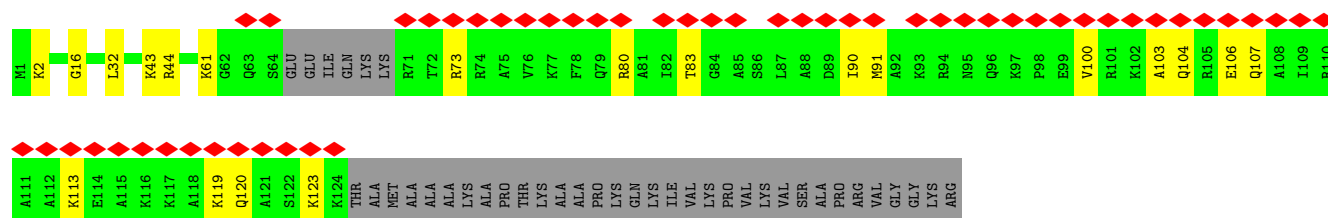
- Molecule 59: 60S ribosomal protein L23a



- Molecule 60: 60S ribosomal protein L26



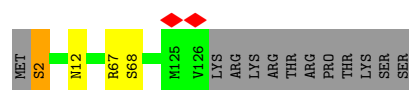
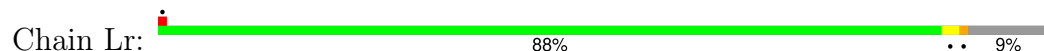
- Molecule 61: 60S ribosomal protein L24



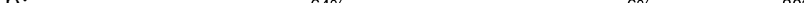
- Molecule 62: 60S ribosomal protein L27

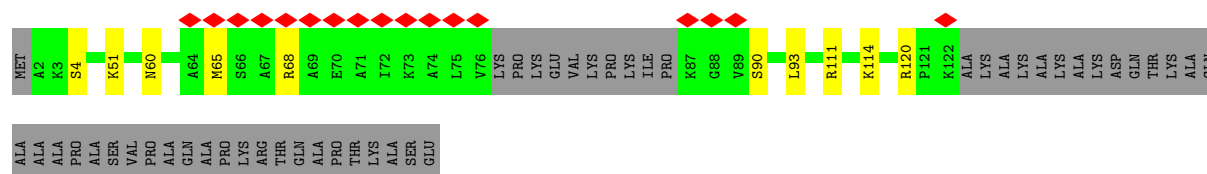


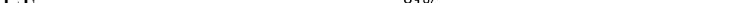
- Molecule 63: 60S ribosomal protein L28

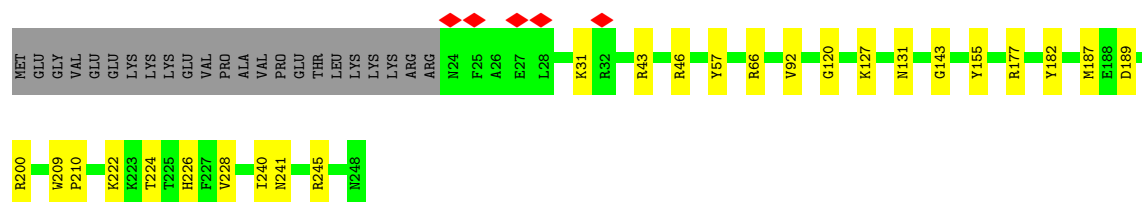


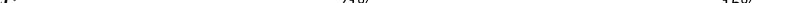
- Molecule 64: 60S ribosomal protein L35

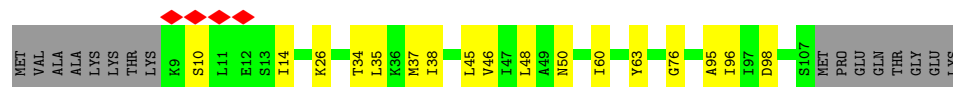
- Chain Lb: 

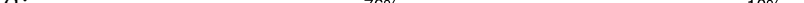


- Chain LF: 



- Chain Lc: 



- Chain Ld: 

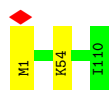


- Chain Le: 86% 9% 5%



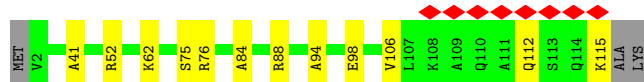
- 

Chain Lf:  98% .



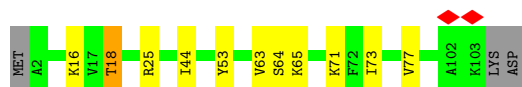
- Molecule 71: 60S ribosomal protein L34

Chain Lg:  7% 87% 10% .



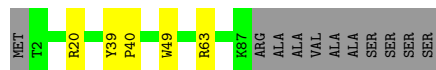
- Molecule 72: 60S ribosomal protein L36

Chain Li:  87% 10% . .



- Molecule 73: 60S ribosomal protein L37

Chain Lj:  84% 5% 11%



- Molecule 74: 60S ribosomal protein L38

Chain Lk:  86% 13% .



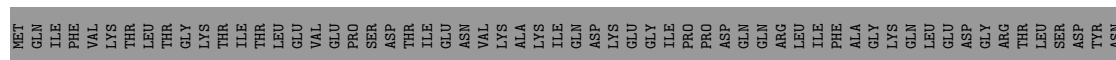
- Molecule 75: 60S ribosomal protein L39

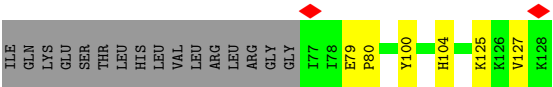
Chain Ll:  78% 20% .



- Molecule 76: 60S ribosomal protein L40 (eL40)

Chain Lm:  36% 5% 59%

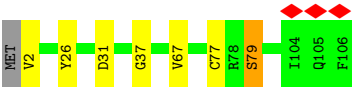




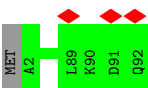
• Molecule 77: 60S ribosomal protein L41



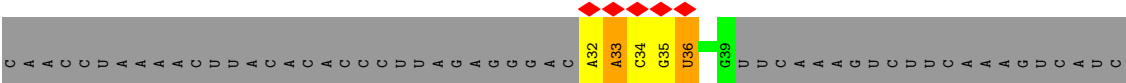
• Molecule 78: 60S ribosomal protein L36a



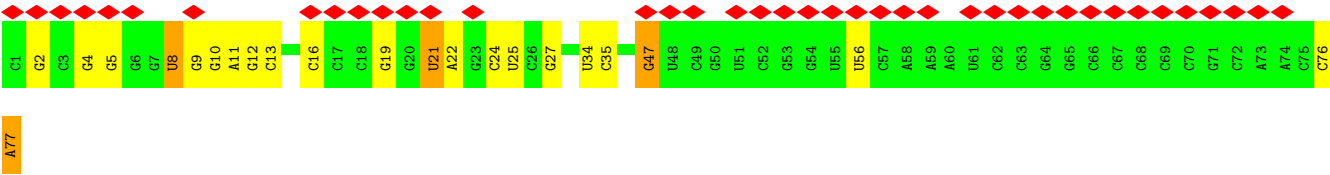
• Molecule 79: 60S ribosomal protein L37a



• Molecule 80: mRNA



• Molecule 81: P-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	845750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	79	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	528.64, 528.64, 528.64	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82600003, 0.82600003, 0.82600003	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, 6MZ, HIC, G7M, A2M, 1MA, OMG, PSU, SPD, HY3, MLZ, PUT, SAC, MG, UR3, TRS, B8N, OMU, ANM, UY1, V5N, H2U, 4SU, MA6, K, 3H3, 5MC, M3L, ZN, AME, OMC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	S2	0.21	0/37935	0.28	0/59125
2	L8	0.28	0/3609	0.31	0/5623
3	L5	0.29	0/82080	0.34	0/128048
4	L7	0.27	0/2858	0.29	0/4455
5	SB	0.15	0/1832	0.29	0/2449
6	SA	0.15	0/1778	0.29	0/2416
7	SD	0.12	0/1784	0.28	0/2403
8	SJ	0.13	0/1550	0.28	0/2069
9	SE	0.13	0/2118	0.30	0/2849
10	SC	0.22	0/1762	0.41	1/2381 (0.0%)
11	SG	0.13	0/1946	0.27	0/2590
12	SF	0.29	0/1515	0.52	1/2037 (0.0%)
13	SH	0.26	0/1540	0.44	0/2064
14	SW	0.17	0/1051	0.36	0/1406
15	SI	0.19	0/1715	0.36	0/2287
16	SQ	0.13	0/1141	0.32	0/1528
17	SU	0.24	0/813	0.47	0/1092
18	SK	0.13	0/834	0.33	0/1125
19	SO	0.16	0/1022	0.33	0/1372
20	SX	0.14	0/1096	0.27	0/1461
21	SM	0.17	0/960	0.53	0/1286
22	SS	0.15	0/1232	0.32	0/1651
23	Sd	0.12	0/469	0.27	0/623
24	SN	0.15	0/1242	0.26	0/1671
25	SL	0.19	0/1221	0.30	0/1632
26	SR	0.16	0/1097	0.43	1/1474 (0.1%)
27	SP	0.19	0/1100	0.36	0/1470
28	ST	0.14	0/1148	0.36	0/1540
29	SV	0.14	0/635	0.27	0/850
30	SY	0.11	0/1083	0.27	0/1438
31	SZ	0.11	0/682	0.29	0/911

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sa	0.18	0/816	0.32	0/1093
33	Sb	0.15	0/665	0.32	0/891
34	Sc	0.14	0/514	0.31	0/688
35	Se	0.10	0/396	0.27	0/519
36	Sf	0.12	0/525	0.36	0/695
37	Sg	0.12	0/2493	0.34	0/3394
38	LA	0.23	0/1958	0.39	0/2623
39	LB	0.23	0/3294	0.34	0/4406
40	LC	0.23	0/2968	0.34	0/3985
41	LJ	0.18	0/1385	0.32	0/1852
42	LH	0.23	0/1537	0.34	0/2066
43	LE	0.19	0/1820	0.32	0/2442
44	LG	0.20	0/1959	0.34	0/2637
45	LO	0.25	0/1686	0.35	0/2257
46	LL	0.20	0/1706	0.33	0/2284
47	LV	0.21	0/1002	0.34	0/1345
48	LM	0.21	0/1142	0.31	0/1527
49	La	0.23	0/1178	0.34	0/1573
50	LN	0.28	0/1745	0.40	1/2338 (0.0%)
51	LI	0.20	0/1683	0.31	0/2247
52	LD	0.19	0/2437	0.31	0/3263
53	LQ	0.24	0/1536	0.37	0/2052
54	LR	0.20	0/1582	0.36	0/2091
55	LS	0.24	0/1500	0.33	0/2013
56	LT	0.25	0/1345	0.39	0/1795
57	LP	0.31	0/1279	0.47	2/1716 (0.1%)
58	LU	0.21	0/822	0.39	0/1103
59	LX	0.21	0/983	0.33	0/1323
60	LY	0.21	0/1132	0.32	0/1504
61	LW	0.19	0/964	0.34	0/1278
62	LZ	0.20	0/1141	0.29	0/1521
63	Lr	0.23	0/1020	0.32	0/1367
64	Lh	0.20	0/1022	0.27	0/1351
65	Lb	0.19	0/900	0.36	0/1187
66	LF	0.24	0/1926	0.34	0/2567
67	Lc	0.20	0/780	0.35	0/1046
68	Ld	0.21	0/903	0.34	0/1216
69	Le	0.23	0/1082	0.32	0/1443
70	Lf	0.24	0/902	0.32	0/1208
71	Lg	0.21	0/916	0.31	0/1220
72	Li	0.18	0/843	0.28	0/1115
73	Lj	0.24	0/731	0.36	0/967
74	Lk	0.19	0/574	0.32	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Ll	0.23	0/453	0.32	0/599
76	Lm	0.20	0/433	0.31	0/575
77	Ln	0.21	0/240	0.26	0/305
78	Lo	0.22	0/877	0.29	0/1156
79	Lp	0.22	0/728	0.34	0/967
80	mR	0.09	0/192	0.18	0/297
81	Pt	0.27	0/1721	0.30	0/2679
All	All	0.24	0/222284	0.33	6/325873 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	SR	81	ARG	CB-CG-CD	7.09	127.61	111.30
50	LN	123	GLU	CB-CA-C	-5.92	99.20	109.86
57	LP	93[A]	HIS	CA-C-O	5.68	126.57	120.55
57	LP	93[B]	HIS	CA-C-O	5.68	126.57	120.55
10	SC	275	LYS	N-CA-C	-5.16	105.57	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	35736	0	18087	538	0
2	L8	3316	0	1687	39	0
3	L5	76116	0	38517	709	0
4	L7	2558	0	1295	17	0
5	SB	1806	0	1888	25	0
6	SA	1750	0	1755	35	0
7	SD	1756	0	1852	34	0
8	SJ	1525	0	1640	25	0
9	SE	2076	0	2177	31	0
10	SC	1725	0	1813	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	SG	1923	0	2089	52	0
12	SF	1494	0	1549	25	0
13	SH	1517	0	1605	38	0
14	SW	1034	0	1080	11	0
15	SI	1686	0	1772	33	0
16	SQ	1123	0	1193	24	0
17	SU	803	0	873	27	0
18	SK	810	0	836	25	0
19	SO	1009	0	1034	18	0
20	SX	1088	0	1149	13	0
21	SM	950	0	987	35	0
22	SS	1214	0	1275	21	0
23	Sd	458	0	448	8	0
24	SN	1214	0	1300	8	0
25	SL	1200	0	1271	8	0
26	SR	1082	0	1137	34	0
27	SP	1078	0	1121	19	0
28	ST	1121	0	1151	27	0
29	SV	639	0	638	7	0
30	SY	1065	0	1142	30	0
31	SZ	674	0	748	10	0
32	Sa	800	0	854	10	0
33	Sb	651	0	672	8	0
34	Sc	512	0	541	11	0
35	Se	394	0	434	9	0
36	Sf	515	0	521	21	0
37	Sg	2436	0	2393	68	0
38	LA	1930	0	2028	14	0
39	LB	3239	0	3377	25	0
40	LC	2914	0	3087	18	0
41	LJ	1362	0	1399	15	0
42	LH	1518	0	1600	15	0
43	LE	1786	0	1945	16	0
44	LG	1926	0	2074	16	0
45	LO	1654	0	1799	13	0
46	LL	1672	0	1786	16	0
47	LV	988	0	1047	7	0
48	LM	1120	0	1187	9	0
49	La	1162	0	1206	8	0
50	LN	1700	0	1749	20	0
51	LI	1645	0	1693	11	0
52	LD	2391	0	2426	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	LQ	1512	0	1628	3	0
54	LR	1566	0	1728	16	0
55	LS	1460	0	1502	10	0
56	LT	1311	0	1392	16	0
57	LP	1249	0	1276	11	0
58	LU	808	0	831	13	0
59	LX	966	0	1040	6	0
60	LY	1115	0	1205	11	0
61	LW	950	0	999	17	0
62	LZ	1115	0	1195	9	0
63	Lr	1011	0	1085	5	0
64	Lh	1014	0	1148	7	0
65	Lb	898	0	983	10	0
66	LF	1885	0	2022	19	0
67	Lc	770	0	809	10	0
68	Ld	888	0	930	7	0
69	Le	1061	0	1160	10	0
70	Lf	883	0	923	2	0
71	Lg	906	0	998	8	0
72	Li	832	0	917	9	0
73	Lj	712	0	744	3	0
74	Lk	568	0	637	6	0
75	Ll	443	0	482	8	0
76	Lm	436	0	477	4	0
77	Ln	239	0	289	1	0
78	Lo	870	0	936	5	0
79	Lp	715	0	769	0	0
80	mR	172	0	87	4	0
81	Pt	1645	0	843	11	0
82	L5	130	0	246	27	0
82	S2	20	0	38	2	0
83	L5	48	0	96	3	0
83	S2	6	0	12	0	0
84	L5	117	0	0	0	0
84	L7	4	0	0	0	0
84	L8	4	0	0	0	0
84	LA	3	0	0	0	0
84	LH	1	0	0	0	0
84	LI	1	0	0	0	0
84	LL	1	0	0	0	0
84	LN	1	0	0	0	0
84	LQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Lb	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lf	1	0	0	0	0
84	Ll	1	0	0	0	0
84	S2	12	0	0	0	0
84	SL	1	0	0	0	0
84	SO	1	0	0	0	0
84	Sa	1	0	0	0	0
85	L5	463	0	0	0	0
85	L7	15	0	0	0	0
85	L8	16	0	0	0	0
85	LB	1	0	0	0	0
85	LC	1	0	0	0	0
85	LD	1	0	0	0	0
85	LF	1	0	0	0	0
85	LG	1	0	0	0	0
85	LH	1	0	0	0	0
85	LL	1	0	0	0	0
85	LN	3	0	0	0	0
85	LO	2	0	0	0	0
85	LP	2	0	0	0	0
85	LQ	2	0	0	0	0
85	LR	1	0	0	0	0
85	LS	1	0	0	0	0
85	LV	1	0	0	0	0
85	La	1	0	0	0	0
85	Lc	1	0	0	0	0
85	Lf	1	0	0	0	0
85	Lg	1	0	0	0	0
85	Lj	2	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	2	0	0	0	0
85	Lr	3	0	0	0	0
85	Pt	2	0	0	0	0
85	S2	137	0	0	0	0
85	SG	1	0	0	0	0
85	SN	1	0	0	0	0
85	SS	2	0	0	0	0
85	ST	1	0	0	0	0
85	SX	1	0	0	0	0
85	Sd	1	0	0	0	0
86	L5	19	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	L5	33	0	35	2	0
88	L5	16	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	0	0
89	Sf	1	0	0	0	0
90	Pt	8	0	8	2	0
91	L5	5661	0	0	7	0
91	L7	133	0	0	0	0
91	L8	189	0	0	0	0
91	LA	93	0	0	0	0
91	LB	113	0	0	0	0
91	LC	137	0	0	1	0
91	LD	37	0	0	0	0
91	LE	28	0	0	0	0
91	LF	77	0	0	0	0
91	LG	28	0	0	0	0
91	LH	14	0	0	0	0
91	LI	33	0	0	0	0
91	LJ	4	0	0	0	0
91	LL	62	0	0	1	0
91	LM	10	0	0	0	0
91	LN	112	0	0	0	0
91	LO	69	0	0	0	0
91	LP	44	0	0	1	0
91	LQ	81	0	0	0	0
91	LR	34	0	0	0	0
91	LS	51	0	0	1	0
91	LT	58	0	0	1	0
91	LU	1	0	0	0	0
91	LV	25	0	0	0	0
91	LW	8	0	0	0	0
91	LX	15	0	0	0	0
91	LY	23	0	0	0	0
91	LZ	7	0	0	0	0
91	La	71	0	0	0	0
91	Lb	21	0	0	0	0
91	Lc	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	Ld	20	0	0	0	0
91	Le	71	0	0	2	0
91	Lf	45	0	0	0	0
91	Lg	39	0	0	0	0
91	Lh	10	0	0	0	0
91	Li	15	0	0	0	0
91	Lj	36	0	0	0	0
91	Lk	2	0	0	0	0
91	Ll	14	0	0	0	0
91	Lm	8	0	0	0	0
91	Ln	4	0	0	0	0
91	Lo	37	0	0	0	0
91	Lp	24	0	0	0	0
91	Lr	53	0	0	0	0
91	Pt	1	0	0	1	0
91	S2	266	0	0	1	0
91	SA	1	0	0	0	0
91	SE	1	0	0	1	0
91	SF	1	0	0	0	0
91	SL	2	0	0	0	0
91	SN	3	0	0	0	0
91	SO	3	0	0	0	0
91	Sa	4	0	0	0	0
91	Sb	1	0	0	0	0
All	All	220877	0	158440	2229	0

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

The worst 5 of 2229 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)
50:LN:123:GLU:HG2	50:LN:128:LYS:HG2	1.38	1.06
1:S2:394:G:H5"	25:SL:81:LYS:HB3	1.45	0.96
1:S2:928:G:H1	1:S2:1013:U:H3	1.16	0.91
27:SP:28:MET:HE3	27:SP:29:SER:H	1.36	0.89
1:S2:925:G:H1	1:S2:1017:U:H3	1.20	0.88

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
5	SB	219/264 (83%)	217 (99%)	2 (1%)	0	100	100
6	SA	220/295 (75%)	214 (97%)	6 (3%)	0	100	100
7	SD	224/243 (92%)	213 (95%)	11 (5%)	0	100	100
8	SJ	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
9	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
10	SC	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
11	SG	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
12	SF	187/204 (92%)	179 (96%)	6 (3%)	2 (1%)	11	1
13	SH	187/194 (96%)	176 (94%)	9 (5%)	2 (1%)	11	1
14	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
15	SI	204/208 (98%)	198 (97%)	6 (3%)	0	100	100
16	SQ	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
17	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
18	SK	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
19	SO	133/151 (88%)	128 (96%)	4 (3%)	1 (1%)	16	4
20	SX	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
21	SM	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
22	SS	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
23	Sd	53/56 (95%)	53 (100%)	0	0	100	100
24	SN	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
25	SL	142/158 (90%)	139 (98%)	3 (2%)	0	100	100
26	SR	132/135 (98%)	121 (92%)	11 (8%)	0	100	100
27	SP	129/145 (89%)	126 (98%)	3 (2%)	0	100	100
28	ST	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
29	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	SY	129/133 (97%)	126 (98%)	3 (2%)	0	100	100
31	SZ	82/125 (66%)	78 (95%)	4 (5%)	0	100	100
32	Sa	98/115 (85%)	98 (100%)	0	0	100	100
33	Sb	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
34	Sc	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
35	Se	46/133 (35%)	45 (98%)	0	1 (2%)	5	0
36	Sf	61/156 (39%)	53 (87%)	8 (13%)	0	100	100
37	Sg	311/317 (98%)	292 (94%)	19 (6%)	0	100	100
38	LA	249/257 (97%)	240 (96%)	9 (4%)	0	100	100
39	LB	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
40	LC	364/427 (85%)	361 (99%)	3 (1%)	0	100	100
41	LJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
42	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
43	LE	217/288 (75%)	212 (98%)	5 (2%)	0	100	100
44	LG	239/266 (90%)	230 (96%)	9 (4%)	0	100	100
45	LO	200/203 (98%)	199 (100%)	1 (0%)	0	100	100
46	LL	205/211 (97%)	198 (97%)	7 (3%)	0	100	100
47	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
48	LM	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
49	La	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	5
50	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
51	LI	199/214 (93%)	198 (100%)	1 (0%)	0	100	100
52	LD	292/297 (98%)	288 (99%)	4 (1%)	0	100	100
53	LQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
54	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
55	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
56	LT	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
57	LP	152/184 (83%)	150 (99%)	2 (1%)	0	100	100
58	LU	97/128 (76%)	95 (98%)	1 (1%)	1 (1%)	12	2
59	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
60	LY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	LW	114/157 (73%)	109 (96%)	5 (4%)	0	100	100
62	LZ	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
63	Lr	124/137 (90%)	124 (100%)	0	0	100	100
64	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
65	Lb	106/159 (67%)	103 (97%)	3 (3%)	0	100	100
66	LF	225/248 (91%)	219 (97%)	6 (3%)	0	100	100
67	Lc	97/115 (84%)	97 (100%)	0	0	100	100
68	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
69	Le	127/135 (94%)	127 (100%)	0	0	100	100
70	Lf	108/110 (98%)	108 (100%)	0	0	100	100
71	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
72	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
73	Lj	85/97 (88%)	85 (100%)	0	0	100	100
74	Lk	67/70 (96%)	67 (100%)	0	0	100	100
75	Ll	48/51 (94%)	48 (100%)	0	0	100	100
76	Lm	50/128 (39%)	50 (100%)	0	0	100	100
77	Ln	23/25 (92%)	23 (100%)	0	0	100	100
78	Lo	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
79	Lp	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	11301/12762 (89%)	11033 (98%)	260 (2%)	8 (0%)	49	31

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	Se	119	VAL
19	SO	138	ASP
13	SH	18	GLU
12	SF	79	HIS
12	SF	80	GLY

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	
5	SB	202/231 (87%)	197 (98%)	5 (2%)	42	16
6	SA	183/242 (76%)	182 (100%)	1 (0%)	81	72
7	SD	189/202 (94%)	181 (96%)	8 (4%)	26	5
8	SJ	161/168 (96%)	159 (99%)	2 (1%)	63	43
9	SE	224/225 (100%)	219 (98%)	5 (2%)	45	19
10	SC	188/225 (84%)	186 (99%)	2 (1%)	65	47
11	SG	207/218 (95%)	206 (100%)	1 (0%)	81	72
12	SF	159/170 (94%)	152 (96%)	7 (4%)	25	4
13	SH	168/174 (97%)	157 (94%)	11 (6%)	15	1
14	SW	112/113 (99%)	112 (100%)	0	100	100
15	SI	178/180 (99%)	173 (97%)	5 (3%)	38	12
16	SQ	117/121 (97%)	109 (93%)	8 (7%)	14	1
17	SU	93/107 (87%)	90 (97%)	3 (3%)	34	9
18	SK	87/136 (64%)	87 (100%)	0	100	100
19	SO	105/119 (88%)	104 (99%)	1 (1%)	68	52
20	SX	111/114 (97%)	107 (96%)	4 (4%)	31	6
21	SM	104/108 (96%)	99 (95%)	5 (5%)	23	4
22	SS	128/132 (97%)	123 (96%)	5 (4%)	28	6
23	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	21
24	SN	131/131 (100%)	128 (98%)	3 (2%)	44	18
25	SL	132/142 (93%)	131 (99%)	1 (1%)	73	59
26	SR	121/122 (99%)	115 (95%)	6 (5%)	22	3
27	SP	117/130 (90%)	112 (96%)	5 (4%)	26	5
28	ST	114/115 (99%)	109 (96%)	5 (4%)	25	4
29	SV	66/66 (100%)	65 (98%)	1 (2%)	57	34
30	SY	113/115 (98%)	109 (96%)	4 (4%)	32	7
31	SZ	74/103 (72%)	71 (96%)	3 (4%)	27	5
32	Sa	87/98 (89%)	83 (95%)	4 (5%)	24	4
33	Sb	75/76 (99%)	72 (96%)	3 (4%)	28	5
34	Sc	58/62 (94%)	56 (97%)	2 (3%)	32	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Se	40/104 (38%)	40 (100%)	0	100	100
36	Sf	56/140 (40%)	54 (96%)	2 (4%)	31	6
37	Sg	272/275 (99%)	261 (96%)	11 (4%)	28	5
38	LA	193/198 (98%)	192 (100%)	1 (0%)	81	72
39	LB	347/348 (100%)	347 (100%)	0	100	100
40	LC	305/348 (88%)	303 (99%)	2 (1%)	76	62
41	LJ	143/149 (96%)	143 (100%)	0	100	100
42	LH	169/171 (99%)	169 (100%)	0	100	100
43	LE	196/252 (78%)	195 (100%)	1 (0%)	81	72
44	LG	203/223 (91%)	202 (100%)	1 (0%)	81	72
45	LO	173/174 (99%)	173 (100%)	0	100	100
46	LL	173/177 (98%)	172 (99%)	1 (1%)	78	67
47	LV	102/107 (95%)	102 (100%)	0	100	100
48	LM	116/161 (72%)	115 (99%)	1 (1%)	70	55
49	La	119/120 (99%)	119 (100%)	0	100	100
50	LN	171/172 (99%)	169 (99%)	2 (1%)	63	43
51	LI	173/181 (96%)	171 (99%)	2 (1%)	63	43
52	LD	247/250 (99%)	245 (99%)	2 (1%)	73	59
53	LQ	164/165 (99%)	161 (98%)	3 (2%)	51	27
54	LR	166/175 (95%)	164 (99%)	2 (1%)	63	43
55	LS	157/157 (100%)	157 (100%)	0	100	100
56	LT	141/140 (101%)	141 (100%)	0	100	100
57	LP	135/163 (83%)	135 (100%)	0	100	100
58	LU	89/115 (77%)	87 (98%)	2 (2%)	45	19
59	LX	106/133 (80%)	106 (100%)	0	100	100
60	LY	124/135 (92%)	121 (98%)	3 (2%)	43	17
61	LW	95/126 (75%)	93 (98%)	2 (2%)	47	21
62	LZ	118/118 (100%)	117 (99%)	1 (1%)	73	59
63	Lr	109/120 (91%)	109 (100%)	0	100	100
64	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	55
65	Lb	90/125 (72%)	89 (99%)	1 (1%)	65	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	LF	196/215 (91%)	196 (100%)	0	100	100
67	Lc	84/97 (87%)	84 (100%)	0	100	100
68	Ld	98/110 (89%)	98 (100%)	0	100	100
69	Le	115/121 (95%)	115 (100%)	0	100	100
70	Lf	89/89 (100%)	89 (100%)	0	100	100
71	Lg	98/100 (98%)	97 (99%)	1 (1%)	68	52
72	Li	86/89 (97%)	85 (99%)	1 (1%)	63	43
73	Lj	74/80 (92%)	73 (99%)	1 (1%)	59	36
74	Lk	64/65 (98%)	64 (100%)	0	100	100
75	Ll	47/48 (98%)	46 (98%)	1 (2%)	47	21
76	Lm	48/115 (42%)	47 (98%)	1 (2%)	47	21
77	Ln	24/24 (100%)	24 (100%)	0	100	100
78	Lo	93/93 (100%)	92 (99%)	1 (1%)	65	47
79	Lp	75/75 (100%)	75 (100%)	0	100	100
All	All	9844/10847 (91%)	9686 (98%)	158 (2%)	54	32

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	Sg	113	PHE
58	LU	107	LYS
37	Sg	160	SER
48	LM	136	LEU
64	Lh	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
58	LU	94	ASN
69	Le	107	ASN
59	LX	107	HIS
60	LY	96	HIS
28	ST	12	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1667/1869 (89%)	255 (15%)	1 (0%)
2	L8	155/156 (99%)	19 (12%)	0
3	L5	3530/5069 (69%)	504 (14%)	15 (0%)
4	L7	119/120 (99%)	8 (6%)	0
80	mR	7/60 (11%)	3 (42%)	0
81	Pt	76/77 (98%)	8 (10%)	0
All	All	5554/7351 (75%)	797 (14%)	16 (0%)

5 of 797 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C
1	S2	4	C
1	S2	17	C
1	S2	33	G
1	S2	41	G

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4699	U
3	L5	3876	A
3	L5	1754	U
3	L5	2489	C
3	L5	1633	G

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

233 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	OMU	L5	2415	3	19,22,23	1.26	3 (15%)	25,31,34	1.81	5 (20%)
1	PSU	S2	1347	1	18,21,22	1.36	3 (16%)	21,30,33	2.04	4 (19%)
3	A2M	L5	1871	85,3	22,25,26	1.47	5 (22%)	30,36,39	2.17	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3825	3	22,25,26	1.46	5 (22%)	30,36,39	2.09	10 (33%)
3	OMG	L5	3899	3	23,26,27	1.20	4 (17%)	32,38,41	2.02	7 (21%)
3	PSU	L5	3920	85,3	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
1	A2M	S2	468	1	22,25,26	1.49	5 (22%)	30,36,39	2.15	10 (33%)
3	PSU	L5	4423	3	18,21,22	1.41	3 (16%)	21,30,33	2.11	4 (19%)
81	4SU	Pt	8	81	18,21,22	1.83	4 (22%)	25,30,33	2.26	5 (20%)
3	OMC	L5	3808	3	19,22,23	0.77	0	25,31,34	0.72	0
3	OMG	L5	4623	3	23,26,27	1.18	4 (17%)	32,38,41	2.01	6 (18%)
3	A2M	L5	400	3	22,25,26	1.48	5 (22%)	30,36,39	2.01	8 (26%)
3	OMC	L5	2861	3	19,22,23	0.77	0	25,31,34	0.69	0
3	PSU	L5	2508	3	18,21,22	1.37	3 (16%)	21,30,33	2.10	4 (19%)
3	OMU	L5	4620	3	19,22,23	1.28	3 (15%)	25,31,34	1.83	5 (20%)
65	MLZ	Lb	5	84,65	8,9,10	0.83	0	4,9,11	0.68	0
3	A2M	L5	3724	3	22,25,26	1.48	5 (22%)	30,36,39	2.01	8 (26%)
1	OMU	S2	116	1	19,22,23	1.20	3 (15%)	25,31,34	1.79	5 (20%)
1	MA6	S2	1850	1	23,26,27	1.48	4 (17%)	33,38,41	2.09	10 (30%)
1	UY1	S2	1326	85,1	19,22,23	1.33	2 (10%)	21,31,34	2.05	4 (19%)
3	PSU	L5	4312	85,3	18,21,22	1.39	3 (16%)	21,30,33	2.05	4 (19%)
1	A2M	S2	159	1	22,25,26	1.50	4 (18%)	30,36,39	2.11	9 (30%)
3	A2M	L5	2401	85,3	22,25,26	1.46	4 (18%)	30,36,39	2.11	10 (33%)
3	PSU	L5	4579	3	18,21,22	1.40	4 (22%)	21,30,33	2.06	3 (14%)
3	5MC	L5	4447	84,3	19,22,23	1.51	3 (15%)	26,32,35	1.28	2 (7%)
3	PSU	L5	4299	3	18,21,22	1.40	3 (16%)	21,30,33	2.11	4 (19%)
1	PSU	S2	1367	1	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
1	OMC	S2	517	1	19,22,23	0.78	0	25,31,34	0.79	0
1	PSU	S2	1232	1	18,21,22	1.40	2 (11%)	21,30,33	2.07	3 (14%)
3	A2M	L5	1534	85,3	22,25,26	1.49	4 (18%)	30,36,39	2.06	10 (33%)
3	UR3	L5	4530	3	19,22,23	0.92	0	26,32,35	1.97	3 (11%)
3	PSU	L5	4353	3	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
3	PSU	L5	3853	85,84,3	18,21,22	1.40	3 (16%)	21,30,33	2.09	3 (14%)
1	PSU	S2	609	1	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
3	PSU	L5	3729	3	18,21,22	1.39	3 (16%)	21,30,33	2.10	4 (19%)
3	OMG	L5	3792	3	23,26,27	1.21	3 (13%)	32,38,41	1.97	6 (18%)
3	PSU	L5	4552	3	18,21,22	1.40	4 (22%)	21,30,33	2.06	4 (19%)
3	A2M	L5	2815	85,3	22,25,26	1.47	5 (22%)	30,36,39	2.07	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	4392	3	23,26,27	1.21	3 (13%)	32,38,41	2.01	6 (18%)
3	OMU	L5	3925	3	19,22,23	1.29	3 (15%)	25,31,34	1.89	5 (20%)
3	A2M	L5	3785	3	22,25,26	1.46	4 (18%)	30,36,39	2.45	12 (40%)
3	PSU	L5	4532	3	18,21,22	1.50	3 (16%)	21,30,33	2.38	4 (19%)
3	PSU	L5	4403	84,3	18,21,22	1.41	3 (16%)	21,30,33	2.15	5 (23%)
1	PSU	S2	815	1	18,21,22	1.36	3 (16%)	21,30,33	2.05	3 (14%)
3	PSU	L5	4457	3	18,21,22	1.35	3 (16%)	21,30,33	2.17	3 (14%)
3	PSU	L5	4673	85,3	18,21,22	1.41	3 (16%)	21,30,33	2.14	3 (14%)
1	PSU	S2	1243	1	18,21,22	1.39	3 (16%)	21,30,33	2.06	4 (19%)
1	PSU	S2	966	1	18,21,22	1.38	3 (16%)	21,30,33	2.03	3 (14%)
20	HY3	SX	62	20	7,8,9	1.27	1 (14%)	7,10,12	1.61	2 (28%)
3	UY1	L5	3818	84,3	19,22,23	1.40	4 (21%)	21,31,34	2.23	4 (19%)
3	OMC	L5	2804	3	19,22,23	0.77	0	25,31,34	0.65	0
63	SAC	Lr	2	63	7,8,9	3.86	2 (28%)	7,9,11	4.05	3 (42%)
1	OMU	S2	172	1	19,22,23	1.23	2 (10%)	25,31,34	1.87	5 (20%)
1	A2M	S2	512	1	22,25,26	1.47	4 (18%)	30,36,39	2.18	9 (30%)
3	PSU	L5	2632	3	18,21,22	1.42	4 (22%)	21,30,33	1.99	3 (14%)
3	PSU	L5	4293	3	18,21,22	1.36	3 (16%)	21,30,33	2.06	4 (19%)
76	M3L	Lm	98	76	10,11,12	0.52	0	9,14,16	0.46	0
1	PSU	S2	1056	1	18,21,22	1.36	3 (16%)	21,30,33	2.10	4 (19%)
1	PSU	S2	1625	1	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
3	OMG	L5	1316	3	23,26,27	1.21	4 (17%)	32,38,41	1.90	5 (15%)
3	OMC	L5	4536	3	19,22,23	0.76	0	25,31,34	0.82	0
6	SAC	SA	2	6	7,8,9	3.84	2 (28%)	7,9,11	4.38	3 (42%)
1	OMG	S2	683	1	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
1	OMG	S2	436	1	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
1	PSU	S2	1445	1	18,21,22	1.35	2 (11%)	21,30,33	2.11	5 (23%)
1	4AC	S2	1842	1	21,24,25	0.98	1 (4%)	28,34,37	1.15	3 (10%)
2	OMU	L8	14	84,3,2	19,22,23	1.27	3 (15%)	25,31,34	1.76	5 (20%)
1	PSU	S2	105	1	18,21,22	1.39	3 (16%)	21,30,33	2.08	4 (19%)
1	PSU	S2	572	1	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
1	OMC	S2	462	1	19,22,23	0.86	0	25,31,34	0.99	1 (4%)
3	A2M	L5	4571	3	22,25,26	1.50	5 (22%)	30,36,39	2.00	8 (26%)
1	A2M	S2	1031	1	22,25,26	1.48	5 (22%)	30,36,39	2.08	10 (33%)
3	PSU	L5	4628	3	18,21,22	1.40	4 (22%)	21,30,33	1.99	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	S2	1639	81,1	23,26,27	2.37	5 (21%)	34,39,42	3.03	10 (29%)
3	OMG	L5	3944	3	23,26,27	1.18	3 (13%)	32,38,41	2.01	6 (18%)
38	V5N	LA	216	38	8,11,12	1.46	1 (12%)	8,14,16	1.76	2 (25%)
1	PSU	S2	651	1	18,21,22	1.37	3 (16%)	21,30,33	2.07	4 (19%)
2	PSU	L8	55	2	18,21,22	1.39	3 (16%)	21,30,33	2.05	4 (19%)
1	A2M	S2	99	85,1	22,25,26	1.48	4 (18%)	30,36,39	2.09	8 (26%)
1	OMU	S2	121	1	19,22,23	1.23	3 (15%)	25,31,34	1.82	5 (20%)
1	PSU	S2	863	1	18,21,22	1.39	3 (16%)	21,30,33	2.09	3 (14%)
3	OMG	L5	3744	3	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
3	PSU	L5	4420	3	18,21,22	1.47	4 (22%)	21,30,33	2.01	3 (14%)
2	PSU	L8	69	85,2	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)
1	PSU	S2	686	1	18,21,22	1.38	2 (11%)	21,30,33	2.09	4 (19%)
1	4AC	S2	1337	1	21,24,25	1.05	1 (4%)	28,34,37	1.04	2 (7%)
3	A2M	L5	1326	3	22,25,26	1.51	4 (18%)	30,36,39	1.96	7 (23%)
3	PSU	L5	1744	84,3	18,21,22	1.41	3 (16%)	21,30,33	2.03	3 (14%)
1	PSU	S2	119	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	4 (19%)
1	PSU	S2	34	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
3	PSU	L5	3695	84,3	18,21,22	1.39	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.40	3 (16%)	21,30,33	2.04	4 (19%)
3	OMG	L5	4637	84,3	23,26,27	1.20	3 (13%)	32,38,41	1.93	6 (18%)
1	PSU	S2	573	1	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
3	OMC	L5	3887	85,3	19,22,23	0.79	0	25,31,34	0.80	0
3	OMG	L5	2424	3	23,26,27	1.21	3 (13%)	32,38,41	1.93	6 (18%)
3	PSU	L5	4569	3	18,21,22	1.42	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	1536	3	18,21,22	1.44	3 (16%)	21,30,33	2.13	3 (14%)
1	A2M	S2	484	1	22,25,26	1.49	4 (18%)	30,36,39	2.11	8 (26%)
1	PSU	S2	918	1	18,21,22	1.44	3 (16%)	21,30,33	2.02	3 (14%)
1	PSU	S2	814	1	18,21,22	1.37	3 (16%)	21,30,33	2.00	3 (14%)
1	PSU	S2	296	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
1	PSU	S2	1244	1	18,21,22	1.37	2 (11%)	21,30,33	2.11	4 (19%)
1	PSU	S2	1238	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	4 (19%)
3	OMC	L5	3869	3	19,22,23	0.78	0	25,31,34	0.77	0
3	OMG	L5	1625	84,3	23,26,27	1.21	3 (13%)	32,38,41	1.97	6 (18%)
1	PSU	S2	218	1	18,21,22	1.37	3 (16%)	21,30,33	2.03	4 (19%)
1	PSU	S2	866	1	18,21,22	1.37	2 (11%)	21,30,33	2.10	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	S2	1391	1	19,22,23	0.80	0	25,31,34	0.80	0
1	A2M	S2	590	1	22,25,26	1.51	4 (18%)	30,36,39	2.08	7 (23%)
3	OMC	L5	2422	85,3	19,22,23	0.79	0	25,31,34	0.69	0
3	1MA	L5	1322	85,3	21,25,26	1.32	4 (19%)	30,37,40	1.66	5 (16%)
1	PSU	S2	1174	85,1	18,21,22	1.40	3 (16%)	21,30,33	2.05	4 (19%)
1	OMG	S2	644	1	23,26,27	1.19	3 (13%)	32,38,41	2.00	6 (18%)
1	OMU	S2	1442	85,1	19,22,23	1.23	3 (15%)	25,31,34	1.80	5 (20%)
3	OMG	L5	2364	3	23,26,27	1.20	4 (17%)	32,38,41	1.92	6 (18%)
3	A2M	L5	3718	3	22,25,26	1.50	5 (22%)	30,36,39	1.94	8 (26%)
3	OMU	L5	4227	3	19,22,23	1.26	3 (15%)	25,31,34	1.89	5 (20%)
3	PSU	L5	4531	3	18,21,22	1.33	3 (16%)	21,30,33	2.15	5 (23%)
3	PSU	L5	3768	3	18,21,22	1.37	3 (16%)	21,30,33	2.08	4 (19%)
1	PSU	S2	1004	1	18,21,22	1.37	2 (11%)	21,30,33	2.06	3 (14%)
3	OMU	L5	2837	3	19,22,23	1.27	3 (15%)	25,31,34	1.89	5 (20%)
3	OMG	L5	4618	84,3	23,26,27	1.18	4 (17%)	32,38,41	2.00	6 (18%)
3	PSU	L5	1860	3	18,21,22	1.43	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.40	3 (16%)	21,30,33	1.92	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.43	3 (16%)	21,30,33	2.14	4 (19%)
3	PSU	L5	5001	85,3	18,21,22	1.44	4 (22%)	21,30,33	2.03	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.43	3 (16%)	21,30,33	2.05	4 (19%)
3	OMU	L5	4498	84,3	19,22,23	1.26	3 (15%)	25,31,34	1.81	5 (20%)
3	A2M	L5	3760	85,3	22,25,26	1.52	4 (18%)	30,36,39	2.07	7 (23%)
3	OMU	L5	4306	3	19,22,23	1.28	3 (15%)	25,31,34	1.76	4 (16%)
1	OMU	S2	428	1	19,22,23	1.21	3 (15%)	25,31,34	1.83	5 (20%)
1	PSU	S2	36	1	18,21,22	1.37	3 (16%)	21,30,33	2.08	4 (19%)
1	A2M	S2	576	1	22,25,26	1.50	4 (18%)	30,36,39	2.20	10 (33%)
1	PSU	S2	1692	1	18,21,22	1.40	3 (16%)	21,30,33	2.08	4 (19%)
81	OMC	Pt	33	81	19,22,23	0.78	0	25,31,34	0.77	0
81	PSU	Pt	56	81	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
3	PSU	L5	2839	3	18,21,22	1.43	3 (16%)	21,30,33	2.15	4 (19%)
1	OMG	S2	601	1	23,26,27	1.19	3 (13%)	32,38,41	1.95	6 (18%)
3	PSU	L5	3715	3	18,21,22	1.37	3 (16%)	21,30,33	2.09	5 (23%)
3	PSU	L5	2843	3	18,21,22	1.38	3 (16%)	21,30,33	2.06	5 (23%)
3	5MC	L5	3782	85,3	19,22,23	1.51	3 (15%)	26,32,35	1.15	2 (7%)
81	G7M	Pt	47	81	23,26,27	1.88	2 (8%)	34,39,42	1.07	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	L8	75	2	23,26,27	1.18	3 (13%)	32,38,41	1.97	6 (18%)
3	PSU	L5	3639	3	18,21,22	1.42	3 (16%)	21,30,33	2.05	3 (14%)
1	OMG	S2	1328	1	23,26,27	1.19	3 (13%)	32,38,41	1.96	6 (18%)
3	A2M	L5	1524	3	22,25,26	1.49	4 (18%)	30,36,39	2.03	10 (33%)
1	PSU	S2	1643	85,1	18,21,22	1.40	3 (16%)	21,30,33	2.06	5 (23%)
1	PSU	S2	1239	1	18,21,22	1.37	3 (16%)	21,30,33	2.05	4 (19%)
3	A2M	L5	3723	3	22,25,26	1.49	5 (22%)	30,36,39	2.05	9 (30%)
78	MLZ	Lo	53	78	8,9,10	0.76	0	4,9,11	0.63	0
1	PSU	S2	801	1	18,21,22	1.35	3 (16%)	21,30,33	2.05	4 (19%)
3	A2M	L5	398	3	22,25,26	1.49	4 (18%)	30,36,39	2.11	9 (30%)
3	PSU	L5	4972	84,3	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
3	PSU	L5	4521	85,84,3	18,21,22	1.43	3 (16%)	21,30,33	2.10	5 (23%)
3	PSU	L5	3851	3	18,21,22	1.43	3 (16%)	21,30,33	2.07	4 (19%)
3	6MZ	L5	4220	3	22,25,26	1.44	4 (18%)	29,36,39	2.12	10 (34%)
3	PSU	L5	4576	3	18,21,22	1.39	3 (16%)	21,30,33	2.09	3 (14%)
3	PSU	L5	1862	3	18,21,22	1.38	3 (16%)	21,30,33	2.14	4 (19%)
3	PSU	L5	3758	3	18,21,22	1.38	3 (16%)	21,30,33	2.05	4 (19%)
1	A2M	S2	166	1	22,25,26	1.49	4 (18%)	30,36,39	2.16	10 (33%)
49	V5N	La	39	49	8,11,12	1.51	1 (12%)	8,14,16	1.70	2 (25%)
1	MA6	S2	1851	85,1	23,26,27	1.46	5 (21%)	33,38,41	2.12	10 (30%)
1	PSU	S2	1177	1	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
1	A2M	S2	1383	1	22,25,26	1.46	4 (18%)	30,36,39	2.25	10 (33%)
1	A2M	S2	27	85,1	22,25,26	1.49	4 (18%)	30,36,39	2.08	9 (30%)
3	OMC	L5	4456	3	19,22,23	0.79	0	25,31,34	0.77	1 (4%)
1	A2M	S2	1678	1	22,25,26	1.51	4 (18%)	30,36,39	2.06	8 (26%)
1	OMG	S2	1490	85,1	23,26,27	1.20	3 (13%)	32,38,41	1.94	6 (18%)
3	PSU	L5	1779	3	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
3	PSU	L5	3844	3	18,21,22	1.46	3 (16%)	21,30,33	2.07	3 (14%)
3	PSU	L5	1781	3	18,21,22	1.38	3 (16%)	21,30,33	2.04	4 (19%)
3	OMC	L5	2365	85,3	19,22,23	0.76	0	25,31,34	0.77	0
1	B8N	S2	1248	1	25,29,30	0.90	1 (4%)	28,42,45	1.68	6 (21%)
3	PSU	L5	1582	3	18,21,22	1.43	3 (16%)	21,30,33	2.09	4 (19%)
3	OMG	L5	1522	3	23,26,27	1.19	4 (17%)	32,38,41	2.04	8 (25%)
3	OMG	L5	4499	3	23,26,27	1.20	3 (13%)	32,38,41	1.96	6 (18%)
3	A2M	L5	3867	3	22,25,26	1.51	4 (18%)	30,36,39	2.04	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3762	3	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
3	OMG	L5	4370	3	23,26,27	1.22	3 (13%)	32,38,41	1.97	6 (18%)
3	OMC	L5	1340	3	19,22,23	0.76	0	25,31,34	0.73	0
1	PSU	S2	109	1	18,21,22	1.37	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	1677	3	18,21,22	1.44	4 (22%)	21,30,33	2.09	4 (19%)
3	PSU	L5	3770	3	18,21,22	1.54	5 (27%)	21,30,33	2.17	5 (23%)
3	PSU	L5	4493	84,3	18,21,22	1.43	3 (16%)	21,30,33	2.07	4 (19%)
1	PSU	S2	1081	1	18,21,22	1.45	4 (22%)	21,30,33	2.05	4 (19%)
3	PSU	L5	1782	3	18,21,22	1.40	3 (16%)	21,30,33	2.07	4 (19%)
1	OMU	S2	354	1	19,22,23	1.26	3 (15%)	25,31,34	1.86	5 (20%)
1	6MZ	S2	1832	85,84,1	22,25,26	1.50	4 (18%)	29,36,39	2.10	9 (31%)
3	OMC	L5	2824	3	19,22,23	0.78	0	25,31,34	0.78	0
3	PSU	L5	4689	3	18,21,22	1.40	3 (16%)	21,30,33	2.07	3 (14%)
1	PSU	S2	649	1	18,21,22	1.38	3 (16%)	21,30,33	2.09	4 (19%)
1	OMU	S2	1288	1	19,22,23	1.27	4 (21%)	25,31,34	1.76	5 (20%)
3	OMG	L5	2876	3	23,26,27	1.21	3 (13%)	32,38,41	1.99	6 (18%)
81	H2U	Pt	21	81	18,21,22	0.96	2 (11%)	19,30,33	1.00	1 (5%)
3	PSU	L5	4636	85,3	18,21,22	1.43	3 (16%)	21,30,33	2.04	4 (19%)
1	OMC	S2	174	85,1	19,22,23	0.78	0	25,31,34	0.82	0
3	PSU	L5	3764	85,3	18,21,22	1.39	3 (16%)	21,30,33	2.07	4 (19%)
3	PSU	L5	4442	3	18,21,22	1.39	3 (16%)	21,30,33	2.13	5 (23%)
3	OMC	L5	2351	85,3	19,22,23	0.79	0	25,31,34	0.98	1 (4%)
1	PSU	S2	1136	1	18,21,22	1.37	3 (16%)	21,30,33	2.07	4 (19%)
3	PSU	L5	1792	84,3	18,21,22	1.36	3 (16%)	21,30,33	2.09	4 (19%)
3	OMG	L5	4494	85,3	23,26,27	1.20	3 (13%)	32,38,41	2.01	6 (18%)
1	OMG	S2	509	85,1	23,26,27	1.21	3 (13%)	32,38,41	1.99	6 (18%)
1	OMC	S2	1703	85,1	19,22,23	0.77	0	25,31,34	0.72	0
29	AME	SV	1	29	9,10,11	3.40	2 (22%)	9,11,13	3.64	3 (33%)
1	OMU	S2	1804	1	19,22,23	1.23	3 (15%)	25,31,34	1.85	5 (20%)
3	OMC	L5	3701	84,3	19,22,23	0.79	0	25,31,34	0.88	0
3	OMC	L5	3841	3	19,22,23	0.77	0	25,31,34	0.67	0
3	A2M	L5	4590	3	22,25,26	1.49	5 (22%)	30,36,39	2.11	11 (36%)
1	A2M	S2	668	85,1	22,25,26	1.46	5 (22%)	30,36,39	2.03	10 (33%)
1	PSU	S2	406	1	18,21,22	1.39	3 (16%)	21,30,33	2.09	4 (19%)
1	PSU	S2	681	1	18,21,22	1.42	3 (16%)	21,30,33	2.07	4 (19%)
3	OMG	L5	4196	81,3	23,26,27	1.21	3 (13%)	32,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3830	3	22,25,26	1.49	5 (22%)	30,36,39	2.13	8 (26%)
3	PSU	L5	4471	85,3	18,21,22	1.41	3 (16%)	21,30,33	2.11	5 (23%)
3	PSU	L5	3637	84,3	18,21,22	1.43	3 (16%)	21,30,33	2.11	5 (23%)
3	PSU	L5	1683	84,3	18,21,22	1.44	4 (22%)	21,30,33	2.16	4 (19%)
1	OMG	S2	867	1	23,26,27	1.17	3 (13%)	32,38,41	1.95	6 (18%)
1	PSU	S2	93	1	18,21,22	1.39	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	3734	3	18,21,22	1.36	3 (16%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4500	85,3	18,21,22	1.38	2 (11%)	21,30,33	2.15	3 (14%)
3	OMG	L5	3627	3	23,26,27	1.19	4 (17%)	32,38,41	2.04	7 (21%)
3	A2M	L5	2363	85,3	22,25,26	1.49	5 (22%)	30,36,39	2.01	9 (30%)
3	PSU	L5	5010	3	18,21,22	1.38	3 (16%)	21,30,33	2.06	4 (19%)
3	A2M	L5	2787	85,3	22,25,26	1.50	3 (13%)	30,36,39	2.10	8 (26%)
3	A2M	L5	4523	85,3	22,25,26	1.48	5 (22%)	30,36,39	2.15	9 (30%)
39	HIC	LB	245	39	10,11,12	1.39	1 (10%)	9,14,16	1.32	2 (22%)
1	OMU	S2	627	1	19,22,23	1.20	3 (15%)	25,31,34	1.83	5 (20%)
1	PSU	S2	822	1	18,21,22	1.39	3 (16%)	21,30,33	2.11	5 (23%)
3	OMG	L5	4228	3	23,26,27	1.18	4 (17%)	32,38,41	1.98	6 (18%)
3	OMC	L5	1881	85,3	19,22,23	0.78	0	25,31,34	0.94	0
1	OMG	S2	1447	1	23,26,27	1.21	3 (13%)	32,38,41	2.00	6 (18%)

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	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	85,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3920	85,3	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
81	4SU	Pt	8	81	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
65	MLZ	Lb	5	84,65	-	1/7/8/10	-
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	1/9/27/28	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
1	UY1	S2	1326	85,1	-	2/9/27/28	0/2/2/2
3	PSU	L5	4312	85,3	-	0/7/25/26	0/2/2/2
1	A2M	S2	159	1	-	1/9/27/28	0/3/3/3
3	A2M	L5	2401	85,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	84,3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	85,3	-	1/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	85,84,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	85,3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3785	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	84,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	85,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
3	UY1	L5	3818	84,3	-	2/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
63	SAC	Lr	2	63	-	2/7/8/10	-
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	512	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
76	M3L	Lm	98	76	-	0/9/10/12	-
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
6	SAC	SA	2	6	-	5/7/8/10	-
1	OMG	S2	683	1	-	1/9/27/28	0/3/3/3
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
2	OMU	L8	14	84,3,2	-	1/9/27/28	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
1	G7M	S2	1639	81,1	-	0/7/25/26	0/3/3/3
3	OMG	L5	3944	3	-	1/9/27/28	0/3/3/3
38	V5N	LA	216	38	-	1/9/10/12	0/1/1/1
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
1	A2M	S2	99	85,1	-	0/9/27/28	0/3/3/3
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4420	3	-	3/7/25/26	0/2/2/2
2	PSU	L8	69	85,2	-	0/7/25/26	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
3	A2M	L5	1326	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1744	84,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	84,3	-	1/9/27/28	0/3/3/3
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	85,3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	918	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	1625	84,3	-	1/9/27/28	0/3/3/3
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	590	1	-	4/9/27/28	0/3/3/3
3	OMC	L5	2422	85,3	-	2/9/27/28	0/2/2/2
3	1MA	L5	1322	85,3	-	2/7/25/26	0/3/3/3
1	PSU	S2	1174	85,1	-	0/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
1	OMU	S2	1442	85,1	-	2/9/27/28	0/2/2/2
3	OMG	L5	2364	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4531	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4618	84,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	84,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3760	85,3	-	2/9/27/28	0/3/3/3
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	OMC	Pt	33	81	-	0/9/27/28	0/2/2/2
81	PSU	Pt	56	81	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	85,3	-	0/7/25/26	0/2/2/2
81	G7M	Pt	47	81	-	0/7/25/26	0/3/3/3
2	OMG	L8	75	2	-	0/9/27/28	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	1328	1	-	1/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	1643	85,1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
78	MLZ	Lo	53	78	-	1/7/8/10	-
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4972	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	85,84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
49	V5N	La	39	49	-	0/9/10/12	0/1/1/1
1	MA6	S2	1851	85,1	-	3/11/29/30	0/3/3/3
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	27	85,1	-	1/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	OMG	S2	1490	85,1	-	3/9/27/28	0/3/3/3
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	2365	85,3	-	0/9/27/28	0/2/2/2
1	B8N	S2	1248	1	-	1/16/34/35	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3867	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	84,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
1	6MZ	S2	1832	85,84,1	-	0/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1288	1	-	2/9/27/28	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
81	H2U	Pt	21	81	-	2/7/38/39	0/2/2/2
3	PSU	L5	4636	85,3	-	2/7/25/26	0/2/2/2
1	OMC	S2	174	85,1	-	0/9/27/28	0/2/2/2
3	PSU	L5	3764	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	85,3	-	2/9/27/28	0/2/2/2
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	84,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	85,3	-	1/9/27/28	0/3/3/3
1	OMG	S2	509	85,1	-	0/9/27/28	0/3/3/3
1	OMC	S2	1703	85,1	-	0/9/27/28	0/2/2/2
29	AME	SV	1	29	-	1/9/10/12	-
1	OMU	S2	1804	1	-	1/9/27/28	0/2/2/2
3	OMC	L5	3701	84,3	-	4/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	668	85,1	-	4/9/27/28	0/3/3/3
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	81,3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4471	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	84,3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	85,3	-	1/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	85,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	85,3	-	3/9/27/28	0/3/3/3
3	A2M	L5	4523	85,3	-	0/9/27/28	0/3/3/3
39	HIC	LB	245	39	-	0/5/6/8	0/1/1/1
1	OMU	S2	627	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1881	85,3	-	0/9/27/28	0/2/2/2
1	OMG	S2	1447	1	-	2/9/27/28	0/3/3/3

The worst 5 of 663 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	Lr	2	SAC	OAC-C1A	9.06	1.43	1.23
6	SA	2	SAC	OAC-C1A	9.05	1.43	1.23
29	SV	1	AME	OT-CT1	9.01	1.43	1.23
81	Pt	47	G7M	C8-N7	7.50	1.45	1.33
1	S2	1639	G7M	C8-N7	7.48	1.45	1.33

The worst 5 of 1085 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1639	G7M	CN7-N7-C8	-8.02	112.64	124.79
6	SA	2	SAC	OAC-C1A-C2A	-7.95	107.89	122.05
3	L5	4530	UR3	C4-N3-C2	-7.75	118.34	124.58
3	L5	4532	PSU	N1-C2-N3	7.59	123.17	115.17
63	Lr	2	SAC	OAC-C1A-N	-7.20	109.27	121.98

There are no chirality outliers.

5 of 128 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L8	14	OMU	C1'-C2'-O2'-CM2
6	SA	2	SAC	OAC-C1A-N-CA
6	SA	2	SAC	CB-CA-N-C1A

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Mol	Chain	Res	Type	Atoms
6	SA	2	SAC	O-C-CA-CB
29	SV	1	AME	OT-CT1-N-CA

There are no ring outliers.

88 monomers are involved in 120 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2415	OMU	2	0
1	S2	1347	PSU	1	0
3	L5	1871	A2M	1	0
1	S2	468	A2M	2	0
81	Pt	8	4SU	1	0
3	L5	4620	OMU	1	0
3	L5	3724	A2M	2	0
1	S2	116	OMU	2	0
1	S2	159	A2M	3	0
3	L5	4579	PSU	1	0
3	L5	4447	5MC	1	0
1	S2	1232	PSU	1	0
3	L5	4530	UR3	2	0
3	L5	2815	A2M	1	0
3	L5	4392	OMG	1	0
3	L5	3925	OMU	1	0
3	L5	3785	A2M	1	0
1	S2	815	PSU	1	0
3	L5	4457	PSU	1	0
3	L5	3818	UY1	1	0
63	Lr	2	SAC	1	0
1	S2	512	A2M	2	0
3	L5	2632	PSU	1	0
3	L5	4536	OMC	1	0
6	SA	2	SAC	2	0
1	S2	683	OMG	1	0
1	S2	436	OMG	2	0
1	S2	1445	PSU	1	0
2	L8	14	OMU	1	0
1	S2	462	OMC	2	0
1	S2	1031	A2M	1	0
3	L5	4628	PSU	1	0
3	L5	3944	OMG	1	0
1	S2	99	A2M	2	0
1	S2	1337	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1326	A2M	1	0
1	S2	119	PSU	1	0
3	L5	4637	OMG	3	0
1	S2	573	PSU	1	0
3	L5	3887	OMC	4	0
3	L5	2424	OMG	1	0
1	S2	484	A2M	1	0
1	S2	918	PSU	2	0
1	S2	814	PSU	1	0
3	L5	3869	OMC	5	0
1	S2	1391	OMC	1	0
1	S2	644	OMG	1	0
1	S2	1442	OMU	1	0
3	L5	2364	OMG	1	0
3	L5	3718	A2M	3	0
3	L5	4531	PSU	2	0
3	L5	4618	OMG	1	0
3	L5	5001	PSU	1	0
3	L5	4306	OMU	1	0
1	S2	576	A2M	3	0
1	S2	1692	PSU	1	0
1	S2	601	OMG	1	0
2	L8	75	OMG	1	0
1	S2	1643	PSU	1	0
1	S2	1239	PSU	1	0
3	L5	3723	A2M	3	0
3	L5	398	A2M	1	0
3	L5	4521	PSU	1	0
3	L5	4220	6MZ	1	0
1	S2	1851	MA6	1	0
1	S2	1383	A2M	1	0
3	L5	4456	OMC	1	0
1	S2	1678	A2M	3	0
1	S2	1490	OMG	2	0
1	S2	1248	B8N	1	0
3	L5	3867	A2M	2	0
3	L5	1340	OMC	2	0
3	L5	1677	PSU	1	0
3	L5	3770	PSU	1	0
1	S2	354	OMU	1	0
1	S2	1288	OMU	2	0
3	L5	2876	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4636	PSU	2	0
1	S2	174	OMC	1	0
3	L5	2351	OMC	1	0
1	S2	509	OMG	1	0
1	S2	1804	OMU	1	0
3	L5	3701	OMC	1	0
1	S2	681	PSU	1	0
1	S2	867	OMG	2	0
3	L5	3734	PSU	1	0
3	L5	1881	OMC	2	0
1	S2	1447	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 860 ligands modelled in this entry, 831 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	$\# Z > 2$
83	PUT	L5	5121	-	5,5,5	0.14	0	4,4,4	0.23	0
82	SPD	L5	5111	-	9,9,9	0.14	0	8,8,8	0.21	0
82	SPD	L5	5104	-	9,9,9	0.15	0	8,8,8	0.31	0
83	PUT	L5	5119	-	5,5,5	0.08	0	4,4,4	0.13	0
86	ANM	L5	5101	84	20,20,20	1.18	1 (5%)	24,27,27	1.32	2 (8%)
88	TRS	L5	5124	-	7,7,7	0.39	0	9,9,9	0.59	0
82	SPD	L5	5107	-	9,9,9	0.31	0	8,8,8	0.91	0
82	SPD	L5	5105	-	9,9,9	0.18	0	8,8,8	0.26	0
83	PUT	L5	5116	-	5,5,5	0.08	0	4,4,4	0.14	0
87	3H3	L5	5102	-	34,34,34	3.49	12 (35%)	36,45,45	3.81	16 (44%)
82	SPD	L5	5114	-	9,9,9	0.18	0	8,8,8	0.30	0
90	MET	Pt	78	81	6,7,8	0.66	0	2,7,9	1.91	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	SPD	L5	5113	-	9,9,9	0.15	0	8,8,8	0.21	0
83	PUT	L5	5117	-	5,5,5	0.08	0	4,4,4	0.12	0
82	SPD	L5	5103	-	9,9,9	0.30	0	8,8,8	0.83	0
82	SPD	S2	1902	-	9,9,9	0.32	0	8,8,8	0.76	0
83	PUT	S2	1903	-	5,5,5	0.10	0	4,4,4	0.12	0
82	SPD	S2	1901	-	9,9,9	0.32	0	8,8,8	0.75	0
83	PUT	L5	5118	-	5,5,5	0.08	0	4,4,4	0.15	0
82	SPD	L5	5115	-	9,9,9	0.19	0	8,8,8	0.26	0
83	PUT	L5	5123	-	5,5,5	0.12	0	4,4,4	0.13	0
82	SPD	L5	5112	-	9,9,9	0.18	0	8,8,8	0.27	0
83	PUT	L5	5122	-	5,5,5	0.10	0	4,4,4	0.13	0
82	SPD	L5	5108	-	9,9,9	0.32	0	8,8,8	1.00	0
82	SPD	L5	5106	-	9,9,9	0.21	0	8,8,8	0.24	0
82	SPD	L5	5110	-	9,9,9	0.32	0	8,8,8	0.97	0
88	TRS	L5	5125	-	7,7,7	0.09	0	9,9,9	0.28	0
82	SPD	L5	5109	-	9,9,9	0.15	0	8,8,8	0.24	0
83	PUT	L5	5120	-	5,5,5	0.10	0	4,4,4	0.12	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
83	PUT	L5	5121	-	-	1/3/3/3	-
82	SPD	L5	5111	-	-	3/7/7/7	-
82	SPD	L5	5104	-	-	4/7/7/7	-
83	PUT	L5	5119	-	-	1/3/3/3	-
86	ANM	L5	5101	84	-	0/10/23/23	0/2/2/2
88	TRS	L5	5124	-	-	0/9/9/9	-
82	SPD	L5	5107	-	-	3/7/7/7	-
82	SPD	L5	5105	-	-	5/7/7/7	-
83	PUT	L5	5116	-	-	0/3/3/3	-
87	3H3	L5	5102	-	-	14/39/51/51	0/1/2/2
82	SPD	L5	5114	-	-	5/7/7/7	-
90	MET	Pt	78	81	-	4/5/6/8	-
82	SPD	L5	5113	-	-	6/7/7/7	-
83	PUT	L5	5117	-	-	1/3/3/3	-
82	SPD	L5	5103	-	-	0/7/7/7	-
82	SPD	S2	1902	-	-	5/7/7/7	-
83	PUT	S2	1903	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	SPD	S2	1901	-	-	2/7/7/7	-
83	PUT	L5	5118	-	-	0/3/3/3	-
82	SPD	L5	5115	-	-	1/7/7/7	-
83	PUT	L5	5123	-	-	0/3/3/3	-
82	SPD	L5	5112	-	-	5/7/7/7	-
83	PUT	L5	5122	-	-	0/3/3/3	-
82	SPD	L5	5108	-	-	4/7/7/7	-
82	SPD	L5	5106	-	-	2/7/7/7	-
82	SPD	L5	5110	-	-	3/7/7/7	-
88	TRS	L5	5125	-	-	6/9/9/9	-
82	SPD	L5	5109	-	-	4/7/7/7	-
83	PUT	L5	5120	-	-	1/3/3/3	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L5	5102	3H3	C13-C12	9.17	1.53	1.33
87	L5	5102	3H3	O3-C22	8.10	1.39	1.23
87	L5	5102	3H3	O4-C23	7.74	1.38	1.23
87	L5	5102	3H3	C23-N	7.47	1.50	1.37
87	L5	5102	3H3	C22-N	6.59	1.48	1.37

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	L5	5102	3H3	C22-N-C23	-12.74	110.52	125.87
87	L5	5102	3H3	O3-C22-N	-7.90	108.12	120.30
87	L5	5102	3H3	O4-C23-N	-7.72	108.39	120.30
87	L5	5102	3H3	O4-C23-C24	-7.07	109.12	122.62
87	L5	5102	3H3	O3-C22-C21	-6.87	109.51	122.62

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

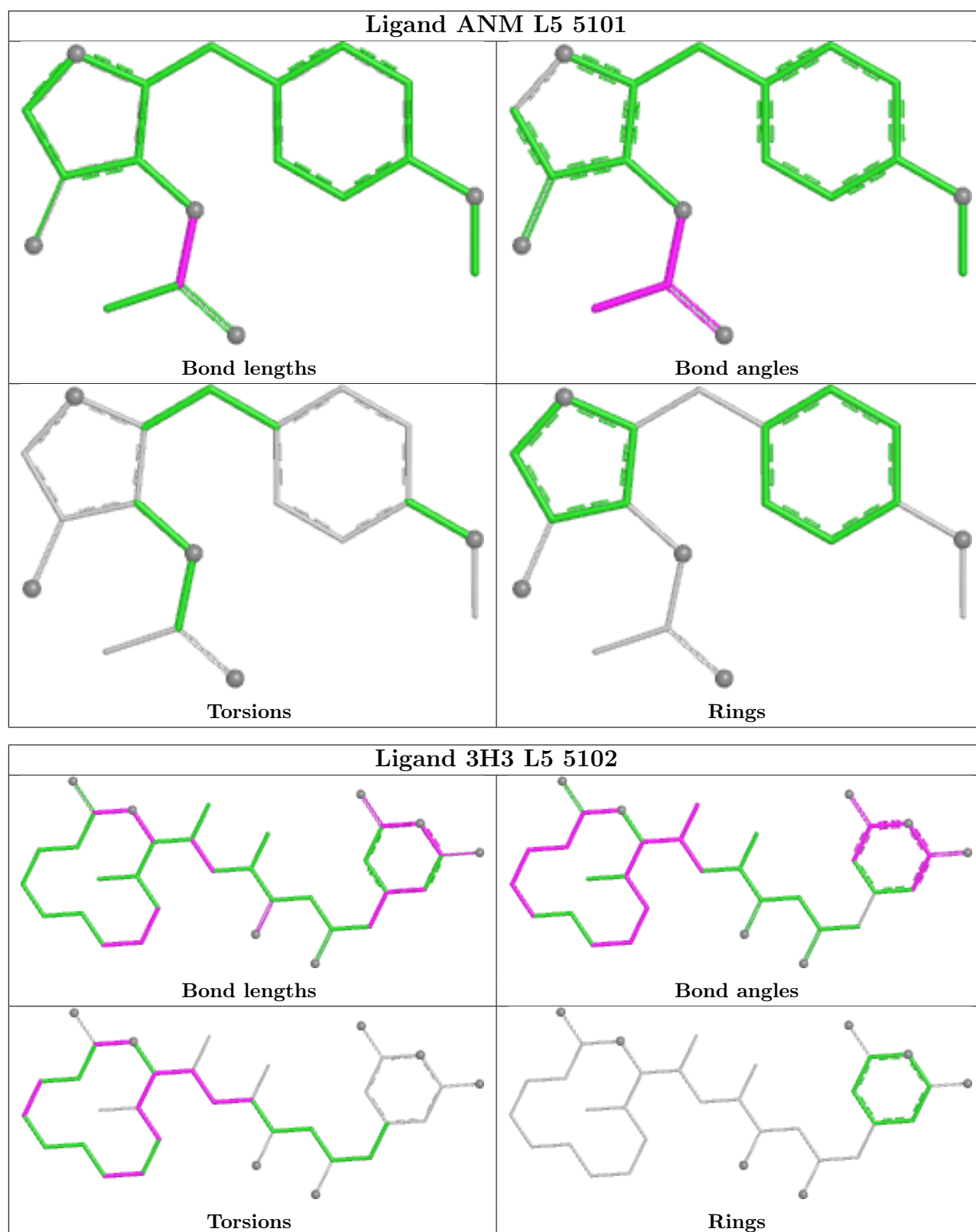
Mol	Chain	Res	Type	Atoms
82	L5	5114	SPD	C4-C5-N6-C7
87	L5	5102	3H3	C2-C1-C11-O1
87	L5	5102	3H3	C2-C1-C11-C12
87	L5	5102	3H3	C-C1-C11-O1
87	L5	5102	3H3	C-C1-C11-C12

There are no ring outliers.

13 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	L5	5121	PUT	1	0
86	L5	5101	ANM	1	0
87	L5	5102	3H3	2	0
82	L5	5114	SPD	16	0
90	Pt	78	MET	2	0
83	L5	5117	PUT	2	0
82	L5	5103	SPD	1	0
82	S2	1902	SPD	1	0
82	S2	1901	SPD	1	0
82	L5	5115	SPD	2	0
82	L5	5112	SPD	6	0
82	L5	5110	SPD	1	0
82	L5	5109	SPD	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

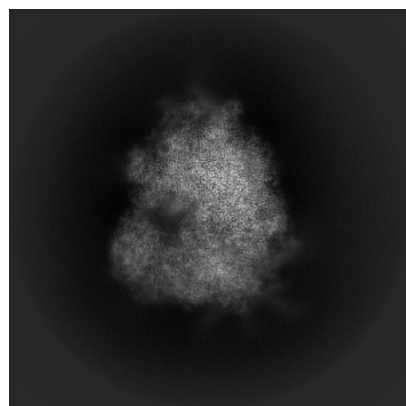
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40205. These allow visual inspection of the internal detail of the map and identification of artifacts.

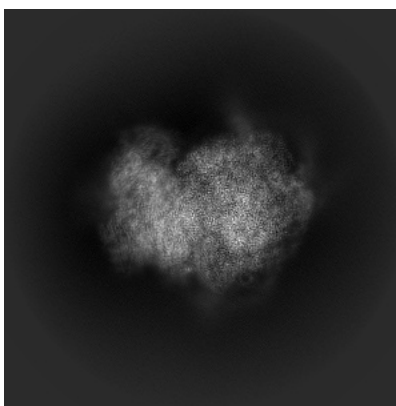
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

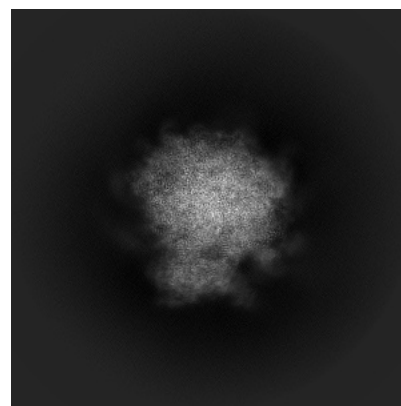
6.1.1 Primary map



X

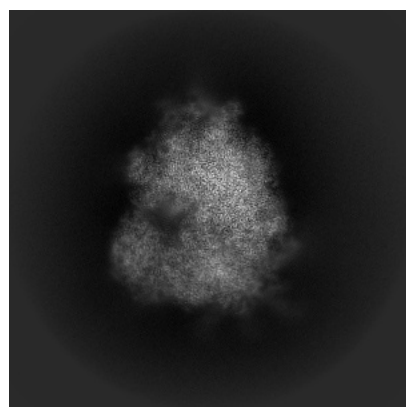


Y

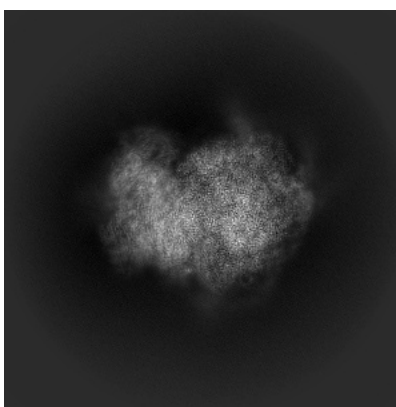


Z

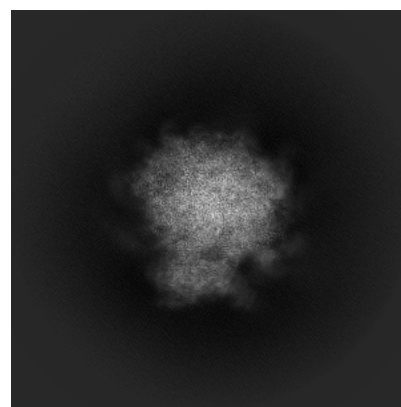
6.1.2 Raw map



X



Y

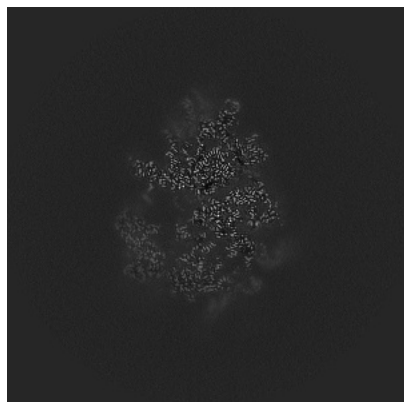


Z

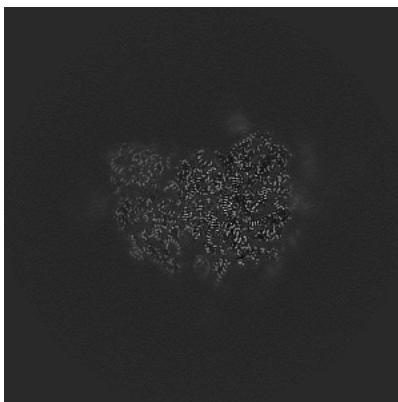
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

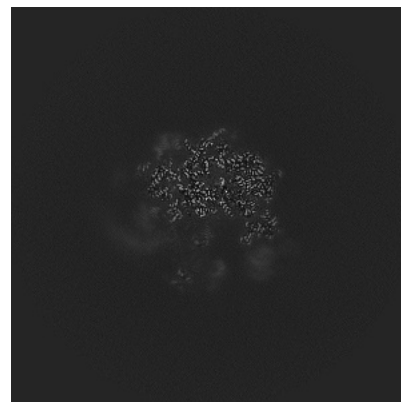
6.2.1 Primary map



X Index: 320

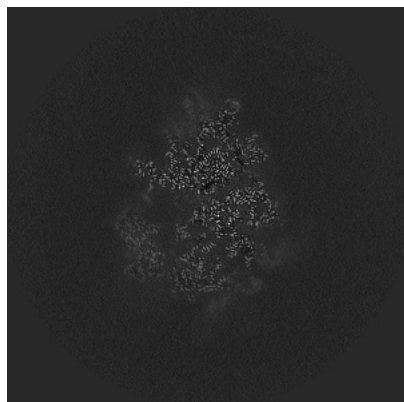


Y Index: 320

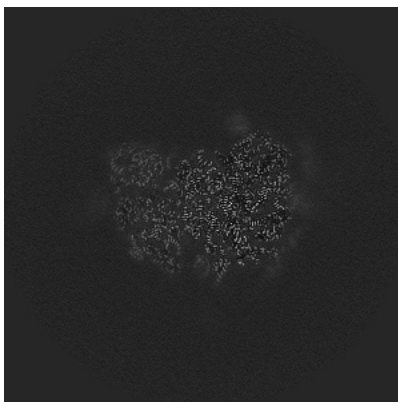


Z Index: 320

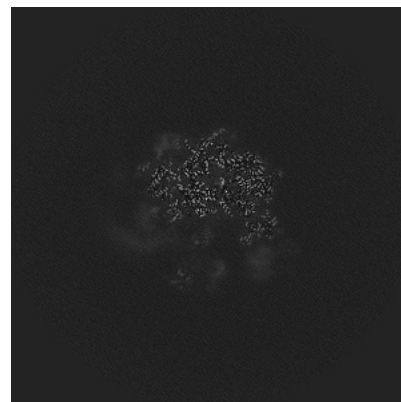
6.2.2 Raw map



X Index: 320



Y Index: 320

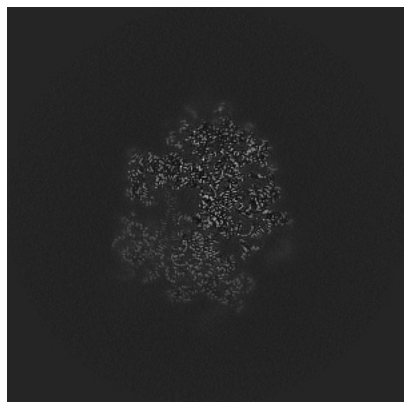


Z Index: 320

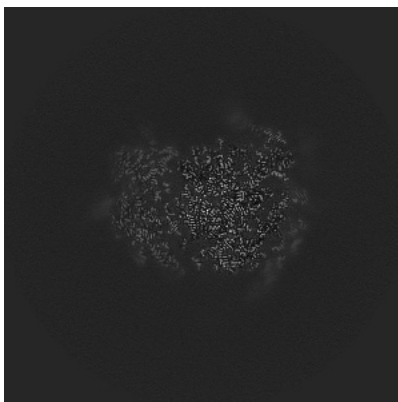
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 299

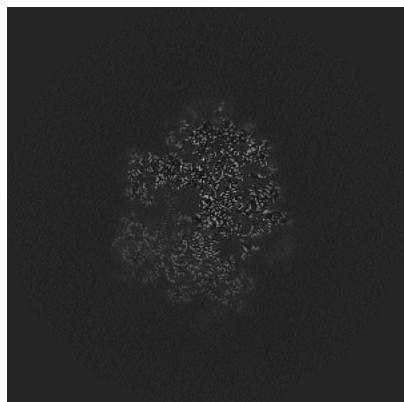


Y Index: 332

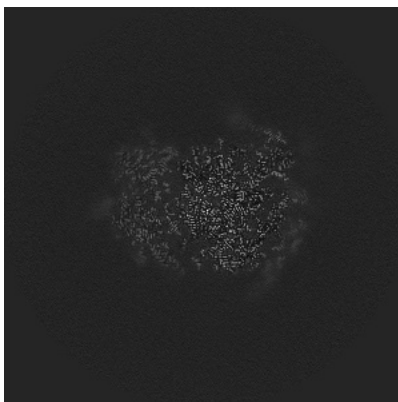


Z Index: 362

6.3.2 Raw map



X Index: 299



Y Index: 332

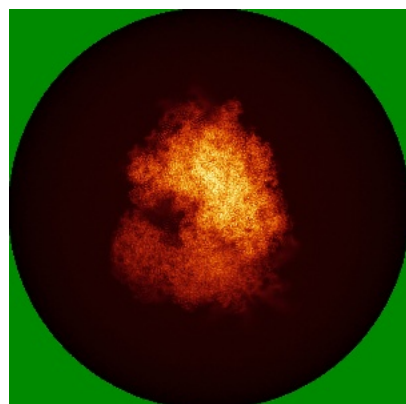


Z Index: 362

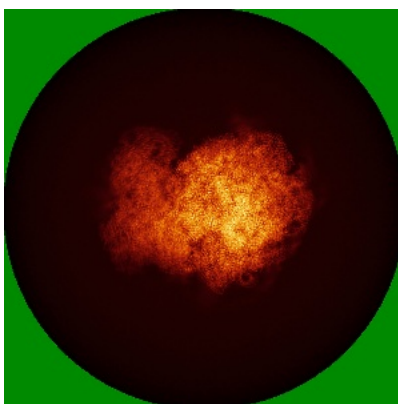
The images above show the largest variance slices of the map in three orthogonal directions.

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

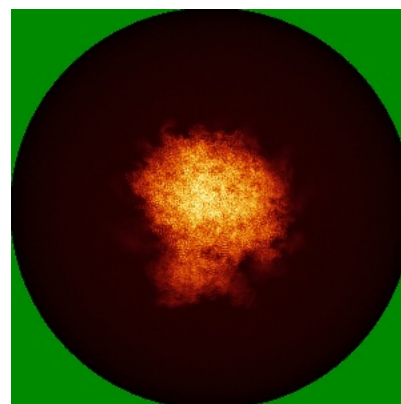
6.4.1 Primary map



X

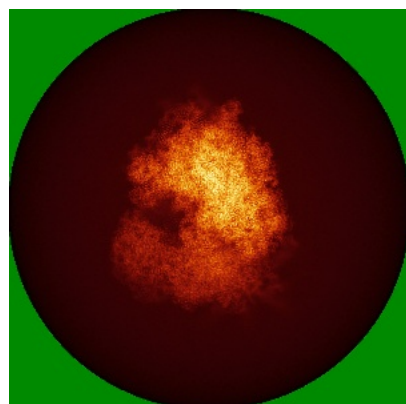


Y

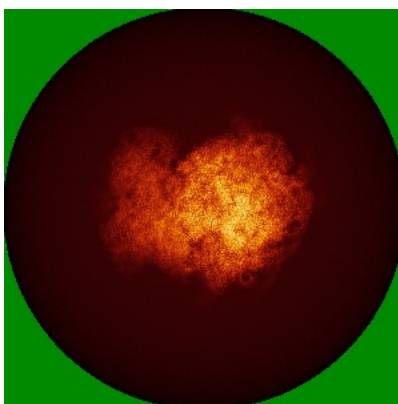


Z

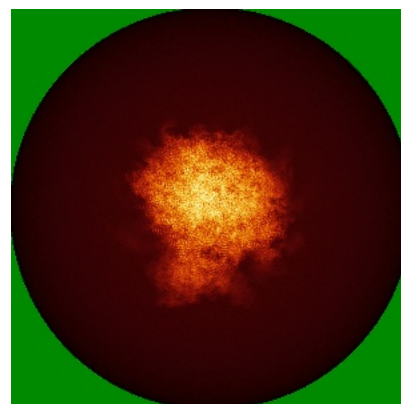
6.4.2 Raw map



X



Y

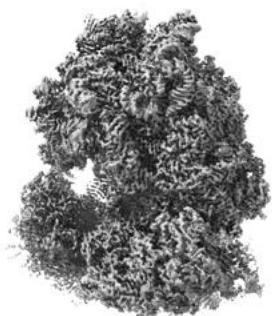


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. 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



X



Y



Z

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.

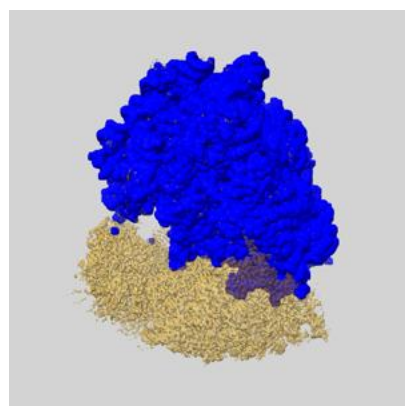
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

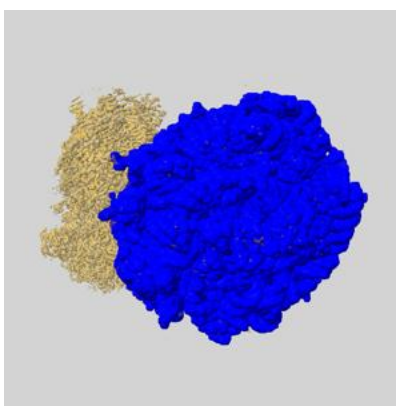
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

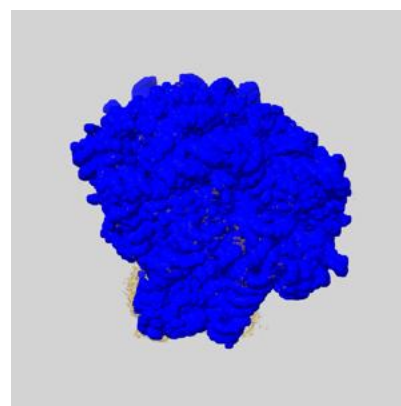
6.6.1 emd_40205_msk_1.map [i](#)



X



Y

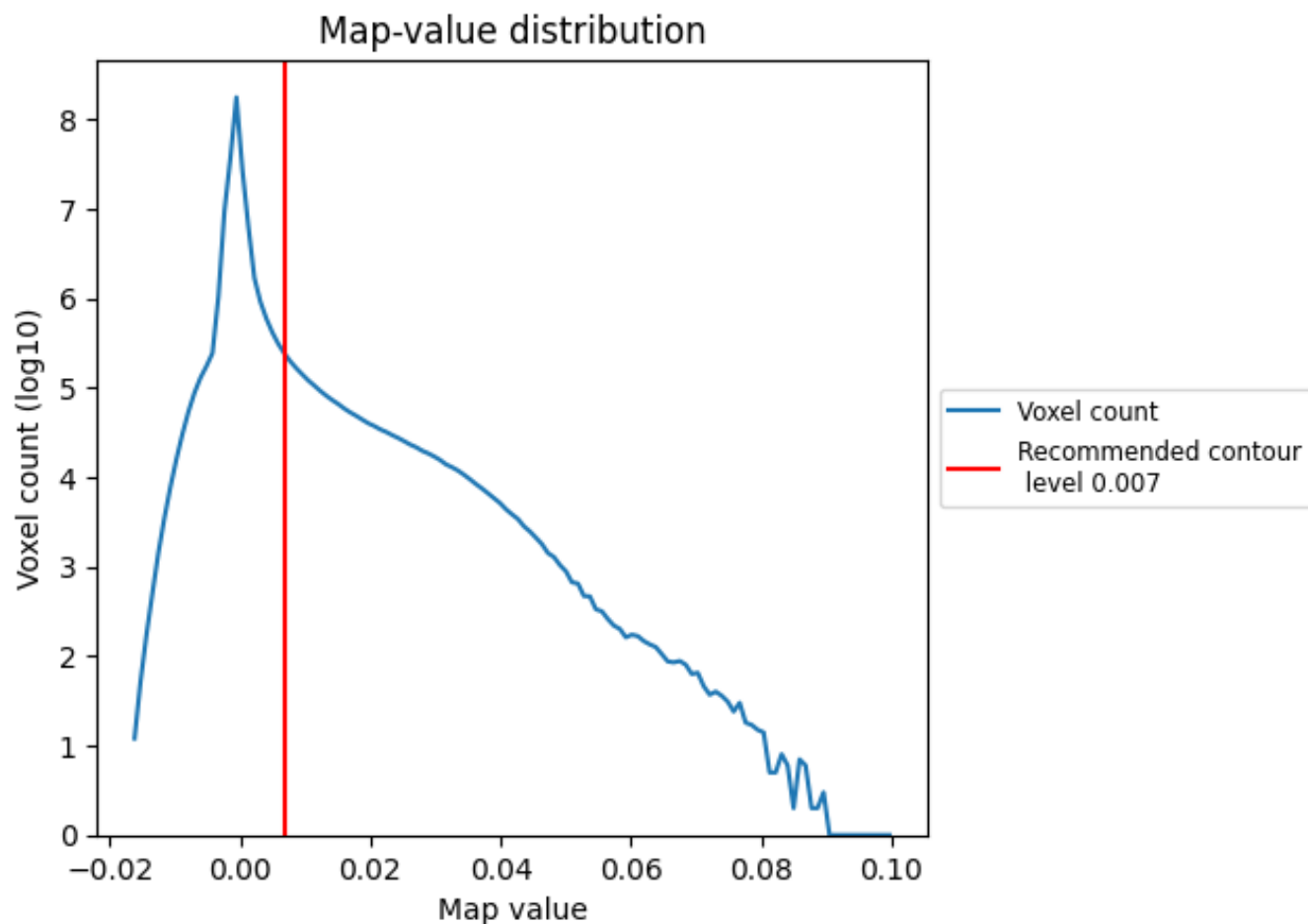


Z

7 Map analysis [i](#)

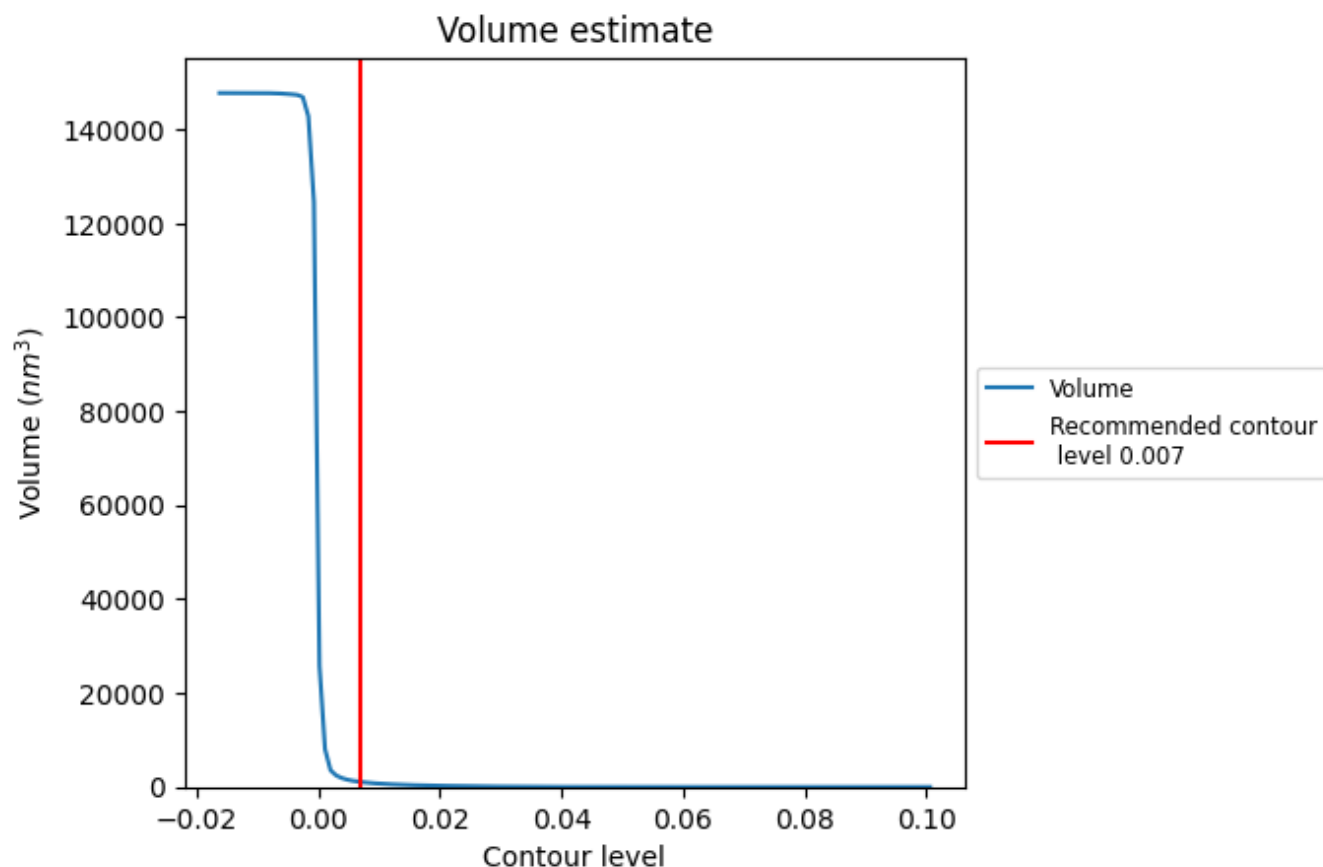
This section contains the results of statistical analysis of the map.

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.

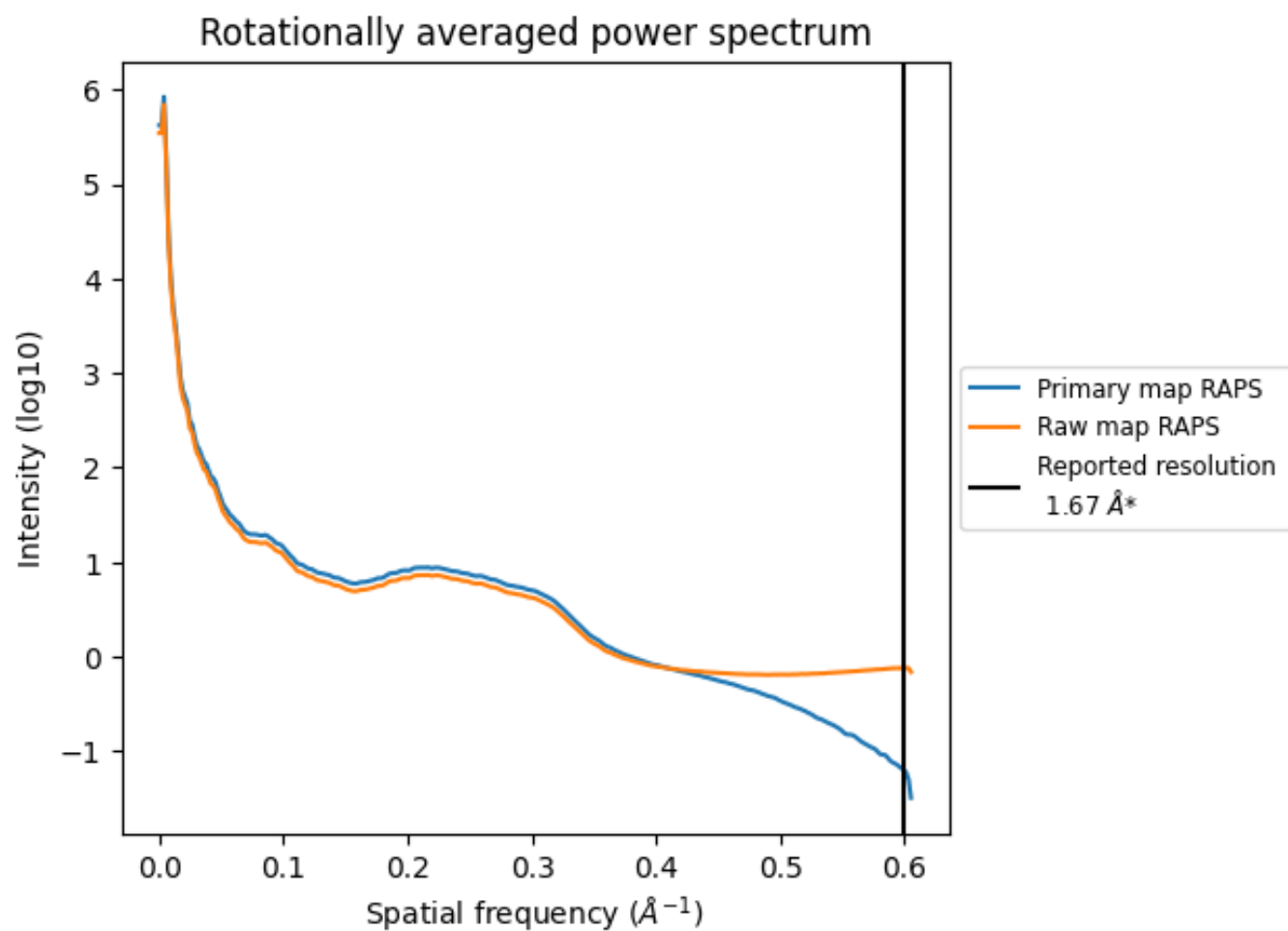
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1063 nm^3 ; this corresponds to an approximate mass of 960 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 ⓘ

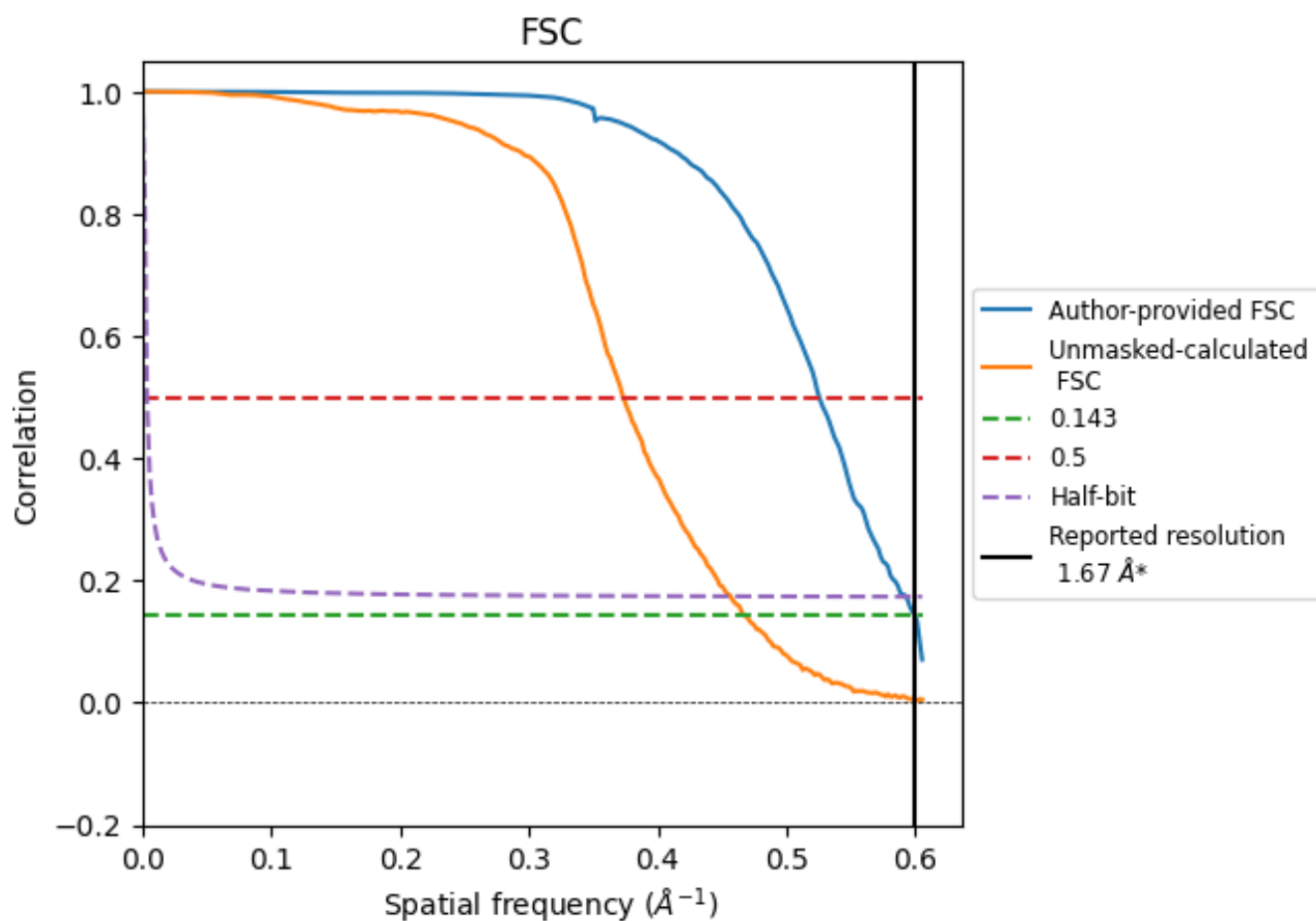


*Reported resolution corresponds to spatial frequency of 0.599 Å⁻¹

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 $0.599 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

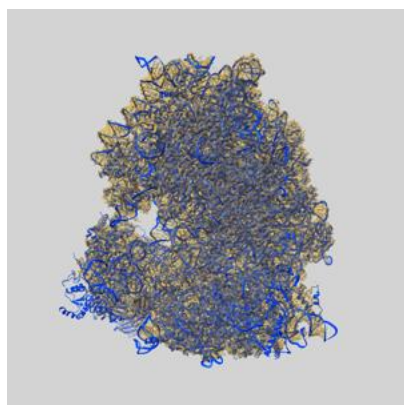
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.67	-	-
Author-provided FSC curve	1.67	1.90	1.69
Unmasked-calculated*	2.14	2.68	2.19

*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 2.14 differs from the reported value 1.67 by more than 10 %

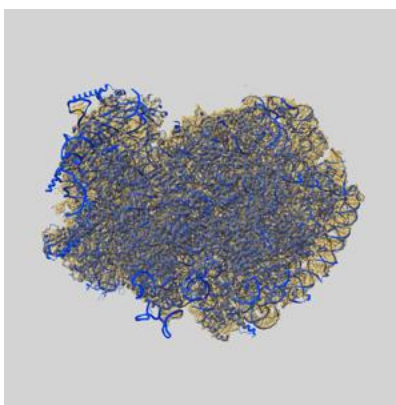
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40205 and PDB model 8GLP. Per-residue inclusion information can be found in section 3 on page 29.

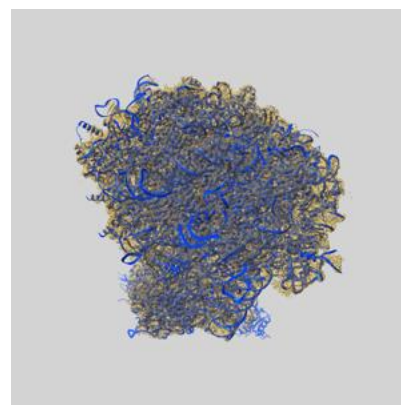
9.1 Map-model overlay [i](#)



X



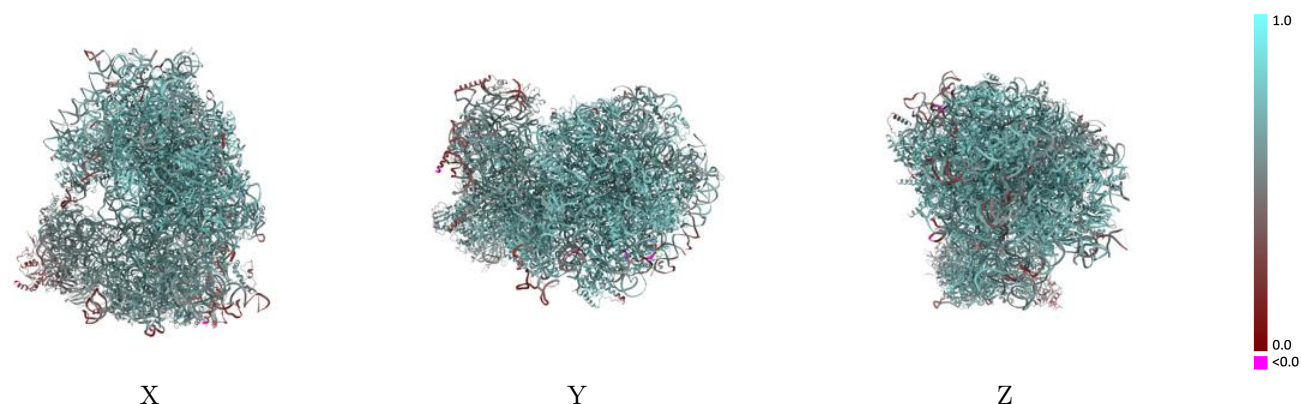
Y



Z

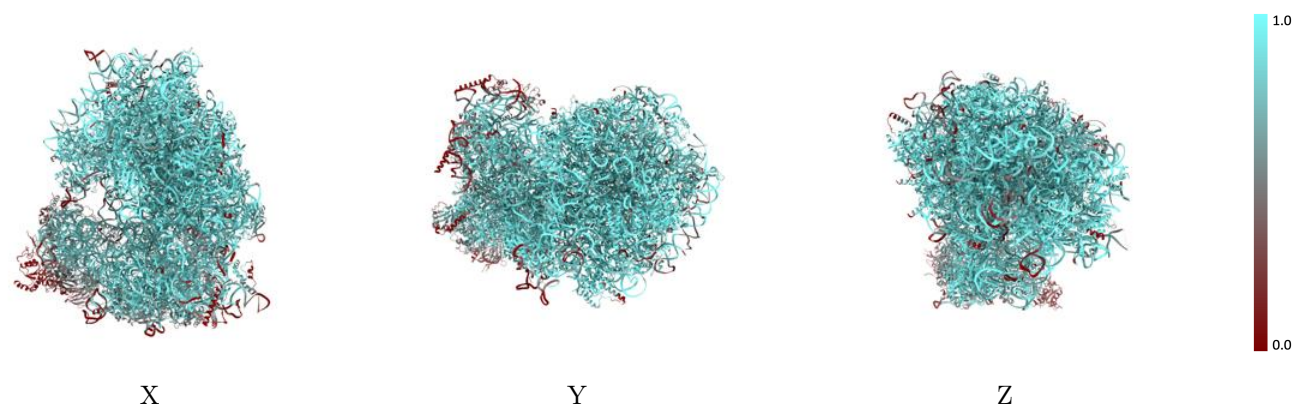
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



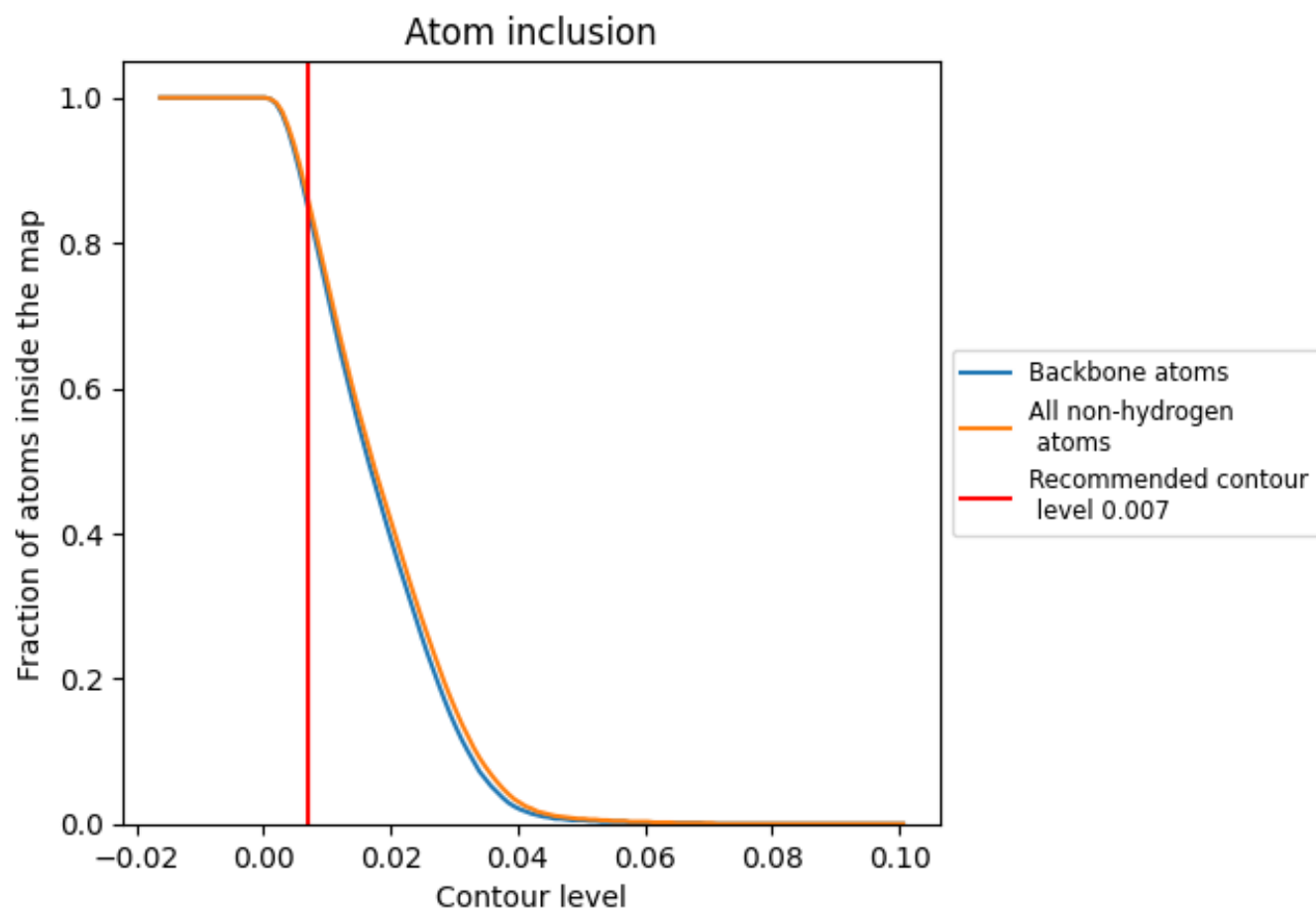
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 86% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.6730
L5	 0.9260	 0.6950
L7	 0.9930	 0.7260
L8	 0.9600	 0.7170
LA	 0.9760	 0.7710
LB	 0.9450	 0.7530
LC	 0.9500	 0.7580
LD	 0.9200	 0.7160
LE	 0.9070	 0.7160
LF	 0.9550	 0.7620
LG	 0.8390	 0.6800
LH	 0.9350	 0.7190
LI	 0.9560	 0.7390
LJ	 0.8800	 0.6850
LL	 0.9100	 0.7240
LM	 0.9490	 0.7300
LN	 0.9980	 0.7780
LO	 0.9540	 0.7570
LP	 0.9600	 0.7640
LQ	 0.9810	 0.7820
LR	 0.8490	 0.6920
LS	 0.9790	 0.7560
LT	 0.9250	 0.7400
LU	 0.8200	 0.6540
LV	 0.9650	 0.7600
LW	 0.5570	 0.5540
LX	 0.9400	 0.7380
LY	 0.9280	 0.7400
LZ	 0.9330	 0.7200
La	 0.9770	 0.7730
Lb	 0.8050	 0.6790
Lc	 0.9110	 0.7260
Ld	 0.9050	 0.7250
Le	 0.9790	 0.7790
Lf	 0.9750	 0.7730



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Chain	Atom inclusion	Q-score
Lg	 0.9050	 0.7370
Lh	 0.9260	 0.7320
Li	 0.9070	 0.7210
Lj	 0.9910	 0.7740
Lk	 0.8270	 0.6840
Ll	 0.9760	 0.7540
Lm	 0.9380	 0.7330
Ln	 0.9500	 0.7320
Lo	 0.9260	 0.7470
Lp	 0.9360	 0.7510
Lr	 0.9660	 0.7620
Pt	 0.4250	 0.6000
S2	 0.8740	 0.6160
SA	 0.7440	 0.6310
SB	 0.7980	 0.6670
SC	 0.8050	 0.6500
SD	 0.5010	 0.5400
SE	 0.7260	 0.6250
SF	 0.6950	 0.6120
SG	 0.5300	 0.5400
SH	 0.5660	 0.5770
SI	 0.7920	 0.6540
SJ	 0.7020	 0.6010
SK	 0.4230	 0.5040
SL	 0.8390	 0.6890
SM	 0.0070	 0.2880
SN	 0.8960	 0.7060
SO	 0.8720	 0.6880
SP	 0.5240	 0.5520
SQ	 0.6820	 0.5980
SR	 0.5890	 0.5660
SS	 0.6750	 0.6080
ST	 0.6510	 0.5890
SU	 0.4910	 0.5240
SV	 0.7630	 0.6480
SW	 0.9200	 0.6950
SX	 0.8780	 0.6760
SY	 0.5720	 0.5590
SZ	 0.5120	 0.5690
Sa	 0.8900	 0.6910
Sb	 0.7210	 0.6440
Sc	 0.5630	 0.5770

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Chain	Atom inclusion	Q-score
Sd	 0.7960	 0.6090
Se	 0.6200	 0.5770
Sf	 0.0620	 0.3100
Sg	 0.2780	 0.4970
mR	 0.2500	 0.4990