



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 08:55 AM EDT

PDB ID : 8G5Y / pdb_00008g5y
EMDB ID : EMD-29757
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (IC state)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-02-14
Resolution : 2.29 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:

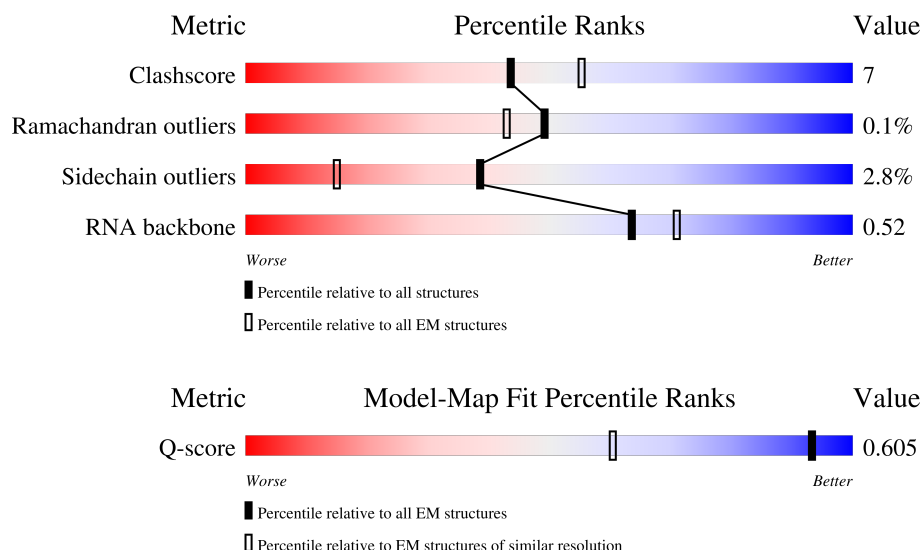
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.29 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.



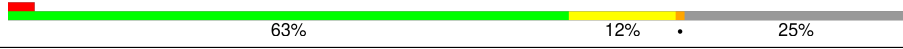
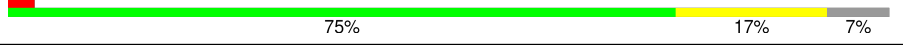
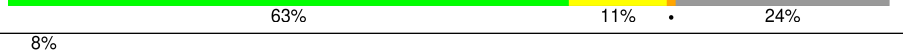
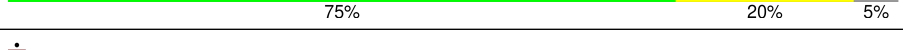
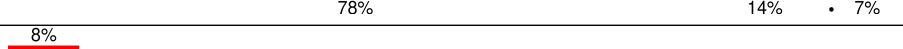
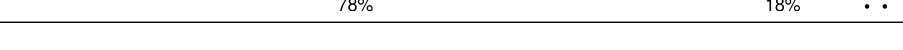
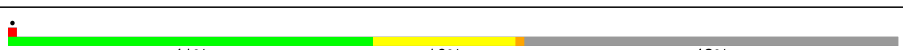
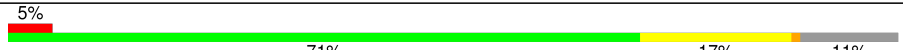
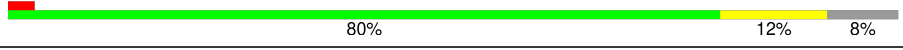
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3699 (1.79 - 2.79)

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	

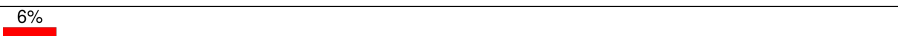
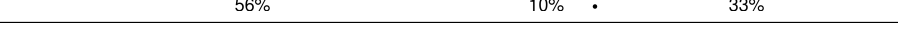
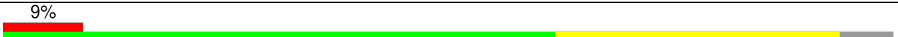
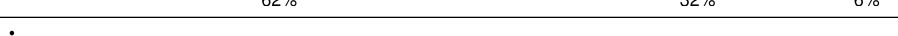
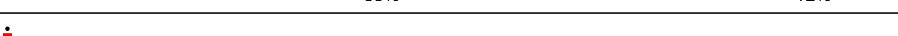
Continued on next page...

Continued from previous page...

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	

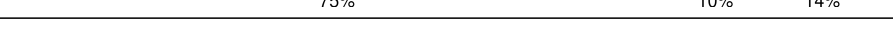
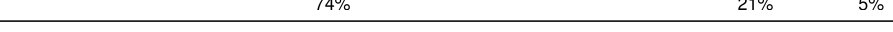
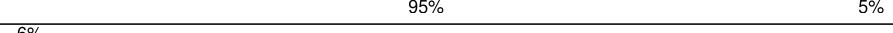
Continued on next page...

Continued from previous page...

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	Lz	217	
39	LA	257	
40	LB	403	
41	LC	427	
42	LJ	178	
43	LH	192	
44	LE	288	
45	LG	266	
46	LO	203	
47	LL	211	
48	LV	140	
49	LM	215	
50	La	148	
51	LN	204	
52	LI	214	
53	LD	297	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	LQ	188	
55	LR	196	
56	LS	176	
57	LT	160	
58	LP	184	
59	LU	128	
60	LX	156	
61	LY	145	
62	LW	157	
63	LZ	136	
64	Lr	137	
65	Lh	123	
66	Lb	159	
67	LF	248	
68	Lc	115	
69	Ld	125	
70	Le	135	
71	Lf	110	
72	Lg	117	
73	Li	105	
74	Lj	97	
75	Lk	70	
76	Ll	51	
77	Lm	128	
78	Ln	25	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	Lo	106	
80	Lp	92	
81	mR	60	
82	Pt	77	
83	5A	154	

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
85	PUT	L5	5518	-	-	X	-

2 Entry composition [i](#)

There are 92 unique types of molecules in this entry. The entry contains 219823 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	1680	Total	C	N	O	P	0	0
			35800	16005	6403	11713	1679		

- 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	3721	Total	C	N	O	P	2	0
			79154	35258	14402	25772	3722		

- 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 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 L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lz	211	Total	C	N	O	S	0	0
			1695	1086	304	297	8		

- Molecule 39 is a protein called uL2.

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

- Molecule 40 is a protein called 60S ribosomal protein L3.

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

- Molecule 41 is a protein called 60S ribosomal protein L4.

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

- Molecule 42 is a protein called 60S ribosomal protein L11.

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

- Molecule 43 is a protein called 60S ribosomal protein L9.

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

- Molecule 44 is a protein called 60S ribosomal protein L6.

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

- Molecule 45 is a protein called 60S ribosomal protein L7a.

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

- Molecule 46 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LO	199	Total	C	N	O	S	0	0
			1633	1053	319	256	5		

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LL	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 48 is a protein called 60S ribosomal protein L23.

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

- Molecule 49 is a protein called 60S ribosomal protein L14.

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

- Molecule 50 is a protein called 60S ribosomal protein L27a.

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

- Molecule 51 is a protein called 60S ribosomal protein L15.

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

- Molecule 52 is a protein called 60S ribosomal protein L10.

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

- Molecule 53 is a protein called 60S ribosomal protein L5.

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

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

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

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

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

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

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

- Molecule 57 is a protein called 60S ribosomal protein L21.

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

- Molecule 58 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LP	153	Total	C	N	O	S	1	0
			1248	780	242	217	9		

- Molecule 59 is a protein called 60S ribosomal protein L22.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L26.

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

- Molecule 62 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LW	118	Total	C	N	O	S	1	0
			955	599	192	159	5		

- Molecule 63 is a protein called 60S ribosomal protein L27.

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

- Molecule 64 is a protein called 60S ribosomal protein L28.

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

- Molecule 65 is a protein called 60S ribosomal protein L35.

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

- Molecule 66 is a protein called 60S ribosomal protein L29.

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

- Molecule 67 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	LF	225	Total	C	N	O	S	0	0
			1869	1202	358	300	9		

- Molecule 68 is a protein called 60S ribosomal protein L30.

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

- Molecule 69 is a protein called 60S ribosomal protein L31.

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

- Molecule 70 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 71 is a protein called 60S ribosomal protein L35a.

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

- Molecule 72 is a protein called 60S ribosomal protein L34.

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

- Molecule 73 is a protein called 60S ribosomal protein L36.

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

- Molecule 74 is a protein called 60S ribosomal protein L37.

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

- Molecule 75 is a protein called 60S ribosomal protein L38.

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

- Molecule 76 is a protein called 60S ribosomal protein L39.

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

- Molecule 77 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Lm	52	Total	C	N	O	S	0	0
			431	269	90	66	6		

- Molecule 78 is a protein called 60S ribosomal protein L41.

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

- Molecule 79 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lo	105	Total	C	N	O	S	2	0
			878	553	180	139	6		

- Molecule 80 is a protein called 60S ribosomal protein L37a.

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

- Molecule 81 is a RNA chain called mRNA.

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

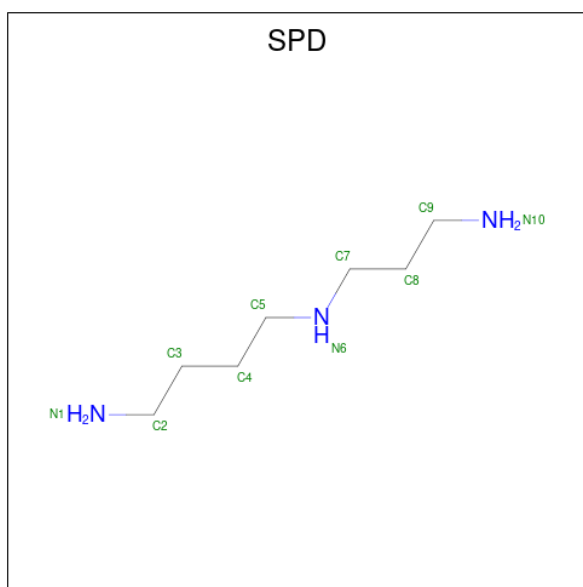
- Molecule 82 is a RNA chain called P-site tRNA.

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

- Molecule 83 is a protein called eIF5A1.

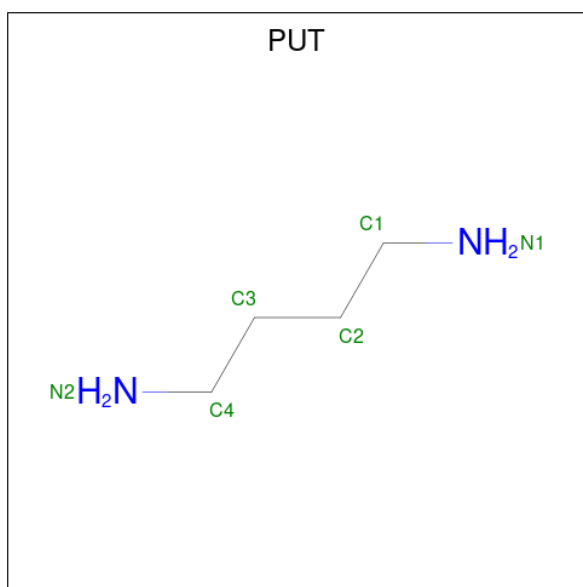
Mol	Chain	Residues	Atoms					AltConf	Trace
83	5A	138	Total	C	N	O	S	1	0
			1073	676	184	204	9		

- Molecule 84 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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

- Molecule 85 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

- Molecule 86 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
86	S2	17	Total	K	0
			17	17	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
86	L8	1	Total K 1 1	0
86	L5	52	Total K 52 52	0
86	L7	1	Total K 1 1	0
86	SL	1	Total K 1 1	0
86	Sa	1	Total K 1 1	0
86	LA	1	Total K 1 1	0
86	LH	1	Total K 1 1	0
86	Lf	1	Total K 1 1	0
86	Lg	1	Total K 1 1	0

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
87	S2	124	Total Mg 124 124	0
87	L8	10	Total Mg 10 10	0
87	L5	344	Total Mg 344 344	0
87	L7	5	Total Mg 5 5	0
87	SJ	1	Total Mg 1 1	0
87	SE	1	Total Mg 1 1	0
87	SC	1	Total Mg 1 1	0
87	SX	1	Total Mg 1 1	0
87	Sd	1	Total Mg 1 1	0
87	SN	1	Total Mg 1 1	0

Continued on next page...

Continued from previous page...

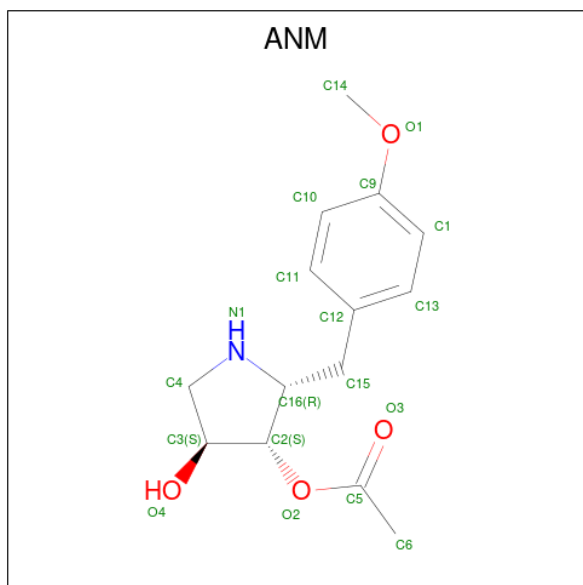
Mol	Chain	Residues	Atoms		AltConf
87	ST	1	Total 1	Mg 1	0
87	Sb	1	Total 1	Mg 1	0
87	LA	2	Total 2	Mg 2	0
87	LB	2	Total 2	Mg 2	0
87	LC	2	Total 2	Mg 2	0
87	LO	1	Total 1	Mg 1	0
87	LL	2	Total 2	Mg 2	0
87	LV	1	Total 1	Mg 1	0
87	LN	1	Total 1	Mg 1	0
87	LI	1	Total 1	Mg 1	0
87	LD	1	Total 1	Mg 1	0
87	LQ	1	Total 1	Mg 1	0
87	LR	2	Total 2	Mg 2	0
87	LS	2	Total 2	Mg 2	0
87	LP	3	Total 3	Mg 3	0
87	Lr	1	Total 1	Mg 1	0
87	Lc	1	Total 1	Mg 1	0
87	Le	1	Total 1	Mg 1	0
87	Lg	1	Total 1	Mg 1	0
87	Lj	1	Total 1	Mg 1	0
87	Lo	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

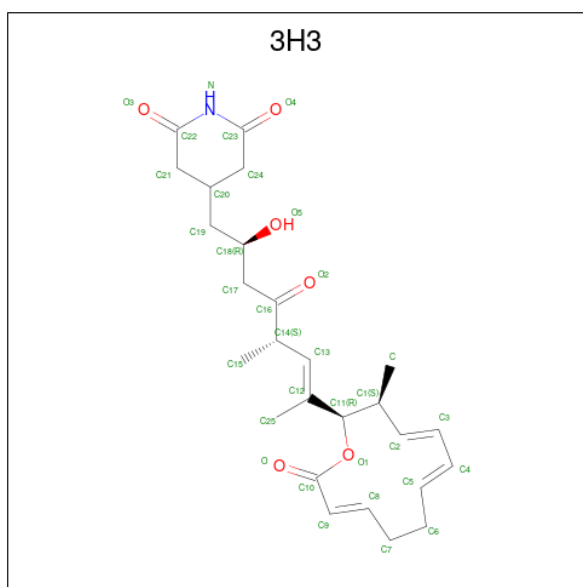
Mol	Chain	Residues	Atoms		AltConf
87	Lp	1	Total	Mg	0
			1	1	
87	Pt	4	Total	Mg	0
			4	4	
87	5A	1	Total	Mg	0
			1	1	

- Molecule 88 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



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

- Molecule 89 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).

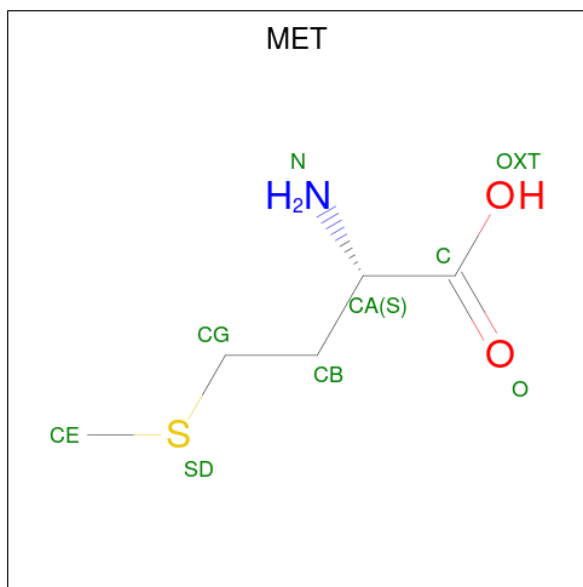


Mol	Chain	Residues	Atoms				AltConf
89	L5	1	Total	C	N	O	0
			33	26	1	6	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 91 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



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

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	S2	123	Total	O	0
			123	123	
92	L8	11	Total	O	0
			11	11	
92	L5	996	Total	O	0
			996	996	
92	L7	8	Total	O	0
			8	8	
92	SA	1	Total	O	0
			1	1	
92	SF	1	Total	O	0
			1	1	
92	SQ	1	Total	O	0
			1	1	
92	SS	1	Total	O	0
			1	1	
92	SN	1	Total	O	0
			1	1	
92	Sa	3	Total	O	0
			3	3	
92	LA	18	Total	O	0
			18	18	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
92	LB	8	Total 8	O 8	0
92	LC	21	Total 21	O 21	0
92	LO	3	Total 3	O 3	0
92	LL	3	Total 3	O 3	0
92	LV	2	Total 2	O 2	0
92	La	10	Total 10	O 10	0
92	LN	4	Total 4	O 4	0
92	LI	2	Total 2	O 2	0
92	LD	1	Total 1	O 1	0
92	LQ	6	Total 6	O 6	0
92	LR	1	Total 1	O 1	0
92	LT	1	Total 1	O 1	0
92	LP	2	Total 2	O 2	0
92	LX	2	Total 2	O 2	0
92	LZ	1	Total 1	O 1	0
92	Lr	1	Total 1	O 1	0
92	Lb	2	Total 2	O 2	0
92	LF	4	Total 4	O 4	0
92	Lc	1	Total 1	O 1	0
92	Ld	1	Total 1	O 1	0
92	Le	14	Total 14	O 14	0

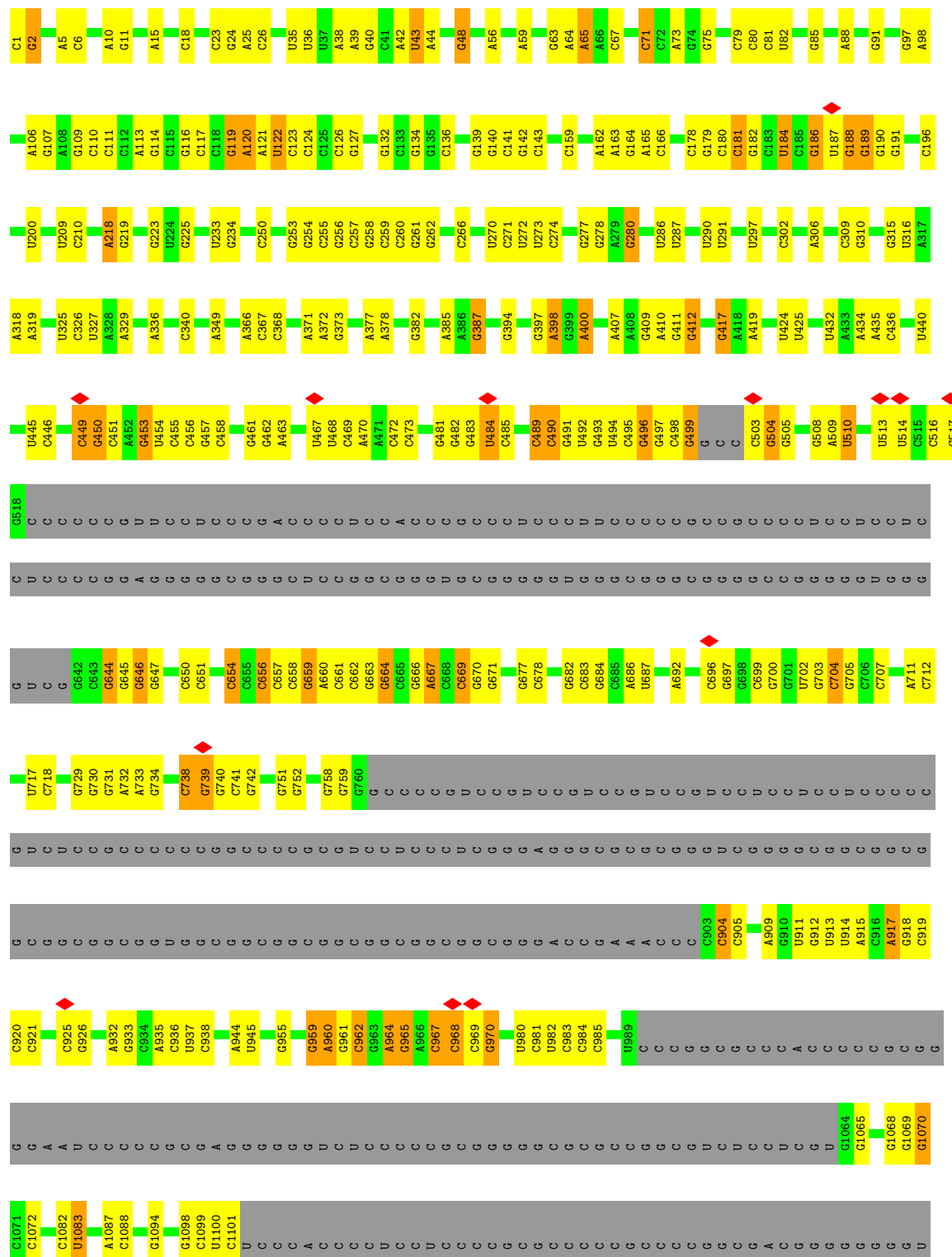
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
92	Lf	3	Total 3	O 3	0
92	Lg	4	Total 4	O 4	0
92	Lj	6	Total 6	O 6	0
92	Ln	1	Total 1	O 1	0
92	Lo	1	Total 1	O 1	0
92	Lp	2	Total 2	O 2	0
92	Pt	1	Total 1	O 1	0
92	5A	1	Total 1	O 1	0

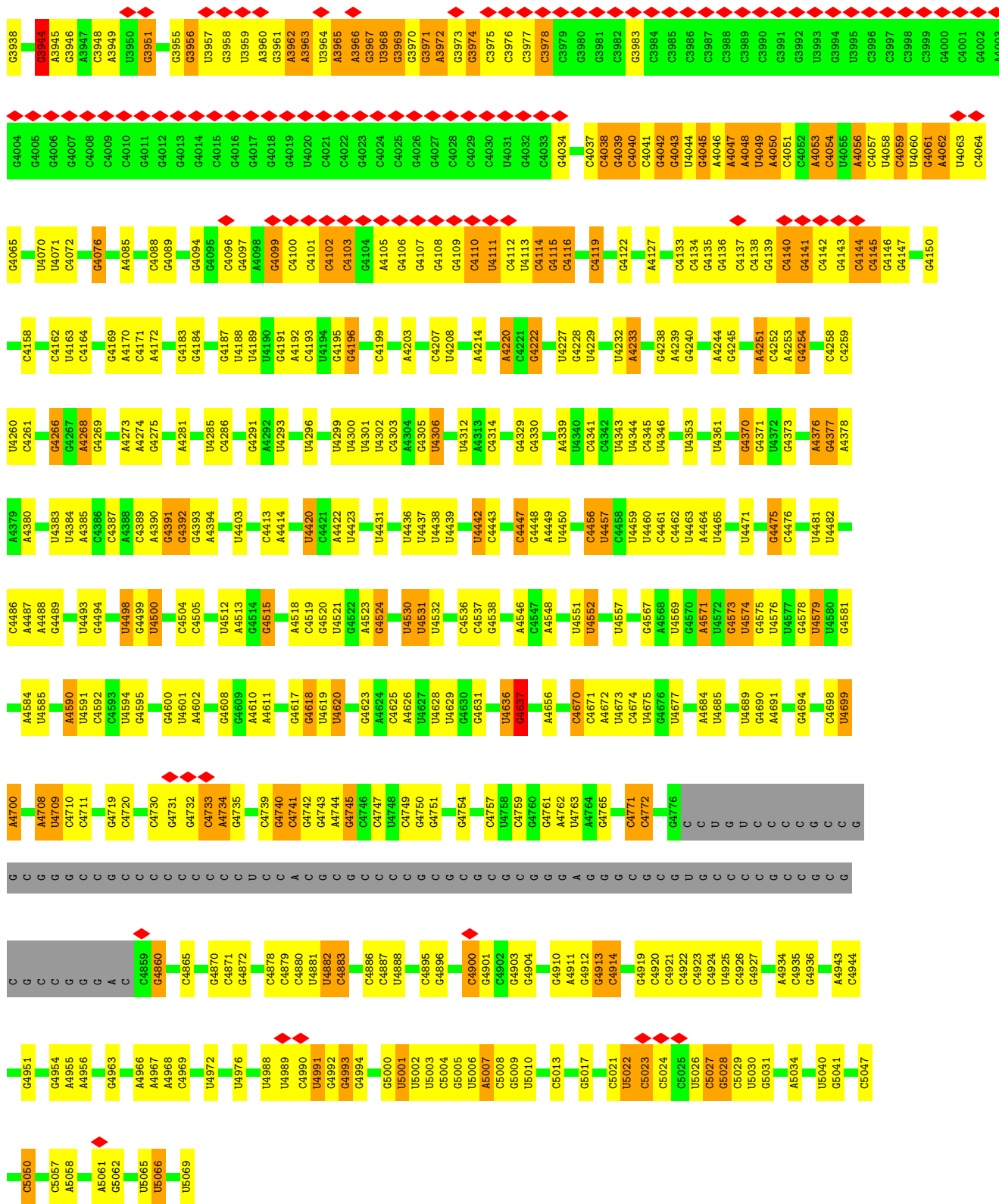


• Molecule 3: 28S rRNA



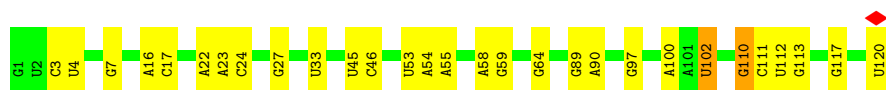






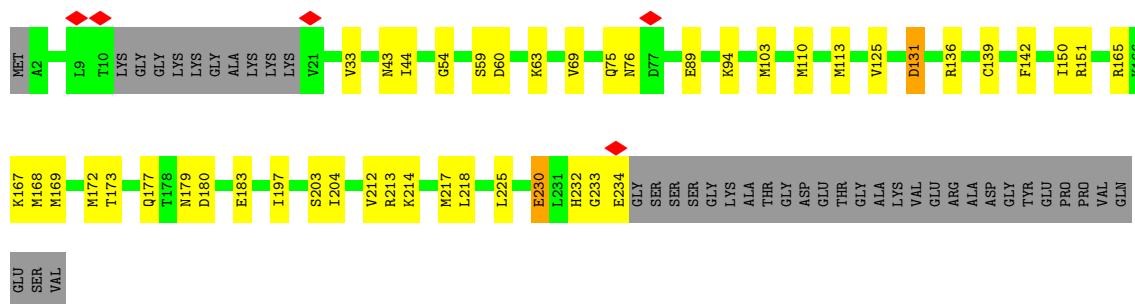
• Molecule 4: 5S rRNA

Chain L7:



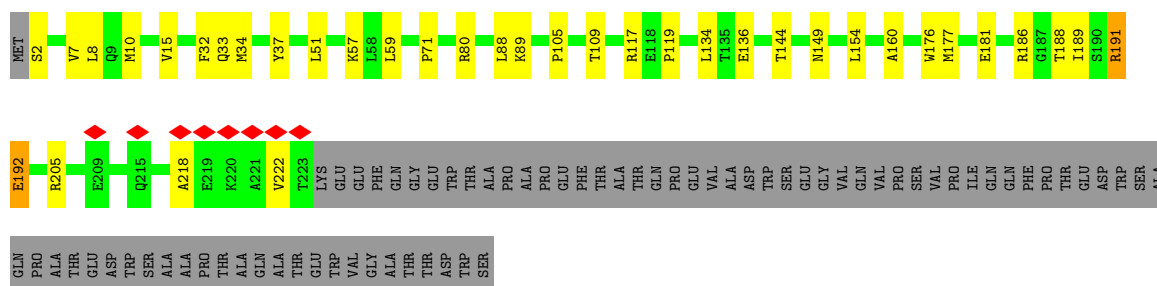
- Molecule 5: 40S ribosomal protein S3a

Chain SB: 67% 16% 16%



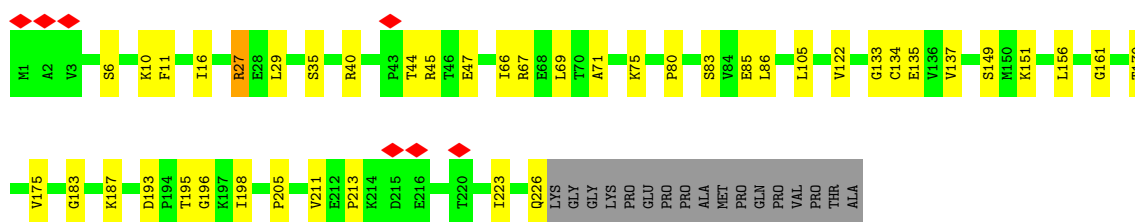
- Molecule 6: 40S ribosomal protein SA

Chain SA: 63% 12% 25%



- Molecule 7: 40S ribosomal protein S3

Chain SD: 75% 17% 7%



- Molecule 8: 40S ribosomal protein S9

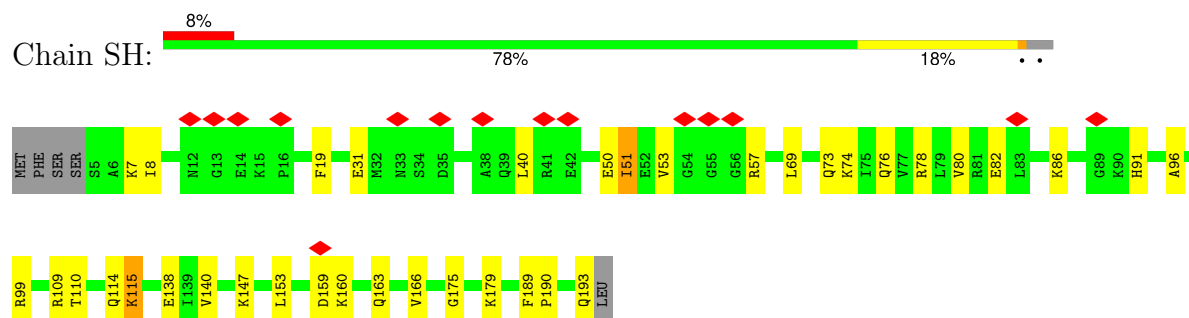
Chain SJ: 74% 20% 5%



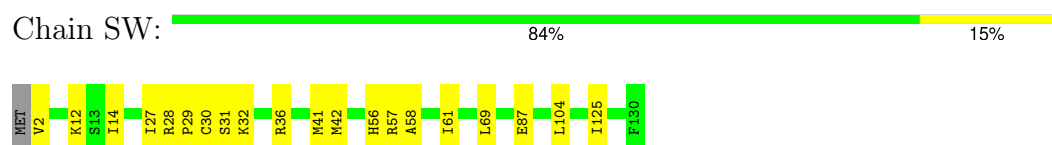




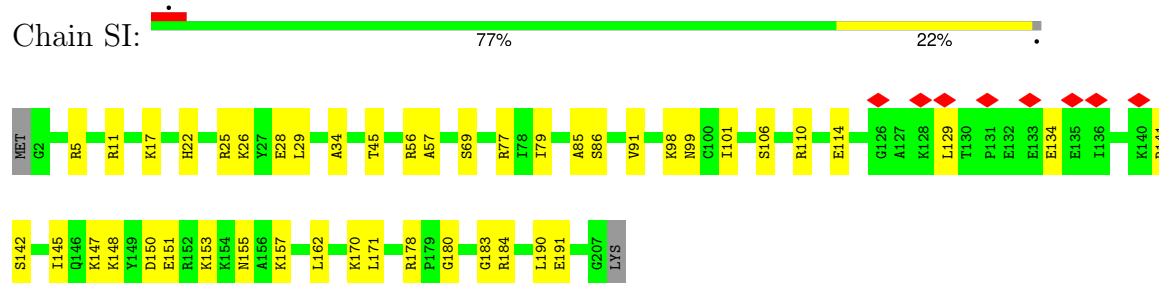
- Molecule 13: 40S ribosomal protein S7



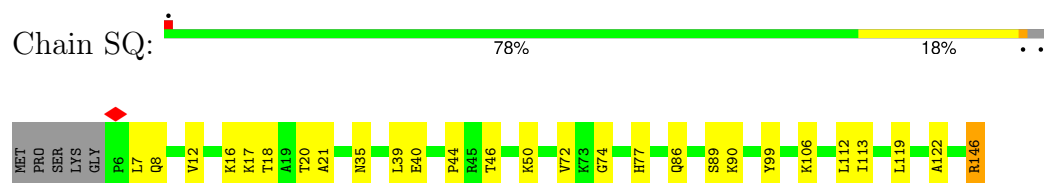
- Molecule 14: 40S ribosomal protein S15a



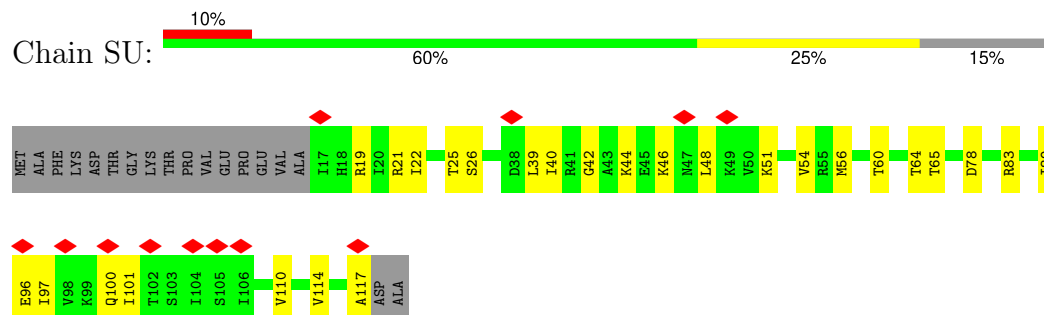
- Molecule 15: 40S ribosomal protein S8



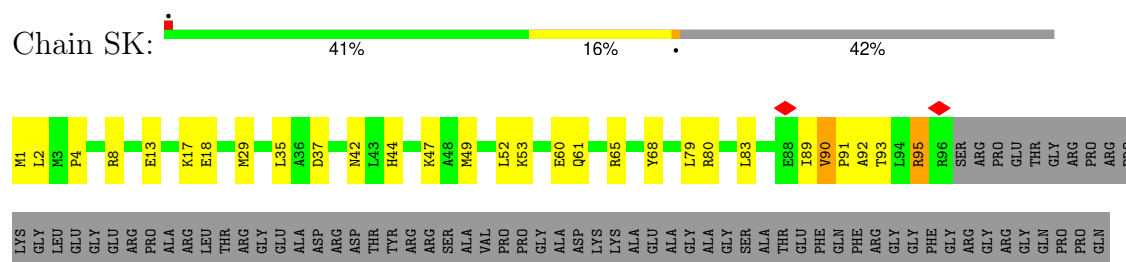
- Molecule 16: 40S ribosomal protein S16



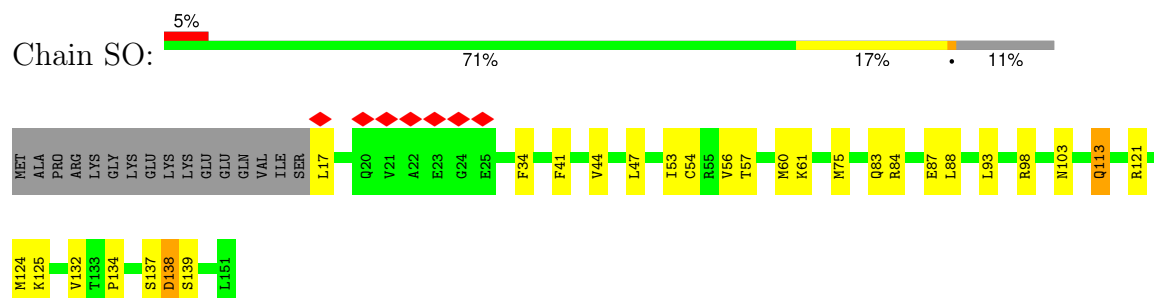
- Molecule 17: 40S ribosomal protein S20



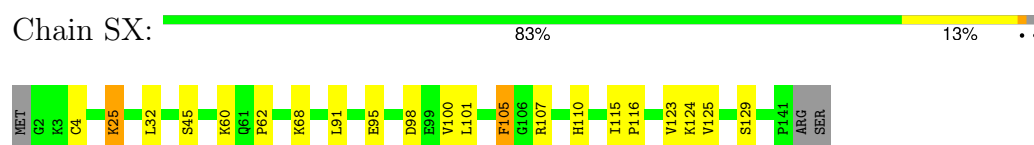
- Molecule 18: 40S ribosomal protein S10



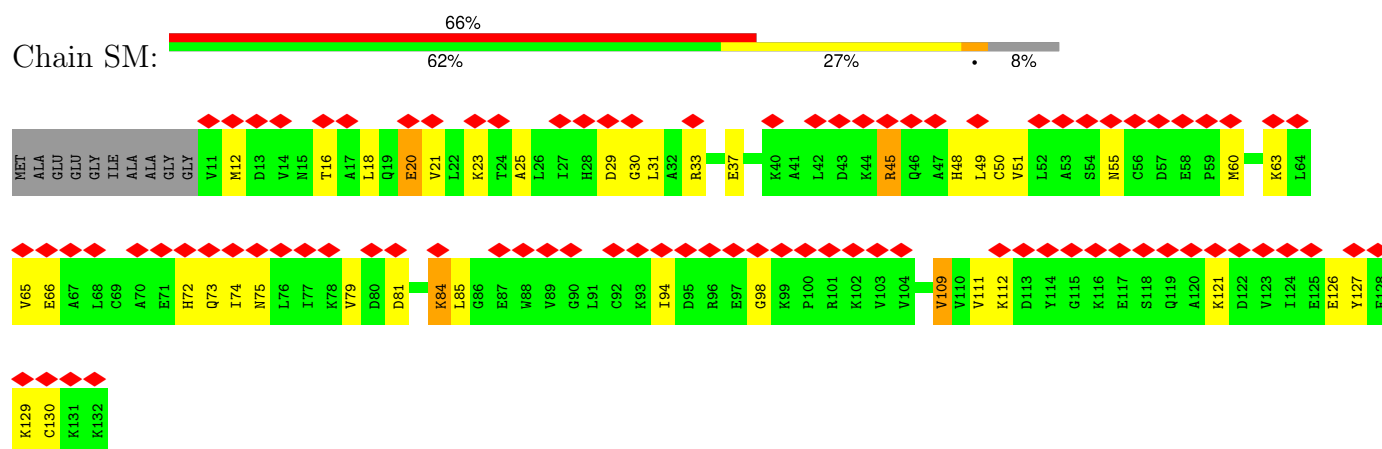
- Molecule 19: 40S ribosomal protein S14



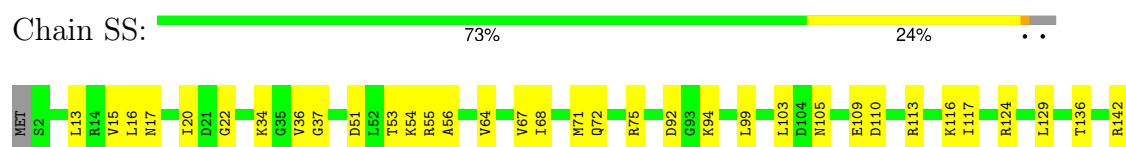
- Molecule 20: uS12

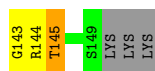


- Molecule 21: 40S ribosomal protein S12



- Molecule 22: 40S ribosomal protein S18





- Molecule 23: 40S ribosomal protein S29

Chain Sd: 79% 18% ..



- Molecule 24: 40S ribosomal protein S13

Chain SN: 79% 20% ..



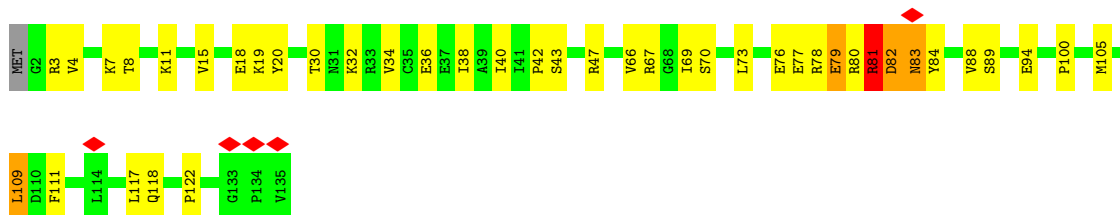
- Molecule 25: 40S ribosomal protein S11

Chain SL: 80% 12% 8%



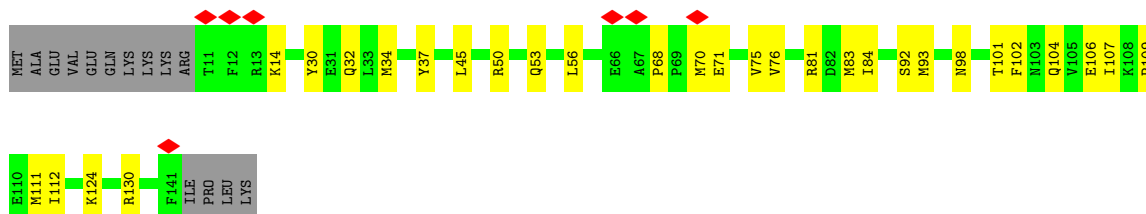
- Molecule 26: 40S ribosomal protein S17

Chain SR: 68% 27% ..



- Molecule 27: 40S ribosomal protein S15

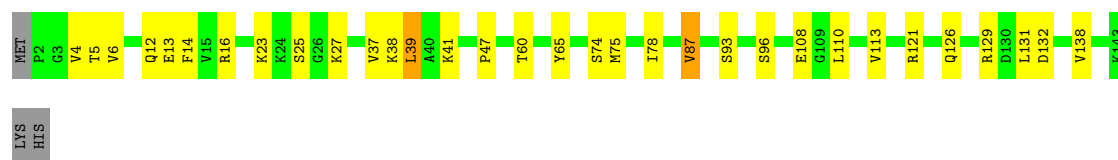
Chain SP: 5% 70% 21% 10%



- Molecule 28: 40S ribosomal protein S19

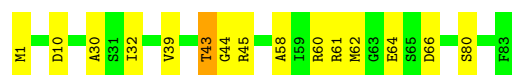


Chain ST:  76% 21% ..



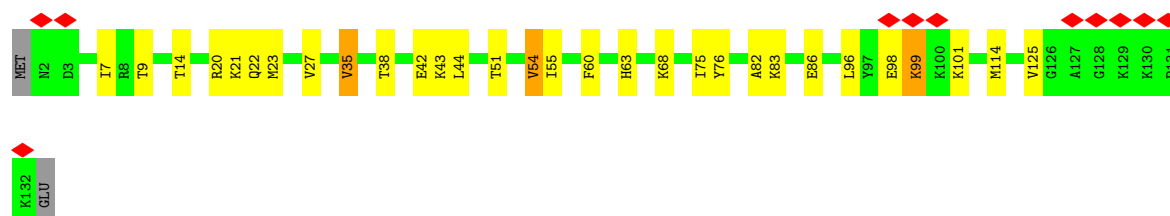
- Molecule 29: 40S ribosomal protein S21

Chain SV:  82% 17% .



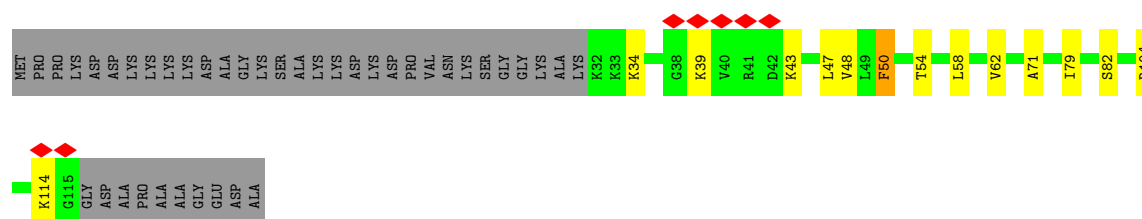
- Molecule 30: 40S ribosomal protein S24

Chain SY:  8% 76% 20% ..



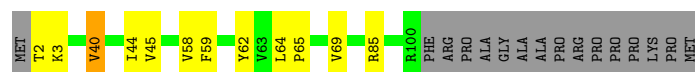
- Molecule 31: 40S ribosomal protein S25

Chain SZ:  6% 56% 10% 33%

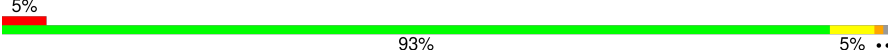


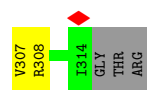
- Molecule 32: 40S ribosomal protein S26

Chain Sa:  76% 10% 14%



- Molecule 33: 40S ribosomal protein S27

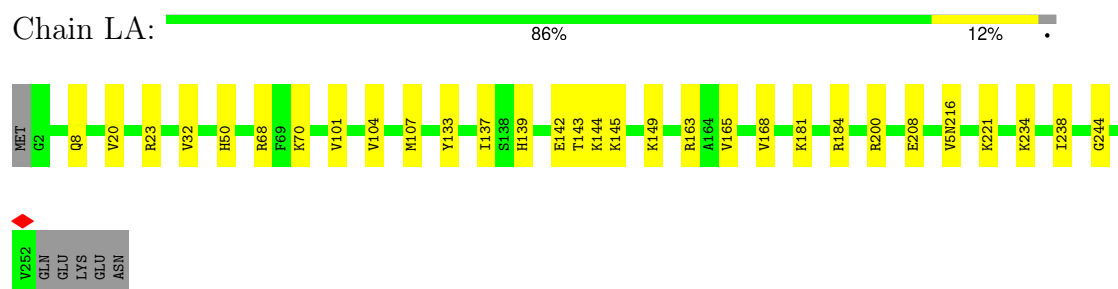
Chain Sb:  5% 93% 5% ..



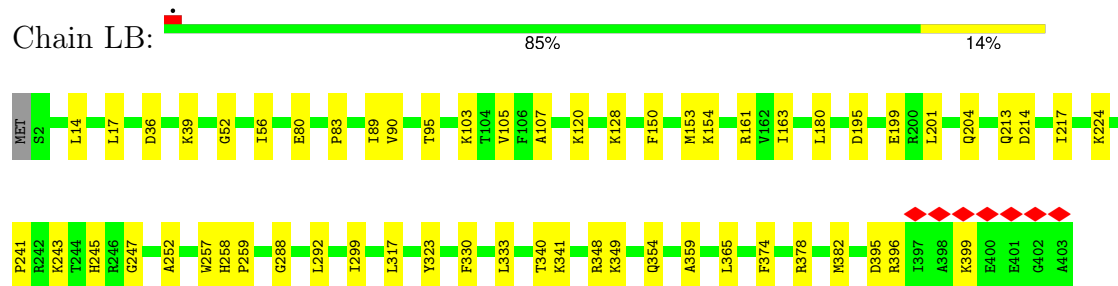
• Molecule 38: 60S ribosomal protein L10a



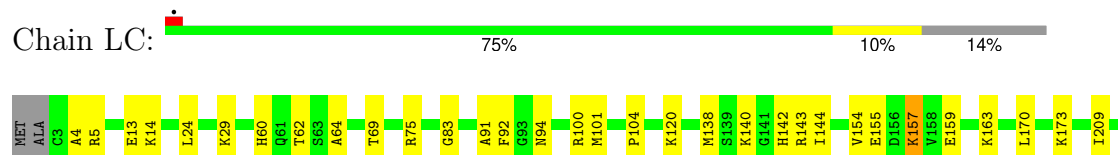
• Molecule 39: uL2

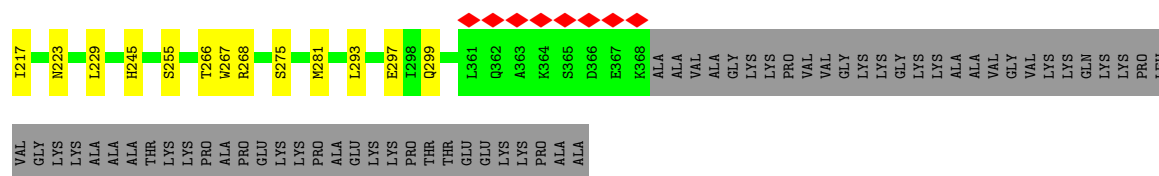


• Molecule 40: 60S ribosomal protein L3

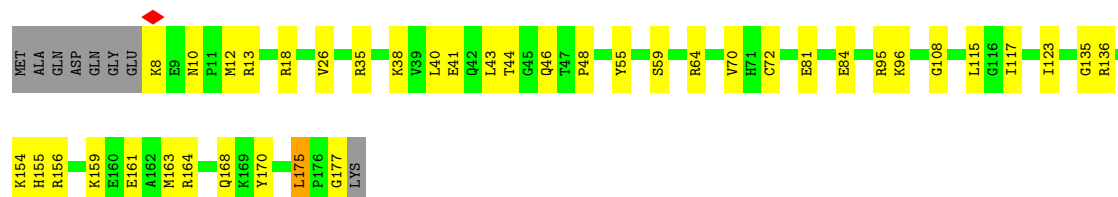


• Molecule 41: 60S ribosomal protein L4

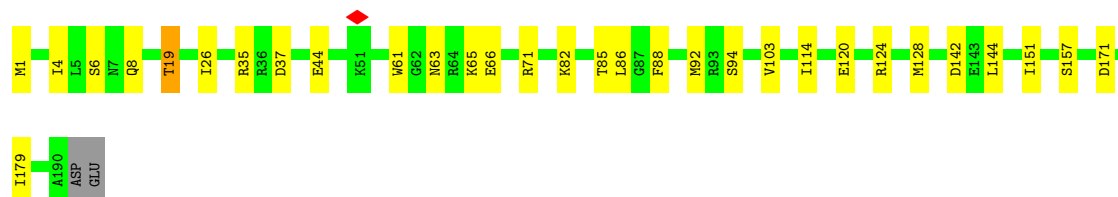
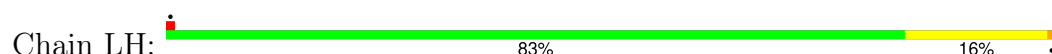




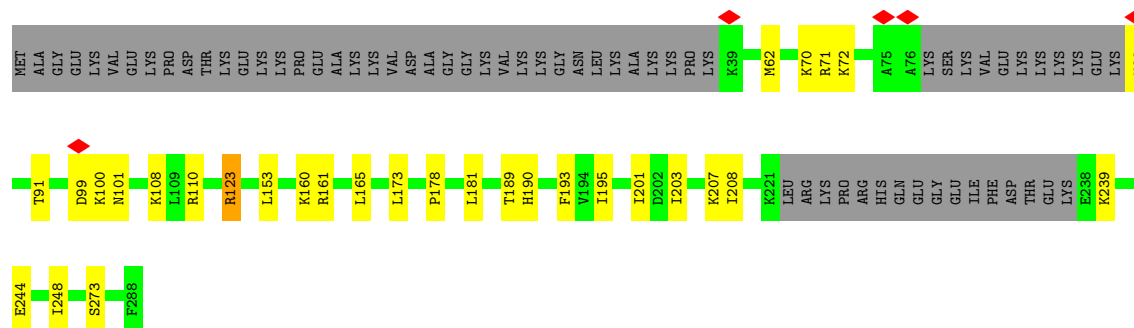
• Molecule 42: 60S ribosomal protein L11



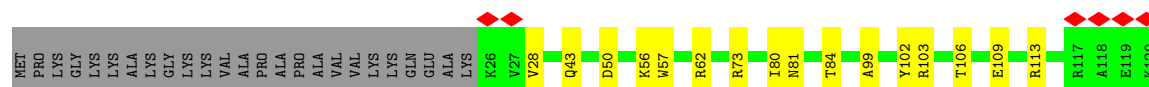
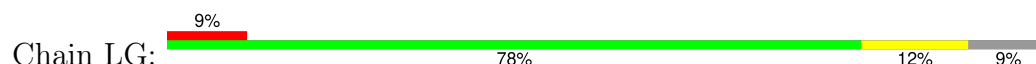
• Molecule 43: 60S ribosomal protein L9



• Molecule 44: 60S ribosomal protein L6

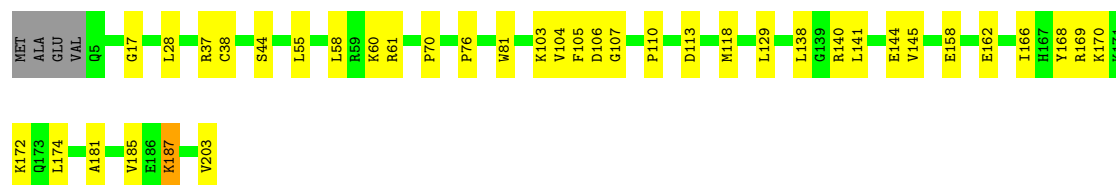


• Molecule 45: 60S ribosomal protein L7a



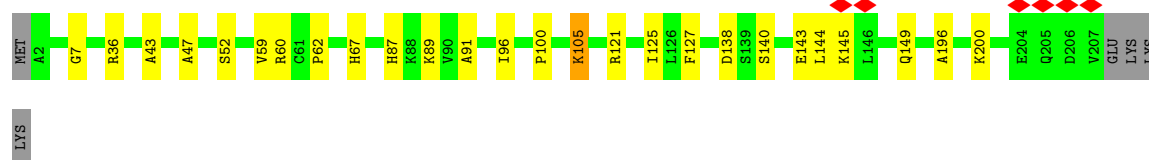
- Molecule 46: 60S ribosomal protein L13a

Chain LO:  79% 18%

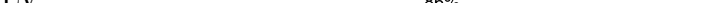


- Molecule 47: 60S ribosomal protein L13

Chain LL: 85% 12% 3%

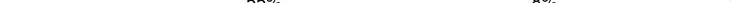


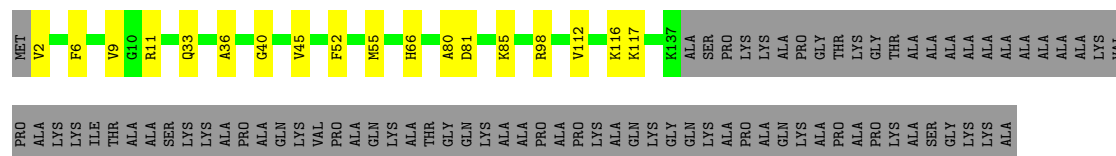
- Molecule 48: 60S ribosomal protein L23

Chain LV:  86% 9% 5%

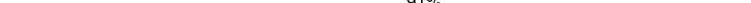


- Molecule 49: 60S ribosomal protein L14

Chain LM: 



- Molecule 50: 60S ribosomal protein L27a

Chain La:  91% 8%



- Molecule 51: 60S ribosomal protein L15

Chain LN:  88% 11%



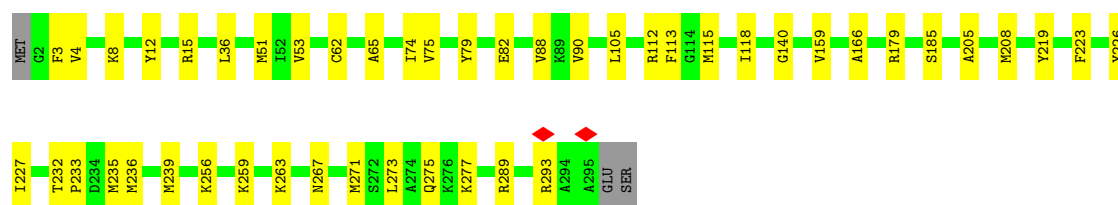
- Molecule 52: 60S ribosomal protein L10

Chain LI:  77% 17% 5%



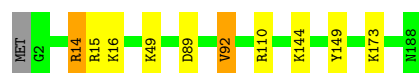
- Molecule 53: 60S ribosomal protein L5

Chain LD:  83% 16%



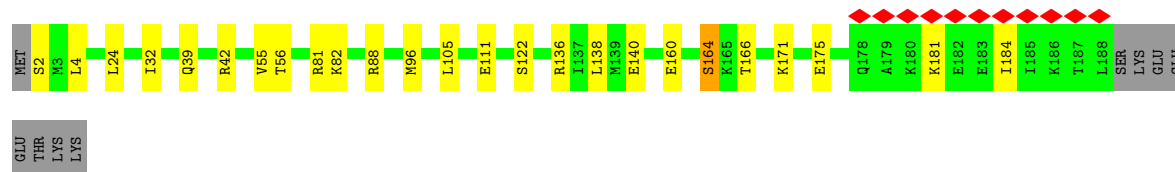
- Molecule 54: 60S ribosomal protein L18

Chain LQ:  94%



- Molecule 55: 60S ribosomal protein L19

Chain LR:  6% 83% 12% 5%

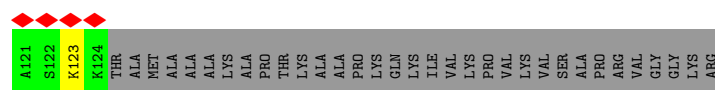


- Molecule 56: 60S ribosomal protein L18a

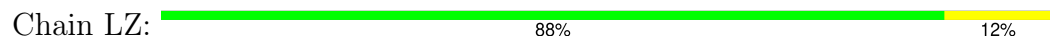
Chain LS:  90% 10%



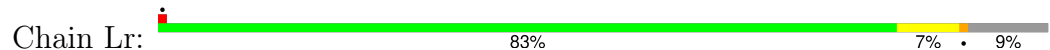
- | | | | | | | | | | | | | | | | | |
|----|----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| M1 | K2 | P15 | R19 | K27 | L32 | R44 | L49 | L54 | K61 | G62 | Q63 | G64 | GLU | GLU | ILE | GLN | LYS | LYS | R71 | T72 | R73 | R74 | A75 | V76 | K77 | F78 | T83 | I90 | M91 | F98 | E99 | V100 | Q104 | A108 | I109 | R110 | A111 | A112 | K113 | E114 | A115 | K116 | K117 | A118 | K119 | P120 |
|----|----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|



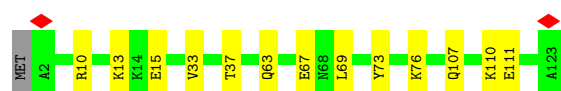
- Molecule 63: 60S ribosomal protein L27



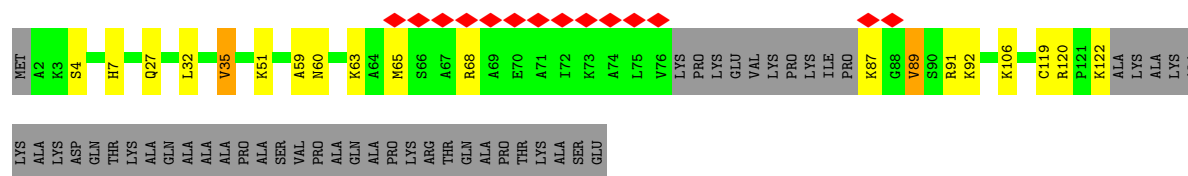
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L35

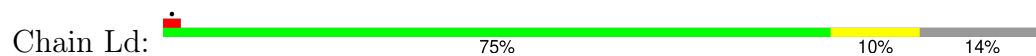


- Molecule 66: 60S ribosomal protein L29

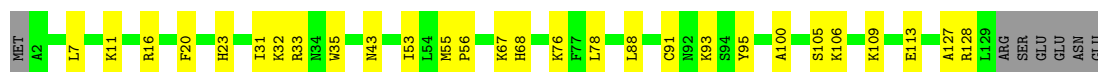




- Molecule 69: 60S ribosomal protein L31



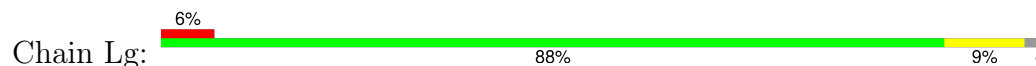
- Molecule 70: 60S ribosomal protein L32



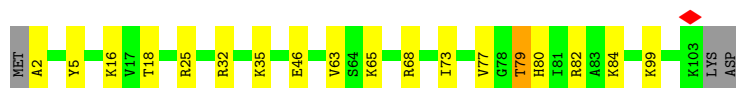
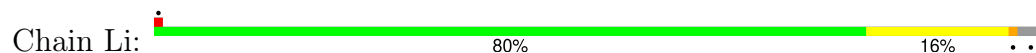
- Molecule 71: 60S ribosomal protein L35a



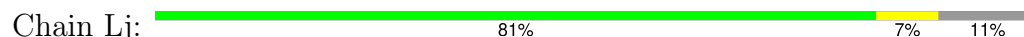
- Molecule 72: 60S ribosomal protein L34



- Molecule 73: 60S ribosomal protein L36



- Molecule 74: 60S ribosomal protein L37



- Molecule 75: 60S ribosomal protein L38

Chain Lk:  74% 23% ..



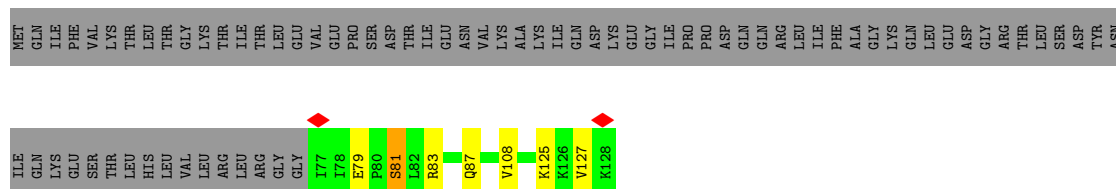
- Molecule 76: 60S ribosomal protein L39

Chain Ll:  90% 8% .



- Molecule 77: eL40

Chain Lm:  35% 5% 59%



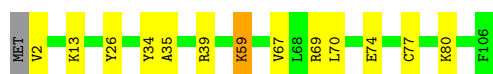
- Molecule 78: 60S ribosomal protein L41

Chain Ln:  84% 16%

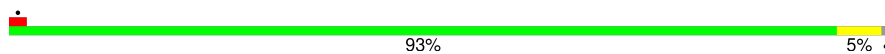


- Molecule 79: 60S ribosomal protein L36a

Chain Lo:  87% 11% ..



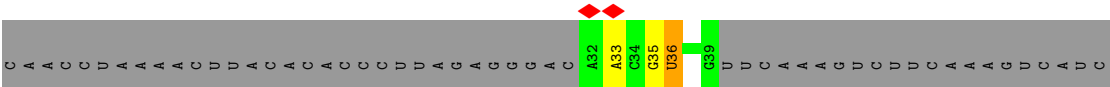
- Molecule 80: 60S ribosomal protein L37a

Chain Lp:  93% 5% .

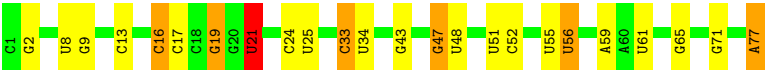


- Molecule 81: mRNA

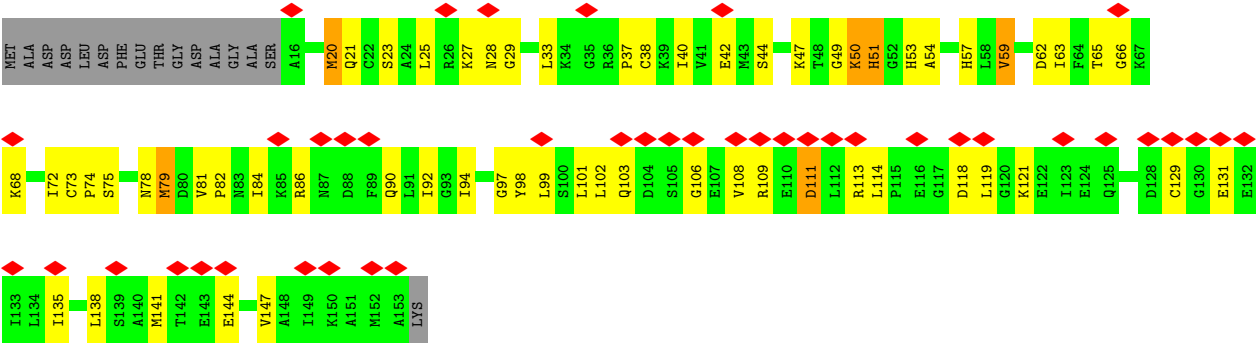
Chain mR:  8% 87%



• Molecule 82: P-site tRNA



• Molecule 83: eIF5A1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55836	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	0.053	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	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: AME, ANM, SAC, HIC, MLZ, ZN, PSU, A2M, H2U, 1MA, 5MC, 4AC, HY3, MA6, 3H3, 6MZ, UR3, MG, PUT, K, 4SU, B8N, G7M, OMU, OMG, UY1, SPD, V5N, 5CT, OMC, M3L

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	0.38	1/38000 (0.0%)	0.37	0/59217
2	L8	0.44	0/3609	0.42	0/5623
3	L5	0.44	3/85432 (0.0%)	0.44	2/133204 (0.0%)
4	L7	0.43	0/2858	0.37	0/4455
5	SB	0.27	0/1832	0.39	0/2449
6	SA	0.31	0/1778	0.39	0/2416
7	SD	0.27	0/1784	0.37	0/2403
8	SJ	0.25	0/1550	0.30	0/2069
9	SE	0.28	0/2118	0.37	0/2849
10	SC	0.29	0/1762	0.35	0/2381
11	SG	0.23	0/1946	0.41	0/2590
12	SF	0.28	0/1515	0.40	0/2037
13	SH	0.23	0/1540	0.42	0/2064
14	SW	0.34	0/1051	0.50	0/1406
15	SI	0.30	0/1715	0.40	0/2287
16	SQ	0.28	0/1141	0.38	0/1528
17	SU	0.28	0/813	0.38	0/1092
18	SK	0.27	0/834	0.47	0/1125
19	SO	0.29	0/1022	0.43	1/1372 (0.1%)
20	SX	0.31	0/1096	0.36	0/1461
21	SM	0.18	0/960	0.49	0/1286
22	SS	0.25	0/1232	0.37	0/1651
23	Sd	0.29	0/469	0.41	0/623
24	SN	0.30	0/1242	0.35	0/1671
25	SL	0.32	0/1221	0.38	0/1632
26	SR	0.40	0/1097	0.57	1/1474 (0.1%)
27	SP	0.25	0/1100	0.39	0/1470
28	ST	0.26	0/1148	0.39	0/1540
29	SV	0.33	0/635	0.40	0/850
30	SY	0.24	0/1083	0.38	0/1438
31	SZ	0.22	0/682	0.33	0/911

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sa	0.31	0/816	0.37	0/1093
33	Sb	0.28	0/665	0.39	0/891
34	Sc	0.26	0/514	0.42	0/688
35	Se	0.22	0/396	0.29	0/519
36	Sf	0.44	0/525	0.69	0/695
37	Sg	0.26	0/2493	0.47	0/3394
38	Lz	0.20	0/1723	0.45	0/2313
39	LA	0.38	0/1958	0.48	0/2623
40	LB	0.33	0/3294	0.40	0/4406
41	LC	0.38	0/2968	0.46	0/3985
42	LJ	0.27	0/1385	0.37	0/1852
43	LH	0.29	0/1537	0.32	0/2066
44	LE	0.28	0/1820	0.35	0/2442
45	LG	0.29	0/1959	0.37	0/2637
46	LO	0.35	0/1665	0.41	0/2228
47	LL	0.34	0/1695	0.46	0/2270
48	LV	0.32	0/1002	0.41	0/1345
49	LM	0.30	0/1142	0.32	0/1527
50	La	0.41	0/1178	0.50	0/1573
51	LN	0.43	0/1745	0.51	0/2338
52	LI	0.30	0/1683	0.36	0/2247
53	LD	0.29	0/2437	0.35	0/3263
54	LQ	0.37	0/1536	0.49	0/2052
55	LR	0.29	0/1582	0.34	0/2091
56	LS	0.36	0/1500	0.39	0/2013
57	LT	0.35	0/1345	0.38	0/1795
58	LP	0.35	0/1277	0.41	0/1713
59	LU	0.22	0/822	0.31	0/1103
60	LX	0.33	0/983	0.35	0/1323
61	LY	0.31	0/1132	0.34	0/1504
62	LW	0.28	0/972	0.38	0/1288
63	LZ	0.30	0/1141	0.31	0/1521
64	Lr	0.34	0/1020	0.36	0/1367
65	Lh	0.28	0/1022	0.34	0/1351
66	Lb	0.33	0/900	0.44	0/1187
67	LF	0.36	0/1904	0.43	0/2539
68	Lc	0.29	0/780	0.34	0/1046
69	Ld	0.33	0/903	0.42	0/1216
70	Le	0.41	0/1071	0.48	0/1429
71	Lf	0.36	0/902	0.42	0/1208
72	Lg	0.33	0/916	0.38	0/1220
73	Li	0.29	0/843	0.42	0/1115
74	Lj	0.41	0/731	0.50	0/967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lk	0.26	0/574	0.29	0/761
76	Ll	0.35	0/453	0.40	0/599
77	Lm	0.42	0/425	0.50	1/564 (0.2%)
78	Ln	0.39	0/240	0.45	0/305
79	Lo	0.34	0/888	0.43	0/1170
80	Lp	0.32	0/728	0.41	0/967
81	mR	0.22	0/192	0.33	0/297
82	Pt	0.39	1/1721 (0.1%)	0.37	0/2679
83	5A	0.27	0/1060	0.56	0/1425
All	All	0.38	5/228428 (0.0%)	0.41	5/334784 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	SO	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1383	A2M	O3'-P	5.34	1.61	1.56
3	L5	3760	A2M	O3'-P	5.17	1.61	1.56
3	L5	1871	A2M	O3'-P	5.12	1.61	1.56
82	Pt	47	G7M	O3'-P	5.06	1.61	1.56
3	L5	2415	OMU	O3'-P	5.02	1.61	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1670	G	C2'-C3'-O3'	-6.25	104.32	113.70
19	SO	139	SER	N-CA-C	5.84	115.80	108.45
26	SR	81	ARG	CB-CA-C	-5.55	101.36	110.08
3	L5	1624	G	C2'-C3'-O3'	-5.12	101.82	109.50
77	Lm	108	VAL	N-CA-C	-5.05	107.81	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	SO	138	ASP	Peptide

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	35800	0	18101	445	0
2	L8	3316	0	1687	45	0
3	L5	79154	0	39952	877	0
4	L7	2558	0	1296	16	0
5	SB	1806	0	1888	24	0
6	SA	1750	0	1755	25	0
7	SD	1756	0	1852	27	0
8	SJ	1525	0	1640	29	0
9	SE	2076	0	2177	23	0
10	SC	1725	0	1813	21	0
11	SG	1923	0	2089	40	0
12	SF	1494	0	1549	22	0
13	SH	1517	0	1605	27	0
14	SW	1034	0	1080	13	0
15	SI	1686	0	1772	30	0
16	SQ	1123	0	1193	17	0
17	SU	803	0	873	17	0
18	SK	810	0	836	20	0
19	SO	1009	0	1034	17	0
20	SX	1088	0	1149	12	0
21	SM	950	0	987	29	0
22	SS	1214	0	1275	23	0
23	Sd	458	0	448	10	0
24	SN	1214	0	1300	19	0
25	SL	1200	0	1271	11	0
26	SR	1082	0	1137	29	0
27	SP	1078	0	1121	18	0
28	ST	1121	0	1151	20	0
29	SV	639	0	638	9	0
30	SY	1065	0	1142	17	0
31	SZ	674	0	748	10	0
32	Sa	800	0	854	9	0
33	Sb	651	0	672	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Sc	512	0	541	13	0
35	Se	394	0	434	10	0
36	Sf	515	0	521	23	0
37	Sg	2436	0	2393	65	0
38	Lz	1695	0	1799	51	0
39	LA	1930	0	2028	17	0
40	LB	3239	0	3377	37	0
41	LC	2914	0	3087	32	0
42	LJ	1362	0	1399	25	0
43	LH	1518	0	1600	20	0
44	LE	1786	0	1945	18	0
45	LG	1926	0	2074	19	0
46	LO	1633	0	1779	25	0
47	LL	1664	0	1773	22	0
48	LV	988	0	1047	6	0
49	LM	1120	0	1187	11	0
50	La	1162	0	1206	8	0
51	LN	1700	0	1749	20	0
52	LI	1645	0	1694	26	0
53	LD	2391	0	2426	29	0
54	LQ	1512	0	1628	9	0
55	LR	1566	0	1728	12	0
56	LS	1460	0	1502	11	0
57	LT	1311	0	1392	20	0
58	LP	1248	0	1277	13	0
59	LU	808	0	831	11	0
60	LX	966	0	1040	6	0
61	LY	1115	0	1205	13	0
62	LW	955	0	1010	14	0
63	LZ	1115	0	1195	9	0
64	Lr	1011	0	1085	6	0
65	Lh	1014	0	1148	8	0
66	Lb	898	0	983	16	0
67	LF	1869	0	1996	14	0
68	Lc	770	0	809	10	0
69	Ld	888	0	930	7	0
70	Le	1053	0	1147	22	0
71	Lf	883	0	924	6	0
72	Lg	906	0	998	6	0
73	Li	832	0	917	12	0
74	Lj	712	0	744	6	0
75	Lk	568	0	637	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	Ll	443	0	483	3	0
77	Lm	431	0	471	3	0
78	Ln	239	0	289	4	0
79	Lo	878	0	949	10	0
80	Lp	715	0	769	2	0
81	mR	172	0	87	1	0
82	Pt	1645	0	843	12	0
83	5A	1073	0	1098	53	0
84	L5	120	0	228	11	0
84	S2	10	0	19	1	0
85	L5	54	0	108	7	0
85	S2	12	0	24	2	0
86	L5	52	0	0	0	0
86	L7	1	0	0	0	0
86	L8	1	0	0	0	0
86	LA	1	0	0	0	0
86	LH	1	0	0	0	0
86	Lf	1	0	0	0	0
86	Lg	1	0	0	0	0
86	S2	17	0	0	0	0
86	SL	1	0	0	0	0
86	Sa	1	0	0	0	0
87	5A	1	0	0	0	0
87	L5	344	0	0	0	0
87	L7	5	0	0	0	0
87	L8	10	0	0	0	0
87	LA	2	0	0	0	0
87	LB	2	0	0	0	0
87	LC	2	0	0	0	0
87	LD	1	0	0	0	0
87	LI	1	0	0	0	0
87	LL	2	0	0	0	0
87	LN	1	0	0	0	0
87	LO	1	0	0	0	0
87	LP	3	0	0	0	0
87	LQ	1	0	0	0	0
87	LR	2	0	0	0	0
87	LS	2	0	0	0	0
87	LV	1	0	0	0	0
87	Lc	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lg	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	Lj	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Lr	1	0	0	0	0
87	Pt	4	0	0	0	0
87	S2	124	0	0	0	0
87	SC	1	0	0	0	0
87	SE	1	0	0	0	0
87	SJ	1	0	0	0	0
87	SN	1	0	0	0	0
87	ST	1	0	0	0	0
87	SX	1	0	0	0	0
87	Sb	1	0	0	0	0
87	Sd	1	0	0	0	0
88	L5	19	0	18	0	0
89	L5	33	0	35	3	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
90	Sd	1	0	0	0	0
90	Sf	1	0	0	0	0
91	Pt	8	0	8	1	0
92	5A	1	0	0	0	0
92	L5	996	0	0	3	0
92	L7	8	0	0	0	0
92	L8	11	0	0	0	0
92	LA	18	0	0	0	0
92	LB	8	0	0	0	0
92	LC	21	0	0	0	0
92	LD	1	0	0	0	0
92	LF	4	0	0	0	0
92	LI	2	0	0	0	0
92	LL	3	0	0	0	0
92	LN	4	0	0	0	0
92	LO	3	0	0	0	0
92	LP	2	0	0	0	0
92	LQ	6	0	0	0	0
92	LR	1	0	0	0	0
92	LT	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	LV	2	0	0	0	0
92	LX	2	0	0	0	0
92	LZ	1	0	0	0	0
92	La	10	0	0	0	0
92	Lb	2	0	0	0	0
92	Lc	1	0	0	0	0
92	Ld	1	0	0	0	0
92	Le	14	0	0	0	0
92	Lf	3	0	0	0	0
92	Lg	4	0	0	0	0
92	Lj	6	0	0	0	0
92	Ln	1	0	0	0	0
92	Lo	1	0	0	0	0
92	Lp	2	0	0	0	0
92	Lr	1	0	0	0	0
92	Pt	1	0	0	0	0
92	S2	123	0	0	1	0
92	SA	1	0	0	0	0
92	SF	1	0	0	0	0
92	SN	1	0	0	0	0
92	SQ	1	0	0	0	0
92	SS	1	0	0	0	0
92	Sa	3	0	0	0	0
All	All	219823	0	162699	2463	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 7.

The worst 5 of 2463 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)
37:Sg:212:LYS:HA	37:Sg:235:ILE:HD12	1.34	1.03
1:S2:394:G:H5''	25:SL:81:LYS:HB3	1.39	1.02
3:L5:1194:G:H3'	3:L5:1195:G:H21	1.35	0.91
12:SF:165:ASN:HD21	12:SF:167:LYS:HG2	1.36	0.91
26:SR:79:GLU:HA	26:SR:83:ASN:HD21	1.35	0.90

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%)	213 (97%)	6 (3%)	0	100	100
6	SA	220/295 (75%)	215 (98%)	5 (2%)	0	100	100
7	SD	224/243 (92%)	212 (95%)	12 (5%)	0	100	100
8	SJ	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
9	SE	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
10	SC	220/293 (75%)	215 (98%)	5 (2%)	0	100	100
11	SG	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
12	SF	187/204 (92%)	180 (96%)	6 (3%)	1 (0%)	24	31
13	SH	187/194 (96%)	179 (96%)	8 (4%)	0	100	100
14	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
15	SI	204/208 (98%)	197 (97%)	7 (3%)	0	100	100
16	SQ	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
17	SU	99/119 (83%)	97 (98%)	2 (2%)	0	100	100
18	SK	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
19	SO	133/151 (88%)	129 (97%)	3 (2%)	1 (1%)	16	20
20	SX	137/143 (96%)	134 (98%)	3 (2%)	0	100	100
21	SM	120/132 (91%)	117 (98%)	3 (2%)	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%)	147 (99%)	2 (1%)	0	100	100
25	SL	142/158 (90%)	138 (97%)	4 (3%)	0	100	100
26	SR	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
27	SP	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
28	ST	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
29	SV	81/83 (98%)	81 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	SY	129/133 (97%)	126 (98%)	3 (2%)	0	100	100
31	SZ	82/125 (66%)	79 (96%)	3 (4%)	0	100	100
32	Sa	98/115 (85%)	98 (100%)	0	0	100	100
33	Sb	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
34	Sc	63/69 (91%)	59 (94%)	4 (6%)	0	100	100
35	Se	46/133 (35%)	45 (98%)	0	1 (2%)	5	4
36	Sf	61/156 (39%)	49 (80%)	10 (16%)	2 (3%)	3	2
37	Sg	311/317 (98%)	287 (92%)	23 (7%)	1 (0%)	36	46
38	Lz	209/217 (96%)	201 (96%)	8 (4%)	0	100	100
39	LA	249/257 (97%)	240 (96%)	9 (4%)	0	100	100
40	LB	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
41	LC	364/427 (85%)	359 (99%)	5 (1%)	0	100	100
42	LJ	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
43	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
44	LE	217/288 (75%)	212 (98%)	5 (2%)	0	100	100
45	LG	239/266 (90%)	230 (96%)	9 (4%)	0	100	100
46	LO	197/203 (97%)	194 (98%)	3 (2%)	0	100	100
47	LL	204/211 (97%)	195 (96%)	9 (4%)	0	100	100
48	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
49	LM	134/215 (62%)	130 (97%)	4 (3%)	0	100	100
50	La	144/148 (97%)	143 (99%)	1 (1%)	0	100	100
51	LN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
52	LI	199/214 (93%)	197 (99%)	2 (1%)	0	100	100
53	LD	292/297 (98%)	286 (98%)	6 (2%)	0	100	100
54	LQ	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
55	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
56	LS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
57	LT	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
58	LP	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
59	LU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
60	LX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	LY	132/145 (91%)	132 (100%)	0	0	100	100
62	LW	114/157 (73%)	110 (96%)	4 (4%)	0	100	100
63	LZ	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
64	Lr	124/137 (90%)	124 (100%)	0	0	100	100
65	Lh	120/123 (98%)	120 (100%)	0	0	100	100
66	Lb	106/159 (67%)	104 (98%)	2 (2%)	0	100	100
67	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
68	Lc	97/115 (84%)	97 (100%)	0	0	100	100
69	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
70	Le	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
71	Lf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
72	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
73	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
74	Lj	85/97 (88%)	83 (98%)	2 (2%)	0	100	100
75	Lk	67/70 (96%)	67 (100%)	0	0	100	100
76	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
77	Lm	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
78	Ln	23/25 (92%)	23 (100%)	0	0	100	100
79	Lo	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
80	Lp	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
83	5A	135/154 (88%)	127 (94%)	7 (5%)	1 (1%)	18	23
All	All	11638/13133 (89%)	11331 (97%)	300 (3%)	7 (0%)	49	60

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	SF	79	HIS
35	Se	119	VAL
37	Sg	234	ASP
83	5A	141	MET
19	SO	138	ASP

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%)	190 (94%)	12 (6%)	18	26
6	SA	183/242 (76%)	178 (97%)	5 (3%)	39	58
7	SD	189/202 (94%)	181 (96%)	8 (4%)	26	40
8	SJ	161/168 (96%)	158 (98%)	3 (2%)	50	69
9	SE	224/225 (100%)	216 (96%)	8 (4%)	31	47
10	SC	188/225 (84%)	181 (96%)	7 (4%)	30	45
11	SG	207/218 (95%)	201 (97%)	6 (3%)	37	55
12	SF	159/170 (94%)	156 (98%)	3 (2%)	50	69
13	SH	168/174 (97%)	164 (98%)	4 (2%)	43	62
14	SW	112/113 (99%)	111 (99%)	1 (1%)	70	84
15	SI	178/180 (99%)	173 (97%)	5 (3%)	38	56
16	SQ	117/121 (97%)	112 (96%)	5 (4%)	26	39
17	SU	93/107 (87%)	90 (97%)	3 (3%)	34	51
18	SK	87/136 (64%)	83 (95%)	4 (5%)	24	36
19	SO	105/119 (88%)	101 (96%)	4 (4%)	29	44
20	SX	111/114 (97%)	108 (97%)	3 (3%)	39	58
21	SM	104/108 (96%)	96 (92%)	8 (8%)	12	16
22	SS	128/132 (97%)	124 (97%)	4 (3%)	35	52
23	Sd	48/49 (98%)	46 (96%)	2 (4%)	26	40
24	SN	131/131 (100%)	124 (95%)	7 (5%)	20	30
25	SL	132/142 (93%)	127 (96%)	5 (4%)	29	44
26	SR	121/122 (99%)	106 (88%)	15 (12%)	4	5
27	SP	117/130 (90%)	112 (96%)	5 (4%)	26	39
28	ST	114/115 (99%)	107 (94%)	7 (6%)	17	24
29	SV	66/66 (100%)	62 (94%)	4 (6%)	17	24
30	SY	113/115 (98%)	108 (96%)	5 (4%)	25	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	SZ	74/103 (72%)	72 (97%)	2 (3%)	39	58
32	Sa	87/98 (89%)	84 (97%)	3 (3%)	32	49
33	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	77
34	Sc	58/62 (94%)	54 (93%)	4 (7%)	14	20
35	Se	40/104 (38%)	38 (95%)	2 (5%)	22	33
36	Sf	56/140 (40%)	48 (86%)	8 (14%)	3	3
37	Sg	272/275 (99%)	250 (92%)	22 (8%)	11	14
38	Lz	189/196 (96%)	178 (94%)	11 (6%)	18	26
39	LA	193/198 (98%)	192 (100%)	1 (0%)	81	90
40	LB	347/348 (100%)	345 (99%)	2 (1%)	78	89
41	LC	305/348 (88%)	302 (99%)	3 (1%)	68	82
42	LJ	143/149 (96%)	137 (96%)	6 (4%)	26	40
43	LH	169/171 (99%)	166 (98%)	3 (2%)	51	70
44	LE	196/252 (78%)	192 (98%)	4 (2%)	48	67
45	LG	203/223 (91%)	199 (98%)	4 (2%)	48	67
46	LO	171/174 (98%)	170 (99%)	1 (1%)	78	89
47	LL	172/177 (97%)	169 (98%)	3 (2%)	53	72
48	LV	102/107 (95%)	101 (99%)	1 (1%)	68	82
49	LM	116/161 (72%)	114 (98%)	2 (2%)	53	72
50	La	119/120 (99%)	117 (98%)	2 (2%)	53	72
51	LN	171/172 (99%)	171 (100%)	0	100	100
52	LI	173/181 (96%)	171 (99%)	2 (1%)	63	79
53	LD	247/250 (99%)	239 (97%)	8 (3%)	34	51
54	LQ	164/165 (99%)	162 (99%)	2 (1%)	63	79
55	LR	166/175 (95%)	161 (97%)	5 (3%)	36	53
56	LS	157/157 (100%)	155 (99%)	2 (1%)	61	77
57	LT	141/140 (101%)	141 (100%)	0	100	100
58	LP	135/163 (83%)	133 (98%)	2 (2%)	57	75
59	LU	89/115 (77%)	86 (97%)	3 (3%)	32	49
60	LX	106/133 (80%)	106 (100%)	0	100	100
61	LY	124/135 (92%)	123 (99%)	1 (1%)	73	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	LW	96/126 (76%)	92 (96%)	4 (4%)	26	40
63	LZ	118/118 (100%)	117 (99%)	1 (1%)	73	86
64	Lr	109/120 (91%)	106 (97%)	3 (3%)	38	56
65	Lh	109/110 (99%)	109 (100%)	0	100	100
66	Lb	90/125 (72%)	86 (96%)	4 (4%)	25	38
67	LF	194/215 (90%)	192 (99%)	2 (1%)	68	82
68	Lc	84/97 (87%)	83 (99%)	1 (1%)	63	79
69	Ld	98/110 (89%)	97 (99%)	1 (1%)	68	82
70	Le	114/121 (94%)	113 (99%)	1 (1%)	70	84
71	Lf	89/89 (100%)	89 (100%)	0	100	100
72	Lg	98/100 (98%)	95 (97%)	3 (3%)	35	52
73	Li	86/89 (97%)	84 (98%)	2 (2%)	44	63
74	Lj	74/80 (92%)	72 (97%)	2 (3%)	39	58
75	Lk	64/65 (98%)	62 (97%)	2 (3%)	35	52
76	Ll	47/48 (98%)	47 (100%)	0	100	100
77	Lm	47/115 (41%)	45 (96%)	2 (4%)	26	39
78	Ln	24/24 (100%)	23 (96%)	1 (4%)	26	40
79	Lo	94/93 (101%)	93 (99%)	1 (1%)	65	81
80	Lp	75/75 (100%)	74 (99%)	1 (1%)	61	77
83	5A	114/127 (90%)	107 (94%)	7 (6%)	17	24
All	All	10142/11170 (91%)	9851 (97%)	291 (3%)	38	55

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	LD	36	LEU
83	5A	59	VAL
54	LQ	14	ARG
64	Lr	124	VAL
24	SN	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
41	LC	329	ASN
52	LI	59	GLN
42	LJ	97	ASN
45	LG	206	GLN
53	LD	250	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1667/1869 (89%)	296 (17%)	2 (0%)
2	L8	155/156 (99%)	26 (16%)	0
3	L5	3651/5069 (72%)	642 (17%)	20 (0%)
4	L7	119/120 (99%)	11 (9%)	0
81	mR	7/60 (11%)	2 (28%)	0
82	Pt	76/77 (98%)	11 (14%)	0
All	All	5675/7351 (77%)	988 (17%)	22 (0%)

5 of 988 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C
1	S2	25	A
1	S2	33	G
1	S2	41	G
1	S2	45	A

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	3958	G
3	L5	4449	A
3	L5	4115	G
3	L5	4699	U
3	L5	1482	G

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

235 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
1	6MZ	S2	1832	86,1,87	22,25,26	1.49	5 (22%)	29,36,39	2.20	9 (31%)
3	OMG	L5	4196	82,87,3	23,26,27	1.22	4 (17%)	32,38,41	1.94	6 (18%)
3	A2M	L5	400	3	22,25,26	1.50	4 (18%)	30,36,39	2.03	6 (20%)
3	A2M	L5	4590	3	22,25,26	1.53	4 (18%)	30,36,39	2.02	10 (33%)
1	PSU	S2	1238	1	18,21,22	1.42	4 (22%)	21,30,33	2.06	4 (19%)
1	A2M	S2	1031	1	22,25,26	1.44	4 (18%)	30,36,39	2.18	10 (33%)
1	OMU	S2	354	1	19,22,23	1.28	3 (15%)	25,31,34	1.77	4 (16%)
3	OMG	L5	4499	3	23,26,27	1.27	4 (17%)	32,38,41	2.03	7 (21%)
3	PSU	L5	4673	87,3	18,21,22	1.45	3 (16%)	21,30,33	2.08	5 (23%)
1	G7M	S2	1639	82,1	23,26,27	2.40	6 (26%)	34,39,42	3.00	10 (29%)
3	A2M	L5	3718	3	22,25,26	1.53	4 (18%)	30,36,39	1.97	7 (23%)
1	OMU	S2	116	1	19,22,23	1.29	3 (15%)	25,31,34	1.77	4 (16%)
3	PSU	L5	3851	87,3	18,21,22	1.48	4 (22%)	21,30,33	2.15	6 (28%)
1	B8N	S2	1248	1	25,29,30	0.86	1 (4%)	28,42,45	1.76	6 (21%)
3	OMU	L5	4306	3	19,22,23	1.23	3 (15%)	25,31,34	1.59	5 (20%)
3	OMU	L5	2415	3	19,22,23	1.32	4 (21%)	25,31,34	1.81	5 (20%)
1	PSU	S2	1244	1	18,21,22	1.43	4 (22%)	21,30,33	2.14	3 (14%)
3	PSU	L5	3639	3	18,21,22	1.72	4 (22%)	21,30,33	2.04	5 (23%)
3	A2M	L5	1326	3	22,25,26	1.56	4 (18%)	30,36,39	2.08	12 (40%)
3	UY1	L5	3818	86,87,3	19,22,23	1.51	4 (21%)	21,31,34	2.00	4 (19%)
3	PSU	L5	4457	3	18,21,22	1.55	4 (22%)	21,30,33	1.94	4 (19%)
1	PSU	S2	1692	1	18,21,22	1.46	4 (22%)	21,30,33	2.10	4 (19%)
3	OMG	L5	3744	3	23,26,27	1.20	4 (17%)	32,38,41	2.03	6 (18%)
3	OMU	L5	4227	3	19,22,23	1.27	2 (10%)	25,31,34	1.84	5 (20%)
1	PSU	S2	863	1	18,21,22	1.42	4 (22%)	21,30,33	2.07	3 (14%)
1	PSU	S2	918	1	18,21,22	1.57	5 (27%)	21,30,33	2.30	5 (23%)
1	PSU	S2	109	86,1	18,21,22	1.66	6 (33%)	21,30,33	2.37	4 (19%)
3	PSU	L5	1860	3	18,21,22	1.40	3 (16%)	21,30,33	2.00	5 (23%)
3	A2M	L5	3867	3	22,25,26	1.57	5 (22%)	30,36,39	2.23	11 (36%)
3	PSU	L5	4552	3	18,21,22	1.51	5 (27%)	21,30,33	2.03	4 (19%)
3	OMG	L5	4618	3	23,26,27	1.18	4 (17%)	32,38,41	2.13	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4361	3	18,21,22	1.42	3 (16%)	21,30,33	2.10	5 (23%)
82	OMC	Pt	33	82	19,22,23	0.79	1 (5%)	25,31,34	0.74	0
3	PSU	L5	3844	3	18,21,22	1.51	5 (27%)	21,30,33	2.09	4 (19%)
3	A2M	L5	2363	87,3	22,25,26	1.55	5 (22%)	30,36,39	2.04	9 (30%)
3	OMG	L5	4637	86,3	23,26,27	1.26	3 (13%)	32,38,41	1.94	6 (18%)
2	PSU	L8	55	2	18,21,22	1.45	3 (16%)	21,30,33	2.08	5 (23%)
40	HIC	LB	245	40	10,11,12	1.44	2 (20%)	9,14,16	1.06	1 (11%)
1	A2M	S2	668	1,87	22,25,26	1.51	5 (22%)	30,36,39	2.10	10 (33%)
3	OMG	L5	1316	3	23,26,27	1.32	4 (17%)	32,38,41	2.20	8 (25%)
3	A2M	L5	3723	3	22,25,26	1.47	4 (18%)	30,36,39	2.04	8 (26%)
3	PSU	L5	3920	87,3	18,21,22	1.45	3 (16%)	21,30,33	2.34	4 (19%)
1	PSU	S2	406	1	18,21,22	1.44	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	3729	3	18,21,22	1.42	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	1779	3	18,21,22	1.43	4 (22%)	21,30,33	2.09	4 (19%)
3	A2M	L5	4571	3	22,25,26	1.50	4 (18%)	30,36,39	2.09	7 (23%)
1	A2M	S2	484	1	22,25,26	1.49	4 (18%)	30,36,39	2.03	7 (23%)
1	A2M	S2	1383	1	22,25,26	1.49	5 (22%)	30,36,39	2.26	11 (36%)
3	PSU	L5	4531	3	18,21,22	1.41	4 (22%)	21,30,33	2.11	3 (14%)
3	OMC	L5	3887	3	19,22,23	0.82	0	25,31,34	0.82	0
3	PSU	L5	4353	3	18,21,22	1.53	4 (22%)	21,30,33	2.30	3 (14%)
3	PSU	L5	4576	3	18,21,22	1.43	4 (22%)	21,30,33	2.11	3 (14%)
1	OMC	S2	1703	1,87	19,22,23	0.75	0	25,31,34	0.74	0
3	A2M	L5	3785	3	22,25,26	1.47	5 (22%)	30,36,39	2.30	12 (40%)
1	A2M	S2	159	1	22,25,26	1.46	4 (18%)	30,36,39	2.15	9 (30%)
3	PSU	L5	4521	86,87,3	18,21,22	1.49	3 (16%)	21,30,33	2.20	5 (23%)
1	PSU	S2	1136	1	18,21,22	1.45	3 (16%)	21,30,33	2.23	4 (19%)
1	A2M	S2	590	1	22,25,26	1.47	4 (18%)	30,36,39	2.10	7 (23%)
3	PSU	L5	4500	3	18,21,22	1.39	4 (22%)	21,30,33	2.20	4 (19%)
3	PSU	L5	3715	3	18,21,22	1.42	4 (22%)	21,30,33	2.22	4 (19%)
3	PSU	L5	3762	3	18,21,22	1.40	3 (16%)	21,30,33	2.07	4 (19%)
1	PSU	S2	105	1	18,21,22	1.51	4 (22%)	21,30,33	2.19	4 (19%)
1	OMU	S2	1804	1	19,22,23	1.33	4 (21%)	25,31,34	1.92	5 (20%)
3	OMC	L5	3701	86,3	19,22,23	0.82	0	25,31,34	1.00	1 (4%)
3	6MZ	L5	4220	3	22,25,26	1.42	4 (18%)	29,36,39	2.29	11 (37%)
3	PSU	L5	3637	86,87,3	18,21,22	1.40	3 (16%)	21,30,33	2.44	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	822	1	18,21,22	1.46	3 (16%)	21,30,33	2.29	5 (23%)
3	A2M	L5	2815	87,3	22,25,26	1.34	4 (18%)	30,36,39	2.23	7 (23%)
1	OMG	S2	644	1	23,26,27	1.23	3 (13%)	32,38,41	1.98	6 (18%)
3	OMG	L5	3899	3	23,26,27	1.26	4 (17%)	32,38,41	2.16	8 (25%)
2	PSU	L8	69	2	18,21,22	1.46	4 (22%)	21,30,33	2.10	5 (23%)
3	PSU	L5	2508	3	18,21,22	1.33	3 (16%)	21,30,33	1.98	4 (19%)
1	A2M	S2	99	1,87	22,25,26	1.49	4 (18%)	30,36,39	2.12	7 (23%)
1	OMG	S2	867	1	23,26,27	1.18	3 (13%)	32,38,41	1.94	6 (18%)
3	PSU	L5	1862	3	18,21,22	1.57	3 (16%)	21,30,33	1.99	5 (23%)
3	OMC	L5	2824	3	19,22,23	0.81	1 (5%)	25,31,34	0.84	0
66	MLZ	Lb	5	66	8,9,10	0.94	0	4,9,11	1.13	0
1	PSU	S2	1643	1,87	18,21,22	1.49	3 (16%)	21,30,33	2.16	5 (23%)
3	PSU	L5	2839	3	18,21,22	1.62	3 (16%)	21,30,33	1.94	4 (19%)
79	MLZ	Lo	53	79	8,9,10	0.74	0	4,9,11	0.82	0
3	PSU	L5	3734	3	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
29	AME	SV	1	29	9,10,11	3.24	2 (22%)	9,11,13	3.93	3 (33%)
1	A2M	S2	1678	1	22,25,26	1.46	4 (18%)	30,36,39	2.10	9 (30%)
1	PSU	S2	1232	1	18,21,22	1.51	4 (22%)	21,30,33	2.16	4 (19%)
3	OMU	L5	4498	87,3	19,22,23	1.32	3 (15%)	25,31,34	1.88	5 (20%)
3	OMG	L5	4370	3	23,26,27	1.21	4 (17%)	32,38,41	2.03	6 (18%)
3	PSU	L5	5010	3	18,21,22	1.49	4 (22%)	21,30,33	2.15	4 (19%)
3	PSU	L5	3758	3	18,21,22	1.45	4 (22%)	21,30,33	2.10	4 (19%)
3	OMG	L5	3792	3	23,26,27	1.23	4 (17%)	32,38,41	1.92	6 (18%)
1	PSU	S2	34	1	18,21,22	1.45	4 (22%)	21,30,33	2.20	4 (19%)
3	5MC	L5	4447	86,3	19,22,23	1.71	3 (15%)	26,32,35	1.32	3 (11%)
3	PSU	L5	4431	3	18,21,22	1.43	3 (16%)	21,30,33	2.00	4 (19%)
50	V5N	La	39	50	8,11,12	1.50	1 (12%)	8,14,16	1.93	2 (25%)
3	PSU	L5	4312	3	18,21,22	1.41	3 (16%)	21,30,33	2.02	4 (19%)
3	OMC	L5	4456	3	19,22,23	0.82	1 (5%)	25,31,34	0.71	0
3	OMC	L5	3841	3	19,22,23	0.80	1 (5%)	25,31,34	0.94	0
1	PSU	S2	1056	1	18,21,22	1.44	4 (22%)	21,30,33	2.14	6 (28%)
1	PSU	S2	1367	1	18,21,22	1.48	4 (22%)	21,30,33	2.12	3 (14%)
3	OMG	L5	4392	3	23,26,27	1.24	4 (17%)	32,38,41	2.04	7 (21%)
3	OMC	L5	2861	3	19,22,23	0.73	0	25,31,34	0.73	0
3	A2M	L5	1534	87,3	22,25,26	1.55	5 (22%)	30,36,39	2.12	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	S2	174	1	19,22,23	0.78	0	25,31,34	0.89	1 (4%)
1	OMG	S2	1490	1,87	23,26,27	1.28	4 (17%)	32,38,41	2.17	7 (21%)
3	OMC	L5	2365	87,3	19,22,23	0.77	0	25,31,34	0.79	0
3	OMG	L5	3944	3	23,26,27	1.20	3 (13%)	32,38,41	1.98	6 (18%)
1	OMU	S2	121	1	19,22,23	1.32	3 (15%)	25,31,34	1.80	4 (16%)
1	PSU	S2	866	1	18,21,22	1.43	4 (22%)	21,30,33	2.10	3 (14%)
3	PSU	L5	1536	3	18,21,22	1.40	3 (16%)	21,30,33	2.27	4 (19%)
1	PSU	S2	1174	1,87	18,21,22	1.46	4 (22%)	21,30,33	2.10	4 (19%)
3	OMU	L5	4620	3	19,22,23	1.25	3 (15%)	25,31,34	1.92	5 (20%)
3	PSU	L5	4293	3	18,21,22	1.48	3 (16%)	21,30,33	2.15	5 (23%)
3	PSU	L5	4296	3	18,21,22	1.45	4 (22%)	21,30,33	2.18	4 (19%)
1	OMG	S2	601	1	23,26,27	1.24	3 (13%)	32,38,41	1.93	5 (15%)
2	OMG	L8	75	2	23,26,27	1.23	4 (17%)	32,38,41	1.94	7 (21%)
1	PSU	S2	1004	1	18,21,22	1.60	5 (27%)	21,30,33	2.19	4 (19%)
1	OMG	S2	1447	1	23,26,27	1.22	3 (13%)	32,38,41	2.05	6 (18%)
3	PSU	L5	1677	3	18,21,22	1.53	5 (27%)	21,30,33	2.38	4 (19%)
3	OMG	L5	2876	3	23,26,27	1.29	3 (13%)	32,38,41	2.01	6 (18%)
82	H2U	Pt	21	82	18,21,22	0.98	2 (11%)	19,30,33	0.94	1 (5%)
82	G7M	Pt	47	82	23,26,27	1.83	2 (8%)	34,39,42	1.11	1 (2%)
3	PSU	L5	4689	3	18,21,22	1.49	4 (22%)	21,30,33	2.20	5 (23%)
3	PSU	L5	4532	3	18,21,22	1.58	3 (16%)	21,30,33	1.97	5 (23%)
3	1MA	L5	1322	87,3	21,25,26	1.39	4 (19%)	30,37,40	1.73	6 (20%)
3	OMC	L5	2804	3	19,22,23	0.79	0	25,31,34	0.98	2 (8%)
3	OMC	L5	1881	87,3	19,22,23	0.82	0	25,31,34	1.06	1 (4%)
82	4SU	Pt	8	82	18,21,22	2.14	5 (27%)	25,30,33	2.48	6 (24%)
1	OMU	S2	172	1	19,22,23	1.28	4 (21%)	25,31,34	1.87	5 (20%)
1	PSU	S2	572	1	18,21,22	1.44	3 (16%)	21,30,33	2.13	5 (23%)
1	OMG	S2	1328	86,1	23,26,27	1.21	3 (13%)	32,38,41	1.98	5 (15%)
3	OMU	L5	3925	3	19,22,23	1.33	2 (10%)	25,31,34	2.02	5 (20%)
3	PSU	L5	4636	3	18,21,22	1.52	4 (22%)	21,30,33	2.11	5 (23%)
3	A2M	L5	2401	3	22,25,26	1.48	5 (22%)	30,36,39	2.11	10 (33%)
1	OMU	S2	1288	1	19,22,23	1.29	3 (15%)	25,31,34	1.99	6 (24%)
1	PSU	S2	966	1	18,21,22	1.44	4 (22%)	21,30,33	2.07	3 (14%)
3	PSU	L5	2632	3	18,21,22	1.44	4 (22%)	21,30,33	2.05	5 (23%)
1	PSU	S2	814	1	18,21,22	1.45	3 (16%)	21,30,33	2.04	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	119	1	18,21,22	1.38	4 (22%)	21,30,33	2.13	4 (19%)
1	OMC	S2	517	1	19,22,23	0.77	0	25,31,34	0.70	0
3	A2M	L5	3724	3	22,25,26	1.44	5 (22%)	30,36,39	2.08	11 (36%)
3	PSU	L5	1792	3	18,21,22	1.41	4 (22%)	21,30,33	2.05	3 (14%)
3	OMG	L5	2364	3	23,26,27	1.41	4 (17%)	32,38,41	2.05	8 (25%)
3	OMG	L5	2424	3	23,26,27	1.24	3 (13%)	32,38,41	1.98	6 (18%)
1	PSU	S2	609	1	18,21,22	1.44	4 (22%)	21,30,33	2.10	3 (14%)
1	A2M	S2	576	1	22,25,26	1.51	5 (22%)	30,36,39	2.02	9 (30%)
3	PSU	L5	1782	3	18,21,22	1.41	3 (16%)	21,30,33	2.13	3 (14%)
1	PSU	S2	801	1	18,21,22	1.39	3 (16%)	21,30,33	2.09	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.51	4 (22%)	21,30,33	2.15	3 (14%)
3	PSU	L5	3764	3	18,21,22	1.45	4 (22%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4423	3	18,21,22	1.47	3 (16%)	21,30,33	2.19	5 (23%)
3	A2M	L5	2787	3	22,25,26	1.52	4 (18%)	30,36,39	2.30	8 (26%)
1	PSU	S2	36	1	18,21,22	1.44	4 (22%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4569	3	18,21,22	1.46	4 (22%)	21,30,33	2.30	6 (28%)
83	5CT	5A	50[B]	-	13,14,15	1.10	1 (7%)	8,15,17	0.99	0
1	OMU	S2	428	1	19,22,23	1.25	3 (15%)	25,31,34	1.86	5 (20%)
1	OMC	S2	1391	1	19,22,23	0.79	0	25,31,34	0.83	0
3	PSU	L5	4972	3	18,21,22	1.63	5 (27%)	21,30,33	2.33	5 (23%)
3	PSU	L5	1582	3	18,21,22	1.51	4 (22%)	21,30,33	2.11	5 (23%)
3	PSU	L5	4403	3	18,21,22	1.48	4 (22%)	21,30,33	2.15	5 (23%)
1	PSU	S2	649	1	18,21,22	1.40	4 (22%)	21,30,33	2.19	3 (14%)
1	4AC	S2	1337	1	21,24,25	1.05	1 (4%)	28,34,37	1.17	4 (14%)
3	A2M	L5	1871	87,3	22,25,26	1.35	5 (22%)	30,36,39	2.39	11 (36%)
3	OMC	L5	4536	3	19,22,23	0.87	2 (10%)	25,31,34	0.96	2 (8%)
1	PSU	S2	1177	1	18,21,22	1.56	4 (22%)	21,30,33	2.05	4 (19%)
3	A2M	L5	3830	3	22,25,26	1.47	4 (18%)	30,36,39	2.31	11 (36%)
1	OMG	S2	509	1,87	23,26,27	1.19	3 (13%)	32,38,41	2.03	5 (15%)
3	OMG	L5	4494	87,3	23,26,27	1.27	3 (13%)	32,38,41	2.14	7 (21%)
1	PSU	S2	686	1	18,21,22	1.43	4 (22%)	21,30,33	2.12	3 (14%)
1	4AC	S2	1842	1	21,24,25	1.07	1 (4%)	28,34,37	1.31	6 (21%)
1	A2M	S2	27	1,87	22,25,26	1.46	4 (18%)	30,36,39	2.08	11 (36%)
1	PSU	S2	1081	1	18,21,22	1.47	4 (22%)	21,30,33	2.09	5 (23%)
82	PSU	Pt	56	82	18,21,22	1.35	3 (16%)	21,30,33	2.10	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	L5	2837	3	19,22,23	1.35	3 (15%)	25,31,34	2.04	6 (24%)
3	OMG	L5	3627	3	23,26,27	1.24	4 (17%)	32,38,41	2.09	7 (21%)
3	OMG	L5	1522	3	23,26,27	1.14	2 (8%)	32,38,41	2.08	11 (34%)
1	PSU	S2	1347	1	18,21,22	1.51	4 (22%)	21,30,33	2.11	4 (19%)
3	A2M	L5	3825	3	22,25,26	1.57	4 (18%)	30,36,39	2.01	9 (30%)
1	OMU	S2	1442	1,87	19,22,23	1.28	3 (15%)	25,31,34	1.80	4 (16%)
1	PSU	S2	296	1	18,21,22	1.43	4 (22%)	21,30,33	2.11	4 (19%)
3	PSU	L5	4493	87,3	18,21,22	1.43	4 (22%)	21,30,33	2.03	3 (14%)
3	OMG	L5	4623	3	23,26,27	1.27	4 (17%)	32,38,41	1.99	6 (18%)
3	PSU	L5	1683	86,3	18,21,22	1.45	4 (22%)	21,30,33	2.22	3 (14%)
3	A2M	L5	3760	1,87,3	22,25,26	1.49	5 (22%)	30,36,39	2.12	9 (30%)
3	UR3	L5	4530	3	19,22,23	0.82	1 (5%)	26,32,35	1.83	3 (11%)
3	PSU	L5	5001	87,3	18,21,22	1.55	4 (22%)	21,30,33	2.23	5 (23%)
3	PSU	L5	3770	3	18,21,22	1.49	5 (27%)	21,30,33	2.14	3 (14%)
3	5MC	L5	3782	87,3	19,22,23	1.80	3 (15%)	26,32,35	1.19	3 (11%)
3	OMG	L5	1625	86,87,3	23,26,27	1.28	3 (13%)	32,38,41	2.10	8 (25%)
3	OMG	L5	4228	3	23,26,27	1.19	4 (17%)	32,38,41	2.02	9 (28%)
6	SAC	SA	2	6	7,8,9	3.81	2 (28%)	7,9,11	4.43	3 (42%)
1	PSU	S2	651	1	18,21,22	1.46	4 (22%)	21,30,33	2.14	4 (19%)
1	PSU	S2	681	1	18,21,22	1.48	4 (22%)	21,30,33	2.17	4 (19%)
20	HY3	SX	62	20	7,8,9	1.35	1 (14%)	7,10,12	1.57	2 (28%)
64	SAC	Lr	2	64	7,8,9	3.82	2 (28%)	7,9,11	4.07	3 (42%)
3	OMC	L5	3808	87,3	19,22,23	0.80	1 (5%)	25,31,34	0.82	1 (4%)
3	PSU	L5	1744	87,3	18,21,22	1.45	3 (16%)	21,30,33	2.09	3 (14%)
1	A2M	S2	512	1	22,25,26	1.43	4 (18%)	30,36,39	2.17	9 (30%)
1	PSU	S2	1243	1	18,21,22	1.46	4 (22%)	21,30,33	2.14	4 (19%)
1	PSU	S2	1239	1	18,21,22	1.45	4 (22%)	21,30,33	2.15	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.51	5 (22%)	30,36,39	2.27	9 (30%)
3	PSU	L5	3768	3	18,21,22	1.41	4 (22%)	21,30,33	2.15	4 (19%)
1	OMG	S2	683	1	23,26,27	1.19	4 (17%)	32,38,41	2.01	7 (21%)
1	PSU	S2	218	1	18,21,22	1.42	4 (22%)	21,30,33	2.10	4 (19%)
1	PSU	S2	1445	1	18,21,22	1.38	3 (16%)	21,30,33	2.06	4 (19%)
1	A2M	S2	468	1	22,25,26	1.47	5 (22%)	30,36,39	2.12	10 (33%)
1	A2M	S2	166	1	22,25,26	1.47	4 (18%)	30,36,39	2.25	9 (30%)
1	PSU	S2	815	1	18,21,22	1.41	4 (22%)	21,30,33	2.05	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	398	3	22,25,26	1.48	4 (18%)	30,36,39	2.21	10 (33%)
1	OMG	S2	436	1	23,26,27	1.24	3 (13%)	32,38,41	2.13	6 (18%)
3	PSU	L5	3884	87,3	18,21,22	1.44	3 (16%)	21,30,33	2.30	5 (23%)
1	PSU	S2	573	1	18,21,22	1.43	3 (16%)	21,30,33	2.09	4 (19%)
1	OMU	S2	627	1	19,22,23	1.23	3 (15%)	25,31,34	1.85	5 (20%)
3	PSU	L5	4628	3	18,21,22	1.45	6 (33%)	21,30,33	2.19	5 (23%)
2	OMU	L8	14	2,3	19,22,23	1.30	3 (15%)	25,31,34	1.65	5 (20%)
39	V5N	LA	216	39	8,11,12	1.62	1 (12%)	8,14,16	1.68	1 (12%)
3	PSU	L5	3853	87,3	18,21,22	1.43	3 (16%)	21,30,33	2.30	4 (19%)
3	PSU	L5	4299	3	18,21,22	1.53	5 (27%)	21,30,33	2.12	5 (23%)
3	A2M	L5	4523	87,3	22,25,26	1.42	4 (18%)	30,36,39	2.49	11 (36%)
3	PSU	L5	4442	3	18,21,22	1.48	5 (27%)	21,30,33	2.16	6 (28%)
1	MA6	S2	1851	1	23,26,27	1.44	4 (17%)	33,38,41	2.18	11 (33%)
1	PSU	S2	93	1	18,21,22	1.54	3 (16%)	21,30,33	1.96	5 (23%)
3	PSU	L5	4579	3	18,21,22	1.46	4 (22%)	21,30,33	2.04	3 (14%)
3	PSU	L5	4471	3	18,21,22	1.42	3 (16%)	21,30,33	1.97	3 (14%)
3	PSU	L5	3695	3	18,21,22	1.41	4 (22%)	21,30,33	2.17	5 (23%)
1	UY1	S2	1326	1,87	19,22,23	1.49	4 (21%)	21,31,34	2.32	4 (19%)
1	PSU	S2	1625	1	18,21,22	1.45	4 (22%)	21,30,33	2.11	4 (19%)
1	MA6	S2	1850	1	23,26,27	1.39	5 (21%)	33,38,41	2.21	11 (33%)
77	M3L	Lm	98	77	10,11,12	0.57	0	9,14,16	0.50	0
83	5CT	5A	50[A]	87	13,14,15	1.09	1 (7%)	8,15,17	1.32	1 (12%)
3	PSU	L5	2843	3	18,21,22	1.47	3 (16%)	21,30,33	2.25	5 (23%)
3	PSU	L5	4420	3	18,21,22	1.49	5 (27%)	21,30,33	2.02	3 (14%)
1	OMC	S2	462	1	19,22,23	0.78	0	25,31,34	0.81	0
3	OMC	L5	3869	3	19,22,23	0.81	1 (5%)	25,31,34	1.07	1 (4%)
3	OMC	L5	2351	87,3	19,22,23	0.80	0	25,31,34	1.22	2 (8%)
3	OMC	L5	1340	3	19,22,23	0.73	0	25,31,34	0.95	0
3	OMC	L5	2422	87,3	19,22,23	0.80	0	25,31,34	0.81	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
1	6MZ	S2	1832	86,1,87	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	4196	82,87,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4673	87,3	-	0/7/25/26	0/2/2/2
1	G7M	S2	1639	82,1	-	0/7/25/26	0/3/3/3
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	3851	87,3	-	1/7/25/26	0/2/2/2
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	1/9/27/28	0/3/3/3
3	UY1	L5	3818	86,87,3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	918	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	109	86,1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
82	OMC	Pt	33	82	-	0/9/27/28	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	2363	87,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4637	86,3	-	1/9/27/28	0/3/3/3
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
40	HIC	LB	245	40	-	0/5/6/8	0/1/1/1
1	A2M	S2	668	1,87	-	5/9/27/28	0/3/3/3
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3729	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	1,87	-	0/9/27/28	0/2/2/2
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
1	A2M	S2	159	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4521	86,87,3	-	2/7/25/26	0/2/2/2
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	590	1	-	4/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	0/9/27/28	0/2/2/2
3	OMC	L5	3701	86,3	-	4/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3637	86,87,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2
3	A2M	L5	2815	87,3	-	4/9/27/28	0/3/3/3
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
2	PSU	L8	69	2	-	0/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	99	1,87	-	0/9/27/28	0/3/3/3
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
66	MLZ	Lb	5	66	-	0/7/8/10	-
1	PSU	S2	1643	1,87	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
79	MLZ	Lo	53	79	-	3/7/8/10	-
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
29	AME	SV	1	29	-	3/9/10/12	-
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	87,3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	86,3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
50	V5N	La	39	50	-	0/9/10/12	0/1/1/1
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	1534	87,3	-	2/9/27/28	0/3/3/3
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	1490	1,87	-	3/9/27/28	0/3/3/3
3	OMC	L5	2365	87,3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1174	1,87	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
2	OMG	L8	75	2	-	0/9/27/28	0/3/3/3
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1447	1	-	3/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
82	H2U	Pt	21	82	-	3/7/38/39	0/2/2/2
82	G7M	Pt	47	82	-	1/7/25/26	0/3/3/3
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	1MA	L5	1322	87,3	-	2/7/25/26	0/3/3/3
3	OMC	L5	2804	3	-	1/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	1881	87,3	-	0/9/27/28	0/2/2/2
82	4SU	Pt	8	82	-	0/7/25/26	0/2/2/2
1	OMU	S2	172	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	1328	86,1	-	1/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	1288	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	2/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3764	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	3/9/27/28	0/3/3/3
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
83	5CT	5A	50[B]	-	-	9/13/14/16	-
1	OMU	S2	428	1	-	2/9/27/28	0/2/2/2
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
3	A2M	L5	1871	87,3	-	0/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
1	OMG	S2	509	1,87	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	4494	87,3	-	0/9/27/28	0/3/3/3
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	A2M	S2	27	1,87	-	1/9/27/28	0/3/3/3
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
82	PSU	Pt	56	82	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
1	OMU	S2	1442	1,87	-	3/9/27/28	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1683	86,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3760	1,87,3	-	6/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1625	86,87,3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	1/9/27/28	0/3/3/3
6	SAC	SA	2	6	-	4/7/8/10	-
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
64	SAC	Lr	2	64	-	4/7/8/10	-
3	OMC	L5	3808	87,3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
1	A2M	S2	512	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	166	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	3884	87,3	-	0/7/25/26	0/2/2/2
1	PSU	S2	573	1	-	1/7/25/26	0/2/2/2
1	OMU	S2	627	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
2	OMU	L8	14	2,3	-	1/9/27/28	0/2/2/2
39	V5N	LA	216	39	-	1/9/10/12	0/1/1/1
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	87,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	3/11/29/30	0/3/3/3
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	1/7/25/26	0/2/2/2
1	UY1	S2	1326	1,87	-	1/9/27/28	0/2/2/2
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
77	M3L	Lm	98	77	-	0/9/10/12	-
83	5CT	5A	50[A]	87	-	9/13/14/16	-
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	2/7/25/26	0/2/2/2
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2351	87,3	-	2/9/27/28	0/2/2/2
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2422	87,3	-	2/9/27/28	0/2/2/2

The worst 5 of 776 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	Lr	2	SAC	OAC-C1A	9.03	1.43	1.23
6	SA	2	SAC	OAC-C1A	8.95	1.43	1.23
29	SV	1	AME	OT-CT1	8.80	1.42	1.23
82	Pt	47	G7M	C8-N7	7.19	1.45	1.33
1	S2	1639	G7M	C8-N7	7.09	1.45	1.33

The worst 5 of 1159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	SA	2	SAC	OAC-C1A-C2A	-8.31	107.26	122.05
1	S2	1639	G7M	CN7-N7-C8	-7.92	112.80	124.79
29	SV	1	AME	OT-CT1-N	-7.88	108.06	121.98
3	L5	3637	PSU	N1-C2-N3	7.64	123.23	115.17
64	Lr	2	SAC	OAC-C1A-N	-7.53	108.67	121.98

There are no chirality outliers.

5 of 169 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
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 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1832	6MZ	1	0
3	L5	4196	OMG	2	0
3	L5	400	A2M	1	0
1	S2	354	OMU	1	0
1	S2	1639	G7M	2	0
3	L5	3718	A2M	4	0
1	S2	116	OMU	2	0
3	L5	2415	OMU	3	0
3	L5	4457	PSU	2	0
1	S2	1692	PSU	1	0
1	S2	109	PSU	1	0
3	L5	3867	A2M	2	0
3	L5	4552	PSU	1	0
3	L5	4618	OMG	2	0
82	Pt	33	OMC	1	0
3	L5	2363	A2M	2	0
3	L5	4637	OMG	1	0
1	S2	668	A2M	1	0
3	L5	3723	A2M	3	0
3	L5	3729	PSU	1	0
3	L5	4571	A2M	1	0
1	S2	484	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1383	A2M	3	0
3	L5	4531	PSU	1	0
3	L5	3785	A2M	1	0
1	S2	159	A2M	2	0
3	L5	3762	PSU	1	0
3	L5	3701	OMC	1	0
3	L5	4220	6MZ	1	0
3	L5	2815	A2M	3	0
1	S2	644	OMG	1	0
3	L5	3899	OMG	1	0
3	L5	2508	PSU	2	0
1	S2	99	A2M	2	0
1	S2	867	OMG	1	0
3	L5	3734	PSU	1	0
1	S2	1678	A2M	1	0
1	S2	1232	PSU	1	0
3	L5	4498	OMU	1	0
3	L5	4370	OMG	1	0
3	L5	4447	5MC	1	0
3	L5	4456	OMC	2	0
3	L5	4392	OMG	1	0
3	L5	2861	OMC	1	0
1	S2	1490	OMG	2	0
3	L5	3944	OMG	1	0
3	L5	1536	PSU	1	0
3	L5	4620	OMU	1	0
2	L8	75	OMG	1	0
1	S2	1004	PSU	1	0
1	S2	1447	OMG	1	0
3	L5	2876	OMG	1	0
82	Pt	21	H2U	1	0
3	L5	2804	OMC	1	0
3	L5	1881	OMC	1	0
1	S2	1288	OMU	1	0
3	L5	2632	PSU	1	0
3	L5	3724	A2M	1	0
3	L5	2364	OMG	1	0
1	S2	576	A2M	3	0
3	L5	1781	PSU	1	0
3	L5	2787	A2M	1	0
83	5A	50[B]	5CT	5	0
1	S2	1391	OMC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	649	PSU	1	0
3	L5	1871	A2M	2	0
1	S2	509	OMG	1	0
1	S2	27	A2M	1	0
82	Pt	56	PSU	2	0
1	S2	1442	OMU	1	0
3	L5	1683	PSU	1	0
3	L5	4530	UR3	1	0
3	L5	5001	PSU	1	0
3	L5	3770	PSU	1	0
1	S2	512	A2M	2	0
1	S2	1239	PSU	1	0
3	L5	1524	A2M	1	0
1	S2	218	PSU	1	0
1	S2	166	A2M	2	0
3	L5	398	A2M	1	0
1	S2	573	PSU	2	0
2	L8	14	OMU	1	0
3	L5	4442	PSU	1	0
3	L5	4579	PSU	1	0
83	5A	50[A]	5CT	4	0
1	S2	462	OMC	1	0
3	L5	2351	OMC	1	0
3	L5	1340	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 636 ligands modelled in this entry, 609 are monoatomic - leaving 27 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
91	MET	Pt	78	82	6,7,8	0.65	0	2,7,9	1.36	0
84	SPD	L5	5504	-	9,9,9	0.39	0	8,8,8	1.02	0
85	PUT	L5	5515	-	5,5,5	0.13	0	4,4,4	0.16	0
85	PUT	L5	5518	-	5,5,5	0.18	0	4,4,4	0.22	0
84	SPD	L5	5510	-	9,9,9	0.28	0	8,8,8	0.74	0
84	SPD	L5	5512	-	9,9,9	0.38	0	8,8,8	0.60	0
84	SPD	L5	5505	-	9,9,9	0.42	0	8,8,8	1.10	1 (12%)
85	PUT	L5	5520	-	5,5,5	0.16	0	4,4,4	0.25	0
89	3H3	L5	5523	-	34,34,34	3.30	13 (38%)	36,45,45	3.67	18 (50%)
85	PUT	S2	1903	-	5,5,5	0.07	0	4,4,4	0.15	0
85	PUT	L5	5514	-	5,5,5	0.13	0	4,4,4	0.20	0
84	SPD	L5	5503	-	9,9,9	0.29	0	8,8,8	1.02	1 (12%)
88	ANM	L5	5501	86	20,20,20	1.24	2 (10%)	24,27,27	1.56	6 (25%)
85	PUT	L5	5519	-	5,5,5	0.14	0	4,4,4	0.25	0
84	SPD	L5	5509	-	9,9,9	0.22	0	8,8,8	0.49	0
84	SPD	L5	5506	-	9,9,9	0.16	0	8,8,8	0.22	0
84	SPD	L5	5507	-	9,9,9	0.33	0	8,8,8	0.80	0
84	SPD	L5	5502	-	9,9,9	0.35	0	8,8,8	0.71	0
85	PUT	L5	5517	-	5,5,5	0.11	0	4,4,4	0.13	0
84	SPD	L5	5513	-	9,9,9	0.28	0	8,8,8	0.79	0
85	PUT	L5	5516	-	5,5,5	0.11	0	4,4,4	0.19	0
85	PUT	L5	5522	-	5,5,5	0.07	0	4,4,4	0.14	0
84	SPD	L5	5508	-	9,9,9	0.36	0	8,8,8	0.54	0
84	SPD	L5	5511	-	9,9,9	0.28	0	8,8,8	0.97	1 (12%)
85	PUT	S2	1902	-	5,5,5	0.11	0	4,4,4	0.15	0
84	SPD	S2	1901	-	9,9,9	0.31	0	8,8,8	0.68	0
85	PUT	L5	5521	-	5,5,5	0.07	0	4,4,4	0.21	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
91	MET	Pt	78	82	-	2/5/6/8	-
84	SPD	L5	5504	-	-	4/7/7/7	-
85	PUT	L5	5515	-	-	1/3/3/3	-
85	PUT	L5	5518	-	-	1/3/3/3	-
84	SPD	L5	5510	-	-	4/7/7/7	-
84	SPD	L5	5512	-	-	2/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	SPD	L5	5505	-	-	4/7/7/7	-
85	PUT	L5	5520	-	-	1/3/3/3	-
89	3H3	L5	5523	-	-	15/39/51/51	0/1/2/2
85	PUT	S2	1903	-	-	0/3/3/3	-
85	PUT	L5	5514	-	-	0/3/3/3	-
84	SPD	L5	5503	-	-	2/7/7/7	-
88	ANM	L5	5501	86	-	2/10/23/23	0/2/2/2
85	PUT	L5	5519	-	-	1/3/3/3	-
84	SPD	L5	5509	-	-	3/7/7/7	-
84	SPD	L5	5506	-	-	4/7/7/7	-
84	SPD	L5	5507	-	-	4/7/7/7	-
84	SPD	L5	5502	-	-	0/7/7/7	-
85	PUT	L5	5517	-	-	0/3/3/3	-
84	SPD	L5	5513	-	-	2/7/7/7	-
85	PUT	L5	5516	-	-	2/3/3/3	-
85	PUT	L5	5522	-	-	2/3/3/3	-
84	SPD	L5	5508	-	-	2/7/7/7	-
84	SPD	L5	5511	-	-	3/7/7/7	-
85	PUT	S2	1902	-	-	1/3/3/3	-
84	SPD	S2	1901	-	-	4/7/7/7	-
85	PUT	L5	5521	-	-	0/3/3/3	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	L5	5523	3H3	C13-C12	8.94	1.53	1.33
89	L5	5523	3H3	O3-C22	7.66	1.38	1.23
89	L5	5523	3H3	O4-C23	7.27	1.37	1.23
89	L5	5523	3H3	C23-N	6.65	1.48	1.37
89	L5	5523	3H3	C22-N	5.58	1.46	1.37

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	L5	5523	3H3	O3-C22-N	-10.22	104.55	120.30
89	L5	5523	3H3	C22-N-C23	-9.57	114.34	125.87
89	L5	5523	3H3	O4-C23-N	-8.78	106.76	120.30
89	L5	5523	3H3	O3-C22-C21	-6.56	110.10	122.62
89	L5	5523	3H3	C15-C14-C13	-5.99	104.99	110.73

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

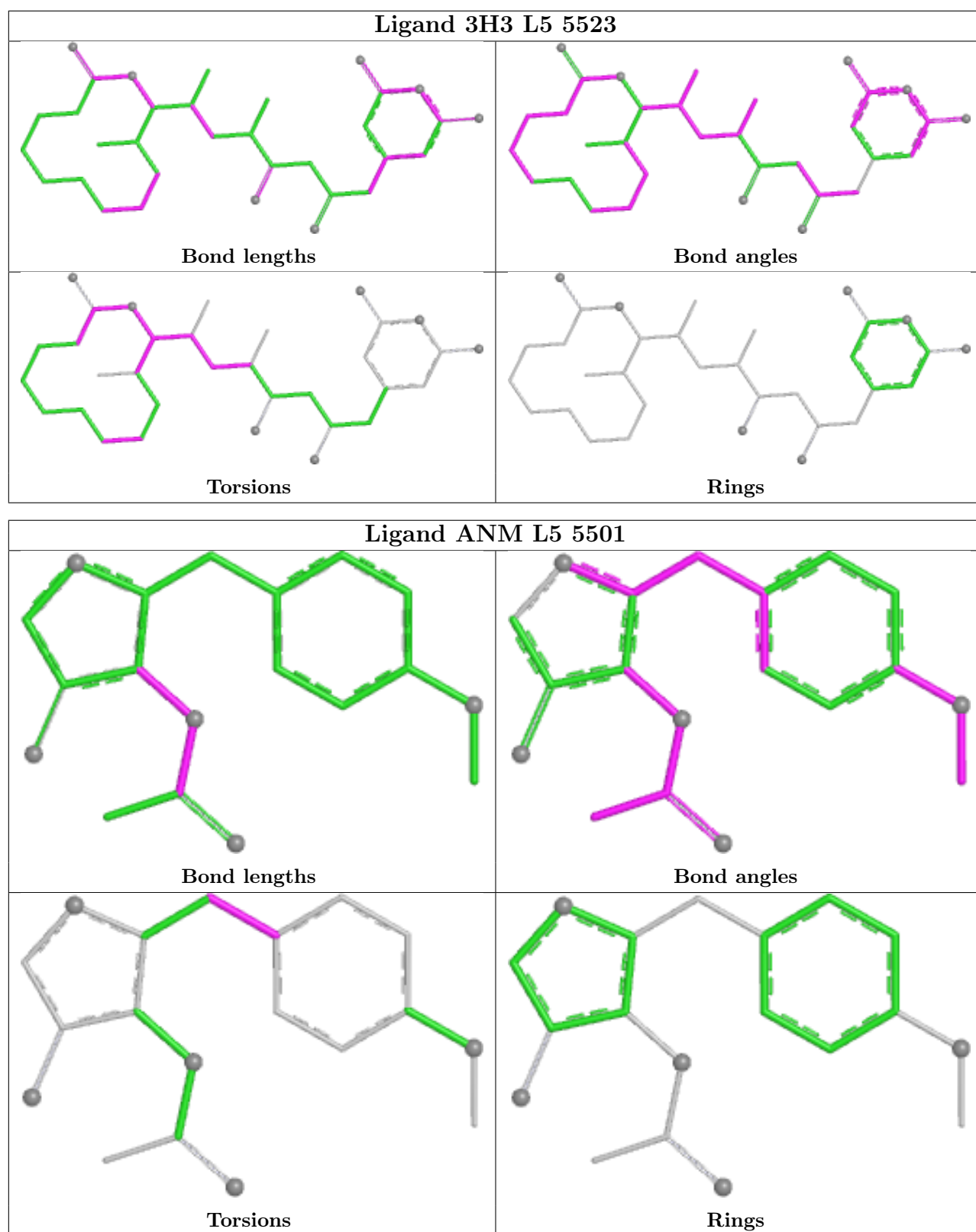
Mol	Chain	Res	Type	Atoms
84	S2	1901	SPD	C4-C5-N6-C7
84	L5	5509	SPD	C8-C7-N6-C5
89	L5	5523	3H3	C2-C1-C11-O1
89	L5	5523	3H3	C2-C1-C11-C12
89	L5	5523	3H3	C-C1-C11-O1

There are no ring outliers.

14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
91	Pt	78	MET	1	0
84	L5	5504	SPD	1	0
85	L5	5515	PUT	1	0
85	L5	5518	PUT	6	0
84	L5	5512	SPD	2	0
89	L5	5523	3H3	3	0
85	S2	1903	PUT	1	0
84	L5	5509	SPD	2	0
84	L5	5506	SPD	1	0
84	L5	5513	SPD	1	0
84	L5	5508	SPD	3	0
84	L5	5511	SPD	1	0
85	S2	1902	PUT	1	0
84	S2	1901	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.

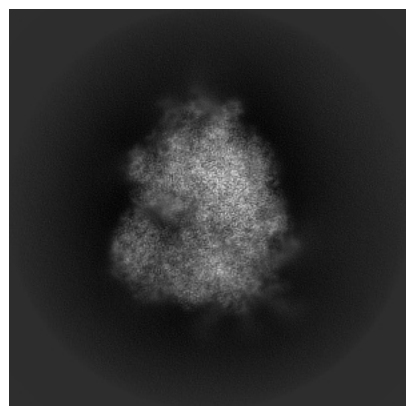
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29757. These allow visual inspection of the internal detail of the map and identification of artifacts.

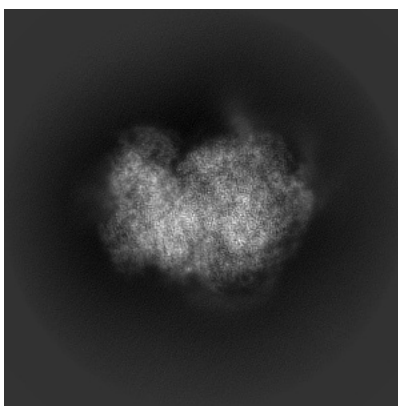
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

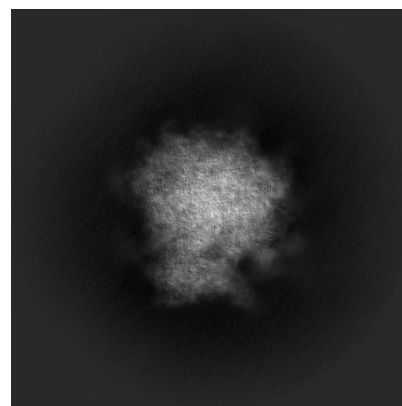
6.1.1 Primary map



X

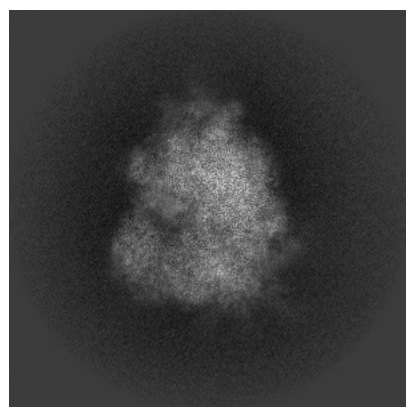


Y

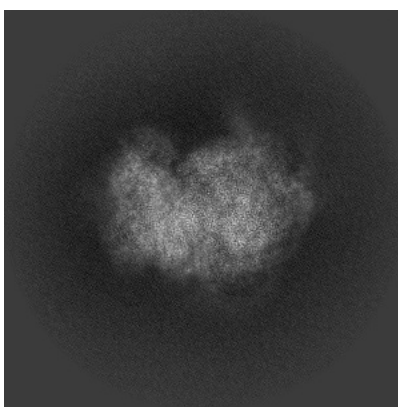


Z

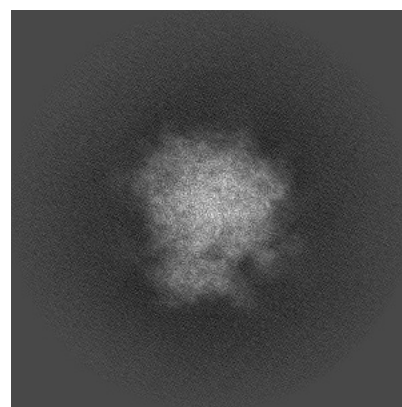
6.1.2 Raw map



X



Y

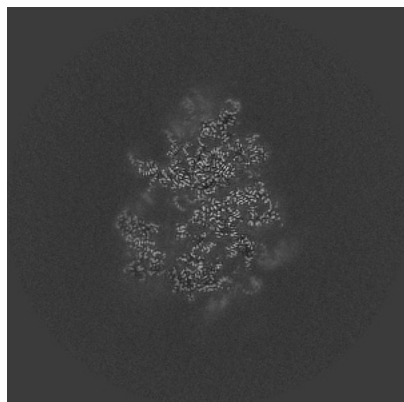


Z

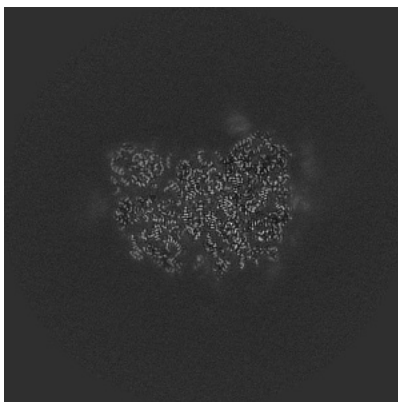
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

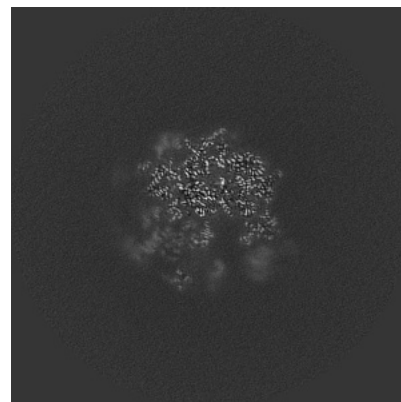
6.2.1 Primary map



X Index: 320

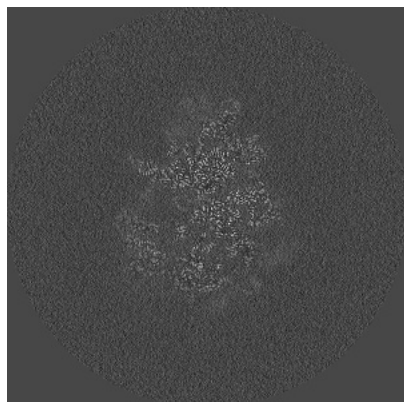


Y Index: 320

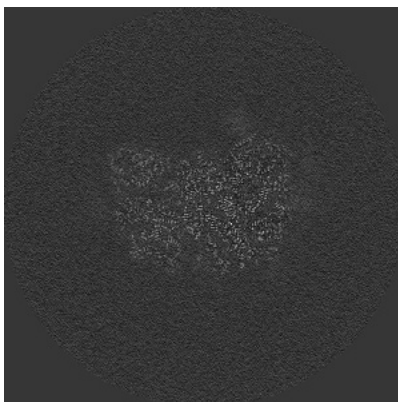


Z Index: 320

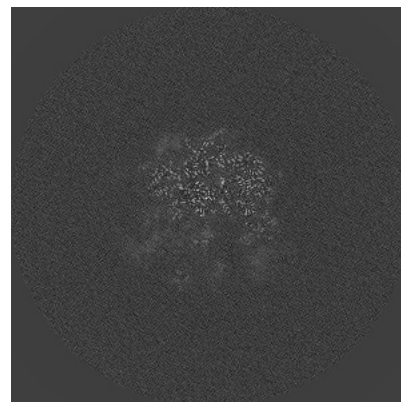
6.2.2 Raw map



X Index: 320



Y Index: 320

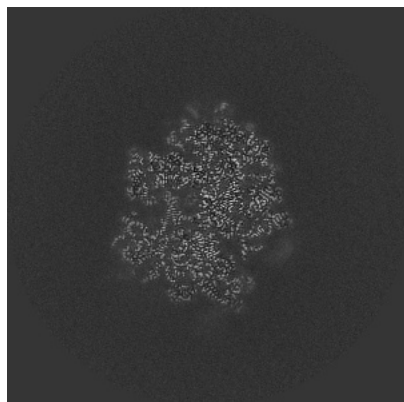


Z Index: 320

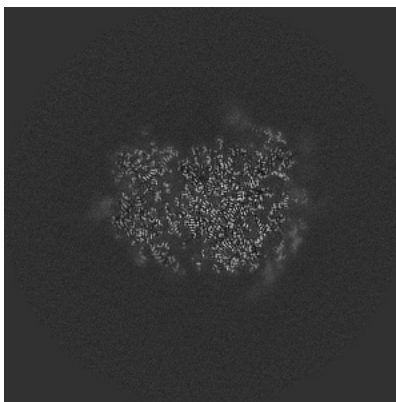
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

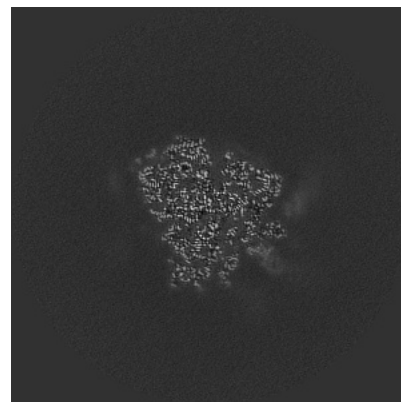
6.3.1 Primary map



X Index: 298

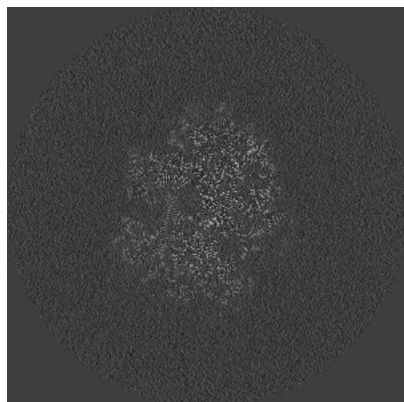


Y Index: 332

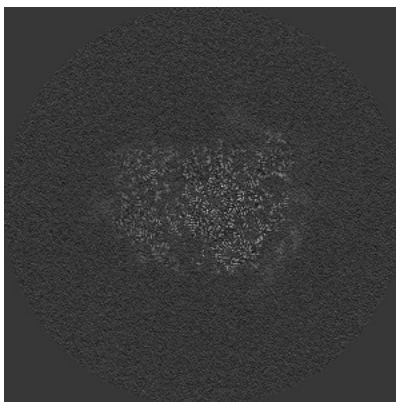


Z Index: 367

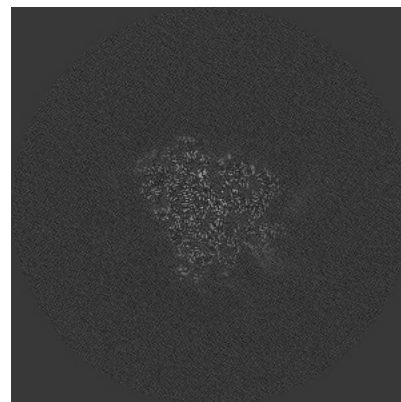
6.3.2 Raw map



X Index: 299



Y Index: 332

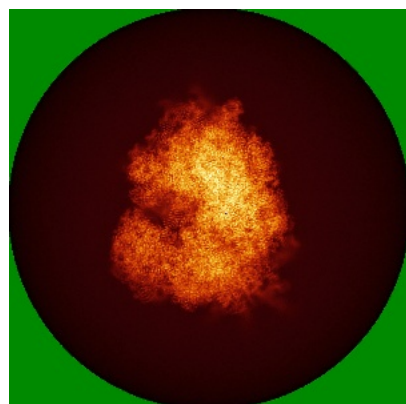


Z Index: 362

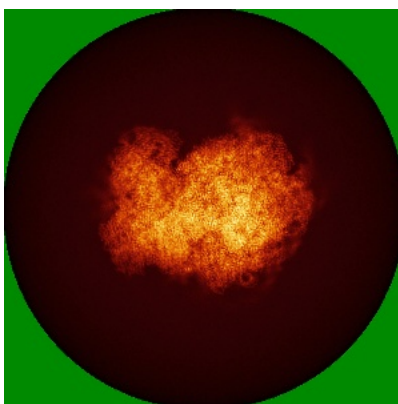
The images above show the largest variance slices of the map in three orthogonal directions.

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

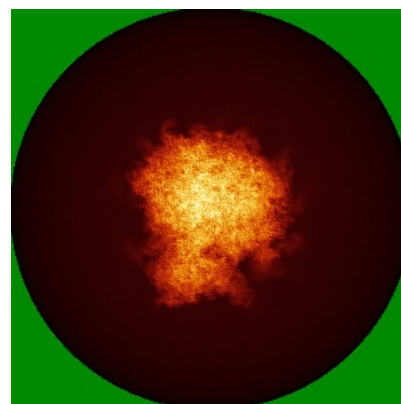
6.4.1 Primary map



X

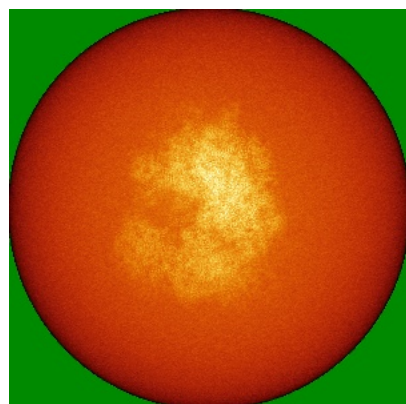


Y

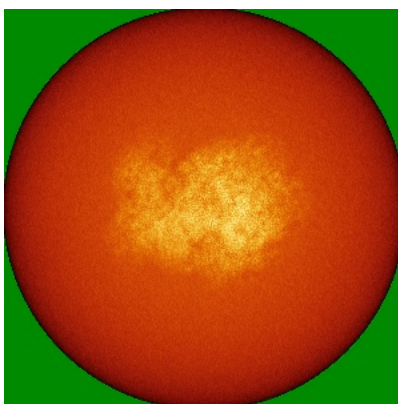


Z

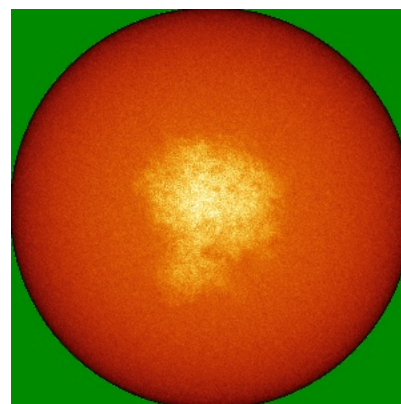
6.4.2 Raw map



X



Y

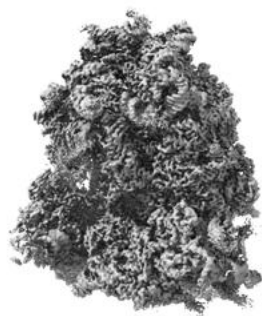


Z

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



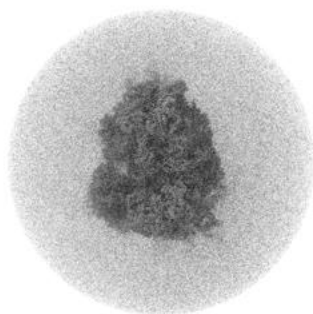
Y



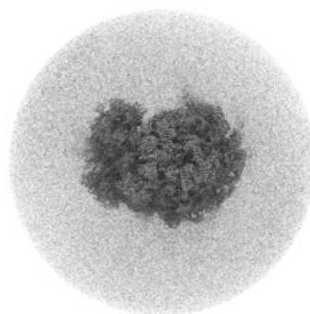
Z

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

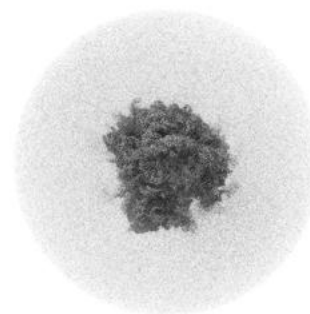
6.5.2 Raw map



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.

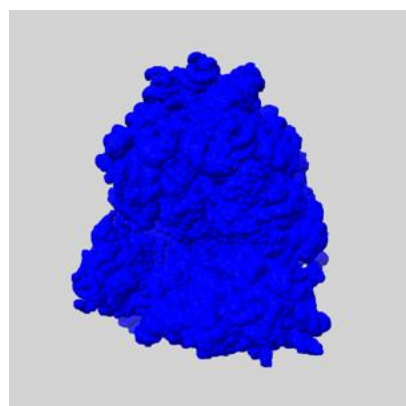
6.6 Mask visualisation [i](#)

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

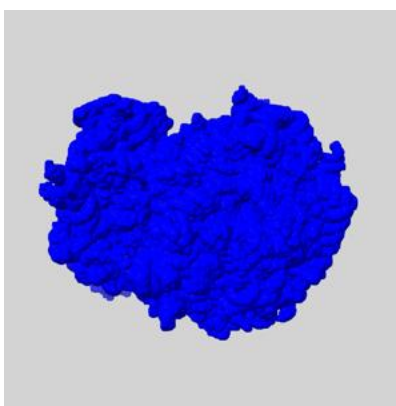
A mask typically either:

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

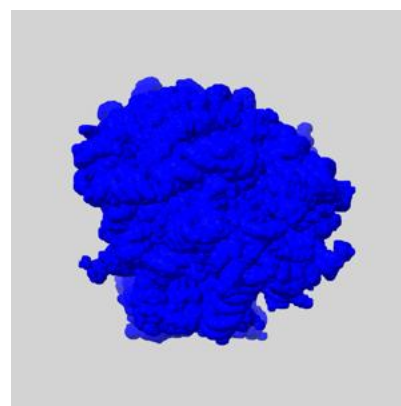
6.6.1 emd_29757_msk_1.map [i](#)



X



Y

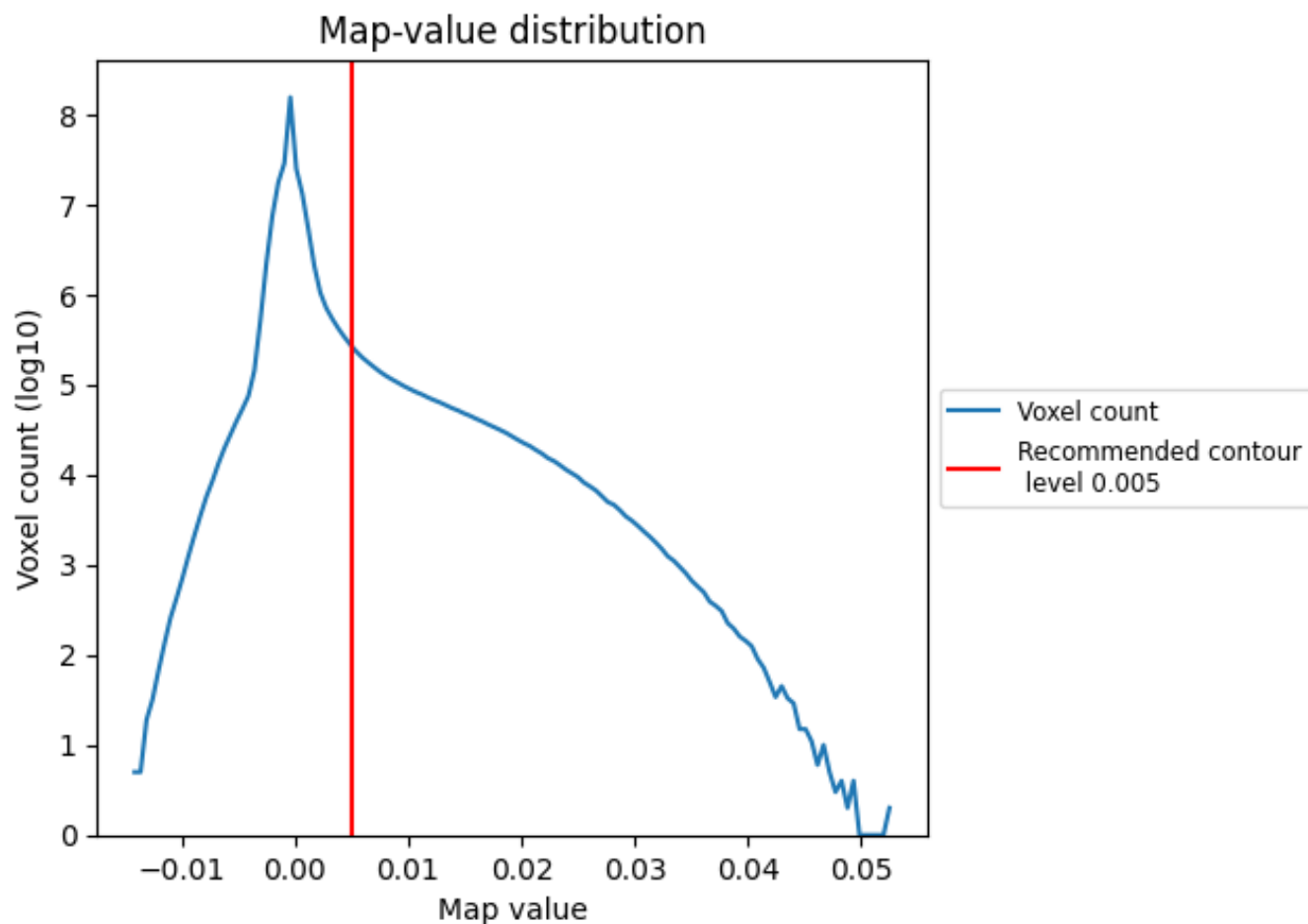


Z

7 Map analysis [i](#)

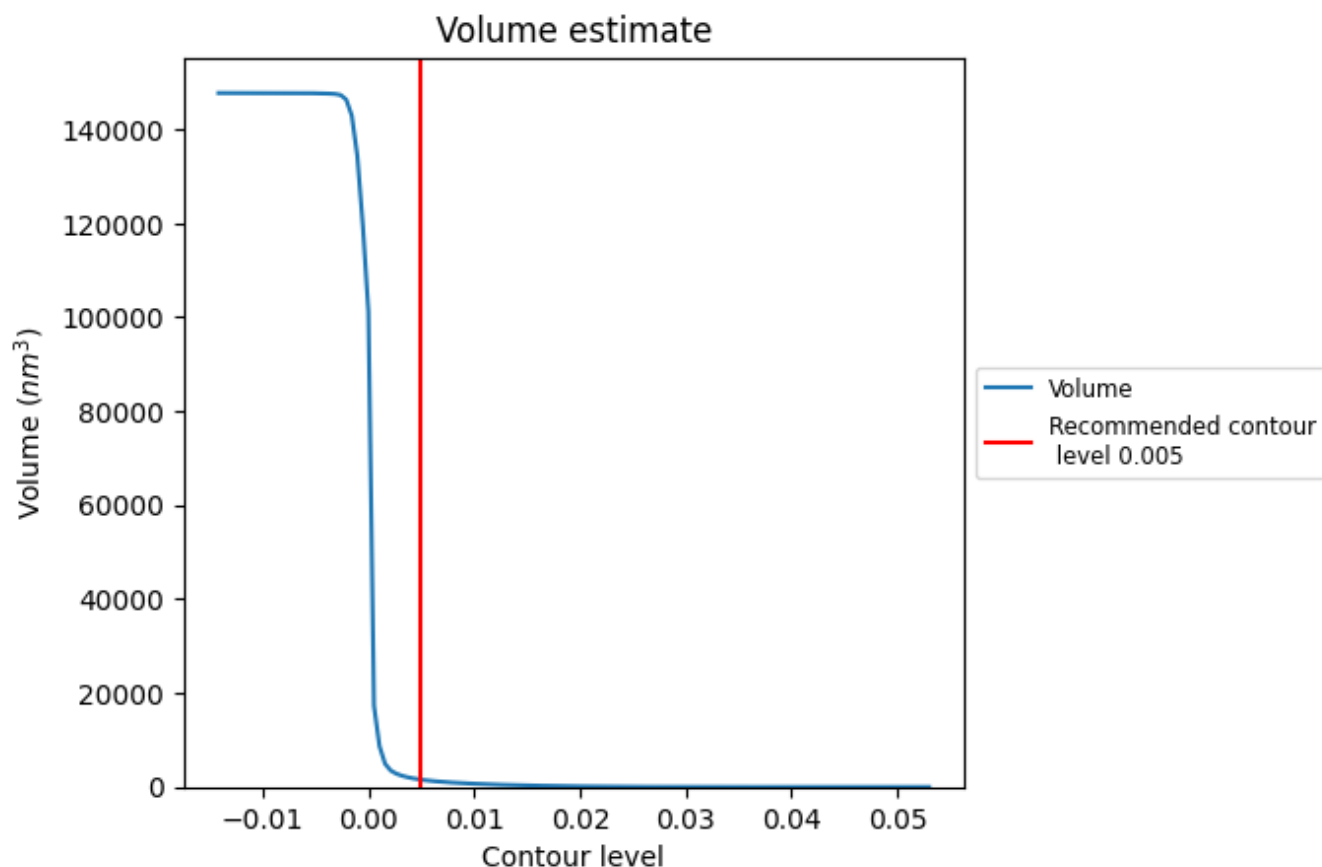
This section contains the results of statistical analysis of the map.

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.

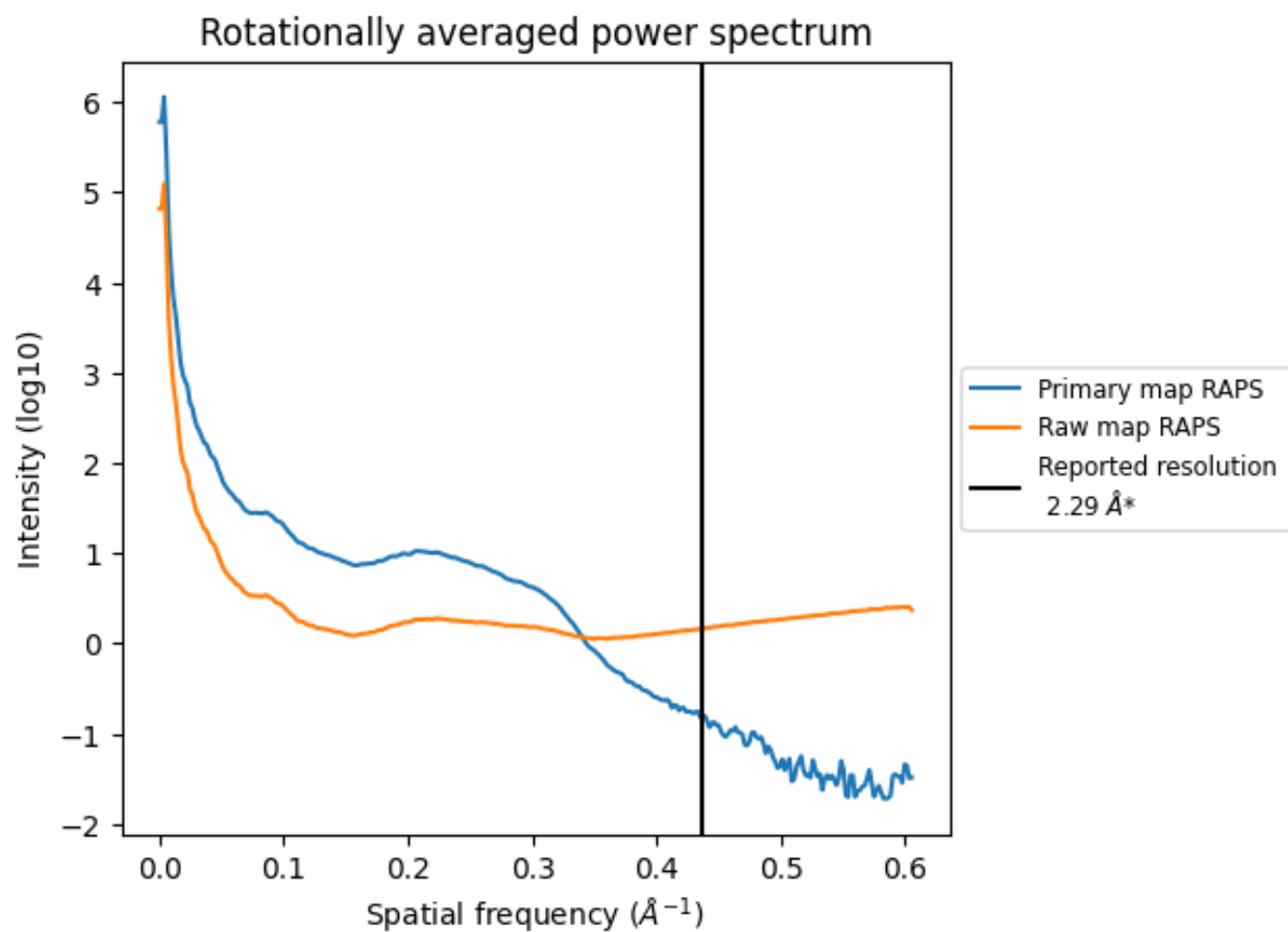
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1549 nm^3 ; this corresponds to an approximate mass of 1399 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 ⓘ

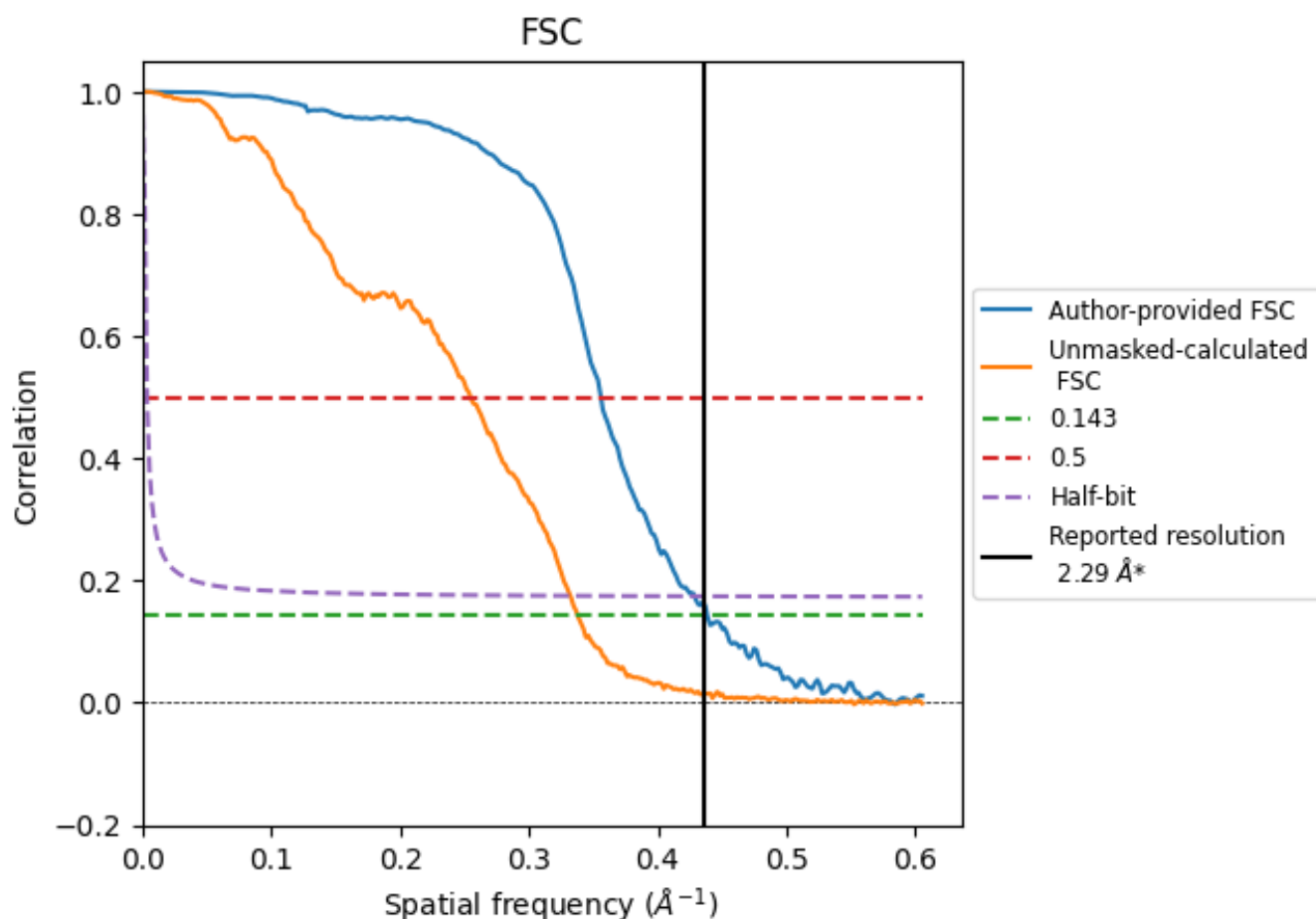


*Reported resolution corresponds to spatial frequency of 0.437 Å⁻¹

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 0.437 Å⁻¹

8.2 Resolution estimates [i](#)

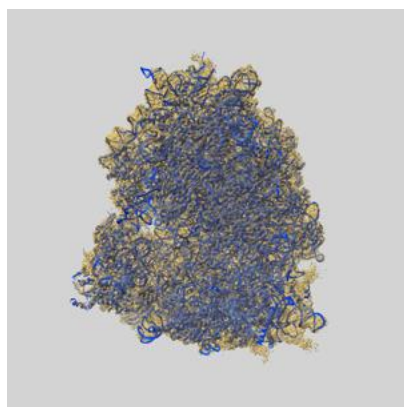
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.28	2.81	2.33
Unmasked-calculated*	2.96	3.92	3.01

*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 2.96 differs from the reported value 2.29 by more than 10 %

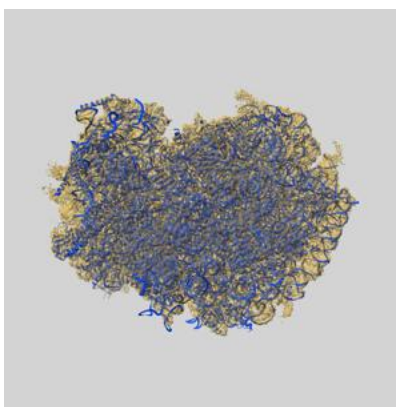
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29757 and PDB model 8G5Y. Per-residue inclusion information can be found in section 3 on page 28.

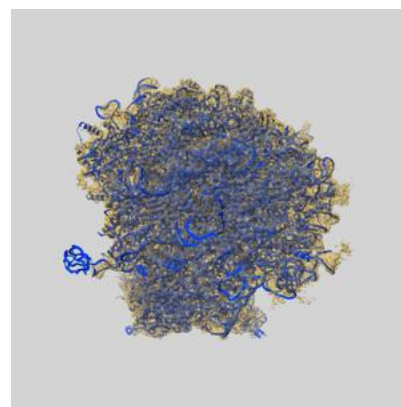
9.1 Map-model overlay [i](#)



X



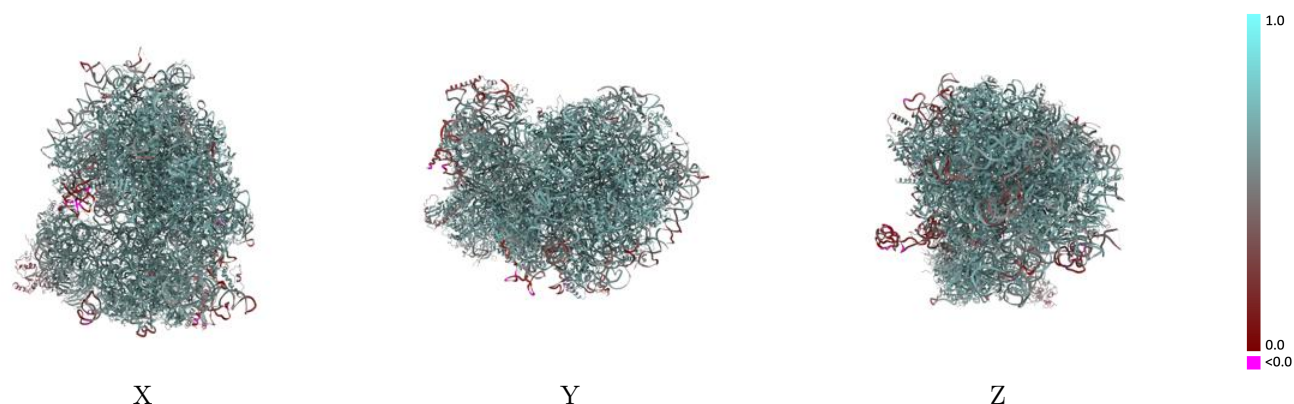
Y



Z

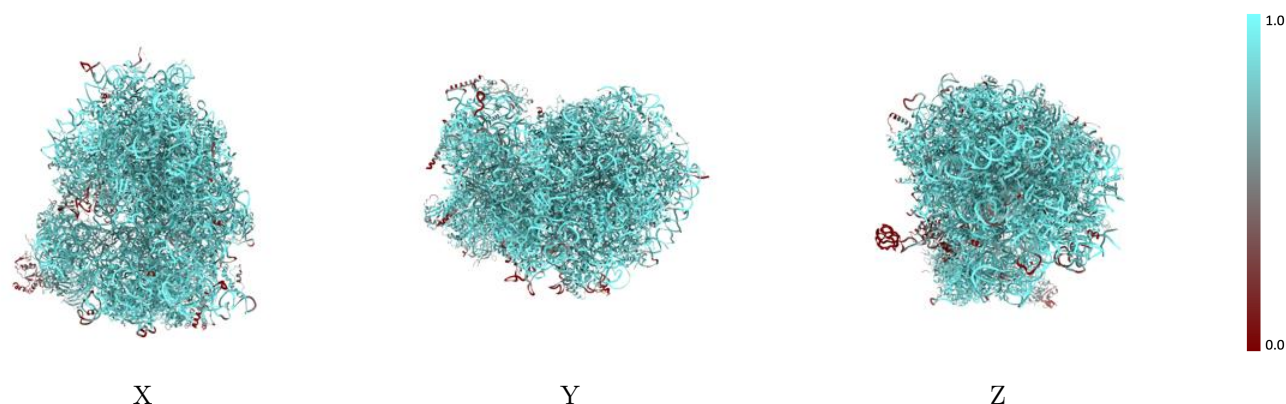
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



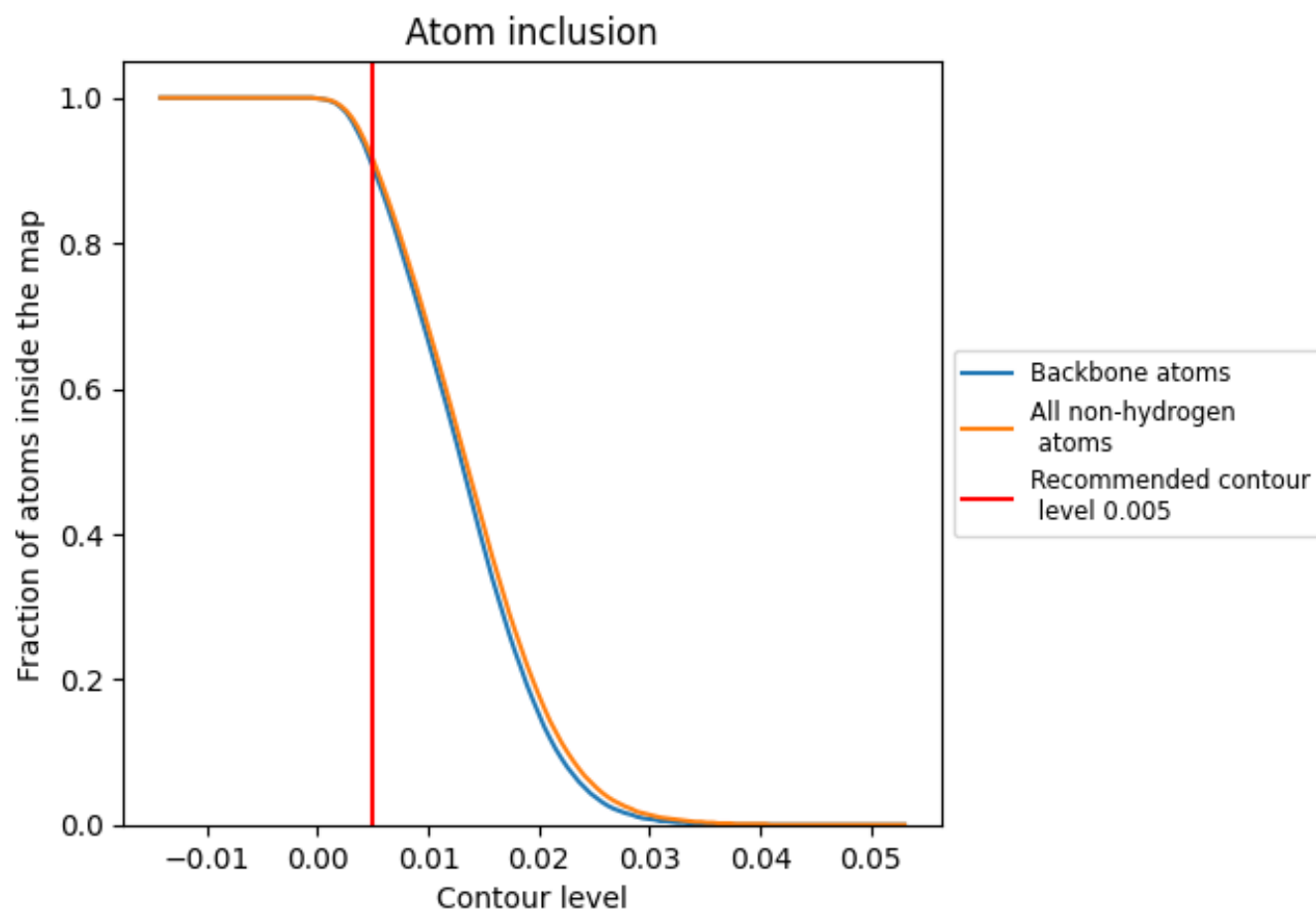
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.6050
5A	 0.5350	 0.4730
L5	 0.9360	 0.5990
L7	 0.9940	 0.6520
L8	 0.9780	 0.6360
LA	 0.9730	 0.6720
LB	 0.9410	 0.6550
LC	 0.9530	 0.6590
LD	 0.9220	 0.6310
LE	 0.9180	 0.6290
LF	 0.9600	 0.6610
LG	 0.8380	 0.5950
LH	 0.9200	 0.6300
LI	 0.9480	 0.6450
LJ	 0.9110	 0.6190
LL	 0.9140	 0.6320
LM	 0.9500	 0.6420
LN	 0.9910	 0.6740
LO	 0.9590	 0.6590
LP	 0.9620	 0.6700
LQ	 0.9780	 0.6750
LR	 0.8830	 0.6220
LS	 0.9750	 0.6590
LT	 0.9380	 0.6500
LU	 0.8470	 0.5820
LV	 0.9540	 0.6580
LW	 0.6950	 0.5080
LX	 0.9400	 0.6470
LY	 0.9260	 0.6400
LZ	 0.9380	 0.6400
La	 0.9810	 0.6760
Lb	 0.8220	 0.5910
Lc	 0.9320	 0.6460
Ld	 0.9240	 0.6330
Le	 0.9800	 0.6750



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lf	 0.9680	 0.6710
Lg	 0.9020	 0.6420
Lh	 0.9280	 0.6430
Li	 0.9010	 0.6210
Lj	 0.9900	 0.6780
Lk	 0.8510	 0.6130
Ll	 0.9620	 0.6510
Lm	 0.9230	 0.6360
Ln	 0.9360	 0.6470
Lo	 0.9480	 0.6490
Lp	 0.9390	 0.6600
Lr	 0.9670	 0.6610
Lz	 0.2670	 0.3690
Pt	 0.9600	 0.5990
S2	 0.9610	 0.5960
SA	 0.9030	 0.6160
SB	 0.8790	 0.6200
SC	 0.9160	 0.6260
SD	 0.8260	 0.5680
SE	 0.9010	 0.6150
SF	 0.8830	 0.6050
SG	 0.7700	 0.5370
SH	 0.7770	 0.5500
SI	 0.8900	 0.6060
SJ	 0.8850	 0.5950
SK	 0.8190	 0.5380
SL	 0.9120	 0.6330
SM	 0.2660	 0.2970
SN	 0.9370	 0.6410
SO	 0.9200	 0.6320
SP	 0.8220	 0.5660
SQ	 0.9090	 0.6100
SR	 0.8150	 0.5660
SS	 0.8920	 0.6040
ST	 0.8930	 0.6030
SU	 0.7750	 0.5470
SV	 0.9090	 0.6230
SW	 0.9680	 0.6480
SX	 0.9460	 0.6390
SY	 0.8040	 0.5550
SZ	 0.7920	 0.5760
Sa	 0.9420	 0.6350

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sb	 0.8420	 0.6070
Sc	 0.8070	 0.5720
Sd	 0.9570	 0.6210
Se	 0.8440	 0.5940
Sf	 0.4420	 0.3830
Sg	 0.7590	 0.5360
mR	 0.6110	 0.5240