



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 08:32 PM EDT

PDB ID : 8G60 / pdb_00008g60
EMDB ID : EMD-29759
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (CR 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 : 2.54 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

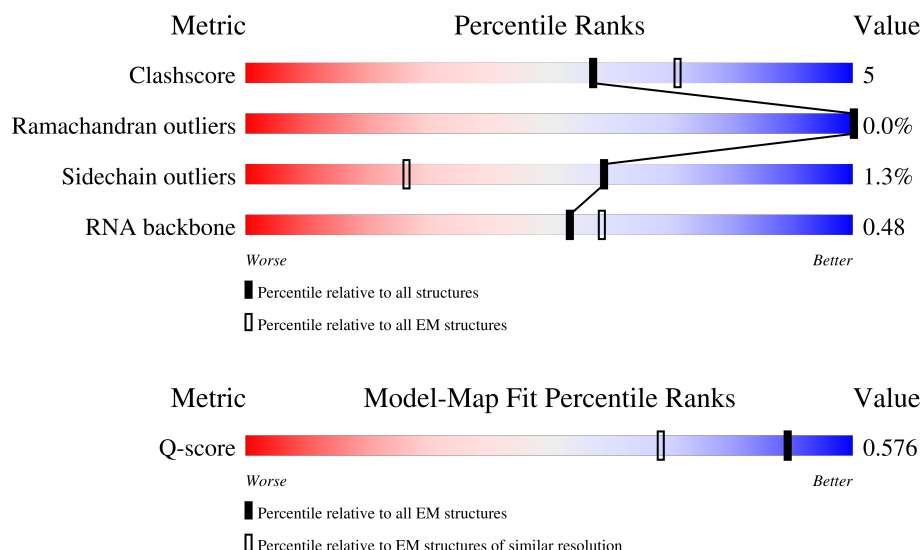
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.54 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.



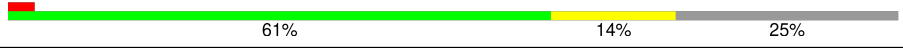
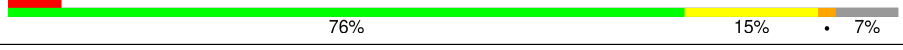
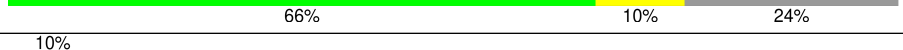
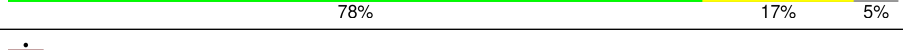
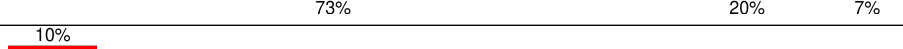
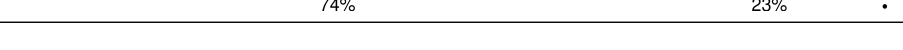
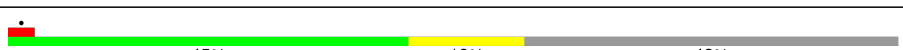
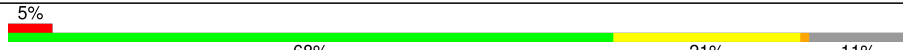
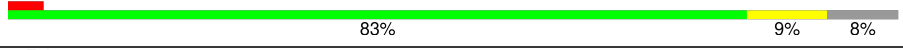
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7403 (2.04 - 3.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S2	1869	
2	L8	156	
3	L5	5069	

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

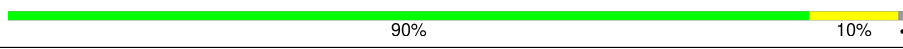
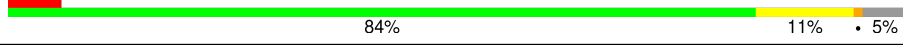
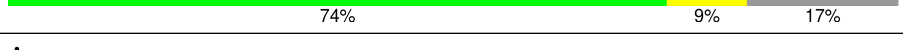
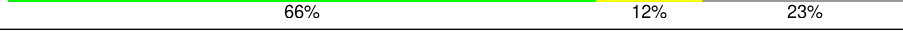
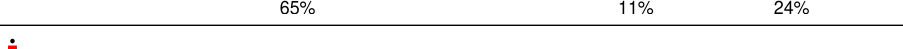
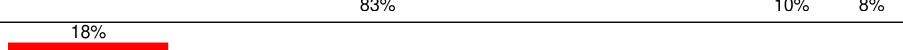
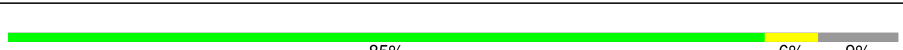
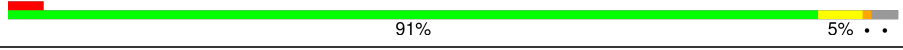
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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	133	
31	SZ	125	
32	Sa	115	
33	Sb	84	
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	Lz	217	
39	LA	257	
40	LB	403	
41	LC	427	
42	LJ	178	
43	LH	192	
44	LE	288	
45	LG	266	
46	Lq	317	
47	LK	165	
48	LO	203	
49	LL	270	
50	LV	140	
51	LM	215	
52	La	148	
53	LN	204	

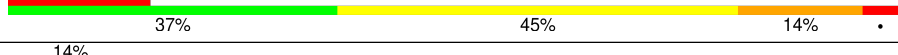
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Mol	Chain	Length	Quality of chain
54	LI	214	
55	LD	297	
56	LQ	188	
57	LR	196	
58	LS	176	
59	LT	160	
60	LP	184	
61	LU	128	
62	LX	156	
63	LY	145	
64	LW	157	
65	LZ	136	
66	Lr	137	
67	Lh	123	
68	Lb	159	
69	LF	248	
70	Lc	115	
71	Ld	125	
72	Le	135	
73	Lf	110	
74	Lg	117	
75	Li	105	
76	Lj	97	
77	Lk	70	
78	Ll	51	

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Mol	Chain	Length	Quality of chain
79	Lm	128	
80	Ln	25	
81	Lo	106	
82	Lp	92	
83	mR	60	
84	At	76	
85	Pt	77	
86	EF	462	

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 223755 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	1654	Total	C	N	O	P	0	0
			35359	15812	6338	11555	1654		

- 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
			3320	1482	585	1097	156		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3637	Total	C	N	O	P	1	0
			78069	34805	14275	25351	3638		

- 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
			2562	1141	456	845	120		

- Molecule 5 is a protein called eS1.

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 uS2.

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 uS3.

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 uS4.

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 eS4.

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 uS5.

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 eS6.

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 uS7.

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 eS7.

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 uS8.

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 eS8.

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 uS9.

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 uS10.

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 eS10.

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 uS11.

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	142	Total	C	N	O	S	0	0
			1105	696	220	186	3		

- Molecule 21 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 22 is a protein called uS13.

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 uS14.

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 uS15.

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 uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SL	145	Total	C	N	O	S	0	0
			1189	757	225	201	6		

- Molecule 26 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	134	Total	C	N	O	S	0	0
			1083	680	201	198	4		

- Molecule 27 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	128	Total	C	N	O	S	0	0
			1050	666	198	179	7		

- Molecule 28 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 29 is a protein called eS21.

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 eS24.

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 eS25.

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 eS26.

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

- Molecule 33 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 34 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 35 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	51	Total	C	N	O	S	0	0
			406	248	92	65	1		

- Molecule 36 is a protein called eS31.

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 RACK1.

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 uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- 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 uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LB	402	Total	C	N	O	S	0	0
			3240	2061	608	557	14		

- Molecule 41 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 42 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LJ	169	Total	C	N	O	S	0	0
			1358	859	253	240	6		

- Molecule 43 is a protein called uL6.

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 eL6.

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 eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LG	239	Total	C	N	O	S	0	0
			1910	1217	368	321	4		

- Molecule 46 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lq	196	Total	C	N	O	S	0	0
			1506	958	263	276	9		

- Molecule 47 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LK	147	Total	C	N	O	S	0	0
			1121	700	211	207	3		

- Molecule 48 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LO	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 49 is a protein called eL13.

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

- Molecule 50 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LV	133	Total	C	N	O	S	0	0
			989	623	186	175	5		

- Molecule 51 is a protein called eL14.

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

- Molecule 52 is a protein called uL15.

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

- Molecule 53 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 54 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LI	208	Total	C	N	O	S	0	0
			1680	1065	323	278	14		

- Molecule 55 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LD	293	Total	C	N	O	S	0	0
			2387	1511	435	427	14		

- Molecule 56 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LQ	187	Total	C	N	O	S	0	0
			1511	944	314	248	5		

- Molecule 57 is a protein called eL19.

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

- Molecule 58 is a protein called eL20.

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

- Molecule 59 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 60 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 61 is a protein called eL22.

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

- Molecule 62 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 63 is a protein called uL24.

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

- Molecule 64 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LW	117	Total	C	N	O	S	0	0
			944	592	191	157	4		

- Molecule 65 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 66 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Lr	125	Total	C	N	O	S	0	0
			1005	624	207	169	5		

- Molecule 67 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 68 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lb	109	Total	C	N	O	S	0	0
			885	552	192	137	4		

- Molecule 69 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 70 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 71 is a protein called eL31.

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

- Molecule 72 is a protein called eL32.

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

- Molecule 73 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 74 is a protein called eL34.

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

- Molecule 75 is a protein called eL36.

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

- Molecule 76 is a protein called eL37.

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

- Molecule 77 is a protein called eL38.

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

- Molecule 78 is a protein called eL39.

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

- Molecule 79 is a protein called eL40.

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

- Molecule 80 is a protein called eL41.

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

- Molecule 81 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lo	104	Total	C	N	O	S	0	0
			852	534	174	138	6		

- Molecule 82 is a protein called eL43.

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

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	mR	9	Total	C	N	O	P	0	0
			188	84	29	66	9		

- Molecule 84 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	At	76	Total	C	N	O	P	S	0	0
			1630	730	290	532	76	2		

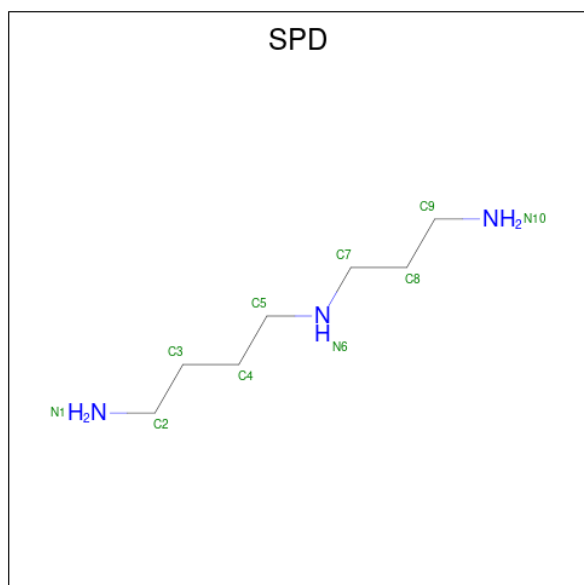
- Molecule 85 is a RNA chain called P-site tRNA.

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

- Molecule 86 is a protein called eEF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	EF	443	Total	C	N	O	S	1	0
			3401	2165	584	635	17		

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



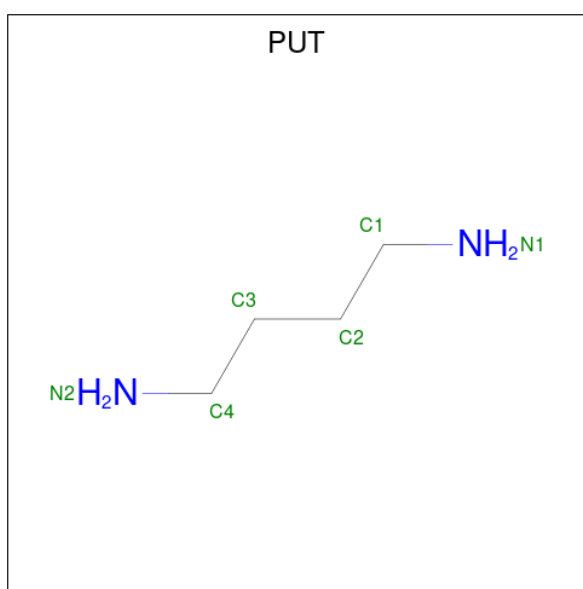
Mol	Chain	Residues	Atoms			AltConf
87	S2	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	

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

- Molecule 88 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

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

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

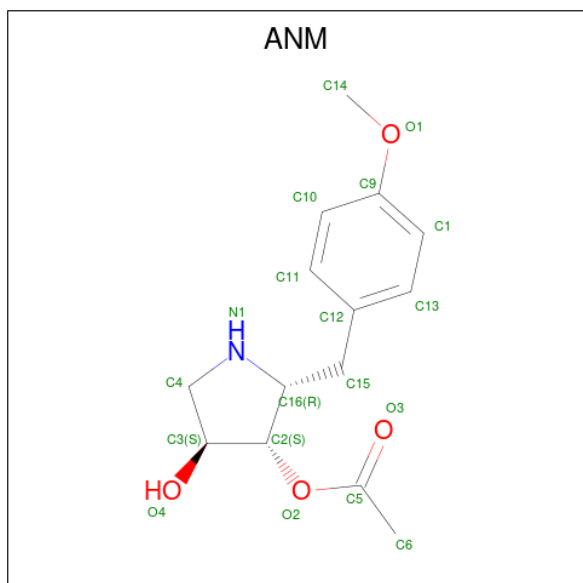
Mol	Chain	Residues	Atoms		AltConf
89	S2	112	Total	Mg	0
			112	112	
89	L8	7	Total	Mg	0
			7	7	
89	L5	307	Total	Mg	0
			307	307	
89	L7	7	Total	Mg	0
			7	7	
89	SG	1	Total	Mg	0
			1	1	
89	SO	1	Total	Mg	0
			1	1	
89	SS	2	Total	Mg	0
			2	2	
89	SN	1	Total	Mg	0
			1	1	
89	SP	1	Total	Mg	0
			1	1	
89	Sa	1	Total	Mg	0
			1	1	
89	LA	1	Total	Mg	0
			1	1	
89	LB	3	Total	Mg	0
			3	3	
89	LC	1	Total	Mg	0
			1	1	
89	LL	1	Total	Mg	0
			1	1	
89	LV	1	Total	Mg	0
			1	1	
89	LN	1	Total	Mg	0
			1	1	

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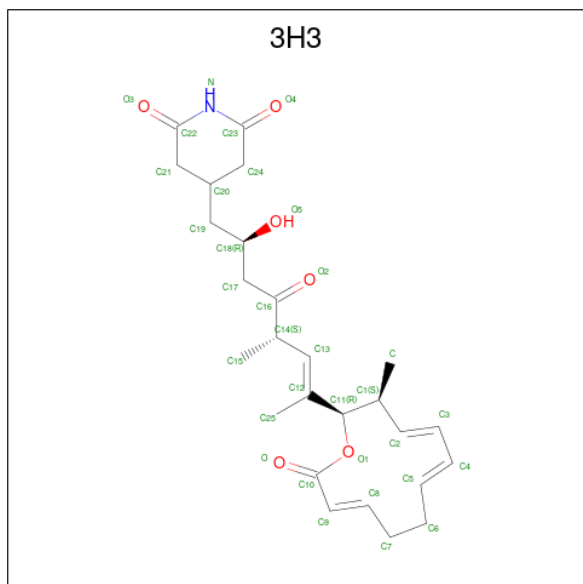
Mol	Chain	Residues	Atoms		AltConf
89	LI	1	Total	Mg	0
			1	1	
89	LR	1	Total	Mg	0
			1	1	
89	LS	1	Total	Mg	0
			1	1	
89	LP	2	Total	Mg	0
			2	2	
89	Le	1	Total	Mg	0
			1	1	
89	Lf	1	Total	Mg	0
			1	1	
89	Lg	2	Total	Mg	0
			2	2	
89	Lj	1	Total	Mg	0
			1	1	
89	Pt	2	Total	Mg	0
			2	2	
89	EF	1	Total	Mg	0
			1	1	

- Molecule 90 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



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

- Molecule 91 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: C₂₆H₃₅NO₆).



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

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
92	L5	10	Total	K	0
			10	10	

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

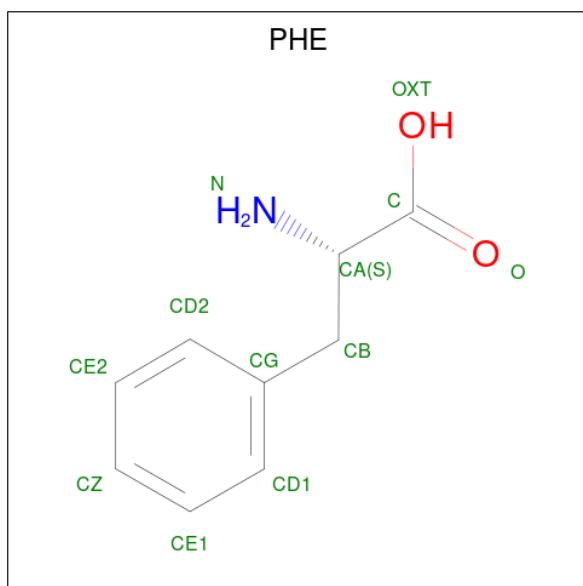
Mol	Chain	Residues	Atoms		AltConf
93	Sd	1	Total	Zn	0
			1	1	
93	Sa	1	Total	Zn	0
			1	1	
93	Lg	1	Total	Zn	0
			1	1	
93	Lj	1	Total	Zn	0
			1	1	
93	Lm	1	Total	Zn	0
			1	1	
93	Lo	1	Total	Zn	0
			1	1	

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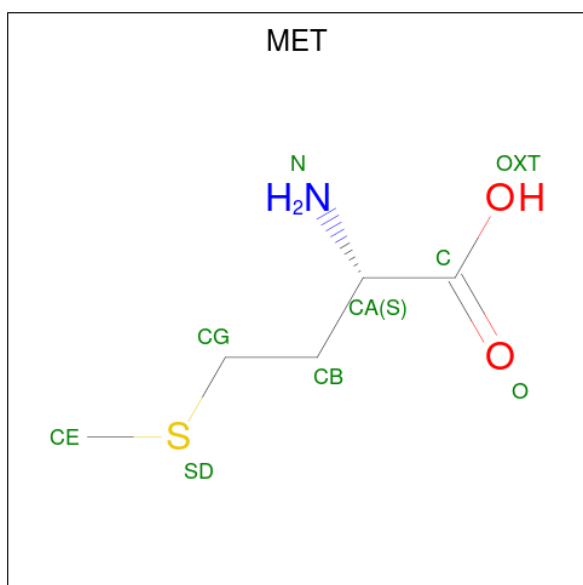
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
93	Lp	1	1	1	0

- Molecule 94 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



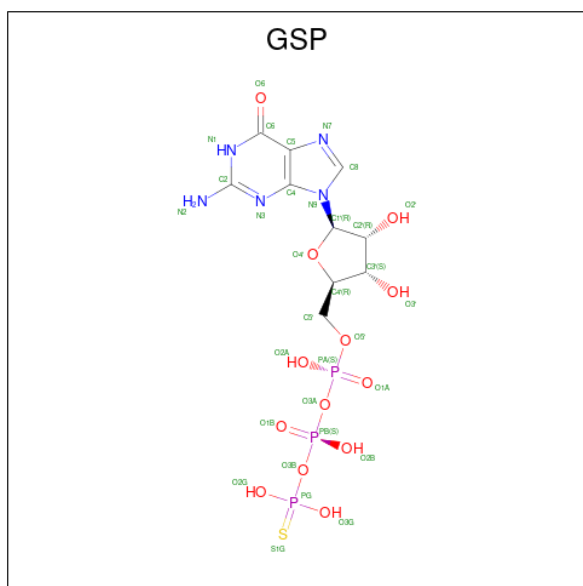
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
94	At	1	11	9	1	1	0

- Molecule 95 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



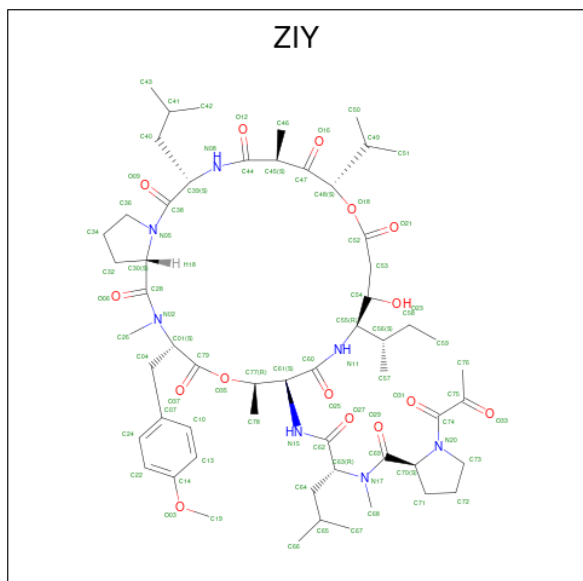
Mol	Chain	Residues	Atoms					AltConf
95	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 96 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms					AltConf
96	EF	1	Total	C	N	O	P	S
			32	10	5	13	3	1

- Molecule 97 is plitidepsin (CCD ID: ZIY) (formula: $C_{57}H_{87}N_7O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
97	EF	1	Total	C	N	O	0
			79	57	7	15	

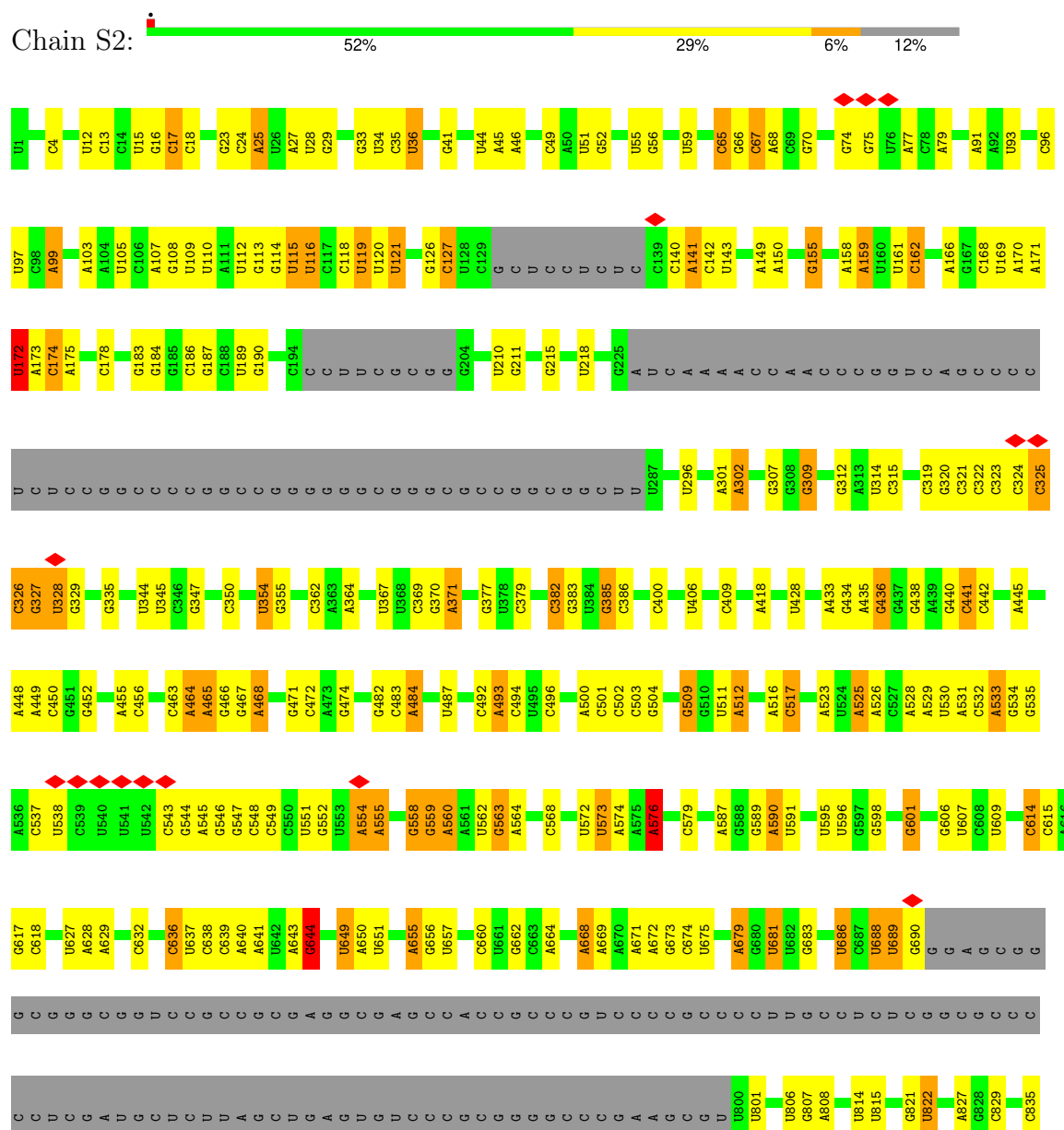
- Molecule 98 is water.

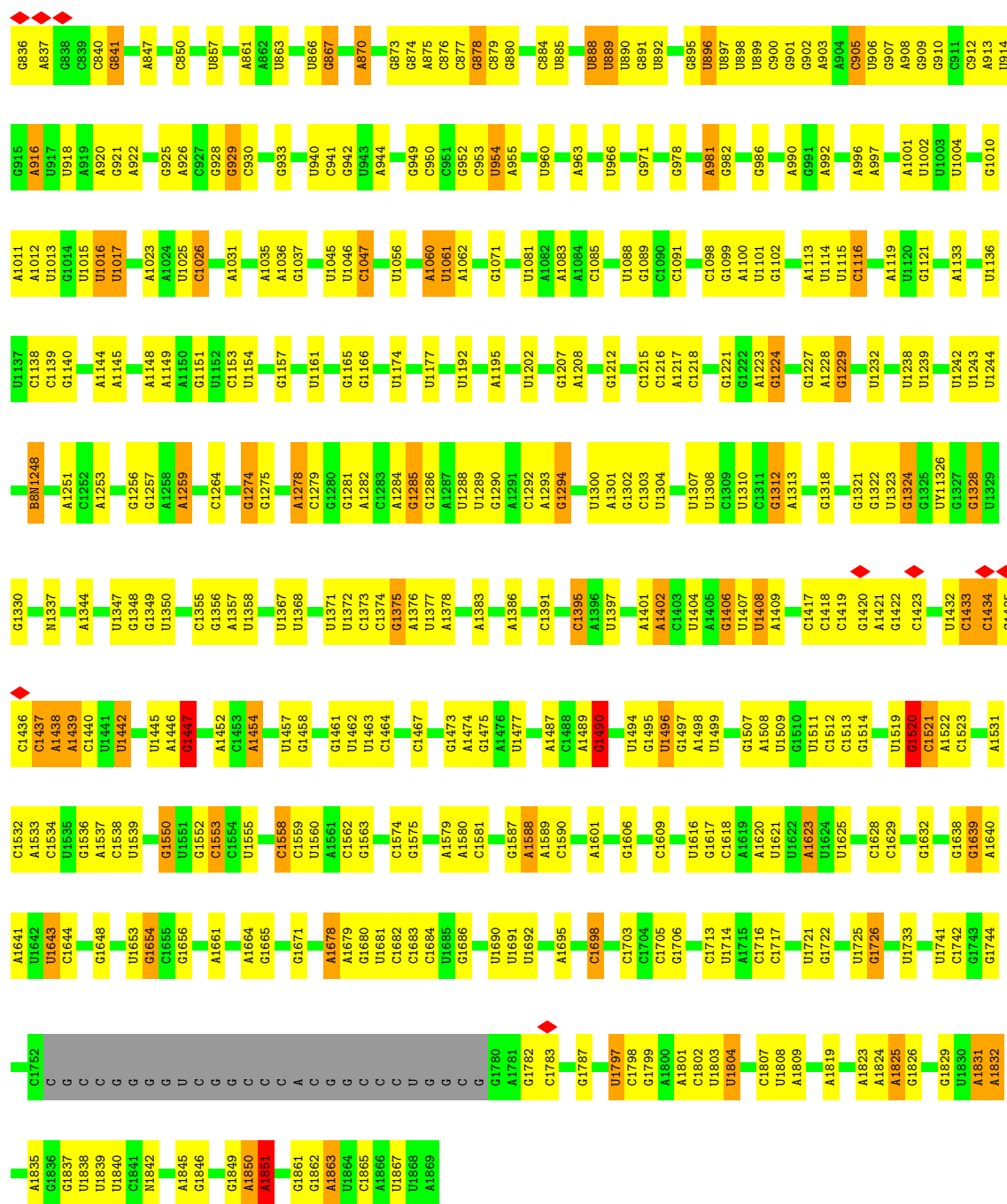
Mol	Chain	Residues	Atoms				AltConf
98	S2	9	Total	O			0
			9	9			
98	L8	3	Total	O			0
			3	3			
98	L5	228	Total	O			0
			228	228			
98	L7	1	Total	O			0
			1	1			
98	SQ	1	Total	O			0
			1	1			
98	SO	1	Total	O			0
			1	1			
98	LA	7	Total	O			0
			7	7			
98	LB	1	Total	O			0
			1	1			
98	LC	1	Total	O			0
			1	1			
98	LH	1	Total	O			0
			1	1			
98	LL	1	Total	O			0
			1	1			
98	LQ	1	Total	O			0
			1	1			
98	LS	1	Total	O			0
			1	1			
98	Lb	2	Total	O			0
			2	2			
98	LF	1	Total	O			0
			1	1			
98	Le	2	Total	O			0
			2	2			
98	Lo	2	Total	O			0
			2	2			

3 Residue-property plots

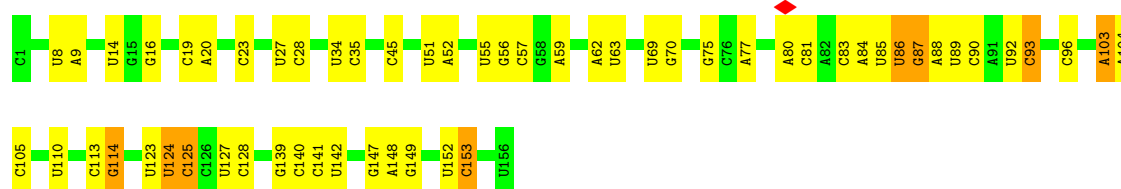
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 18S rRNA





• Molecule 2: 5.8S rRNA

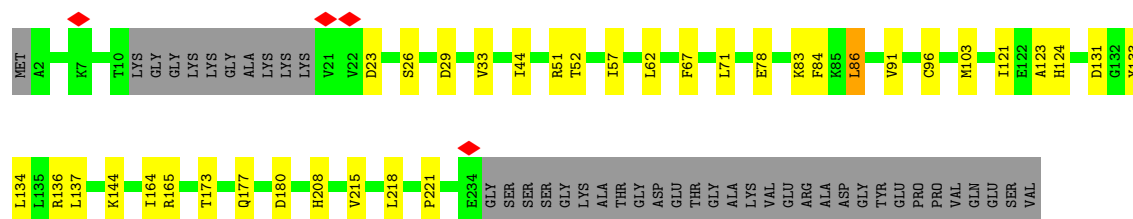


Chain L5: 45% 23% 28%



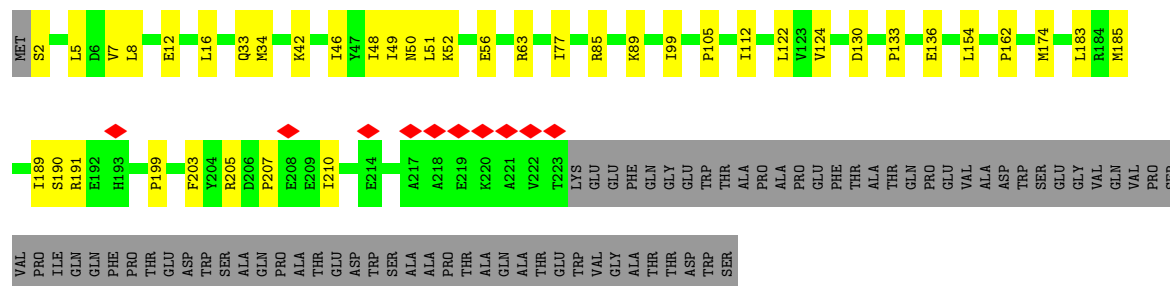


Chain SB:  71% 13% 16%



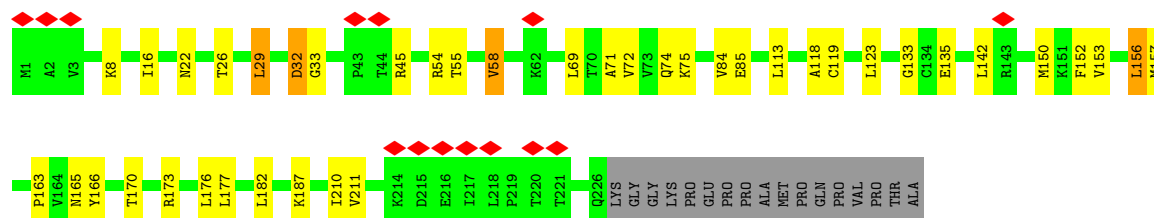
• Molecule 6: uS2

Chain SA:  61% 14% 25%



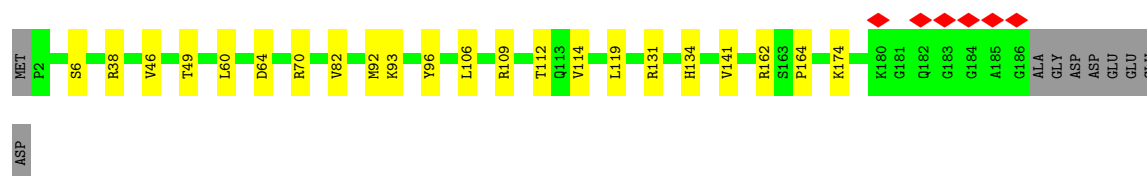
• Molecule 7: uS3

Chain SD:  6% 76% 15% 7%



• Molecule 8: uS4

Chain SJ:  84% 11% 5%



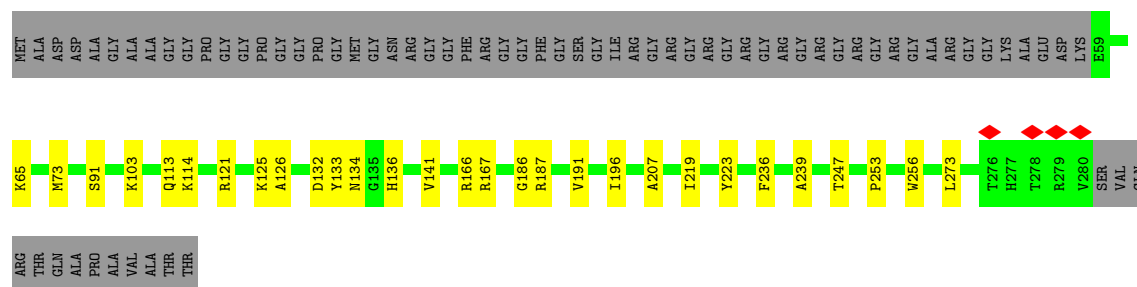
• Molecule 9: eS4

Chain SE:  83% 17%

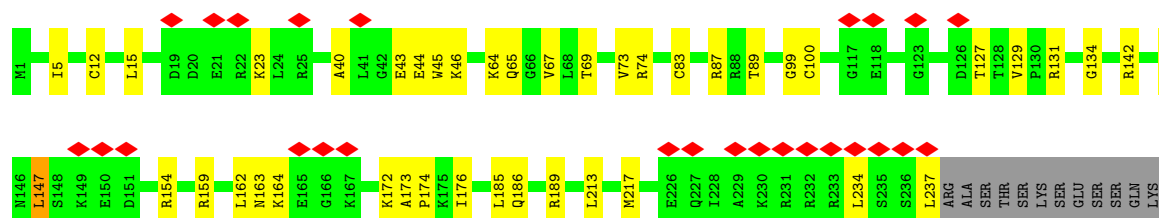
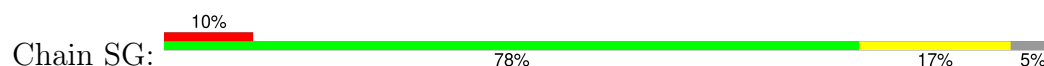




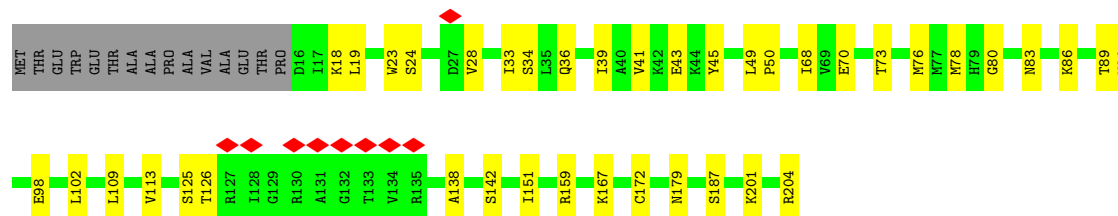
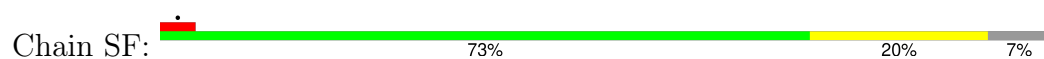
- Molecule 10: uS5



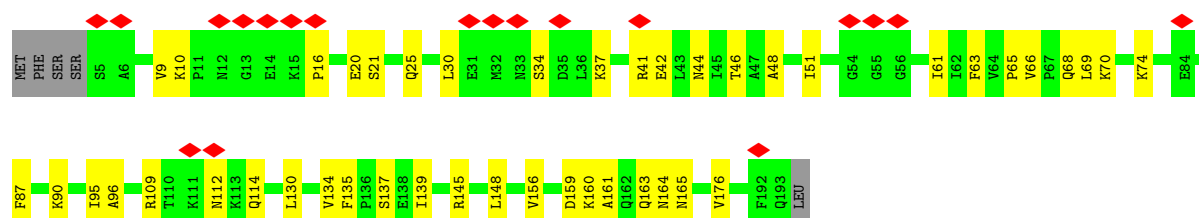
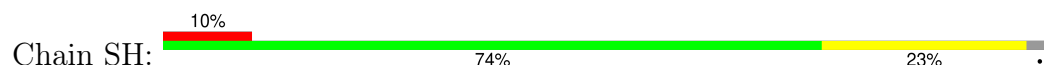
- Molecule 11: eS6



- Molecule 12: uS7

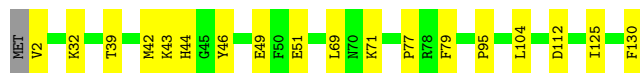


- Molecule 13: eS7



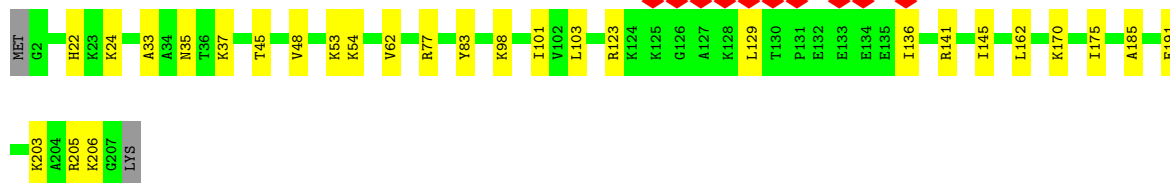
- Molecule 14: uS8

Chain SW:  85% 14%



- Molecule 15: eS8

Chain SI:  5% 86% 13%



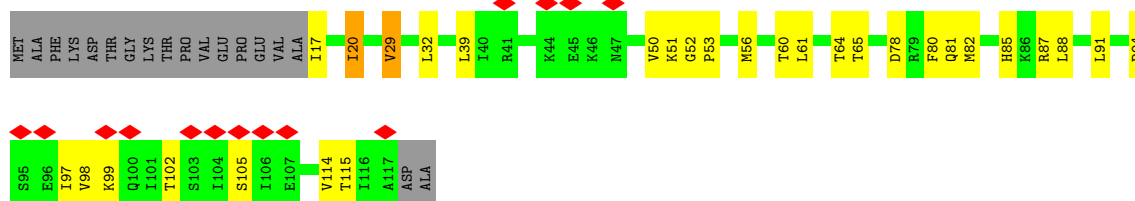
- Molecule 16: uS9

Chain SQ:  83% 14%

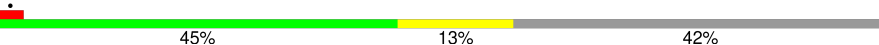


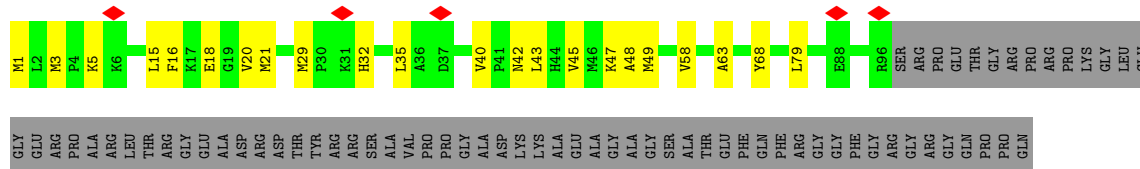
- Molecule 17: uS10

Chain SU:  12% 60% 24% 15%



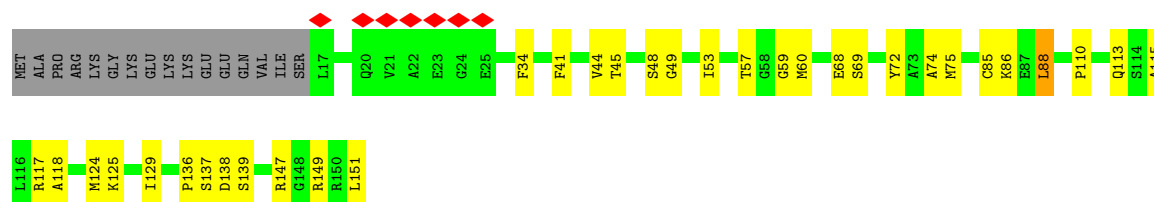
- Molecule 18: eS10

Chain SK:  45% 13% 42%

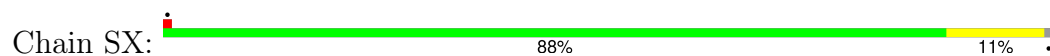


- Molecule 19: uS11

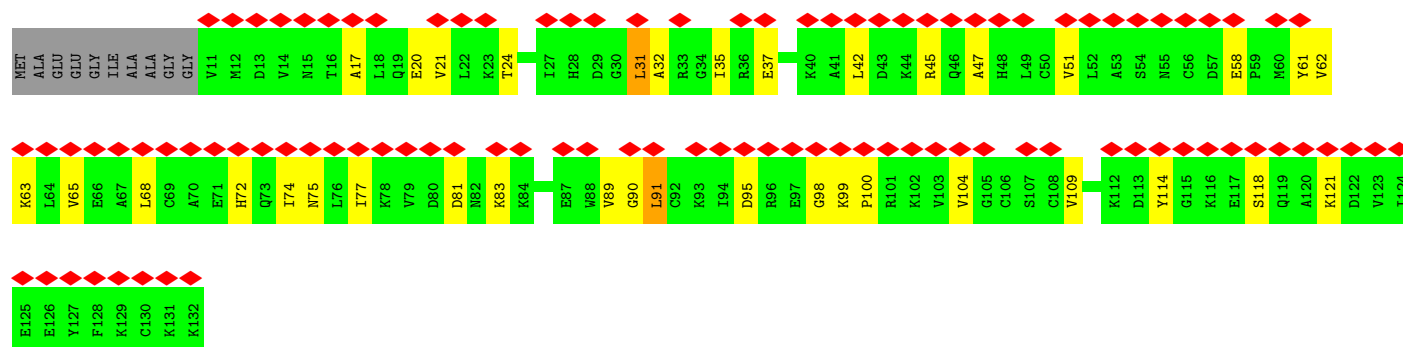
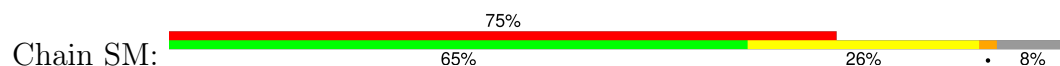
Chain SO:  5% 68% 21% 11%



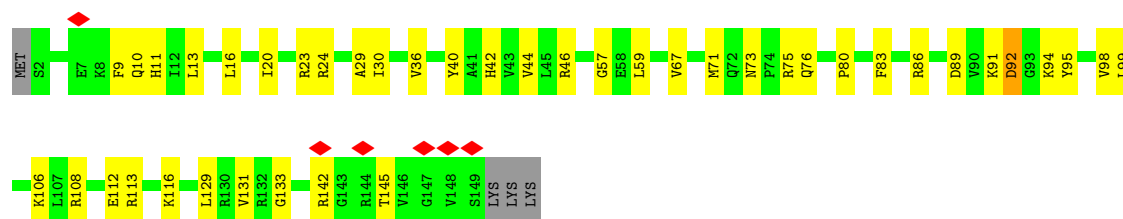
• Molecule 20: uS12



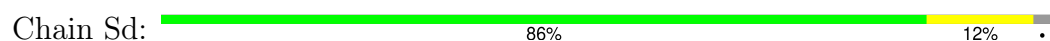
• Molecule 21: eS12



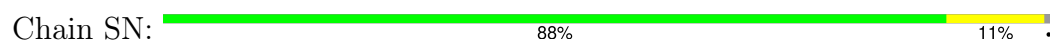
• Molecule 22: uS13



• Molecule 23: uS14

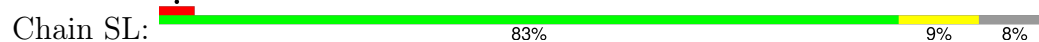


• Molecule 24: uS15

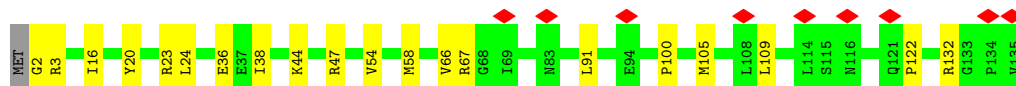
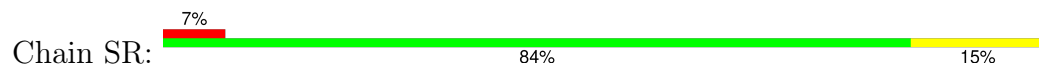




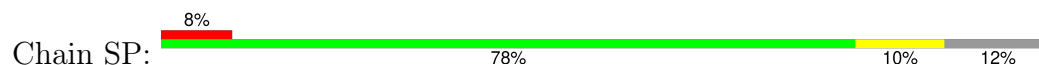
• Molecule 25: uS17



• Molecule 26: eS17



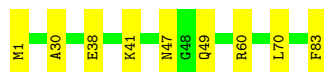
• Molecule 27: uS19



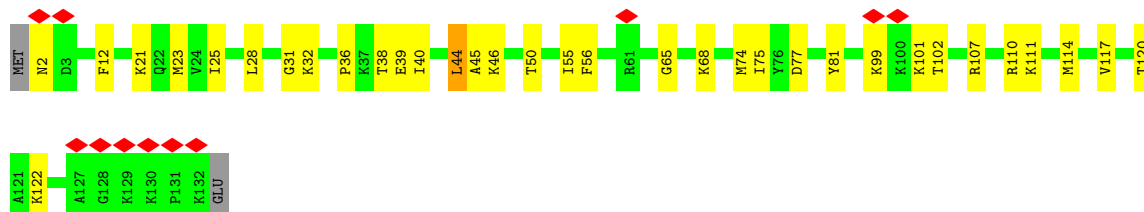
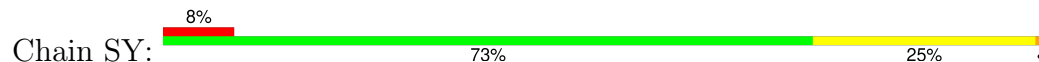
• Molecule 28: eS19



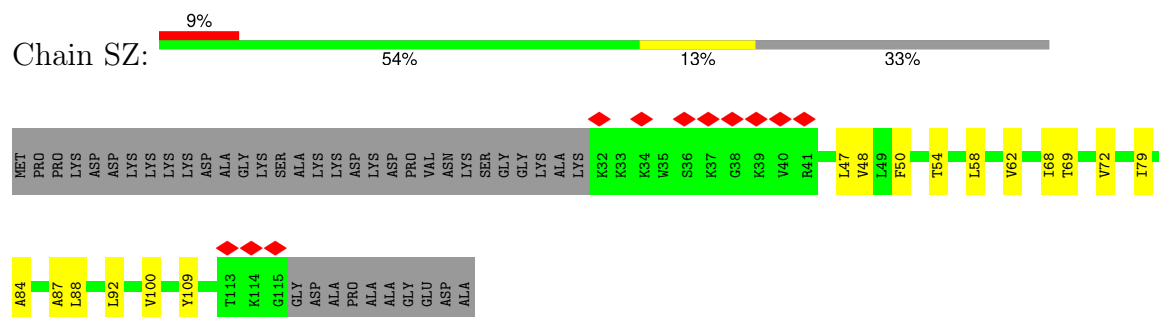
• Molecule 29: eS21



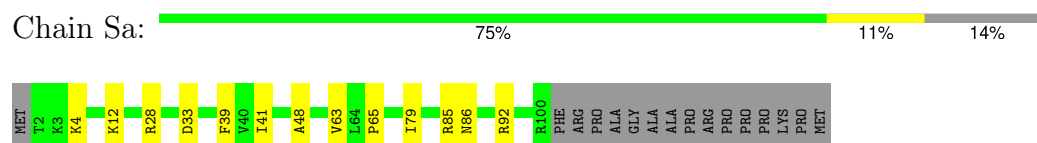
• Molecule 30: eS24



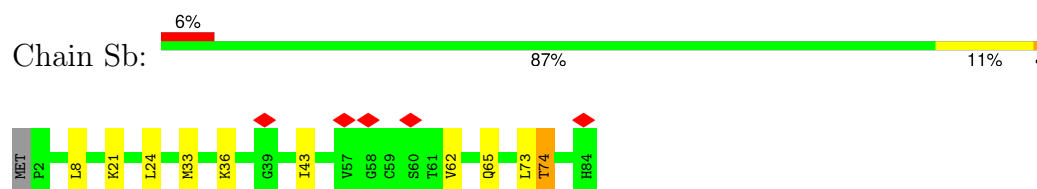
- Molecule 31: eS25



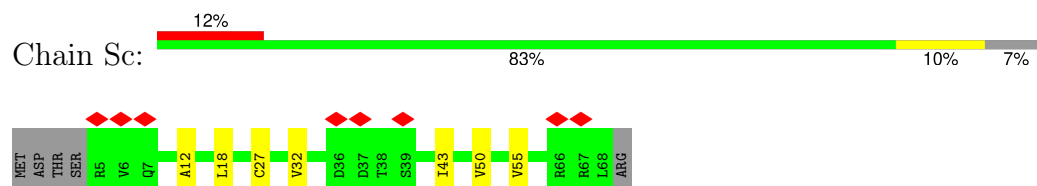
- Molecule 32: eS26



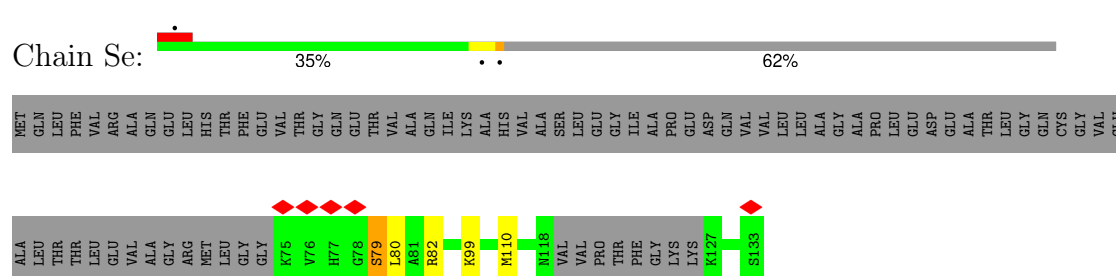
- Molecule 33: eS27



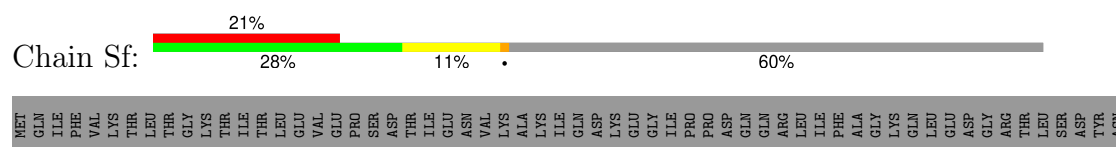
- Molecule 34: eS28

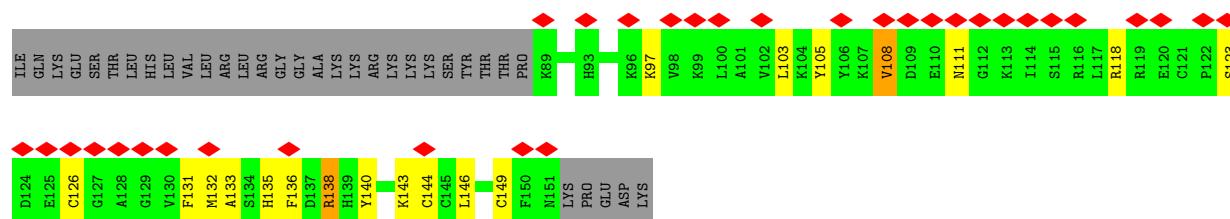


- Molecule 35: eS30

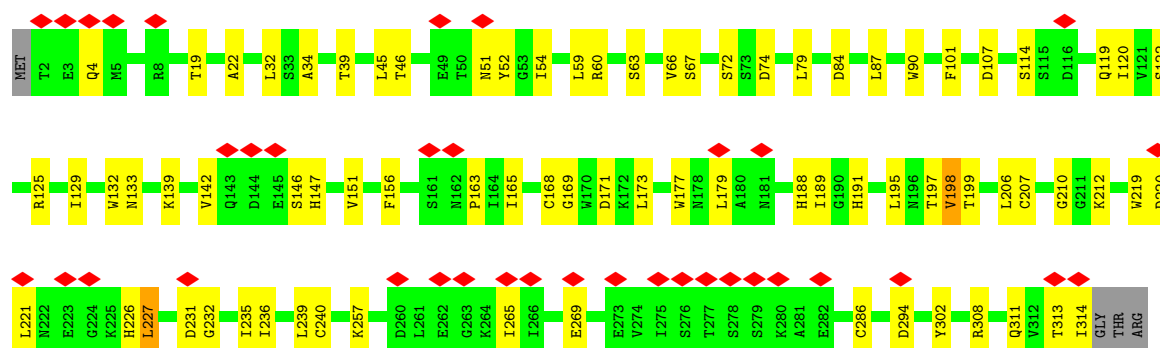
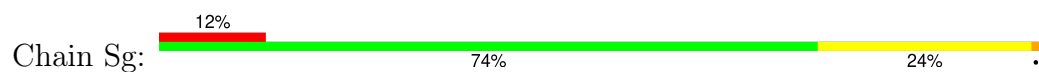


- Molecule 36: eS31

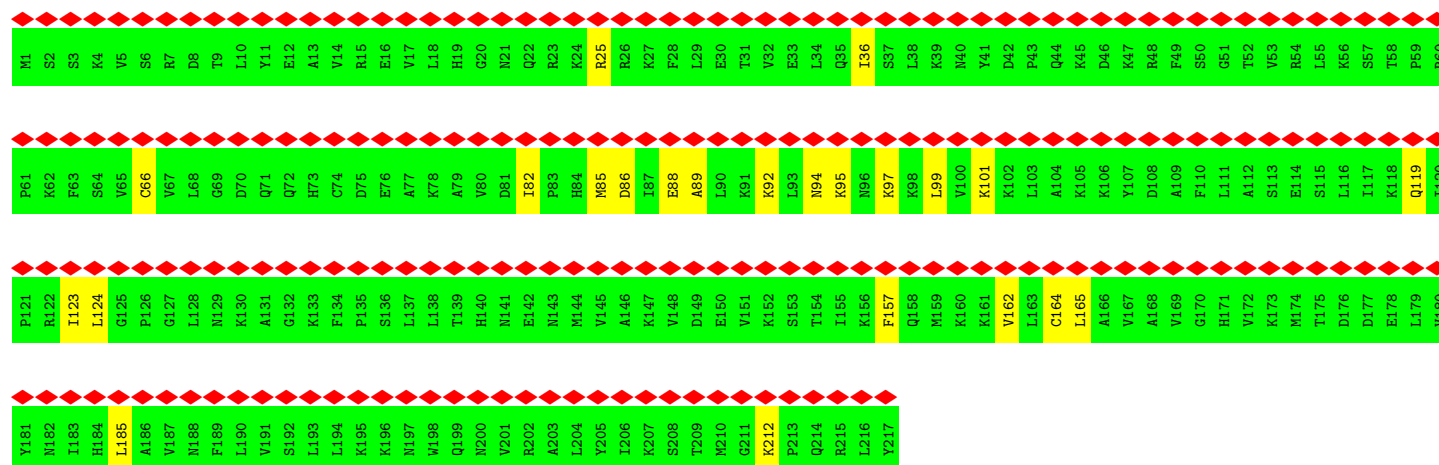
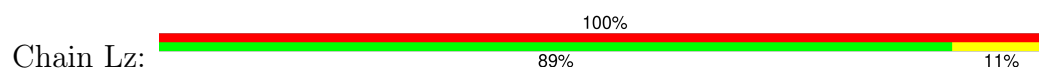




• Molecule 37: RACK1



• Molecule 38: uL1

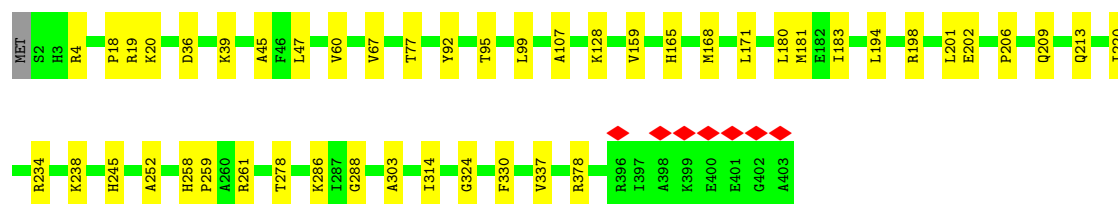


• Molecule 39: uL2



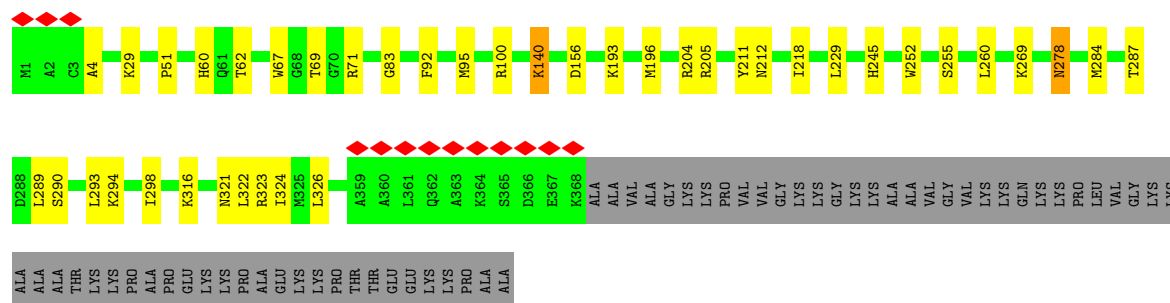
• Molecule 40: uL3

Chain LB:  88% 12%



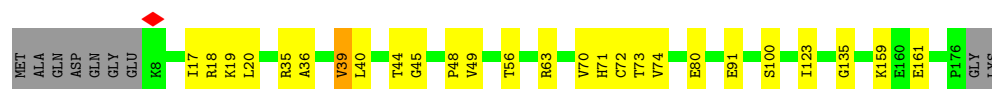
• Molecule 41: uL4

Chain LC:  77% 9% 14%



• Molecule 42: uL5

Chain LJ:  80% 14% 5%



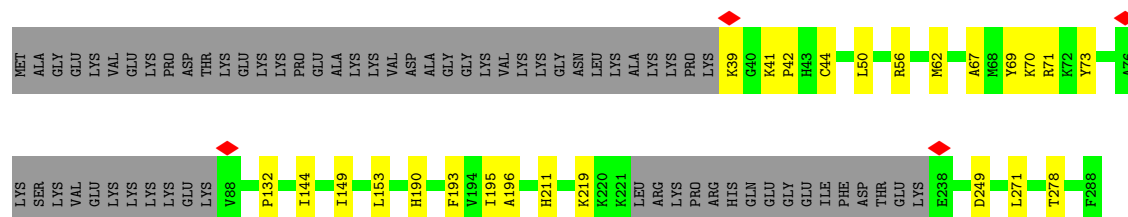
• Molecule 43: uL6

Chain LH:  88% 11%

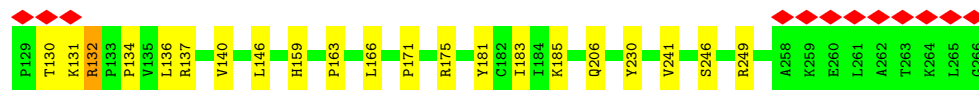
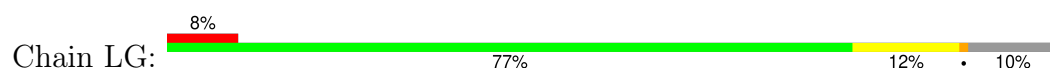


• Molecule 44: eL6

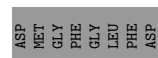
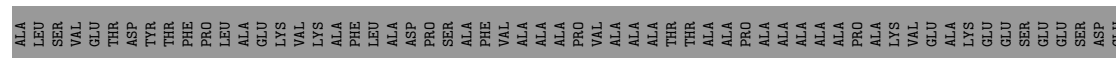
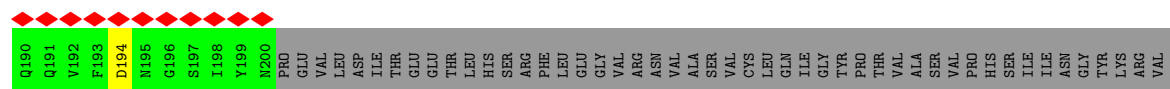
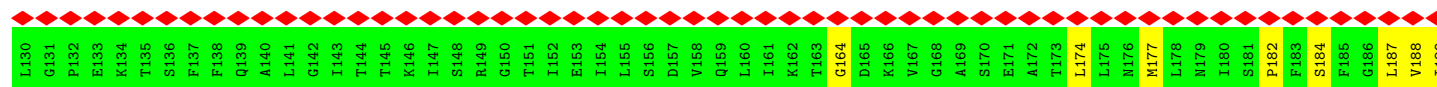
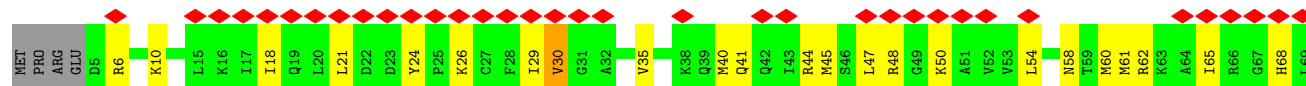
Chain LE:  69% 9% 23%



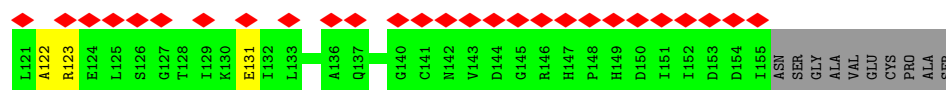
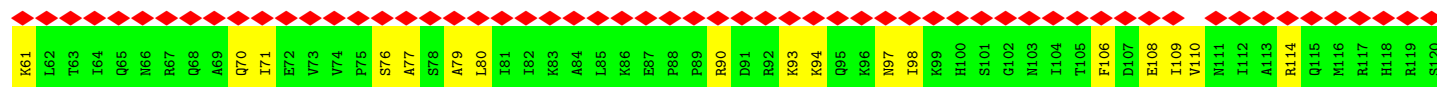
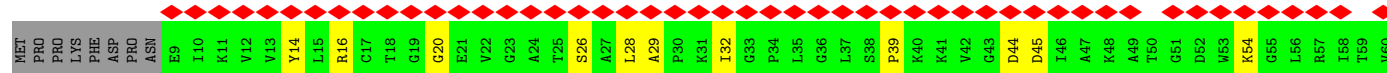
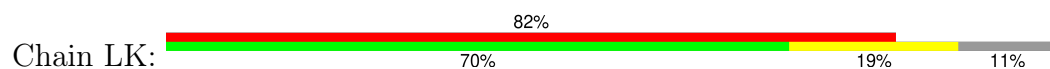
• Molecule 45: eL8



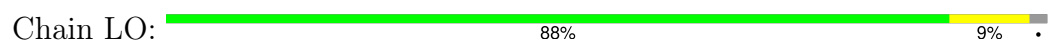
• Molecule 46: uL10



• Molecule 47: uL11

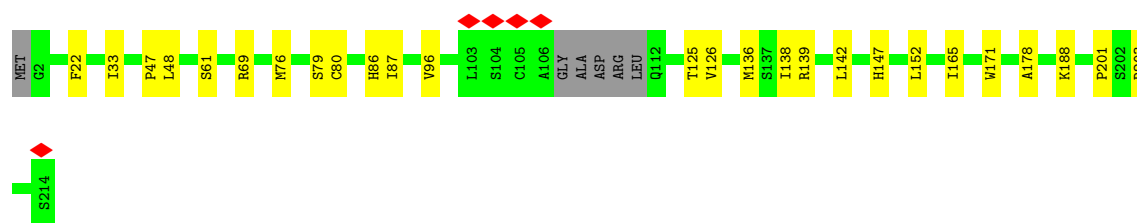


• Molecule 48: uL13

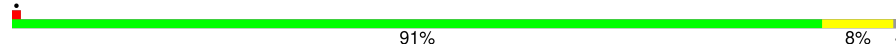




Chain LI:  85% 12%



- Molecule 55: uL18

Chain LD:  91% 8%



- Molecule 56: eL18

Chain LQ:  90% 10%



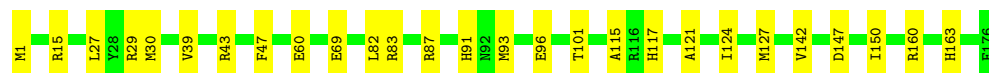
- Molecule 57: eL19

Chain LR:  6% 84% 11% 5%



- Molecule 58: eL20

Chain LS:  85% 15%



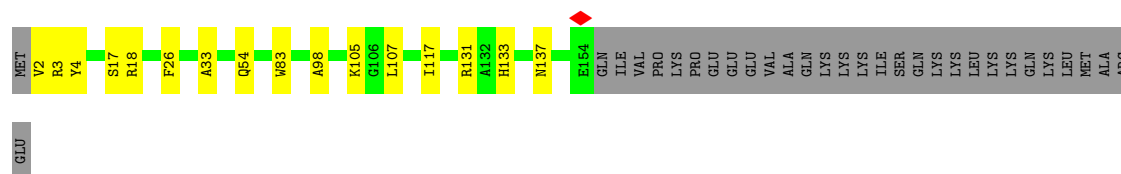
- Molecule 59: eL21

Chain LT:  88% 12%

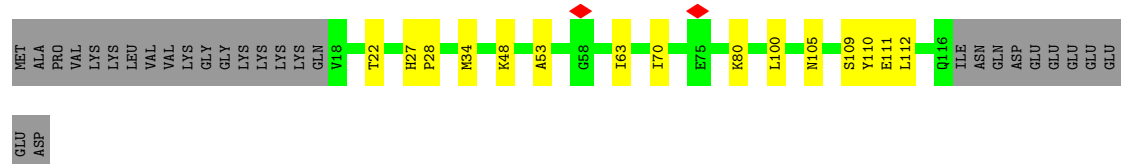


- Molecule 60: uL22

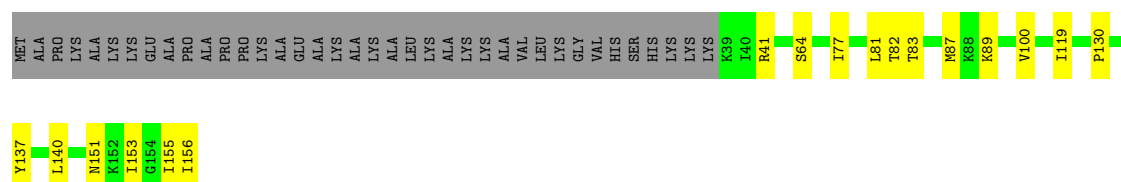
Chain LP:  74% 9% 17%



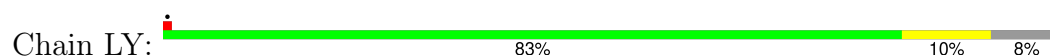
- Molecule 61: eL22



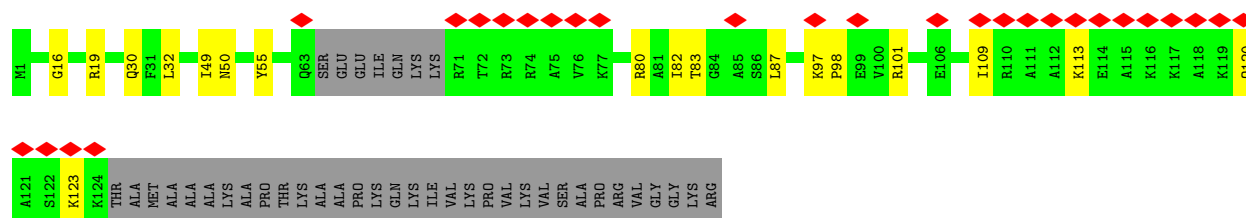
- Molecule 62: uL23



- Molecule 63: uL24



- Molecule 64: eL24

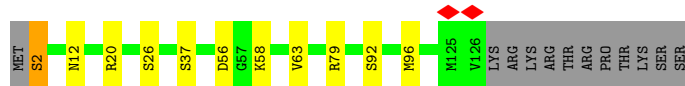


- Molecule 65: eL27

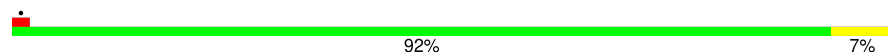


- Molecule 66: eL28

Chain Lr:  83% 7% 9%



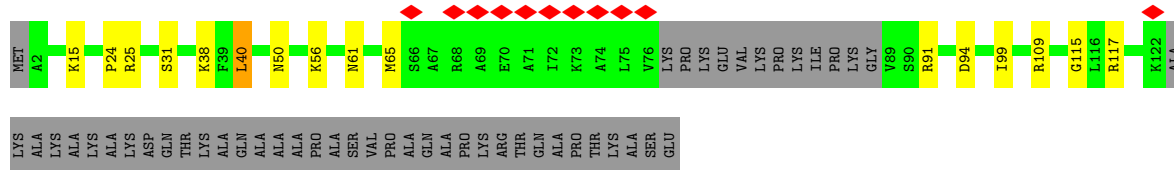
- Molecule 67: uL29

Chain Lh:  92% 7%



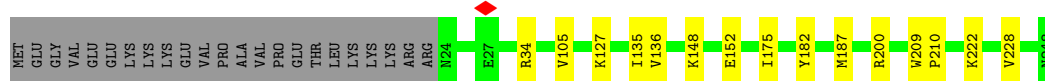
- Molecule 68: eL29

Chain Lb:  7% 58% 9% 31%



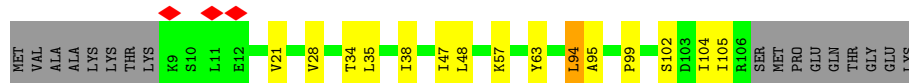
- Molecule 69: uL30

Chain LF:  85% 6% 9%



- Molecule 70: eL30

Chain Lc:  72% 12% 15%



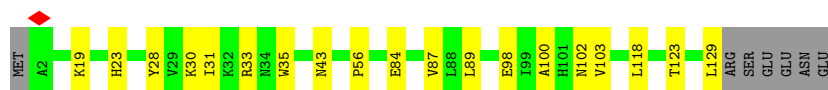
- Molecule 71: eL31

Chain Ld:  78% 8% 14%



- Molecule 72: eL32

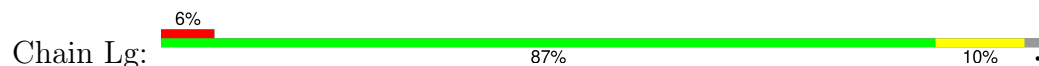
Chain Le:  81% 14% 5%



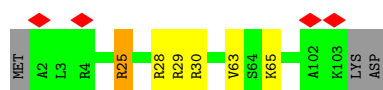
• Molecule 73: eL33



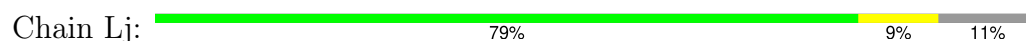
• Molecule 74: eL34



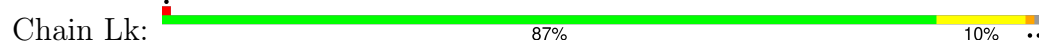
• Molecule 75: eL36



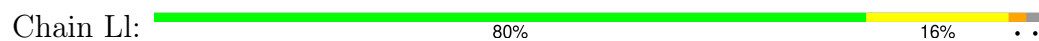
• Molecule 76: eL37



• Molecule 77: eL38

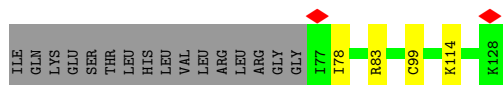


• Molecule 78: eL39

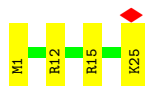
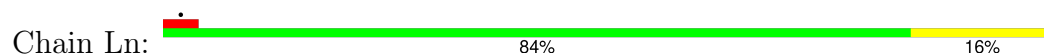


• Molecule 79: eL40

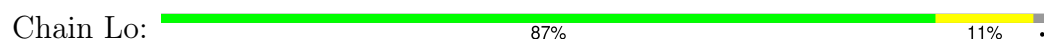




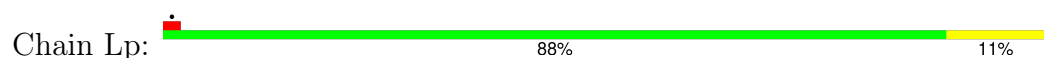
- Molecule 80: eL41



- Molecule 81: eL42



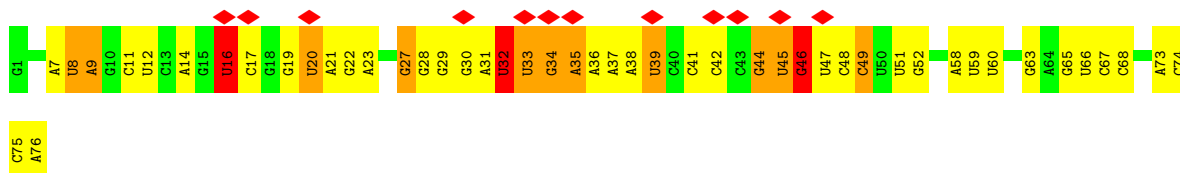
- Molecule 82: eL43



- Molecule 83: mRNA

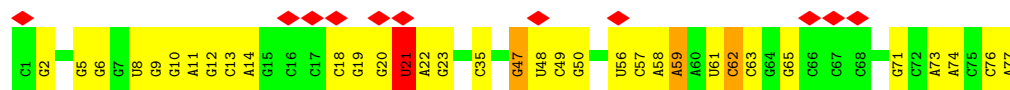


- Molecule 84: A-site tRNA

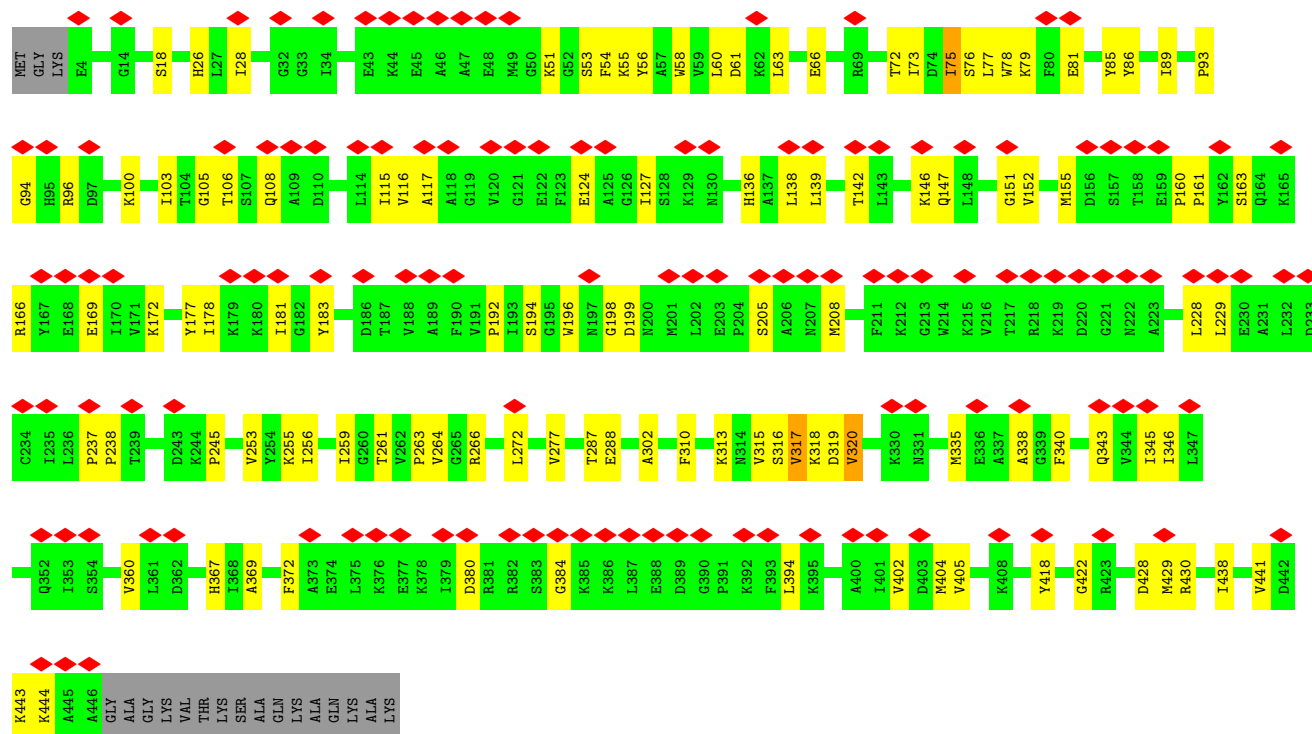
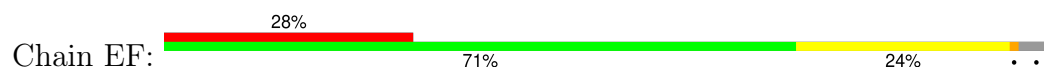


- Molecule 85: P-site tRNA





• Molecule 86: eEF1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21942	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	0.045	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: SPD, B8N, UR3, M3L, OMG, MG, 4SU, ANM, 5MC, ZN, OMU, GSP, 3H3, PUT, ZIY, MLY, 4AC, PSU, H2U, MIA, K, HIC, AME, 6MZ, OMC, SAC, A2M, G7M, 1MA, MA6, V5N, HY3, MLZ, UY1

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	0.42	7/37514 (0.0%)	0.53	1/58464 (0.0%)
2	L8	0.44	0/3613	0.51	0/5627
3	L5	0.45	4/84265 (0.0%)	0.54	5/131451 (0.0%)
4	L7	0.43	0/2862	0.45	0/4459
5	SB	0.37	0/1832	0.52	0/2449
6	SA	0.65	0/1778	0.89	0/2416
7	SD	0.63	0/1784	0.92	1/2403 (0.0%)
8	SJ	0.46	0/1550	0.70	0/2069
9	SE	0.50	0/2118	0.72	0/2849
10	SC	0.45	0/1762	0.62	0/2381
11	SG	0.54	0/1946	0.74	0/2590
12	SF	0.41	0/1515	0.56	0/2037
13	SH	0.37	0/1540	0.56	0/2064
14	SW	0.38	0/1051	0.50	0/1406
15	SI	0.58	0/1715	0.78	0/2287
16	SQ	0.49	0/1141	0.74	0/1528
17	SU	0.71	0/813	1.04	0/1092
18	SK	0.43	0/834	0.59	0/1125
19	SO	0.47	0/1022	0.76	3/1372 (0.2%)
20	SX	0.38	0/1113	0.52	0/1483
21	SM	0.45	0/950	0.70	0/1275
22	SS	0.48	0/1232	0.77	0/1651
23	Sd	0.34	0/469	0.47	0/623
24	SN	0.47	1/1242 (0.1%)	0.62	1/1671 (0.1%)
25	SL	0.35	0/1209	0.40	0/1616
26	SR	0.34	0/1098	0.58	0/1474
27	SP	0.56	0/1071	0.86	0/1432
28	ST	0.64	0/1131	0.95	1/1515 (0.1%)
29	SV	0.54	0/635	0.76	0/850
30	SY	0.66	0/1083	1.04	0/1438

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	SZ	0.57	0/682	0.77	0/911
32	Sa	0.43	0/805	0.65	0/1079
33	Sb	0.42	0/664	0.60	0/891
34	Sc	0.23	0/508	0.30	0/680
35	Se	0.60	0/409	0.97	1/535 (0.2%)
36	Sf	0.79	0/525	1.12	1/695 (0.1%)
37	Sg	0.61	0/2493	0.89	2/3394 (0.1%)
38	Lz	0.30	0/1769	0.51	0/2371
39	LA	0.51	0/1958	0.66	1/2623 (0.0%)
40	LB	0.43	0/3295	0.56	1/4406 (0.0%)
41	LC	0.54	0/2981	0.77	1/4002 (0.0%)
42	LJ	0.48	0/1381	0.71	1/1847 (0.1%)
43	LH	0.38	0/1537	0.52	0/2066
44	LE	0.44	0/1820	0.62	0/2442
45	LG	0.45	0/1943	0.63	0/2616
46	Lq	0.47	0/1529	0.75	0/2063
47	LK	0.45	0/1135	0.64	0/1529
48	LO	0.43	0/1666	0.57	0/2228
49	LL	0.55	0/1695	0.73	0/2270
50	LV	0.38	0/1003	0.52	0/1345
51	LM	0.37	0/1142	0.48	0/1527
52	La	0.56	0/1179	0.77	0/1573
53	LN	0.57	0/1746	0.77	0/2338
54	LI	0.46	0/1718	0.65	0/2293
55	LD	0.51	0/2433	0.74	0/3258
56	LQ	0.39	0/1535	0.52	0/2050
57	LR	0.49	0/1582	0.72	0/2091
58	LS	0.45	0/1500	0.58	0/2013
59	LT	0.48	0/1326	0.64	0/1770
60	LP	0.46	0/1268	0.65	0/1701
61	LU	0.45	0/822	0.75	0/1103
62	LX	0.34	0/984	0.39	0/1323
63	LY	0.56	0/1132	0.86	1/1504 (0.1%)
64	LW	0.48	0/958	0.69	1/1270 (0.1%)
65	LZ	0.57	0/1130	0.80	0/1507
66	Lr	0.50	0/1011	0.67	0/1356
67	Lh	0.42	0/1023	0.56	0/1351
68	Lb	0.53	0/887	0.78	0/1171
69	LF	0.38	0/1905	0.45	0/2539
70	Lc	0.61	0/774	0.87	0/1038
71	Ld	0.37	0/903	0.45	0/1216
72	Le	0.54	0/1071	0.70	0/1429
73	Lf	0.48	0/895	0.57	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Lg	0.39	0/916	0.52	0/1220
75	Li	0.33	0/843	0.46	0/1115
76	Lj	0.50	0/720	0.67	0/952
77	Lk	0.34	0/574	0.41	0/761
78	Ll	0.69	0/453	1.01	1/599 (0.2%)
79	Lm	0.41	0/425	0.58	0/564
80	Ln	0.42	0/240	0.59	0/305
81	Lo	0.39	0/854	0.54	0/1125
82	Lp	0.48	0/718	0.66	0/953
83	mR	0.27	0/208	0.41	0/321
84	At	0.43	0/1650	0.58	0/2566
85	Pt	0.39	1/1721 (0.1%)	0.49	0/2679
86	EF	0.43	1/3424 (0.0%)	0.66	2/4639 (0.0%)
All	All	0.46	14/233356 (0.0%)	0.60	25/341508 (0.0%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1678	A2M	O3'-P	6.93	1.63	1.56
1	S2	166	A2M	O3'-P	6.79	1.63	1.56
3	L5	3760	A2M	O3'-P	6.41	1.62	1.56
1	S2	1442	OMU	O3'-P	6.24	1.62	1.56
1	S2	1031	A2M	O3'-P	5.89	1.62	1.56

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	SO	139	SER	N-CA-C	8.65	119.68	108.34
1	S2	1520	G	C2'-C3'-O3'	-8.26	101.31	113.70
19	SO	138	ASP	CB-CA-C	7.78	125.70	110.30
63	LY	110	LYS	N-CA-C	-6.69	99.99	109.96
3	L5	1590	C	C2'-C3'-O3'	-6.69	103.67	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	35359	0	17896	289	0
2	L8	3320	0	1686	24	0
3	L5	78069	0	39524	572	0
4	L7	2562	0	1295	12	0
5	SB	1806	0	1888	23	0
6	SA	1750	0	1755	24	0
7	SD	1756	0	1852	28	0
8	SJ	1525	0	1640	16	0
9	SE	2076	0	2177	25	0
10	SC	1725	0	1813	16	0
11	SG	1923	0	2088	34	0
12	SF	1494	0	1549	27	0
13	SH	1517	0	1605	27	0
14	SW	1034	0	1080	13	0
15	SI	1686	0	1772	17	0
16	SQ	1123	0	1193	10	0
17	SU	803	0	873	19	0
18	SK	810	0	836	15	0
19	SO	1009	0	1034	21	0
20	SX	1105	0	1167	12	0
21	SM	940	0	965	25	0
22	SS	1214	0	1275	29	0
23	Sd	458	0	448	9	0
24	SN	1214	0	1301	9	0
25	SL	1189	0	1262	8	0
26	SR	1083	0	1137	18	0
27	SP	1050	0	1094	10	0
28	ST	1112	0	1146	10	0
29	SV	639	0	638	6	0
30	SY	1065	0	1142	19	0
31	SZ	674	0	748	10	0
32	Sa	792	0	841	8	0
33	Sb	650	0	672	7	0
34	Sc	506	0	536	5	0
35	Se	406	0	445	4	0
36	Sf	515	0	525	10	0
37	Sg	2436	0	2393	42	0
38	Lz	1741	0	1854	16	0
39	LA	1930	0	2028	13	0
40	LB	3240	0	3377	30	0
41	LC	2927	0	3104	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	LJ	1358	0	1396	12	0
43	LH	1518	0	1601	14	0
44	LE	1786	0	1945	15	0
45	LG	1910	0	2052	19	0
46	Lq	1506	0	1562	27	0
47	LK	1121	0	1184	18	0
48	LO	1634	0	1779	13	0
49	LL	1664	0	1773	22	0
50	LV	989	0	1047	14	0
51	LM	1120	0	1187	7	0
52	La	1163	0	1206	13	0
53	LN	1701	0	1749	16	0
54	LI	1680	0	1728	18	0
55	LD	2387	0	2423	14	0
56	LQ	1511	0	1628	12	0
57	LR	1566	0	1729	10	0
58	LS	1460	0	1502	21	0
59	LT	1298	0	1366	17	0
60	LP	1242	0	1269	10	0
61	LU	808	0	831	8	0
62	LX	967	0	1040	13	0
63	LY	1115	0	1205	8	0
64	LW	944	0	994	15	0
65	LZ	1107	0	1182	10	0
66	Lr	1005	0	1072	9	0
67	Lh	1015	0	1148	8	0
68	Lb	885	0	967	12	0
69	LF	1870	0	1996	10	0
70	Lc	764	0	804	7	0
71	Ld	888	0	930	7	0
72	Le	1053	0	1147	12	0
73	Lf	876	0	912	6	0
74	Lg	906	0	998	10	0
75	Li	832	0	917	4	0
76	Lj	705	0	736	7	0
77	Lk	568	0	637	5	0
78	Ll	443	0	483	5	0
79	Lm	431	0	470	2	0
80	Ln	239	0	289	4	0
81	Lo	852	0	920	7	0
82	Lp	708	0	756	6	0
83	mR	188	0	96	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	At	1630	0	839	32	0
85	Pt	1645	0	843	15	0
86	EF	3401	0	3462	75	0
87	L5	70	0	133	2	0
87	S2	10	0	19	0	0
88	L5	48	0	96	1	0
88	S2	12	0	24	0	0
89	EF	1	0	0	0	0
89	L5	307	0	0	0	0
89	L7	7	0	0	0	0
89	L8	7	0	0	0	0
89	LA	1	0	0	0	0
89	LB	3	0	0	0	0
89	LC	1	0	0	0	0
89	LI	1	0	0	0	0
89	LL	1	0	0	0	0
89	LN	1	0	0	0	0
89	LP	2	0	0	0	0
89	LR	1	0	0	0	0
89	LS	1	0	0	0	0
89	LV	1	0	0	0	0
89	Le	1	0	0	0	0
89	Lf	1	0	0	0	0
89	Lg	2	0	0	0	0
89	Lj	1	0	0	0	0
89	Pt	2	0	0	0	0
89	S2	112	0	0	0	0
89	SG	1	0	0	0	0
89	SN	1	0	0	0	0
89	SO	1	0	0	0	0
89	SP	1	0	0	0	0
89	SS	2	0	0	0	0
89	Sa	1	0	0	0	0
90	L5	19	0	19	0	0
91	L5	33	0	35	4	0
92	L5	10	0	0	0	0
93	Lg	1	0	0	0	0
93	Lj	1	0	0	0	0
93	Lm	1	0	0	0	0
93	Lo	1	0	0	0	0
93	Lp	1	0	0	0	0
93	Sa	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	Sd	1	0	0	0	0
94	At	11	0	8	2	0
95	Pt	8	0	8	0	0
96	EF	32	0	12	1	0
97	EF	79	0	0	1	0
98	L5	228	0	0	2	0
98	L7	1	0	0	0	0
98	L8	3	0	0	0	0
98	LA	7	0	0	0	0
98	LB	1	0	0	0	0
98	LC	1	0	0	0	0
98	LF	1	0	0	0	0
98	LH	1	0	0	0	0
98	LL	1	0	0	0	0
98	LQ	1	0	0	0	0
98	LS	1	0	0	0	0
98	Lb	2	0	0	0	0
98	Le	2	0	0	0	0
98	Lo	2	0	0	0	0
98	S2	9	0	0	0	0
98	SO	1	0	0	0	0
98	SQ	1	0	0	0	0
All	All	223755	0	167808	1884	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1884 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)
84:At:44:G:H1'	84:At:45:U:H2'	1.42	1.01
3:L5:209:U:H5''	63:LY:59:ARG:HD2	1.49	0.93
21:SM:91:LEU:HD21	21:SM:104:VAL:H	1.38	0.88
21:SM:32:ALA:HB1	21:SM:37:GLU:HB3	1.61	0.82
3:L5:4041:C:H1'	38:Lz:101:LYS:HG3	1.60	0.82

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%)	214 (98%)	5 (2%)	0	100	100
6	SA	220/295 (75%)	214 (97%)	6 (3%)	0	100	100
7	SD	224/243 (92%)	219 (98%)	4 (2%)	1 (0%)	30	39
8	SJ	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
9	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
10	SC	220/293 (75%)	216 (98%)	4 (2%)	0	100	100
11	SG	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
12	SF	187/204 (92%)	175 (94%)	12 (6%)	0	100	100
13	SH	187/194 (96%)	178 (95%)	9 (5%)	0	100	100
14	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
15	SI	204/208 (98%)	202 (99%)	2 (1%)	0	100	100
16	SQ	139/146 (95%)	137 (99%)	2 (1%)	0	100	100
17	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
18	SK	94/165 (57%)	86 (92%)	8 (8%)	0	100	100
19	SO	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
20	SX	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
21	SM	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
22	SS	146/152 (96%)	139 (95%)	6 (4%)	1 (1%)	18	25
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	141/158 (89%)	133 (94%)	8 (6%)	0	100	100
26	SR	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
27	SP	126/145 (87%)	117 (93%)	9 (7%)	0	100	100
28	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
29	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	SY	129/133 (97%)	124 (96%)	5 (4%)	0	100	100
31	SZ	82/125 (66%)	78 (95%)	4 (5%)	0	100	100
32	Sa	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
33	Sb	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
34	Sc	62/69 (90%)	59 (95%)	3 (5%)	0	100	100
35	Se	47/133 (35%)	47 (100%)	0	0	100	100
36	Sf	61/156 (39%)	55 (90%)	5 (8%)	1 (2%)	7	9
37	Sg	311/317 (98%)	290 (93%)	21 (7%)	0	100	100
38	Lz	215/217 (99%)	187 (87%)	28 (13%)	0	100	100
39	LA	249/257 (97%)	239 (96%)	10 (4%)	0	100	100
40	LB	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
41	LC	366/427 (86%)	361 (99%)	5 (1%)	0	100	100
42	LJ	167/178 (94%)	166 (99%)	1 (1%)	0	100	100
43	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
44	LE	217/288 (75%)	210 (97%)	7 (3%)	0	100	100
45	LG	237/266 (89%)	227 (96%)	9 (4%)	1 (0%)	30	39
46	Lq	194/317 (61%)	181 (93%)	13 (7%)	0	100	100
47	LK	145/165 (88%)	131 (90%)	14 (10%)	0	100	100
48	LO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
49	LL	204/270 (76%)	196 (96%)	8 (4%)	0	100	100
50	LV	131/140 (94%)	129 (98%)	2 (2%)	0	100	100
51	LM	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
52	La	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	25
53	LN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
54	LI	204/214 (95%)	193 (95%)	11 (5%)	0	100	100
55	LD	291/297 (98%)	287 (99%)	4 (1%)	0	100	100
56	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
57	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
58	LS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
59	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
60	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	LU	97/128 (76%)	90 (93%)	7 (7%)	0	100	100
62	LX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
63	LY	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
64	LW	113/157 (72%)	111 (98%)	2 (2%)	0	100	100
65	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
66	Lr	123/137 (90%)	117 (95%)	6 (5%)	0	100	100
67	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
68	Lb	104/159 (65%)	99 (95%)	5 (5%)	0	100	100
69	LF	223/248 (90%)	215 (96%)	8 (4%)	0	100	100
70	Lc	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
71	Ld	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
72	Le	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
73	Lf	107/110 (97%)	107 (100%)	0	0	100	100
74	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
75	Li	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
76	Lj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
77	Lk	67/70 (96%)	67 (100%)	0	0	100	100
78	Ll	48/51 (94%)	48 (100%)	0	0	100	100
79	Lm	49/128 (38%)	49 (100%)	0	0	100	100
80	Ln	23/25 (92%)	23 (100%)	0	0	100	100
81	Lo	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
82	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
86	EF	437/462 (95%)	413 (94%)	24 (6%)	0	100	100
All	All	12269/13982 (88%)	11858 (97%)	406 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	La	15	VAL
7	SD	157	MET
22	SS	92	ASP
36	Sf	97	LYS
45	LG	132	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SB	202/231 (87%)	201 (100%)	1 (0%)	81	88
6	SA	183/242 (76%)	179 (98%)	4 (2%)	45	64
7	SD	189/202 (94%)	183 (97%)	6 (3%)	34	51
8	SJ	161/168 (96%)	161 (100%)	0	100	100
9	SE	224/225 (100%)	221 (99%)	3 (1%)	61	76
10	SC	188/225 (84%)	186 (99%)	2 (1%)	65	79
11	SG	207/218 (95%)	205 (99%)	2 (1%)	68	80
12	SF	159/170 (94%)	159 (100%)	0	100	100
13	SH	168/174 (97%)	165 (98%)	3 (2%)	51	70
14	SW	112/113 (99%)	112 (100%)	0	100	100
15	SI	178/180 (99%)	177 (99%)	1 (1%)	78	87
16	SQ	117/121 (97%)	116 (99%)	1 (1%)	70	82
17	SU	93/107 (87%)	90 (97%)	3 (3%)	34	51
18	SK	87/136 (64%)	86 (99%)	1 (1%)	65	79
19	SO	105/119 (88%)	104 (99%)	1 (1%)	68	80
20	SX	113/114 (99%)	113 (100%)	0	100	100
21	SM	102/108 (94%)	100 (98%)	2 (2%)	48	67
22	SS	128/132 (97%)	125 (98%)	3 (2%)	44	62
23	Sd	48/49 (98%)	48 (100%)	0	100	100
24	SN	131/131 (100%)	131 (100%)	0	100	100
25	SL	131/142 (92%)	131 (100%)	0	100	100
26	SR	121/122 (99%)	120 (99%)	1 (1%)	73	84
27	SP	114/130 (88%)	113 (99%)	1 (1%)	70	82
28	ST	113/115 (98%)	111 (98%)	2 (2%)	51	70
29	SV	66/66 (100%)	66 (100%)	0	100	100
30	SY	113/115 (98%)	107 (95%)	6 (5%)	20	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	SZ	74/103 (72%)	73 (99%)	1 (1%)	59	75
32	Sa	86/98 (88%)	85 (99%)	1 (1%)	63	78
33	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	76
34	Sc	57/62 (92%)	57 (100%)	0	100	100
35	Se	41/104 (39%)	41 (100%)	0	100	100
36	Sf	56/140 (40%)	50 (89%)	6 (11%)	6	7
37	Sg	272/275 (99%)	260 (96%)	12 (4%)	25	38
38	Lz	195/196 (100%)	195 (100%)	0	100	100
39	LA	193/198 (98%)	192 (100%)	1 (0%)	81	88
40	LB	347/348 (100%)	347 (100%)	0	100	100
41	LC	306/348 (88%)	303 (99%)	3 (1%)	68	80
42	LJ	143/149 (96%)	140 (98%)	3 (2%)	47	66
43	LH	169/171 (99%)	169 (100%)	0	100	100
44	LE	196/252 (78%)	195 (100%)	1 (0%)	81	88
45	LG	201/223 (90%)	199 (99%)	2 (1%)	68	80
46	Lq	164/258 (64%)	157 (96%)	7 (4%)	26	39
47	LK	122/137 (89%)	119 (98%)	3 (2%)	42	60
48	LO	171/174 (98%)	170 (99%)	1 (1%)	78	87
49	LL	172/224 (77%)	167 (97%)	5 (3%)	37	55
50	LV	102/107 (95%)	101 (99%)	1 (1%)	68	80
51	LM	116/161 (72%)	116 (100%)	0	100	100
52	La	119/120 (99%)	118 (99%)	1 (1%)	73	84
53	LN	171/172 (99%)	169 (99%)	2 (1%)	63	78
54	LI	177/181 (98%)	177 (100%)	0	100	100
55	LD	247/250 (99%)	245 (99%)	2 (1%)	73	84
56	LQ	164/165 (99%)	164 (100%)	0	100	100
57	LR	166/175 (95%)	161 (97%)	5 (3%)	36	53
58	LS	157/157 (100%)	157 (100%)	0	100	100
59	LT	139/140 (99%)	139 (100%)	0	100	100
60	LP	134/163 (82%)	134 (100%)	0	100	100
61	LU	89/115 (77%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	LX	106/133 (80%)	106 (100%)	0	100	100
63	LY	124/135 (92%)	123 (99%)	1 (1%)	73	84
64	LW	94/126 (75%)	91 (97%)	3 (3%)	34	51
65	LZ	117/118 (99%)	112 (96%)	5 (4%)	26	39
66	Lr	108/120 (90%)	107 (99%)	1 (1%)	70	82
67	Lh	109/110 (99%)	109 (100%)	0	100	100
68	Lb	89/125 (71%)	86 (97%)	3 (3%)	32	48
69	LF	194/215 (90%)	194 (100%)	0	100	100
70	Lc	83/97 (86%)	80 (96%)	3 (4%)	31	46
71	Ld	98/110 (89%)	98 (100%)	0	100	100
72	Le	114/121 (94%)	111 (97%)	3 (3%)	40	59
73	Lf	88/89 (99%)	88 (100%)	0	100	100
74	Lg	98/100 (98%)	98 (100%)	0	100	100
75	Li	86/89 (97%)	84 (98%)	2 (2%)	44	62
76	Lj	73/80 (91%)	73 (100%)	0	100	100
77	Lk	64/65 (98%)	62 (97%)	2 (3%)	35	53
78	Ll	47/48 (98%)	45 (96%)	2 (4%)	26	39
79	Lm	47/115 (41%)	47 (100%)	0	100	100
80	Ln	24/24 (100%)	24 (100%)	0	100	100
81	Lo	91/93 (98%)	90 (99%)	1 (1%)	65	79
82	Lp	74/75 (99%)	74 (100%)	0	100	100
86	EF	363/375 (97%)	354 (98%)	9 (2%)	42	60
All	All	10665/11860 (90%)	10529 (99%)	136 (1%)	59	76

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	Lc	94	LEU
72	Le	129	LEU
86	EF	228	LEU
36	Sf	140	TYR
36	Sf	138	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
41	LC	321	ASN
73	Lf	21	GLN
47	LK	142	ASN
73	Lf	20	ASN
86	EF	147	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1648/1869 (88%)	327 (19%)	28 (1%)
2	L8	155/156 (99%)	25 (16%)	1 (0%)
3	L5	3621/5069 (71%)	642 (17%)	54 (1%)
4	L7	119/120 (99%)	12 (10%)	0
83	mR	8/60 (13%)	2 (25%)	0
84	At	75/76 (98%)	24 (32%)	0
85	Pt	76/77 (98%)	16 (21%)	0
All	All	5702/7427 (76%)	1048 (18%)	83 (1%)

5 of 1048 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	17	C
1	S2	23	G
1	S2	25	A
1	S2	33	G
1	S2	41	G

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	2091	C
3	L5	3956	G
3	L5	2259	G
3	L5	2724	G
3	L5	4699	U

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

244 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	2632	3	18,21,22	1.45	4 (22%)	21,30,33	2.11	3 (14%)
3	OMG	L5	3899	3	23,26,27	1.23	3 (13%)	32,38,41	2.19	7 (21%)
3	PSU	L5	4500	3	18,21,22	1.59	5 (27%)	21,30,33	2.08	5 (23%)
3	OMC	L5	4456	3	19,22,23	0.94	0	25,31,34	1.00	1 (4%)
3	PSU	L5	2508	3	18,21,22	1.43	3 (16%)	21,30,33	1.98	4 (19%)
3	OMG	L5	4637	3	23,26,27	1.29	4 (17%)	32,38,41	2.11	7 (21%)
3	1MA	L5	1322	89,3	21,25,26	1.34	5 (23%)	30,37,40	1.75	6 (20%)
85	G7M	Pt	47	85	23,26,27	1.87	2 (8%)	34,39,42	1.08	1 (2%)
1	PSU	S2	406	1	18,21,22	1.51	4 (22%)	21,30,33	2.14	3 (14%)
1	UY1	S2	1326	89,1	19,22,23	1.36	3 (15%)	21,31,34	2.22	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.55	3 (16%)	21,30,33	1.77	4 (19%)
3	OMG	L5	4623	3	23,26,27	1.28	4 (17%)	32,38,41	2.04	8 (25%)
3	A2M	L5	1326	3	22,25,26	1.48	4 (18%)	30,36,39	2.09	11 (36%)
1	OMU	S2	627	1	19,22,23	1.26	3 (15%)	25,31,34	1.97	5 (20%)
3	OMC	L5	3869	3	19,22,23	0.81	0	25,31,34	1.05	1 (4%)
3	PSU	L5	5001	3	18,21,22	1.42	4 (22%)	21,30,33	2.13	4 (19%)
29	AME	SV	1	29	9,10,11	3.33	2 (22%)	9,11,13	3.74	3 (33%)
3	OMG	L5	3744	3	23,26,27	1.22	4 (17%)	32,38,41	2.07	7 (21%)
1	A2M	S2	590	1	22,25,26	1.47	3 (13%)	30,36,39	2.12	7 (23%)
3	PSU	L5	4299	3	18,21,22	1.55	4 (22%)	21,30,33	2.08	4 (19%)
3	OMU	L5	4498	3	19,22,23	1.31	3 (15%)	25,31,34	1.97	5 (20%)
3	6MZ	L5	4220	3	22,25,26	1.34	5 (22%)	29,36,39	2.19	10 (34%)
1	PSU	S2	1056	1	18,21,22	1.48	3 (16%)	21,30,33	2.18	4 (19%)
1	OMU	S2	1442	89,1	19,22,23	1.34	3 (15%)	25,31,34	1.93	5 (20%)
3	A2M	L5	400	3	22,25,26	1.46	5 (22%)	30,36,39	2.17	10 (33%)
3	PSU	L5	5010	3	18,21,22	1.52	4 (22%)	21,30,33	2.11	4 (19%)
1	PSU	S2	573	1	18,21,22	1.40	3 (16%)	21,30,33	2.04	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.83	0	25,31,34	1.08	2 (8%)
79	M3L	Lm	98	79	10,11,12	0.38	0	9,14,16	0.09	0
1	PSU	S2	218	1	18,21,22	1.49	4 (22%)	21,30,33	2.15	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3639	3	18,21,22	1.56	5 (27%)	21,30,33	2.00	3 (14%)
1	A2M	S2	468	1	22,25,26	1.48	5 (22%)	30,36,39	2.13	9 (30%)
1	PSU	S2	1232	1	18,21,22	1.54	4 (22%)	21,30,33	2.13	3 (14%)
3	PSU	L5	4532	3	18,21,22	1.57	4 (22%)	21,30,33	2.21	6 (28%)
1	A2M	S2	27	89,1	22,25,26	1.43	4 (18%)	30,36,39	2.09	9 (30%)
1	OMC	S2	1391	1	19,22,23	0.84	0	25,31,34	1.05	2 (8%)
1	PSU	S2	1244	1	18,21,22	1.46	4 (22%)	21,30,33	2.07	3 (14%)
81	MLZ	Lo	53	81	8,9,10	0.63	0	4,9,11	0.89	0
86	M3L	EF	318	86	10,11,12	0.48	0	9,14,16	0.10	0
1	PSU	S2	572	1	18,21,22	1.40	4 (22%)	21,30,33	2.05	4 (19%)
1	OMG	S2	601	1	23,26,27	1.28	3 (13%)	32,38,41	1.90	5 (15%)
1	PSU	S2	681	1	18,21,22	1.55	5 (27%)	21,30,33	2.23	3 (14%)
1	OMU	S2	121	1	19,22,23	1.47	4 (21%)	25,31,34	1.78	5 (20%)
1	OMG	S2	683	1	23,26,27	1.22	4 (17%)	32,38,41	2.09	7 (21%)
3	PSU	L5	3762	3	18,21,22	1.37	2 (11%)	21,30,33	2.15	5 (23%)
3	PSU	L5	4442	3	18,21,22	1.53	5 (27%)	21,30,33	2.27	5 (23%)
3	OMG	L5	4392	3	23,26,27	1.32	4 (17%)	32,38,41	2.02	7 (21%)
3	OMG	L5	4494	3	23,26,27	1.28	4 (17%)	32,38,41	1.98	5 (15%)
3	PSU	L5	4576	3	18,21,22	1.52	3 (16%)	21,30,33	1.87	5 (23%)
1	PSU	S2	34	1	18,21,22	1.43	4 (22%)	21,30,33	2.08	4 (19%)
3	OMC	L5	3841	3	19,22,23	0.81	1 (5%)	25,31,34	0.92	0
1	PSU	S2	1243	1	18,21,22	1.55	4 (22%)	21,30,33	2.30	5 (23%)
86	MLY	EF	55	86	9,10,11	0.48	0	6,11,13	0.89	0
3	PSU	L5	4689	3	18,21,22	1.48	3 (16%)	21,30,33	2.17	5 (23%)
3	A2M	L5	4523	89,3	22,25,26	1.40	4 (18%)	30,36,39	2.22	11 (36%)
1	OMC	S2	517	1	19,22,23	0.83	0	25,31,34	1.03	2 (8%)
1	PSU	S2	1004	1	18,21,22	1.58	4 (22%)	21,30,33	1.97	3 (14%)
3	PSU	L5	1744	3,92	18,21,22	1.45	3 (16%)	21,30,33	2.13	3 (14%)
3	OMC	L5	3808	3	19,22,23	0.77	0	25,31,34	0.86	0
1	PSU	S2	109	1	18,21,22	1.53	4 (22%)	21,30,33	2.17	3 (14%)
2	OMG	L8	75	2	23,26,27	1.22	3 (13%)	32,38,41	2.07	7 (21%)
3	PSU	L5	4531	3	18,21,22	1.46	3 (16%)	21,30,33	2.42	4 (19%)
3	OMC	L5	2422	89,3	19,22,23	0.82	0	25,31,34	0.98	1 (4%)
3	A2M	L5	2815	89,3	22,25,26	1.60	5 (22%)	30,36,39	1.98	9 (30%)
3	PSU	L5	3764	3	18,21,22	1.50	3 (16%)	21,30,33	2.11	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	649	1	18,21,22	1.51	4 (22%)	21,30,33	2.18	4 (19%)
86	M3L	EF	36	86	10,11,12	0.51	0	9,14,16	0.49	0
1	PSU	S2	105	1	18,21,22	1.59	5 (27%)	21,30,33	2.26	5 (23%)
40	HIC	LB	245	40	10,11,12	1.17	1 (10%)	9,14,16	1.33	2 (22%)
1	OMG	S2	436	1	23,26,27	1.24	3 (13%)	32,38,41	1.98	6 (18%)
3	A2M	L5	2363	89,3	22,25,26	1.48	4 (18%)	30,36,39	2.01	9 (30%)
3	OMG	L5	3627	3	23,26,27	1.26	4 (17%)	32,38,41	2.11	8 (25%)
2	PSU	L8	69	2	18,21,22	1.55	6 (33%)	21,30,33	2.27	5 (23%)
3	PSU	L5	1782	3	18,21,22	1.55	4 (22%)	21,30,33	2.07	5 (23%)
3	PSU	L5	4361	3	18,21,22	1.49	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.59	5 (27%)	21,30,33	2.00	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.58	5 (27%)	21,30,33	2.21	3 (14%)
20	HY3	SX	62	20	7,8,9	1.58	1 (14%)	7,10,12	1.29	0
3	A2M	L5	2787	89,3	22,25,26	1.44	5 (22%)	30,36,39	2.26	8 (26%)
3	OMC	L5	2861	3	19,22,23	0.71	0	25,31,34	0.79	1 (4%)
3	A2M	L5	2401	3	22,25,26	1.40	4 (18%)	30,36,39	2.08	11 (36%)
1	OMU	S2	116	1	19,22,23	1.32	3 (15%)	25,31,34	1.84	4 (16%)
1	A2M	S2	1678	1	22,25,26	1.44	4 (18%)	30,36,39	2.10	10 (33%)
1	PSU	S2	686	1	18,21,22	1.49	4 (22%)	21,30,33	2.21	3 (14%)
1	OMU	S2	1288	1	19,22,23	1.24	3 (15%)	25,31,34	1.87	5 (20%)
3	PSU	L5	4423	3	18,21,22	1.40	4 (22%)	21,30,33	2.07	3 (14%)
1	PSU	S2	36	1	18,21,22	1.54	5 (27%)	21,30,33	2.11	3 (14%)
3	PSU	L5	4457	3	18,21,22	1.51	4 (22%)	21,30,33	2.17	5 (23%)
1	OMG	S2	509	89,1	23,26,27	1.22	3 (13%)	32,38,41	2.00	7 (21%)
1	PSU	S2	1625	1	18,21,22	1.40	2 (11%)	21,30,33	2.05	3 (14%)
3	PSU	L5	4420	3	18,21,22	1.55	5 (27%)	21,30,33	2.04	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.48	4 (22%)	21,30,33	1.95	4 (19%)
1	PSU	S2	296	1	18,21,22	1.39	4 (22%)	21,30,33	2.12	4 (19%)
3	OMU	L5	4227	3	19,22,23	1.41	2 (10%)	25,31,34	2.02	5 (20%)
3	PSU	L5	3851	3	18,21,22	1.59	4 (22%)	21,30,33	2.22	6 (28%)
3	A2M	L5	398	3	22,25,26	1.47	4 (18%)	30,36,39	2.07	8 (26%)
3	PSU	L5	4636	3	18,21,22	1.47	3 (16%)	21,30,33	2.17	6 (28%)
85	H2U	Pt	21	85	18,21,22	1.01	2 (11%)	19,30,33	0.91	0
3	OMG	L5	1316	3	23,26,27	1.37	4 (17%)	32,38,41	2.02	7 (21%)
3	A2M	L5	3760	1,3	22,25,26	1.48	5 (22%)	30,36,39	2.22	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3785	3	22,25,26	1.41	5 (22%)	30,36,39	2.48	11 (36%)
3	A2M	L5	1534	89,3	22,25,26	1.54	5 (22%)	30,36,39	2.13	10 (33%)
1	PSU	S2	1445	1	18,21,22	1.56	5 (27%)	21,30,33	2.23	4 (19%)
1	G7M	S2	1639	1,85	23,26,27	2.39	5 (21%)	34,39,42	3.11	10 (29%)
39	V5N	LA	216	39	8,11,12	1.36	1 (12%)	8,14,16	1.92	2 (25%)
3	PSU	L5	1677	3	18,21,22	1.56	4 (22%)	21,30,33	2.28	6 (28%)
84	PSU	At	39	84	18,21,22	1.36	2 (11%)	21,30,33	2.12	4 (19%)
3	A2M	L5	4571	3	22,25,26	1.52	5 (22%)	30,36,39	1.94	9 (30%)
1	PSU	S2	1643	89,1	18,21,22	1.55	5 (27%)	21,30,33	2.16	5 (23%)
1	PSU	S2	93	1	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
1	PSU	S2	1081	1	18,21,22	1.58	5 (27%)	21,30,33	2.20	5 (23%)
1	PSU	S2	1692	1	18,21,22	1.44	4 (22%)	21,30,33	2.18	4 (19%)
3	PSU	L5	4493	3	18,21,22	1.60	4 (22%)	21,30,33	2.26	5 (23%)
1	PSU	S2	863	1	18,21,22	1.47	3 (16%)	21,30,33	2.04	3 (14%)
52	V5N	La	39	52	8,11,12	1.52	1 (12%)	8,14,16	1.95	2 (25%)
1	OMG	S2	1490	89,1	23,26,27	1.28	4 (17%)	32,38,41	2.02	7 (21%)
3	UR3	L5	4530	3	19,22,23	0.86	1 (5%)	26,32,35	2.02	5 (19%)
1	PSU	S2	814	1	18,21,22	1.52	4 (22%)	21,30,33	2.16	5 (23%)
1	6MZ	S2	1832	89,1	22,25,26	1.46	5 (22%)	29,36,39	2.14	10 (34%)
3	OMG	L5	1522	3	23,26,27	0.95	2 (8%)	32,38,41	2.15	9 (28%)
3	5MC	L5	4447	3	19,22,23	1.58	3 (15%)	26,32,35	1.57	3 (11%)
3	OMG	L5	4499	3	23,26,27	1.22	3 (13%)	32,38,41	2.02	6 (18%)
1	A2M	S2	576	1	22,25,26	1.51	6 (27%)	30,36,39	2.11	9 (30%)
3	OMC	L5	2365	89,3	19,22,23	0.82	0	25,31,34	0.93	1 (4%)
3	A2M	L5	3825	3	22,25,26	1.37	4 (18%)	30,36,39	2.24	9 (30%)
3	PSU	L5	1683	89,3	18,21,22	1.67	5 (27%)	21,30,33	2.16	3 (14%)
1	A2M	S2	166	1	22,25,26	1.44	4 (18%)	30,36,39	2.21	11 (36%)
3	PSU	L5	4569	3	18,21,22	1.46	5 (27%)	21,30,33	2.24	4 (19%)
3	PSU	L5	3920	89,3	18,21,22	1.57	4 (22%)	21,30,33	2.31	4 (19%)
3	OMG	L5	3944	3	23,26,27	1.25	3 (13%)	32,38,41	2.19	9 (28%)
3	PSU	L5	3715	3	18,21,22	1.42	4 (22%)	21,30,33	2.06	4 (19%)
3	OMG	L5	2364	3	23,26,27	1.14	3 (13%)	32,38,41	2.22	9 (28%)
3	OMC	L5	1881	89,3	19,22,23	0.78	0	25,31,34	0.90	0
1	PSU	S2	1239	1	18,21,22	1.48	4 (22%)	21,30,33	2.11	4 (19%)
66	SAC	Lr	2	66	7,8,9	3.69	2 (28%)	7,9,11	4.53	4 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	3792	3	23,26,27	1.22	3 (13%)	32,38,41	2.05	5 (15%)
3	UY1	L5	3818	89,3	19,22,23	1.40	4 (21%)	21,31,34	2.12	4 (19%)
85	PSU	Pt	56	85	18,21,22	1.39	3 (16%)	21,30,33	2.08	4 (19%)
3	OMU	L5	4306	3	19,22,23	1.41	3 (15%)	25,31,34	2.10	5 (20%)
1	OMG	S2	1328	1	23,26,27	1.26	4 (17%)	32,38,41	1.97	7 (21%)
1	PSU	S2	651	1	18,21,22	1.44	4 (22%)	21,30,33	2.02	4 (19%)
3	PSU	L5	4579	3	18,21,22	1.52	4 (22%)	21,30,33	2.15	4 (19%)
3	A2M	L5	3830	3	22,25,26	1.48	5 (22%)	30,36,39	2.27	9 (30%)
1	A2M	S2	1383	1	22,25,26	1.41	3 (13%)	30,36,39	2.36	9 (30%)
3	OMC	L5	3701	3,92	19,22,23	0.96	0	25,31,34	1.22	2 (8%)
3	PSU	L5	3768	3	18,21,22	1.53	4 (22%)	21,30,33	1.92	3 (14%)
1	OMU	S2	1804	1	19,22,23	1.34	3 (15%)	25,31,34	1.85	5 (20%)
3	PSU	L5	1536	3	18,21,22	1.68	6 (33%)	21,30,33	2.21	4 (19%)
3	OMG	L5	2876	3	23,26,27	1.26	4 (17%)	32,38,41	2.00	6 (18%)
84	H2U	At	20	84	18,21,22	1.01	2 (11%)	19,30,33	1.17	2 (10%)
3	PSU	L5	2839	3	18,21,22	1.52	6 (33%)	21,30,33	2.18	4 (19%)
1	OMG	S2	1447	1	23,26,27	1.30	4 (17%)	32,38,41	2.11	8 (25%)
3	OMG	L5	1625	89,3	23,26,27	1.27	4 (17%)	32,38,41	1.96	6 (18%)
1	PSU	S2	1174	89,1	18,21,22	1.54	5 (27%)	21,30,33	2.02	4 (19%)
3	OMG	L5	4370	3	23,26,27	1.20	4 (17%)	32,38,41	1.96	5 (15%)
1	OMU	S2	428	1	19,22,23	1.23	2 (10%)	25,31,34	2.06	6 (24%)
1	PSU	S2	815	1	18,21,22	1.48	3 (16%)	21,30,33	2.04	5 (23%)
3	A2M	L5	1871	89,3	22,25,26	1.53	5 (22%)	30,36,39	2.22	11 (36%)
6	SAC	SA	2	6	7,8,9	3.67	2 (28%)	7,9,11	4.12	4 (57%)
3	PSU	L5	3844	3	18,21,22	1.60	5 (27%)	21,30,33	2.14	3 (14%)
3	PSU	L5	1582	3	18,21,22	1.54	5 (27%)	21,30,33	1.96	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.38	3 (16%)	21,30,33	1.86	4 (19%)
3	OMG	L5	4228	3	23,26,27	1.25	4 (17%)	32,38,41	2.07	9 (28%)
1	PSU	S2	609	1	18,21,22	1.41	4 (22%)	21,30,33	2.08	3 (14%)
3	PSU	L5	4628	3	18,21,22	1.43	4 (22%)	21,30,33	1.98	4 (19%)
84	PSU	At	32	84	18,21,22	1.43	3 (16%)	21,30,33	2.06	5 (23%)
1	4AC	S2	1337	1	21,24,25	1.09	1 (4%)	28,34,37	1.25	3 (10%)
3	A2M	L5	3724	3	22,25,26	1.39	4 (18%)	30,36,39	2.13	11 (36%)
1	A2M	S2	668	89,1	22,25,26	1.50	5 (22%)	30,36,39	1.97	8 (26%)
3	PSU	L5	4296	3	18,21,22	1.46	4 (22%)	21,30,33	2.26	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	4SU	At	8	84	18,21,22	1.99	4 (22%)	25,30,33	2.55	7 (28%)
1	OMU	S2	172	1	19,22,23	1.36	4 (21%)	25,31,34	2.14	9 (36%)
3	PSU	L5	3770	3	18,21,22	1.44	2 (11%)	21,30,33	2.07	3 (14%)
1	B8N	S2	1248	1	25,29,30	0.92	1 (4%)	28,42,45	1.58	7 (25%)
3	OMC	L5	2351	3	19,22,23	0.90	1 (5%)	25,31,34	0.99	1 (4%)
1	PSU	S2	119	1	18,21,22	1.47	4 (22%)	21,30,33	2.15	5 (23%)
3	OMU	L5	4620	3	19,22,23	1.37	3 (15%)	25,31,34	2.00	6 (24%)
1	PSU	S2	1238	1	18,21,22	1.52	4 (22%)	21,30,33	2.12	4 (19%)
3	PSU	L5	4312	3	18,21,22	1.55	4 (22%)	21,30,33	2.04	4 (19%)
1	PSU	S2	1347	1	18,21,22	1.44	4 (22%)	21,30,33	2.10	3 (14%)
1	OMC	S2	174	89,1	19,22,23	0.86	0	25,31,34	0.99	1 (4%)
3	OMC	L5	2804	3	19,22,23	0.83	0	25,31,34	1.01	1 (4%)
3	PSU	L5	3729	3	18,21,22	1.49	3 (16%)	21,30,33	2.18	4 (19%)
1	PSU	S2	1136	1	18,21,22	1.50	3 (16%)	21,30,33	2.06	4 (19%)
1	A2M	S2	1031	1	22,25,26	1.47	4 (18%)	30,36,39	2.14	10 (33%)
1	A2M	S2	159	1	22,25,26	1.48	4 (18%)	30,36,39	2.16	8 (26%)
3	A2M	L5	1524	3	22,25,26	1.56	4 (18%)	30,36,39	1.97	8 (26%)
3	PSU	L5	3695	89,3	18,21,22	1.49	3 (16%)	21,30,33	2.22	6 (28%)
3	A2M	L5	3867	3	22,25,26	1.50	5 (22%)	30,36,39	2.04	7 (23%)
3	PSU	L5	4521	89,3	18,21,22	1.60	5 (27%)	21,30,33	2.37	6 (28%)
2	PSU	L8	55	2	18,21,22	1.45	3 (16%)	21,30,33	2.24	4 (19%)
1	PSU	S2	1177	1	18,21,22	1.46	4 (22%)	21,30,33	2.08	3 (14%)
1	MA6	S2	1850	1	23,26,27	1.44	5 (21%)	33,38,41	2.09	10 (30%)
3	PSU	L5	3637	89,3	18,21,22	1.58	3 (16%)	21,30,33	2.25	6 (28%)
3	A2M	L5	3723	3	22,25,26	1.45	5 (22%)	30,36,39	2.04	11 (36%)
84	MIA	At	37	84	28,31,32	2.32	6 (21%)	38,44,47	2.79	14 (36%)
3	PSU	L5	1860	3	18,21,22	1.55	4 (22%)	21,30,33	2.11	4 (19%)
3	OMC	L5	2824	3	19,22,23	0.74	0	25,31,34	0.66	0
3	PSU	L5	4972	3	18,21,22	1.53	4 (22%)	21,30,33	2.06	4 (19%)
3	OMU	L5	2415	3	19,22,23	1.41	3 (15%)	25,31,34	1.94	4 (16%)
2	OMU	L8	14	2,3	19,22,23	1.45	4 (21%)	25,31,34	2.00	6 (24%)
68	MLZ	Lb	5	68	8,9,10	0.94	0	4,9,11	1.00	0
86	M3L	EF	79	86	10,11,12	0.48	0	9,14,16	0.11	0
1	OMG	S2	644	1	23,26,27	1.20	4 (17%)	32,38,41	2.13	7 (21%)
3	PSU	L5	1792	3	18,21,22	1.50	4 (22%)	21,30,33	2.21	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	S2	99	89,1	22,25,26	1.46	4 (18%)	30,36,39	2.08	9 (30%)
3	A2M	L5	4590	3	22,25,26	1.50	5 (22%)	30,36,39	2.10	10 (33%)
1	PSU	S2	918	1	18,21,22	1.45	3 (16%)	21,30,33	2.38	5 (23%)
3	PSU	L5	1781	3	18,21,22	1.39	2 (11%)	21,30,33	2.12	4 (19%)
3	OMG	L5	2424	3	23,26,27	1.23	3 (13%)	32,38,41	1.94	5 (15%)
3	PSU	L5	2843	3	18,21,22	1.55	4 (22%)	21,30,33	2.19	4 (19%)
3	OMC	L5	3887	3	19,22,23	0.83	0	25,31,34	0.87	0
3	OMC	L5	1340	3	19,22,23	0.85	0	25,31,34	0.94	0
3	OMG	L5	4196	89,3,85	23,26,27	1.25	4 (17%)	32,38,41	1.92	5 (15%)
1	OMU	S2	354	1	19,22,23	1.47	3 (15%)	25,31,34	2.10	5 (20%)
1	MA6	S2	1851	1	23,26,27	1.46	5 (21%)	33,38,41	2.04	10 (30%)
1	PSU	S2	966	1	18,21,22	1.53	4 (22%)	21,30,33	1.99	5 (23%)
1	OMC	S2	1703	1	19,22,23	0.81	1 (5%)	25,31,34	0.81	1 (4%)
1	A2M	S2	512	1	22,25,26	1.44	5 (22%)	30,36,39	2.22	9 (30%)
1	OMC	S2	462	1	19,22,23	0.89	0	25,31,34	0.87	0
1	PSU	S2	801	1	18,21,22	1.40	3 (16%)	21,30,33	2.11	3 (14%)
1	A2M	S2	484	1	22,25,26	1.49	5 (22%)	30,36,39	2.02	7 (23%)
3	A2M	L5	3718	3	22,25,26	1.52	4 (18%)	30,36,39	1.88	6 (20%)
1	OMG	S2	867	1	23,26,27	1.21	4 (17%)	32,38,41	1.97	7 (21%)
3	OMU	L5	3925	3	19,22,23	1.39	3 (15%)	25,31,34	1.86	5 (20%)
85	OMC	Pt	33	85	19,22,23	0.82	0	25,31,34	0.82	0
3	5MC	L5	3782	89,3	19,22,23	1.64	3 (15%)	26,32,35	1.35	3 (11%)
84	H2U	At	16	84	18,21,22	1.02	2 (11%)	19,30,33	0.92	1 (5%)
1	4AC	S2	1842	1	21,24,25	1.03	2 (9%)	28,34,37	1.23	4 (14%)
3	PSU	L5	1779	3	18,21,22	1.58	5 (27%)	21,30,33	2.12	3 (14%)
1	PSU	S2	822	1	18,21,22	1.50	4 (22%)	21,30,33	2.25	4 (19%)
3	PSU	L5	4673	3	18,21,22	1.36	3 (16%)	21,30,33	1.87	3 (14%)
1	PSU	S2	1367	1	18,21,22	1.56	3 (16%)	21,30,33	2.15	5 (23%)
85	4SU	Pt	8	85	18,21,22	1.96	4 (22%)	25,30,33	2.24	5 (20%)
3	PSU	L5	4403	3	18,21,22	1.58	4 (22%)	21,30,33	2.17	6 (28%)
3	PSU	L5	3734	3	18,21,22	1.41	4 (22%)	21,30,33	2.26	4 (19%)
3	PSU	L5	3853	89,3	18,21,22	1.60	4 (22%)	21,30,33	1.89	5 (23%)
3	OMG	L5	4618	3	23,26,27	1.27	4 (17%)	32,38,41	2.08	7 (21%)
3	OMU	L5	2837	3	19,22,23	1.31	3 (15%)	25,31,34	2.00	5 (20%)
1	PSU	S2	866	1	18,21,22	1.51	4 (22%)	21,30,33	1.84	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4552	3	18,21,22	1.63	5 (27%)	21,30,33	2.21	3 (14%)
3	PSU	L5	3758	3	18,21,22	1.42	4 (22%)	21,30,33	2.02	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.58	4 (22%)	21,30,33	2.13	4 (19%)
84	G7M	At	46	84	23,26,27	2.39	6 (26%)	34,39,42	2.99	10 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	1MA	L5	1322	89,3	-	1/7/25/26	0/3/3/3
85	G7M	Pt	47	85	-	0/7/25/26	0/3/3/3
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
1	UY1	S2	1326	89,1	-	1/9/27/28	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
1	OMU	S2	627	1	-	0/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
29	AME	SV	1	29	-	2/9/10/12	-
3	OMG	L5	3744	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	590	1	-	4/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1442	89,1	-	2/9/27/28	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
79	M3L	Lm	98	79	-	0/9/10/12	-
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	89,1	-	1/9/27/28	0/3/3/3
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
81	MLZ	Lo	53	81	-	2/7/8/10	-
86	M3L	EF	318	86	-	7/9/10/12	-
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1243	1	-	1/7/25/26	0/2/2/2
86	MLY	EF	55	86	-	3/8/9/11	-
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	89,3	-	0/9/27/28	0/3/3/3
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	3,92	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
2	OMG	L8	75	2	-	0/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	2422	89,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2815	89,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3764	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
86	M3L	EF	36	86	-	0/9/10/12	-
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
40	HIC	LB	245	40	-	0/5/6/8	0/1/1/1
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	89,3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3627	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	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
20	HY3	SX	62	20	-	1/1/12/14	0/1/1/1
3	A2M	L5	2787	89,3	-	5/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	1288	1	-	3/9/27/28	0/2/2/2
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	89,1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3851	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
85	H2U	Pt	21	85	-	3/7/38/39	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3760	1,3	-	3/9/27/28	0/3/3/3
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1534	89,3	-	2/9/27/28	0/3/3/3
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	G7M	S2	1639	1,85	-	0/7/25/26	0/3/3/3
39	V5N	LA	216	39	-	1/9/10/12	0/1/1/1
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
84	PSU	At	39	84	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1643	89,1	-	0/7/25/26	0/2/2/2
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
52	V5N	La	39	52	-	1/9/10/12	0/1/1/1
1	OMG	S2	1490	89,1	-	2/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	6MZ	S2	1832	89,1	-	2/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
1	A2M	S2	576	1	-	3/9/27/28	0/3/3/3
3	OMC	L5	2365	89,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1683	89,3	-	0/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	89,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3944	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	1881	89,3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
66	SAC	Lr	2	66	-	2/7/8/10	-
3	OMG	L5	3792	3	-	1/9/27/28	0/3/3/3
3	UY1	L5	3818	89,3	-	2/9/27/28	0/2/2/2
85	PSU	Pt	56	85	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
1	OMG	S2	1328	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
3	OMC	L5	3701	3,92	-	4/9/27/28	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	1804	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
84	H2U	At	20	84	-	6/7/38/39	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	S2	1447	1	-	1/9/27/28	0/3/3/3
3	OMG	L5	1625	89,3	-	3/9/27/28	0/3/3/3
1	PSU	S2	1174	89,1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
1	OMU	S2	428	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	89,3	-	0/9/27/28	0/3/3/3
6	SAC	SA	2	6	-	1/7/8/10	-
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
84	PSU	At	32	84	-	3/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	4/11/29/30	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
1	A2M	S2	668	89,1	-	3/9/27/28	0/3/3/3
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
84	4SU	At	8	84	-	1/7/25/26	0/2/2/2
1	OMU	S2	172	1	-	4/9/27/28	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
3	OMC	L5	2351	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	174	89,1	-	1/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3729	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	1031	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	159	1	-	0/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3695	89,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4521	89,3	-	0/7/25/26	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
3	PSU	L5	3637	89,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
84	MIA	At	37	84	-	2/15/33/34	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
2	OMU	L8	14	2,3	-	1/9/27/28	0/2/2/2
68	MLZ	Lb	5	68	-	2/7/8/10	-
86	M3L	EF	79	86	-	3/9/10/12	-
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2
1	A2M	S2	99	89,1	-	1/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	918	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4196	89,3,85	-	0/9/27/28	0/3/3/3
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
1	MA6	S2	1851	1	-	2/11/29/30	0/3/3/3
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1703	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	512	1	-	1/9/27/28	0/3/3/3
1	OMC	S2	462	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
85	OMC	Pt	33	85	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	89,3	-	0/7/25/26	0/2/2/2
84	H2U	At	16	84	-	3/7/38/39	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	1/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	4SU	Pt	8	85	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	89,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
84	G7M	At	46	84	-	2/7/25/26	0/3/3/3

The worst 5 of 815 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SV	1	AME	OT-CT1	8.97	1.43	1.23
66	Lr	2	SAC	OAC-C1A	8.84	1.43	1.23
6	SA	2	SAC	OAC-C1A	8.61	1.42	1.23
1	S2	1639	G7M	C8-N7	7.61	1.46	1.33
84	At	46	G7M	C8-N7	7.58	1.46	1.33

The worst 5 of 1204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	At	37	MIA	C12-C13-C14	-9.23	110.44	127.01
1	S2	1639	G7M	CN7-N7-C8	-8.41	112.06	124.79
84	At	46	G7M	CN7-N7-C8	-7.88	112.86	124.79
66	Lr	2	SAC	OAC-C1A-N	-7.87	108.06	121.98
3	L5	4521	PSU	N1-C2-N3	7.75	123.35	115.17

There are no chirality outliers.

5 of 165 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
29	SV	1	AME	OT-CT1-N-CA
66	Lr	2	SAC	C2A-C1A-N-CA
68	Lb	5	MLZ	CD-CE-NZ-CM

There are no ring outliers.

80 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2632	PSU	1	0
3	L5	4456	OMC	1	0
3	L5	4637	OMG	1	0
85	Pt	47	G7M	1	0
3	L5	1326	A2M	1	0
3	L5	4220	6MZ	2	0
1	S2	573	PSU	1	0
1	S2	468	A2M	1	0
86	EF	318	M3L	2	0
1	S2	601	OMG	1	0
1	S2	681	PSU	1	0
1	S2	121	OMU	1	0
3	L5	3762	PSU	1	0
86	EF	55	MLY	2	0
1	S2	649	PSU	2	0
1	S2	436	OMG	1	0
3	L5	2363	A2M	2	0
3	L5	2861	OMC	1	0
1	S2	116	OMU	2	0
1	S2	1678	A2M	1	0
1	S2	686	PSU	1	0
1	S2	36	PSU	2	0
1	S2	509	OMG	2	0
3	L5	4420	PSU	1	0
85	Pt	21	H2U	1	0
3	L5	3760	A2M	3	0
3	L5	1534	A2M	1	0
1	S2	1639	G7M	1	0
84	At	39	PSU	1	0
3	L5	4571	A2M	1	0
1	S2	1643	PSU	1	0
1	S2	1490	OMG	1	0
1	S2	1832	6MZ	1	0
1	S2	576	A2M	2	0
3	L5	2364	OMG	2	0
3	L5	1881	OMC	1	0
66	Lr	2	SAC	1	0
1	S2	1328	OMG	1	0
3	L5	3701	OMC	1	0
1	S2	1804	OMU	1	0
3	L5	2876	OMG	1	0
1	S2	1447	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1625	OMG	1	0
3	L5	4370	OMG	1	0
3	L5	1871	A2M	1	0
3	L5	3884	PSU	1	0
3	L5	4228	OMG	1	0
3	L5	4628	PSU	1	0
84	At	32	PSU	2	0
3	L5	3724	A2M	1	0
84	At	8	4SU	2	0
1	S2	172	OMU	1	0
1	S2	1248	B8N	2	0
3	L5	2351	OMC	2	0
1	S2	119	PSU	1	0
3	L5	4620	OMU	1	0
1	S2	174	OMC	1	0
3	L5	2804	OMC	1	0
1	S2	159	A2M	2	0
3	L5	1524	A2M	1	0
3	L5	3867	A2M	1	0
3	L5	4521	PSU	1	0
1	S2	1850	MA6	1	0
3	L5	3723	A2M	1	0
3	L5	2415	OMU	1	0
86	EF	79	M3L	1	0
1	S2	644	OMG	1	0
1	S2	99	A2M	1	0
3	L5	2424	OMG	2	0
3	L5	1340	OMC	1	0
3	L5	4196	OMG	2	0
1	S2	354	OMU	1	0
1	S2	1851	MA6	2	0
1	S2	512	A2M	2	0
1	S2	484	A2M	1	0
3	L5	3718	A2M	3	0
1	S2	867	OMG	1	0
84	At	16	H2U	2	0
3	L5	4618	OMG	2	0
84	At	46	G7M	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 502 ligands modelled in this entry, 478 are monoatomic - leaving 24 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$
94	PHE	At	77	84	10,11,12	0.36	0	8,13,15	0.72	0
95	MET	Pt	78	85	6,7,8	0.57	0	2,7,9	1.28	0
88	PUT	L5	5115	-	5,5,5	0.14	0	4,4,4	0.21	0
87	SPD	L5	5102	-	9,9,9	0.40	0	8,8,8	0.82	0
87	SPD	L5	5103	-	9,9,9	0.40	0	8,8,8	0.97	1 (12%)
88	PUT	L5	5109	-	5,5,5	0.14	0	4,4,4	0.25	0
88	PUT	L5	5113	-	5,5,5	0.13	0	4,4,4	0.26	0
87	SPD	L5	5108	-	9,9,9	0.33	0	8,8,8	1.03	1 (12%)
96	GSP	EF	501	89	33,34,34	0.63	0	47,54,54	0.60	0
88	PUT	L5	5110	-	5,5,5	0.07	0	4,4,4	0.17	0
90	ANM	L5	5101	-	20,20,20	1.20	1 (5%)	24,27,27	1.34	3 (12%)
87	SPD	L5	5106	-	9,9,9	0.35	0	8,8,8	0.70	0
88	PUT	L5	5114	-	5,5,5	0.16	0	4,4,4	0.28	0
88	PUT	L5	5112	-	5,5,5	0.19	0	4,4,4	0.24	0
87	SPD	L5	5105	-	9,9,9	0.31	0	8,8,8	0.75	0
88	PUT	S2	1902	-	5,5,5	0.15	0	4,4,4	0.14	0
88	PUT	L5	5111	-	5,5,5	0.12	0	4,4,4	0.18	0
91	3H3	L5	5117	-	34,34,34	3.30	13 (38%)	36,45,45	3.67	18 (50%)
97	ZIY	EF	502	-	81,82,82	1.02	4 (4%)	111,117,117	1.42	14 (12%)
87	SPD	S2	1901	-	9,9,9	0.14	0	8,8,8	0.23	0
88	PUT	L5	5116	-	5,5,5	0.13	0	4,4,4	0.21	0
88	PUT	S2	1903	-	5,5,5	0.13	0	4,4,4	0.23	0
87	SPD	L5	5104	-	9,9,9	0.33	0	8,8,8	0.78	0
87	SPD	L5	5107	-	9,9,9	0.43	0	8,8,8	0.93	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
94	PHE	At	77	84	-	4/5/6/8	0/1/1/1
95	MET	Pt	78	85	-	3/5/6/8	-
88	PUT	L5	5115	-	-	1/3/3/3	-
87	SPD	L5	5102	-	-	0/7/7/7	-
87	SPD	L5	5103	-	-	5/7/7/7	-
88	PUT	L5	5109	-	-	0/3/3/3	-
88	PUT	L5	5113	-	-	2/3/3/3	-
87	SPD	L5	5108	-	-	2/7/7/7	-
96	GSP	EF	501	89	-	0/21/38/38	0/3/3/3
88	PUT	L5	5110	-	-	3/3/3/3	-
90	ANM	L5	5101	-	-	4/10/23/23	0/2/2/2
87	SPD	L5	5106	-	-	6/7/7/7	-
88	PUT	L5	5114	-	-	0/3/3/3	-
88	PUT	L5	5112	-	-	0/3/3/3	-
87	SPD	L5	5105	-	-	2/7/7/7	-
88	PUT	S2	1902	-	-	1/3/3/3	-
88	PUT	L5	5111	-	-	0/3/3/3	-
91	3H3	L5	5117	-	-	15/39/51/51	0/1/2/2
97	ZIY	EF	502	-	-	11/120/140/140	0/3/4/4
87	SPD	S2	1901	-	-	0/7/7/7	-
88	PUT	L5	5116	-	-	0/3/3/3	-
88	PUT	S2	1903	-	-	0/3/3/3	-
87	SPD	L5	5104	-	-	4/7/7/7	-
87	SPD	L5	5107	-	-	3/7/7/7	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	L5	5117	3H3	C13-C12	8.93	1.53	1.33
91	L5	5117	3H3	O3-C22	7.72	1.38	1.23
91	L5	5117	3H3	O4-C23	7.24	1.37	1.23
91	L5	5117	3H3	C23-N	6.68	1.48	1.37
91	L5	5117	3H3	C22-N	5.57	1.46	1.37

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	L5	5117	3H3	O3-C22-N	-10.22	104.55	120.30
91	L5	5117	3H3	C22-N-C23	-9.58	114.32	125.87
91	L5	5117	3H3	O4-C23-N	-8.78	106.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	EF	502	ZIY	O33-C75-C74	6.80	126.68	118.96
91	L5	5117	3H3	O3-C22-C21	-6.57	110.08	122.62

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

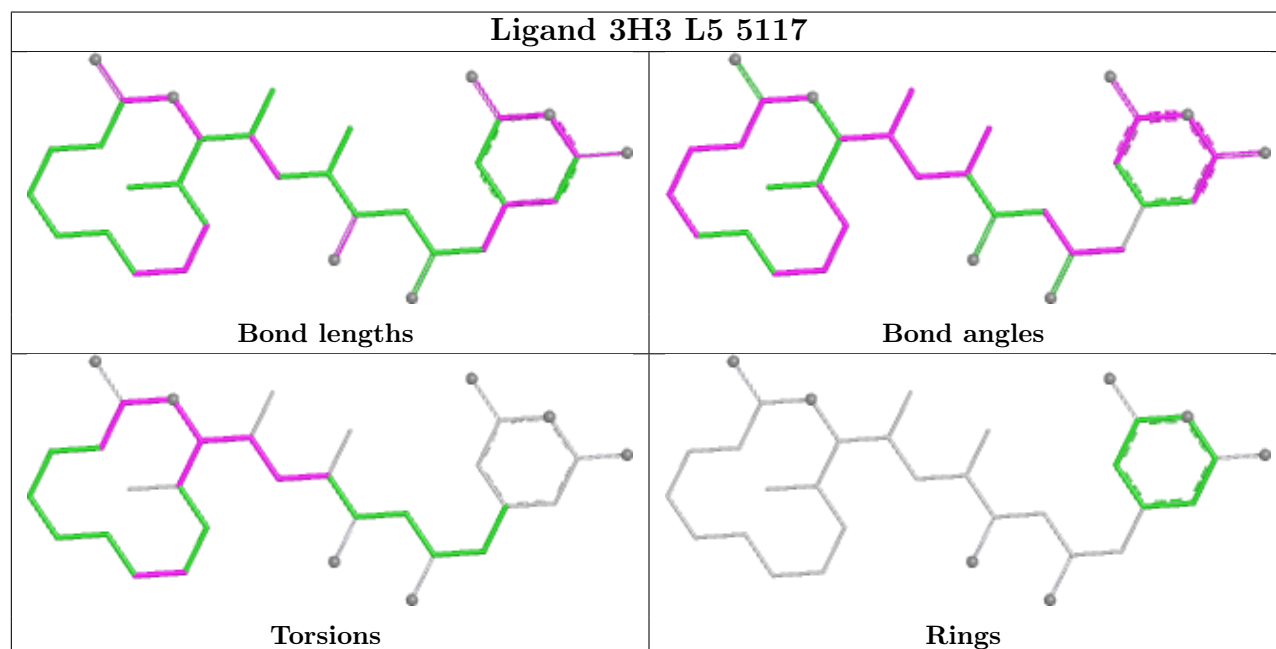
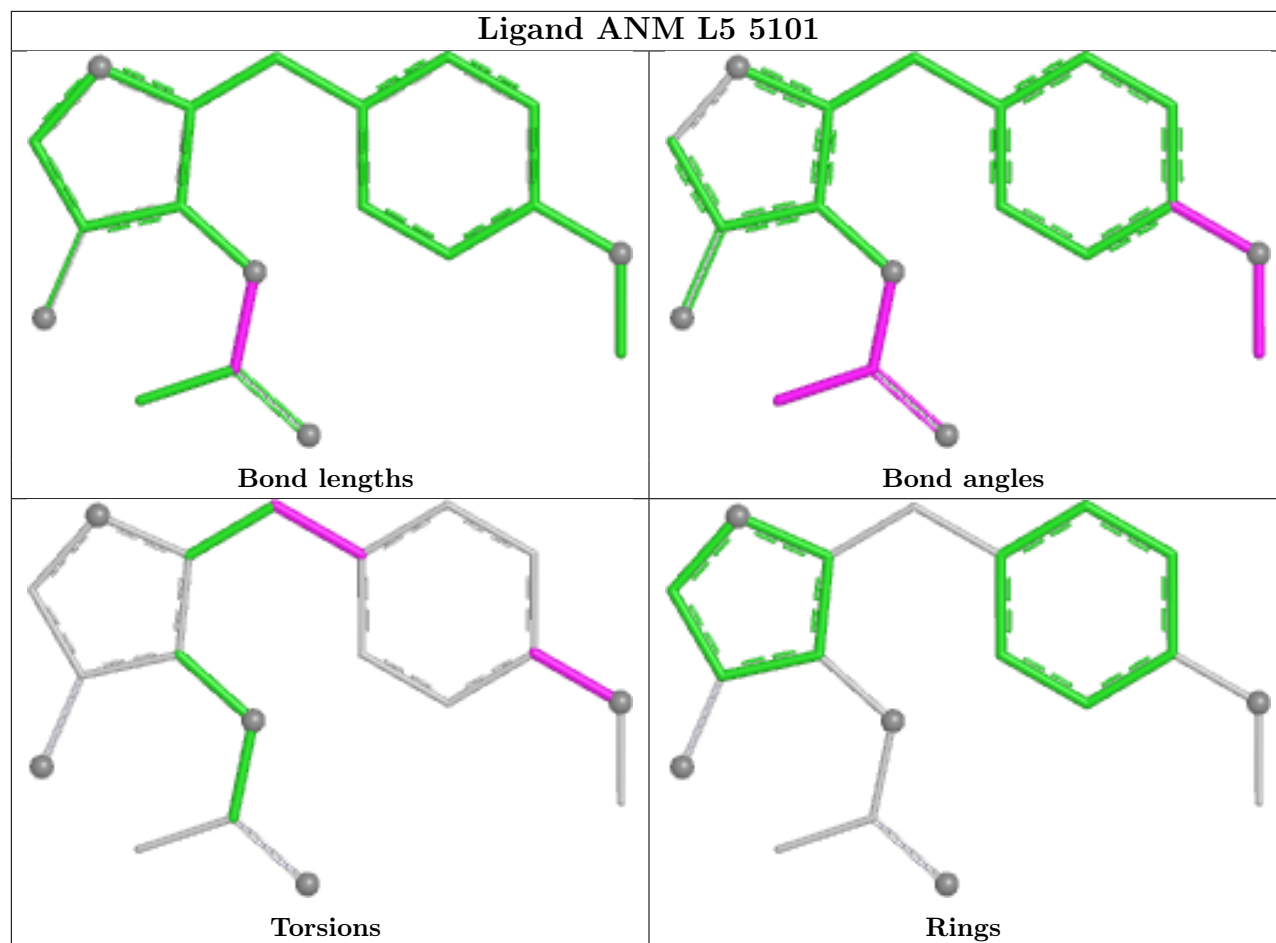
Mol	Chain	Res	Type	Atoms
91	L5	5117	3H3	C2-C1-C11-O1
91	L5	5117	3H3	C2-C1-C11-C12
91	L5	5117	3H3	C-C1-C11-O1
91	L5	5117	3H3	C-C1-C11-C12
91	L5	5117	3H3	C1-C11-O1-C10

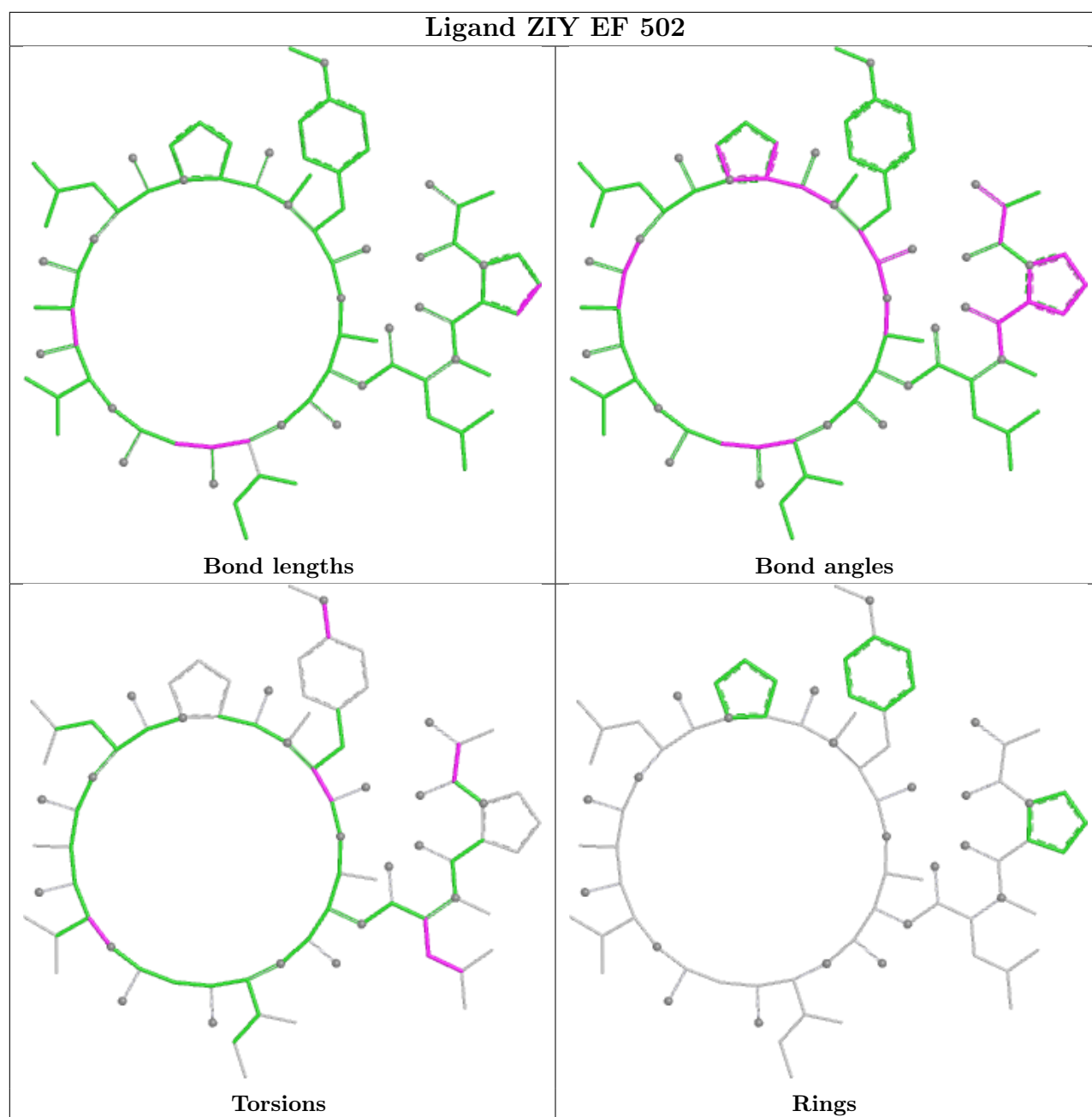
There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	At	77	PHE	2	0
87	L5	5103	SPD	1	0
96	EF	501	GSP	1	0
87	L5	5106	SPD	1	0
91	L5	5117	3H3	4	0
97	EF	502	ZIY	1	0
88	L5	5116	PUT	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

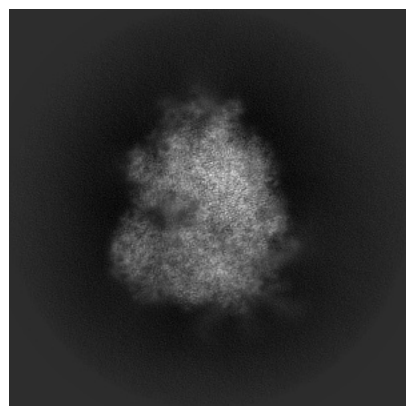
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29759. These allow visual inspection of the internal detail of the map and identification of artifacts.

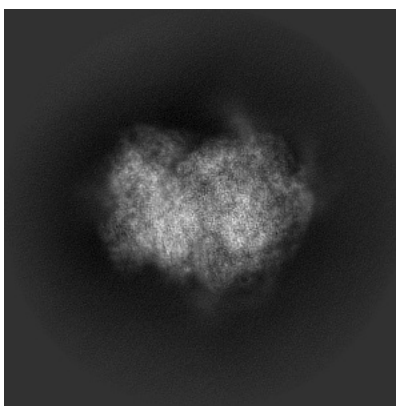
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

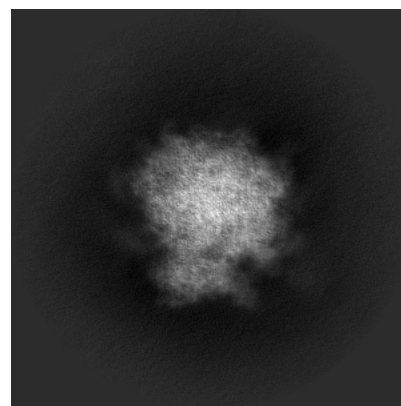
6.1.1 Primary map



X

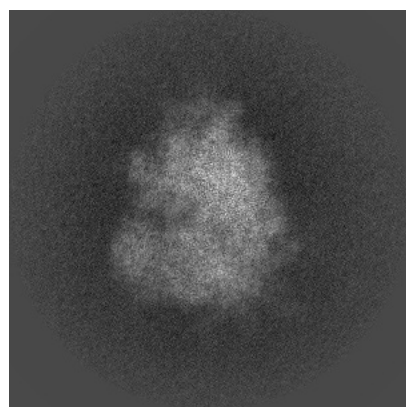


Y

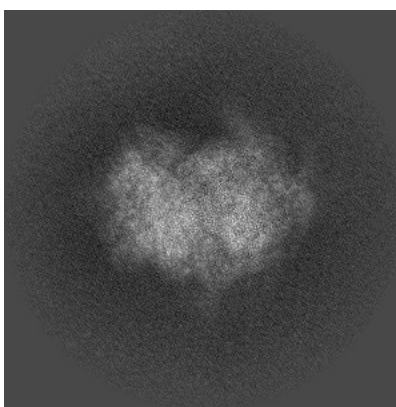


Z

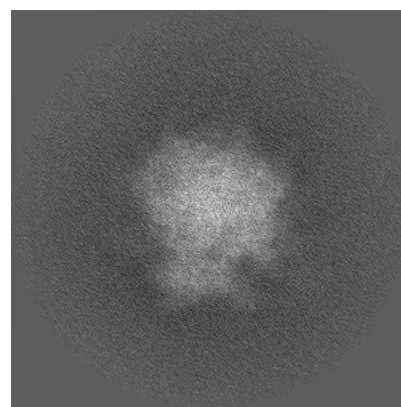
6.1.2 Raw map



X



Y

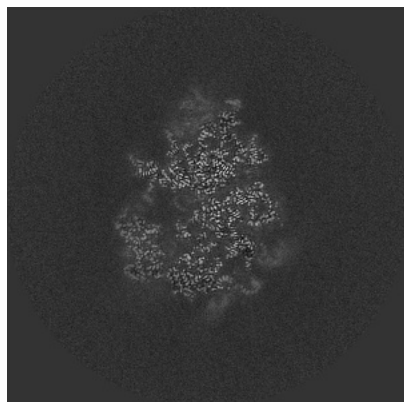


Z

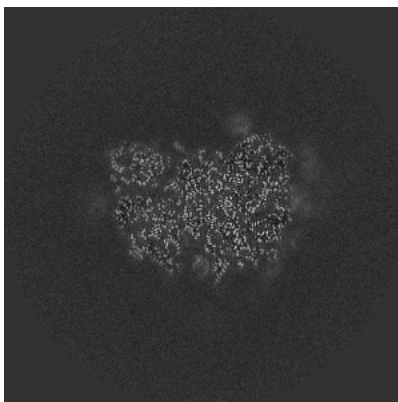
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

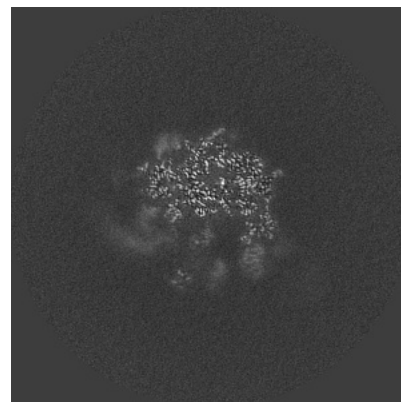
6.2.1 Primary map



X Index: 320

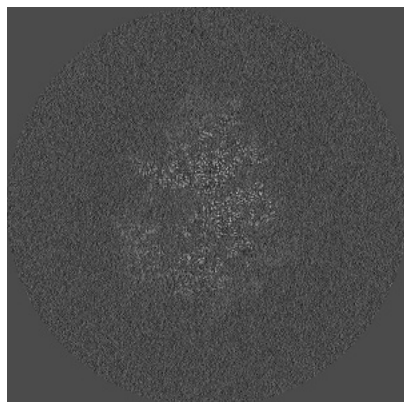


Y Index: 320

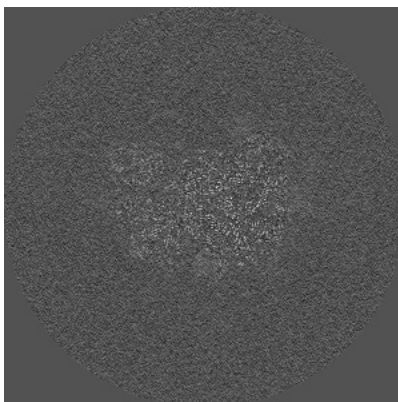


Z Index: 320

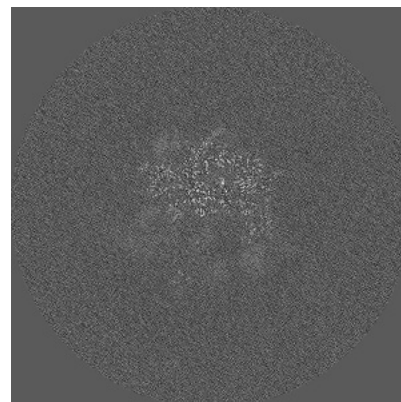
6.2.2 Raw map



X Index: 320



Y Index: 320

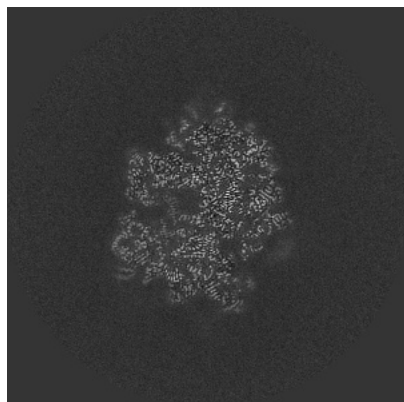


Z Index: 320

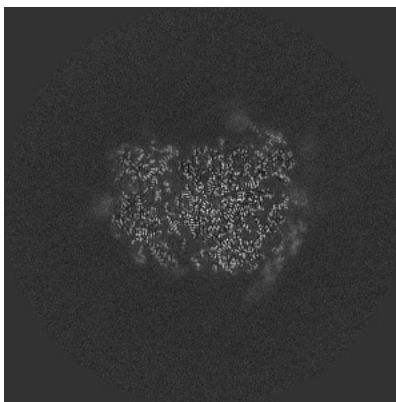
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

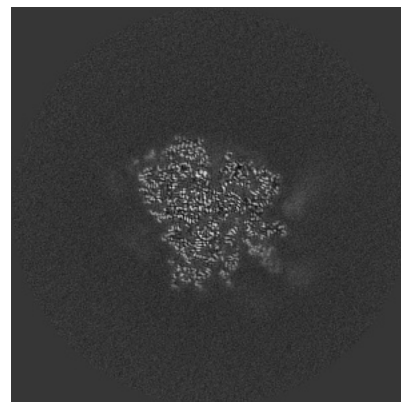
6.3.1 Primary map



X Index: 297

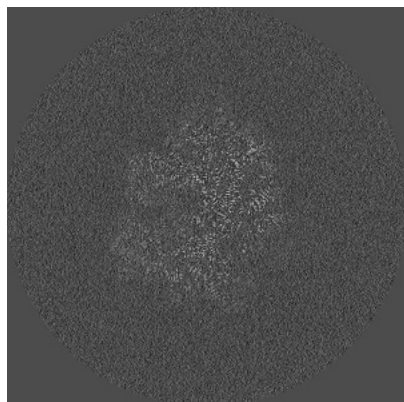


Y Index: 332

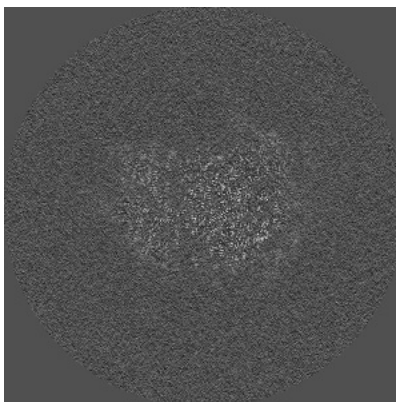


Z Index: 366

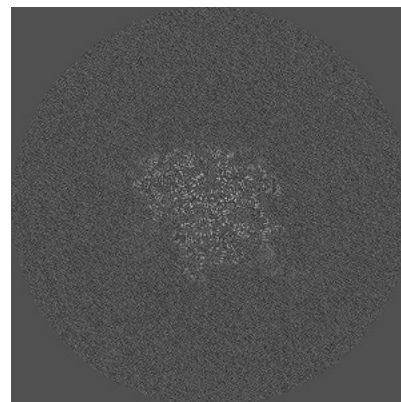
6.3.2 Raw map



X Index: 297



Y Index: 327

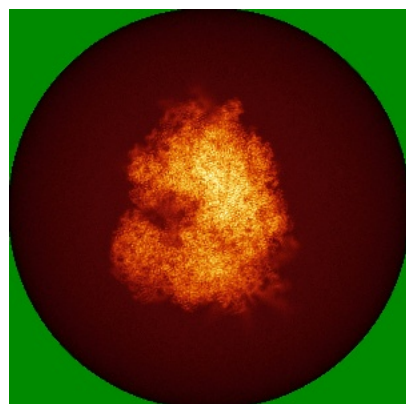


Z Index: 354

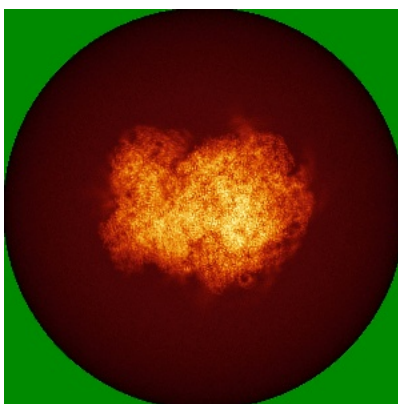
The images above show the largest variance slices of the map in three orthogonal directions.

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

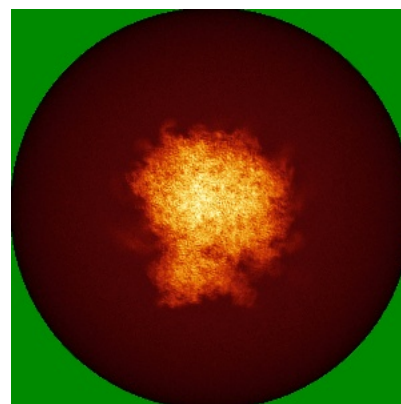
6.4.1 Primary map



X

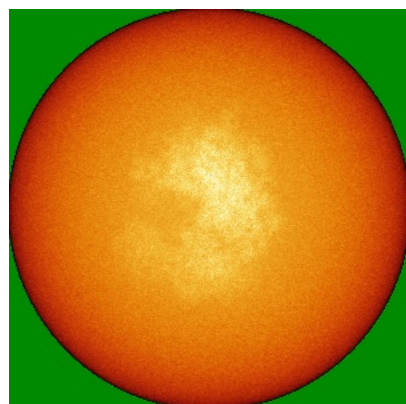


Y

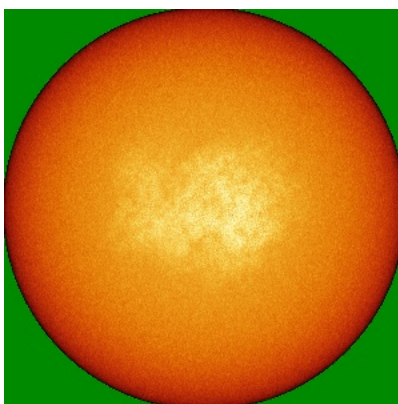


Z

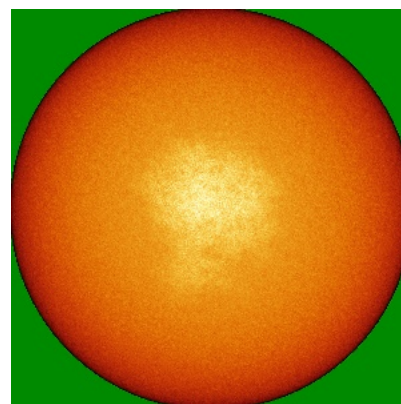
6.4.2 Raw map



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



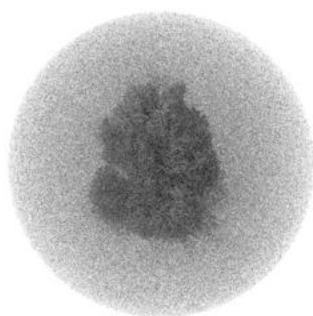
Y



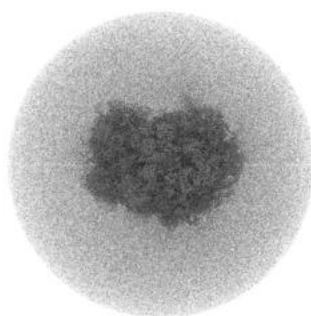
Z

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.

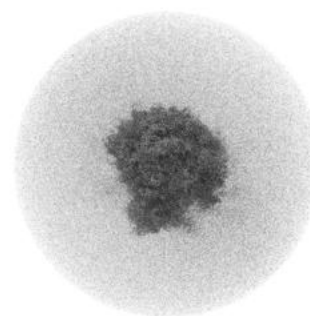
6.5.2 Raw map



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.

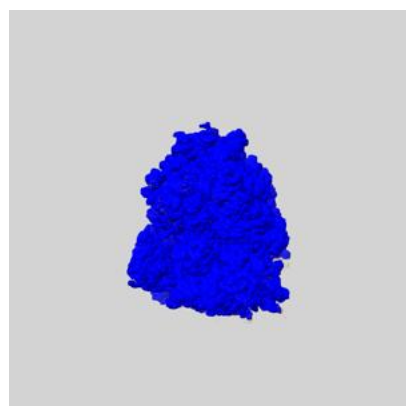
6.6 Mask visualisation [i](#)

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

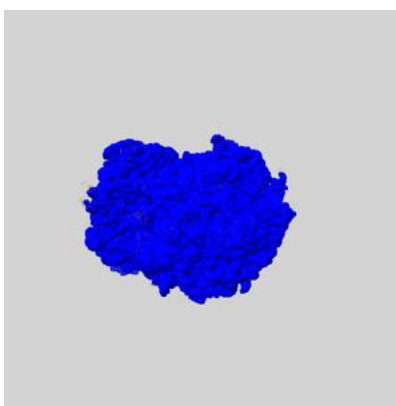
A mask typically either:

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

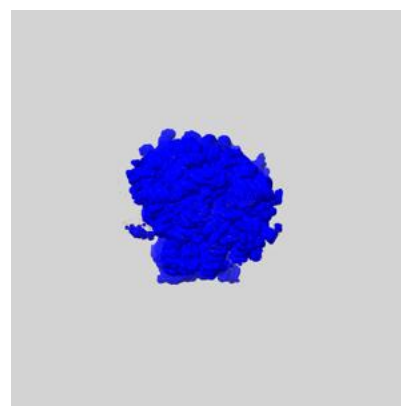
6.6.1 emd_29759_msk_1.map [i](#)



X



Y

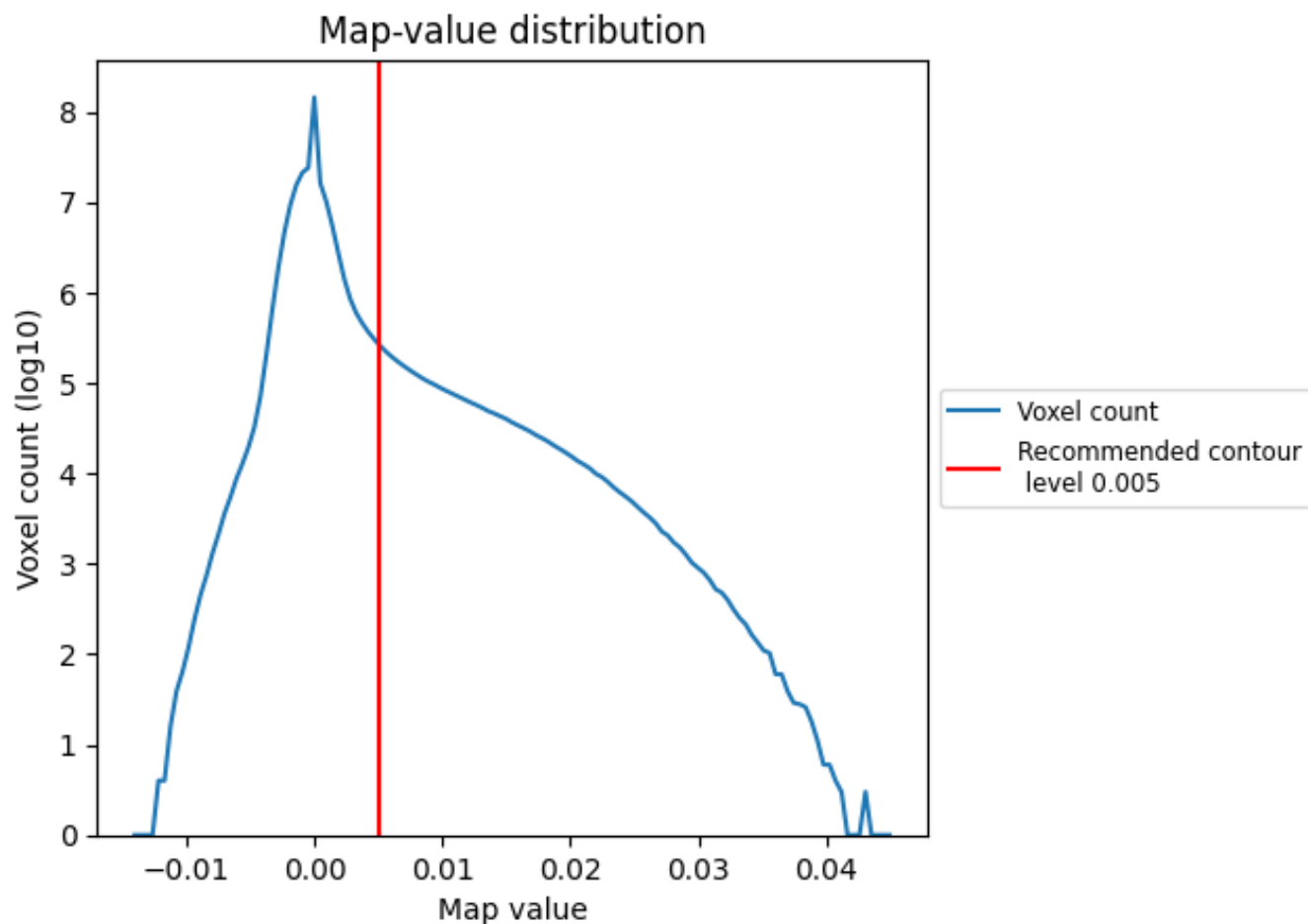


Z

7 Map analysis [i](#)

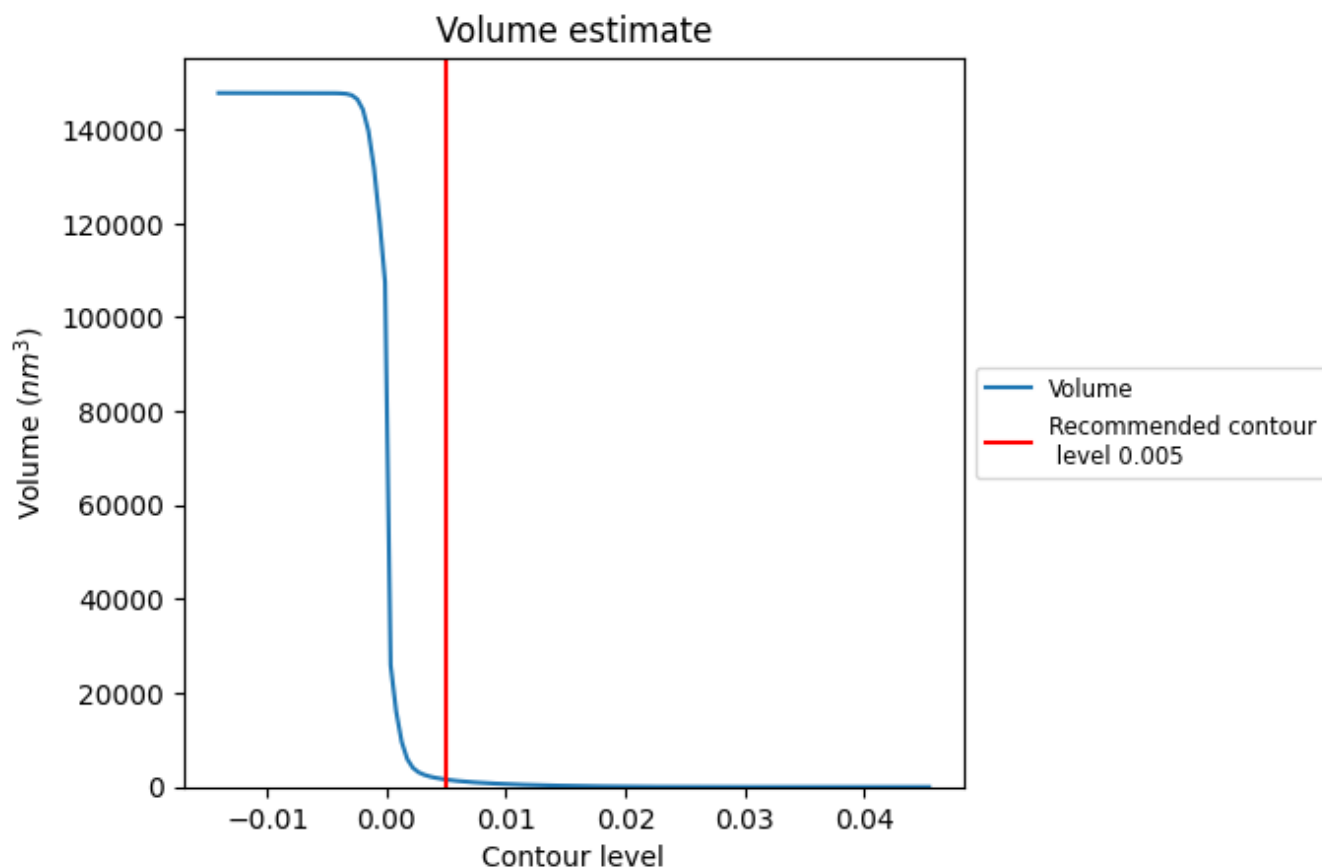
This section contains the results of statistical analysis of the map.

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.

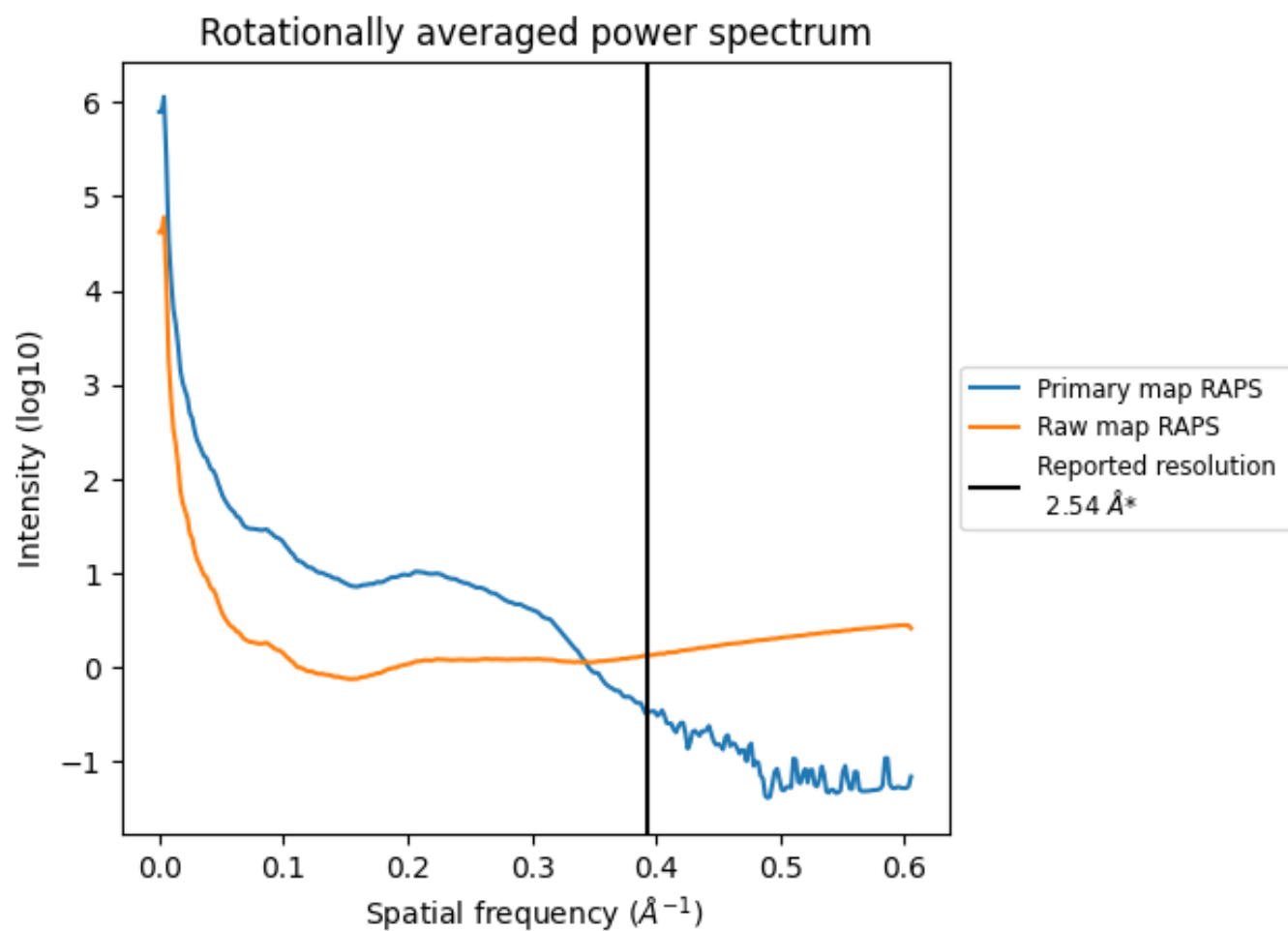
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1563 nm³; this corresponds to an approximate mass of 1412 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 ⓘ

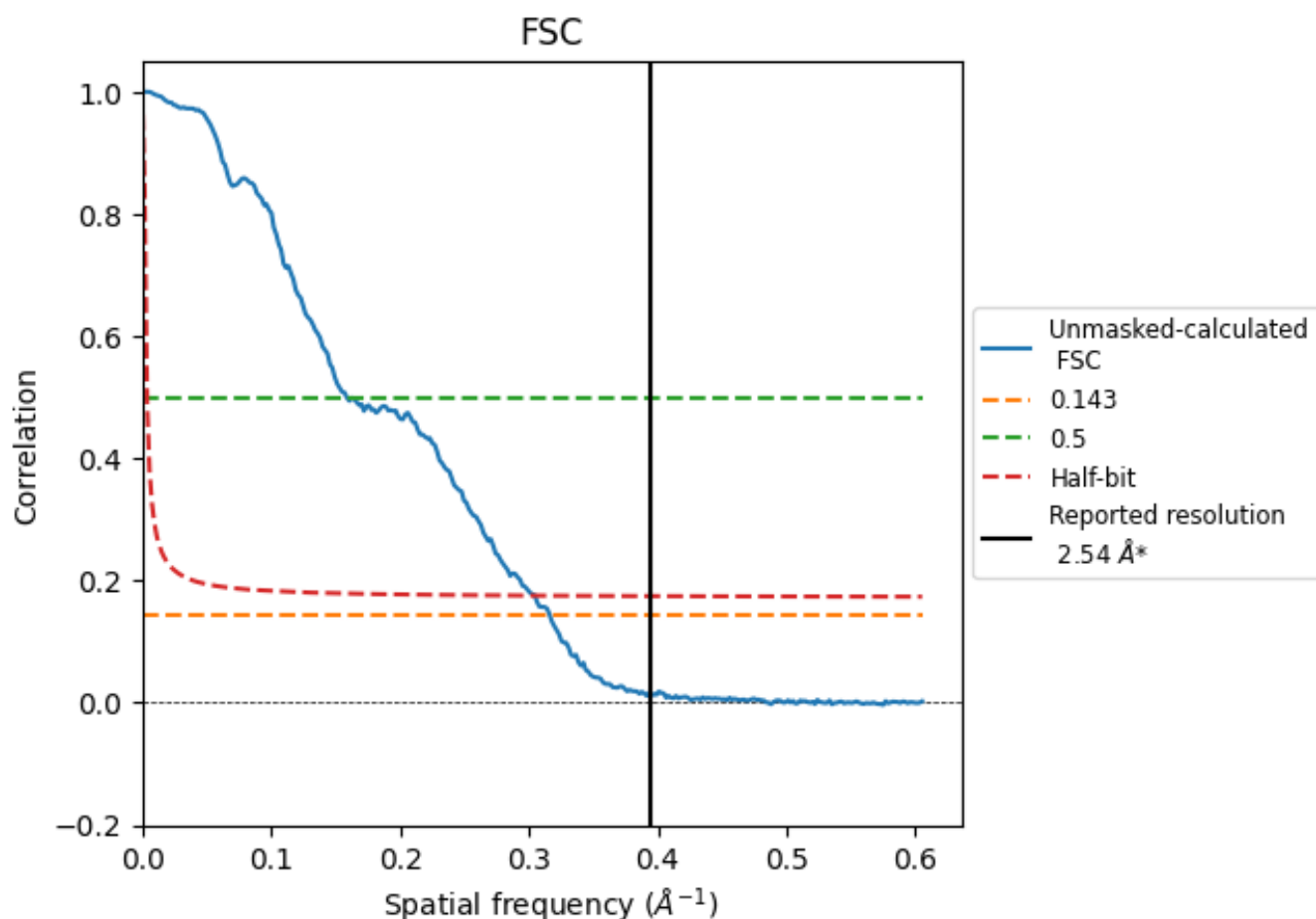


*Reported resolution corresponds to spatial frequency of 0.394 $\text{\AA}^{-1}$

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 0.394 Å⁻¹

8.2 Resolution estimates [i](#)

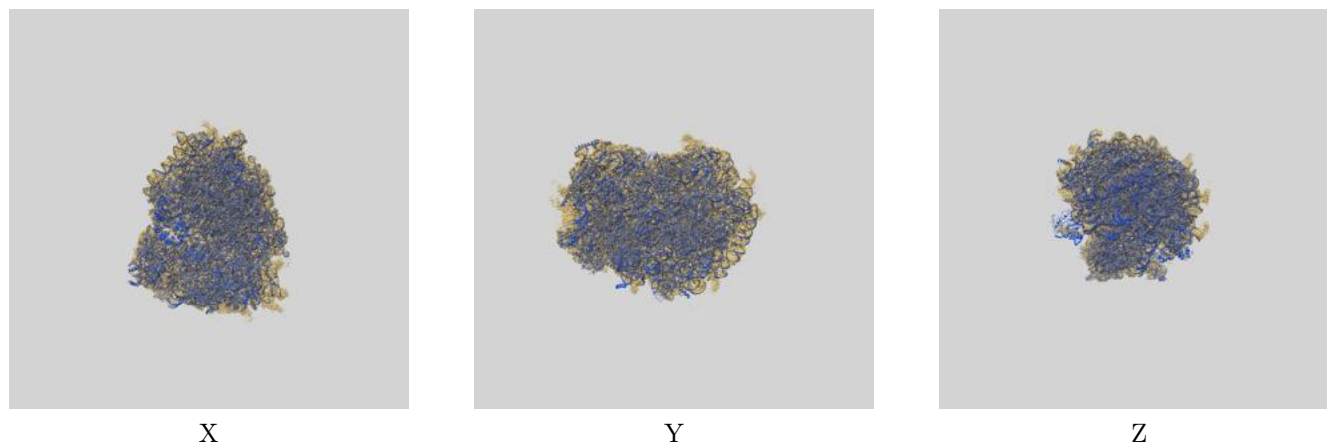
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	6.30	3.28

*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 3.16 differs from the reported value 2.54 by more than 10 %

9 Map-model fit [i](#)

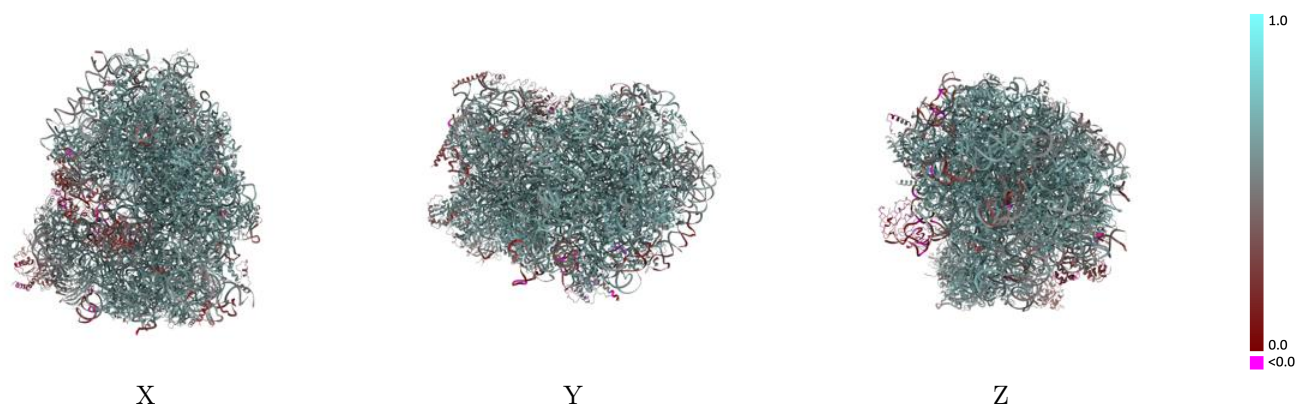
This section contains information regarding the fit between EMDB map EMD-29759 and PDB model 8G60. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



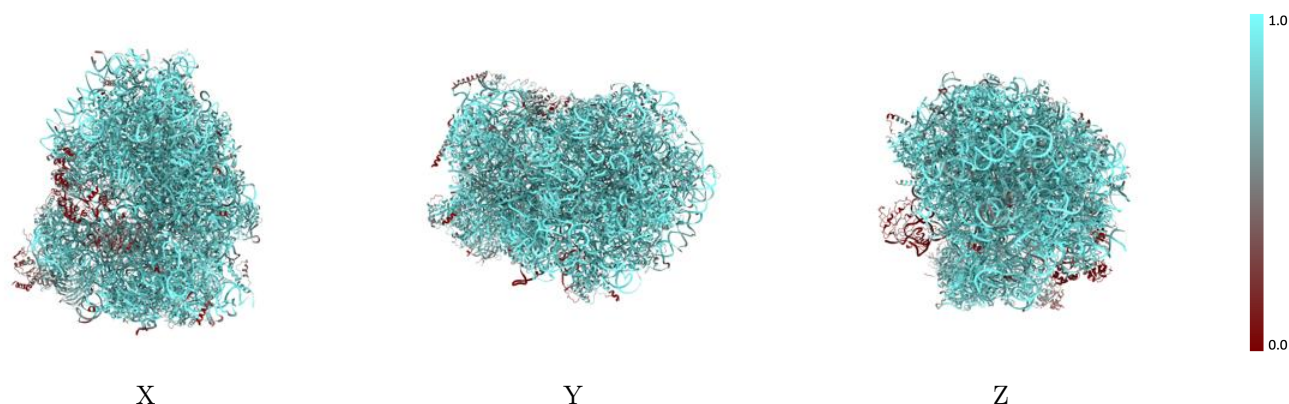
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



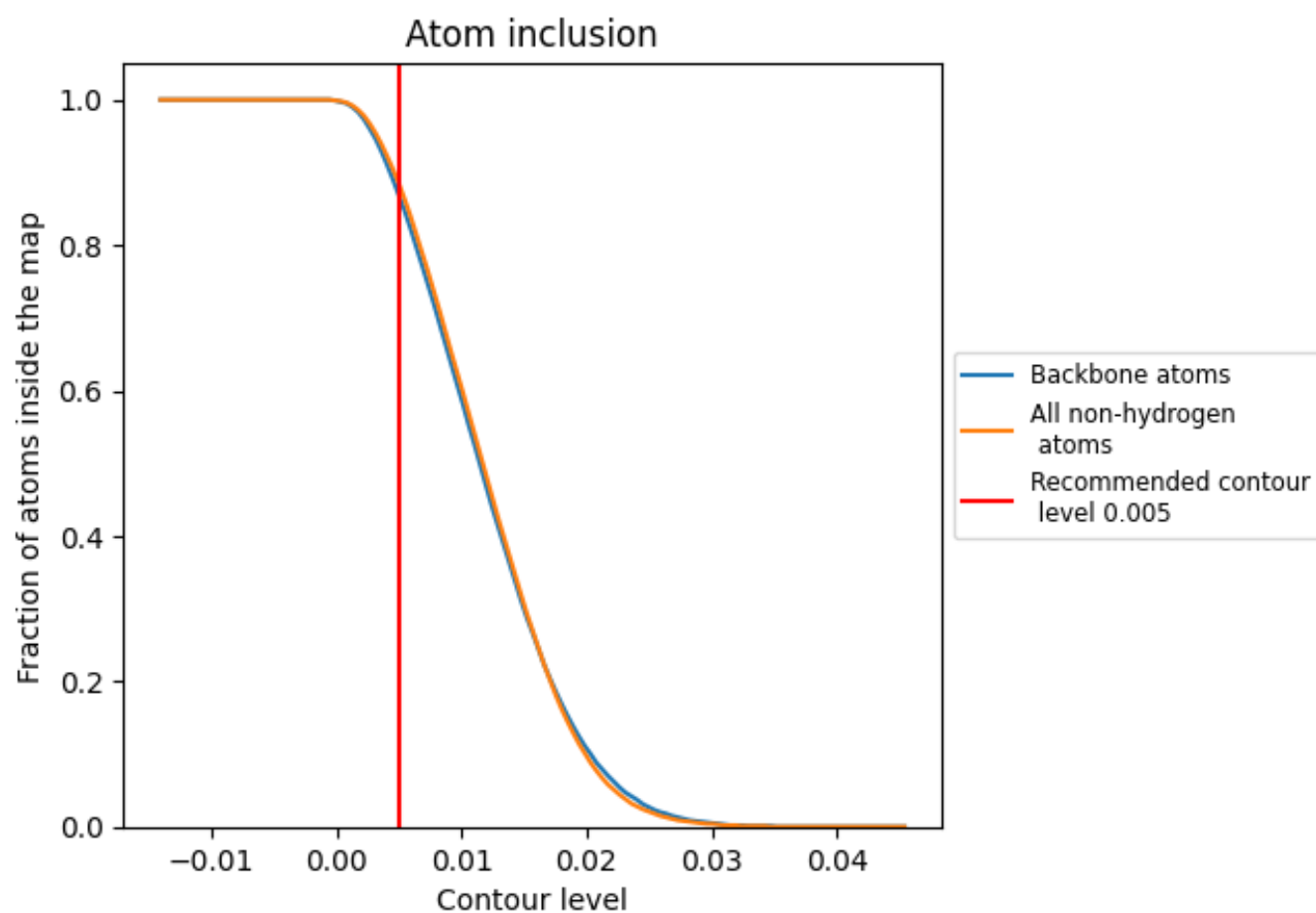
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 88% 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	 0.8840	 0.5760
At	 0.6780	 0.3340
EF	 0.5180	 0.3890
L5	 0.9380	 0.5890
L7	 0.9940	 0.6390
L8	 0.9760	 0.6170
LA	 0.9690	 0.6560
LB	 0.9230	 0.6330
LC	 0.9400	 0.6360
LD	 0.9010	 0.6030
LE	 0.8940	 0.6050
LF	 0.9450	 0.6380
LG	 0.8220	 0.5570
LH	 0.8990	 0.6110
LI	 0.9130	 0.6190
LJ	 0.8600	 0.5920
LK	 0.1030	 0.2140
LL	 0.8950	 0.6090
LM	 0.9250	 0.6150
LN	 0.9820	 0.6550
LO	 0.9440	 0.6370
LP	 0.9460	 0.6470
LQ	 0.9680	 0.6570
LR	 0.8550	 0.5960
LS	 0.9650	 0.6420
LT	 0.9190	 0.6270
LU	 0.8150	 0.5430
LV	 0.9200	 0.6360
LW	 0.6960	 0.4990
LX	 0.9100	 0.6220
LY	 0.9140	 0.6170
LZ	 0.9100	 0.6060
La	 0.9670	 0.6550
Lb	 0.7950	 0.5640
Lc	 0.8940	 0.6130



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Chain	Atom inclusion	Q-score
Ld	 0.8910	 0.6080
Le	 0.9670	 0.6570
Lf	 0.9680	 0.6530
Lg	 0.8990	 0.6190
Lh	 0.9130	 0.6160
Li	 0.8880	 0.5980
Lj	 0.9690	 0.6560
Lk	 0.8220	 0.5690
Ll	 0.9460	 0.6250
Lm	 0.9020	 0.6150
Ln	 0.9080	 0.6230
Lo	 0.9290	 0.6310
Lp	 0.9380	 0.6420
Lq	 0.1600	 0.2630
Lr	 0.9420	 0.6360
Lz	 0.0050	 0.1450
Pt	 0.6650	 0.5440
S2	 0.9600	 0.5840
SA	 0.8660	 0.5840
SB	 0.8560	 0.5930
SC	 0.8940	 0.6050
SD	 0.7650	 0.5270
SE	 0.8670	 0.5900
SF	 0.8350	 0.5640
SG	 0.7440	 0.5050
SH	 0.7420	 0.5270
SI	 0.8670	 0.5860
SJ	 0.8620	 0.5750
SK	 0.7540	 0.4870
SL	 0.8960	 0.6160
SM	 0.2280	 0.2260
SN	 0.9140	 0.6160
SO	 0.8940	 0.6080
SP	 0.7440	 0.5070
SQ	 0.8610	 0.5710
SR	 0.7820	 0.5340
SS	 0.8040	 0.5500
ST	 0.8300	 0.5530
SU	 0.7190	 0.4980
SV	 0.8800	 0.6000
SW	 0.9430	 0.6310
SX	 0.9160	 0.6100

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Chain	Atom inclusion	Q-score
SY	 0.7630	 0.5130
SZ	 0.6950	 0.5130
Sa	 0.9240	 0.6160
Sb	 0.8210	 0.5810
Sc	 0.7330	 0.5380
Sd	 0.9410	 0.5890
Se	 0.7800	 0.5510
Sf	 0.4130	 0.3250
Sg	 0.6850	 0.4910
mR	 0.4470	 0.4820