



wwPDB EM Validation Summary Report ⓘ

Jun 27, 2026 – 12:42 PM EDT

PDB ID : 9PA7 / pdb_00009pa7
EMDB ID : EMD-71435
Title : In situ human 80S consensus ribosome with EBP1
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-25
Resolution : 2.67 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

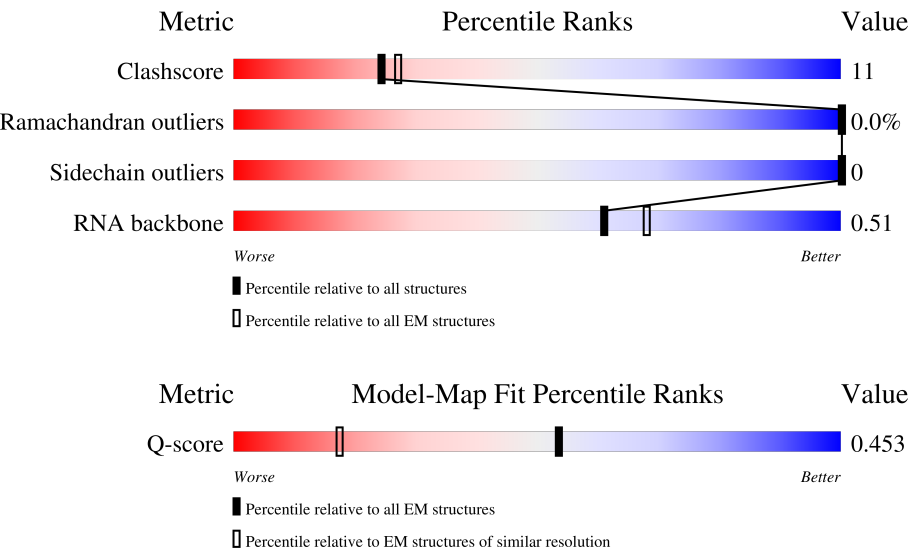
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



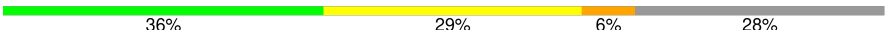
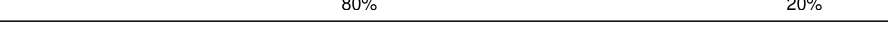
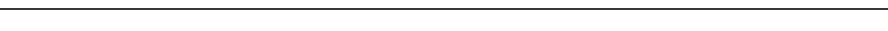
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9182 (2.17 - 3.17)

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

Mol	Chain	Length	Quality of chain
1	CD	36	8% 69% 31%
2	CI	31	65% 35%
3	CF	441	13% 64% 36%

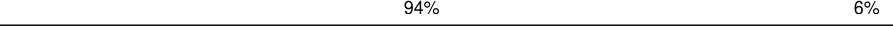
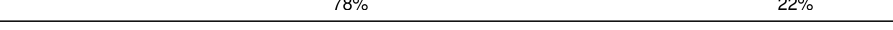
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Mol	Chain	Length	Quality of chain
4	L5	5070	
5	L7	120	
6	L8	156	
7	LA	248	
8	LB	402	
9	LC	368	
10	LD	293	
11	LE	250	
12	LF	225	
13	LG	241	
14	LH	190	
15	LI	213	
16	LJ	176	
17	LL	210	
18	LM	139	
19	LN	203	
20	LO	201	
21	LP	153	
22	LQ	187	
23	LR	187	
24	LS	175	
25	LT	159	
26	LU	101	
27	LV	131	
28	LW	118	

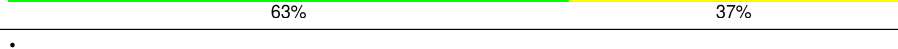
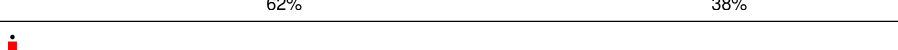
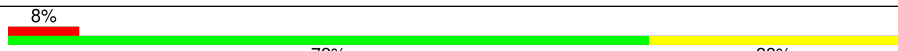
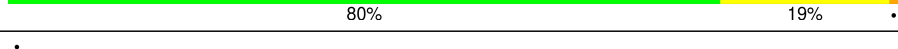
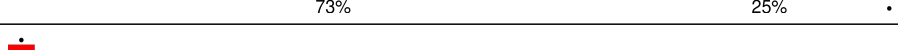
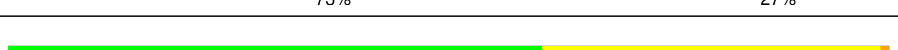
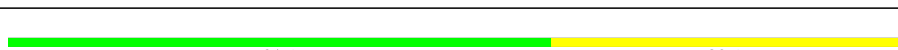
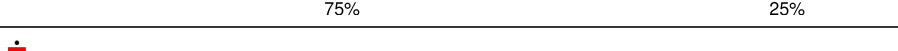
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Mol	Chain	Length	Quality of chain
29	LX	120	
30	LY	134	
31	LZ	135	
32	La	147	
33	Lb	109	
34	Lc	98	
35	Ld	107	
36	Le	128	
37	Lf	109	
38	Lg	114	
39	Lh	122	
40	Li	102	
41	Lj	86	
42	Lk	69	
43	Ll	50	
44	Lm	52	
45	Ln	24	
46	Lo	105	
47	Lp	91	
48	Lr	125	
49	Ls	196	
50	Lt	141	
51	Pt	74	
52	S2	1740	
53	SA	221	

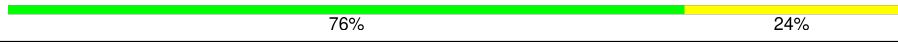
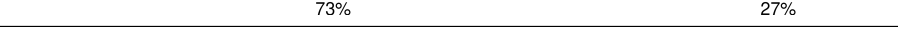
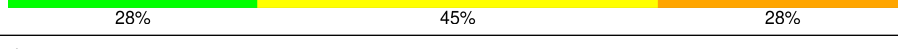
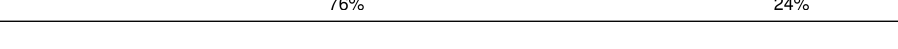
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Mol	Chain	Length	Quality of chain
54	SB	214	
55	SC	222	
56	SD	227	
57	SE	262	
58	SF	189	
59	SG	237	
60	SH	186	
61	SI	206	
62	SJ	185	
63	SK	98	
64	SL	153	
65	SM	122	
66	SN	150	
67	SO	140	
68	SP	121	
69	SQ	144	
70	SR	135	
71	SS	145	
72	ST	143	
73	SU	104	
74	SV	83	
75	SW	129	
76	SX	141	
77	SY	131	
78	SZ	75	

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Mol	Chain	Length	Quality of chain
79	Sa	102	
80	Sb	83	
81	Sc	64	
82	Sd	55	
83	Se	58	
84	Sf	67	
85	Sg	313	
86	AT	76	
87	CA	354	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 231160 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 protein called SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CD	36	Total	C	N	O	S	0	0
			285	179	47	58	1		

- Molecule 2 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CI	31	Total	C	N	O	S	0	0
			247	153	55	38	1		

- Molecule 3 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	CF	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L5	3655	Total	C	N	O	P	1	0
			78445	34968	14346	25476	3655		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 7 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 9 is a protein called 60S ribosomal protein L4.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 11 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LE	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

- Molecule 12 is a protein called 60S ribosomal protein L7.

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

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 14 is a protein called 60S ribosomal protein L9.

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

- Molecule 15 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 16 is a protein called 60S ribosomal protein L11.

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

- Molecule 17 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 18 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 21 is a protein called 60S ribosomal protein L17.

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

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

- Molecule 24 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 27 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LW	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LW	?	-	SER	deletion	UNP A0A994J4A5
LW	?	-	GLU	deletion	UNP A0A994J4A5
LW	?	-	GLU	deletion	UNP A0A994J4A5
LW	?	-	ILE	deletion	UNP A0A994J4A5
LW	?	-	GLN	deletion	UNP A0A994J4A5
LW	?	-	LYS	deletion	UNP A0A994J4A5

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

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

- Molecule 33 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLU	deletion	UNP P47914
Lb	?	-	VAL	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	ILE	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLY	deletion	UNP P47914

- Molecule 34 is a protein called 60S ribosomal protein L30.

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

- Molecule 35 is a protein called 60S ribosomal protein L31.

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

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

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

- Molecule 38 is a protein called 60S ribosomal protein L34.

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

- Molecule 39 is a protein called 60S ribosomal protein L35.

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

- Molecule 40 is a protein called 60S ribosomal protein L36.

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

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 44 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 45 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

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

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 50 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lt	134	Total	C	N	O	S	0	0
			998	626	180	189	3		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lt	?	-	PRO	deletion	UNP P30050
Lt	?	-	PRO	deletion	UNP P30050
Lt	?	-	ARG	deletion	UNP P30050
Lt	?	-	ASP	deletion	UNP P30050
Lt	?	-	ARG	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050

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Chain	Residue	Modelled	Actual	Comment	Reference
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	GLN	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	ASN	deletion	UNP P30050
Lt	?	-	ILE	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	HIS	deletion	UNP P30050
Lt	?	-	SER	deletion	UNP P30050
Lt	?	-	GLY	deletion	UNP P30050
Lt	?	-	ASN	deletion	UNP P30050

- Molecule 51 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Pt	74	Total	C	N	O	P	0	0
			1576	705	285	513	73		

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S2	1740	Total	C	N	O	P	0	0
			36953	16508	6600	12106	1739		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 54 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 55 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SC	220	Total	C	N	O	S	0	0
			1707	1104	293	300	10		

- Molecule 56 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 57 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 58 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 59 is a protein called 40S ribosomal protein S6.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SH	?	-	SER	deletion	UNP P62081
SH	?	-	ARG	deletion	UNP P62081
SH	?	-	THR	deletion	UNP P62081

- Molecule 61 is a protein called 40S ribosomal protein S8.

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

- Molecule 62 is a protein called 40S ribosomal protein S9.

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

- Molecule 63 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 64 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 65 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 66 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 67 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 68 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 69 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 70 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 71 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 72 is a protein called 40S ribosomal protein S19.

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

- Molecule 73 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 74 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 75 is a protein called 40S ribosomal protein S15a.

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

- Molecule 76 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 77 is a protein called 40S ribosomal protein S24.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 79 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 80 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 81 is a protein called 40S ribosomal protein S28.

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

- Molecule 82 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 83 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 84 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 85 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 86 is a RNA chain called A/T site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	AT	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	3	C	U	conflict	GB 28626602
AT	16	C	U	conflict	GB 28626602
AT	51	U	C	conflict	GB 28626602
AT	76	C	A	conflict	GB 28626602
AT	77	A	C	conflict	GB 28626602

- Molecule 87 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

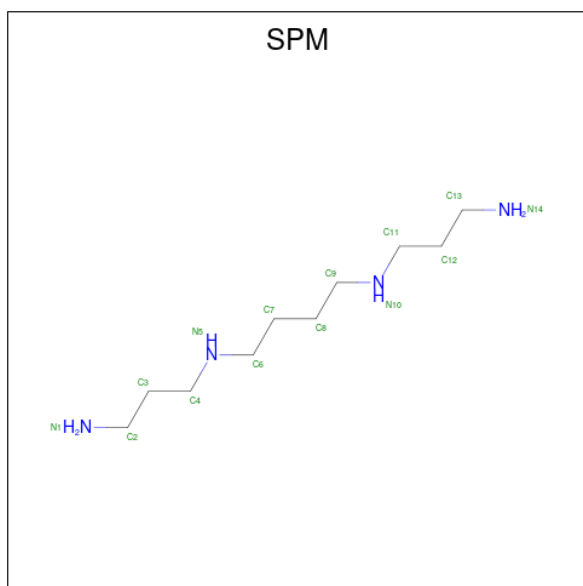
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	?	-	GLU	deletion	UNP Q9UQ80
CA	?	-	ASP	deletion	UNP Q9UQ80

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
88	L5	185	Total	Mg	0
			185	185	
88	L7	3	Total	Mg	0
			3	3	
88	L8	5	Total	Mg	0
			5	5	
88	LA	1	Total	Mg	0
			1	1	
88	LP	1	Total	Mg	0
			1	1	
88	LV	1	Total	Mg	0
			1	1	
88	Le	1	Total	Mg	0
			1	1	
88	S2	28	Total	Mg	0
			28	28	

- Molecule 89 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



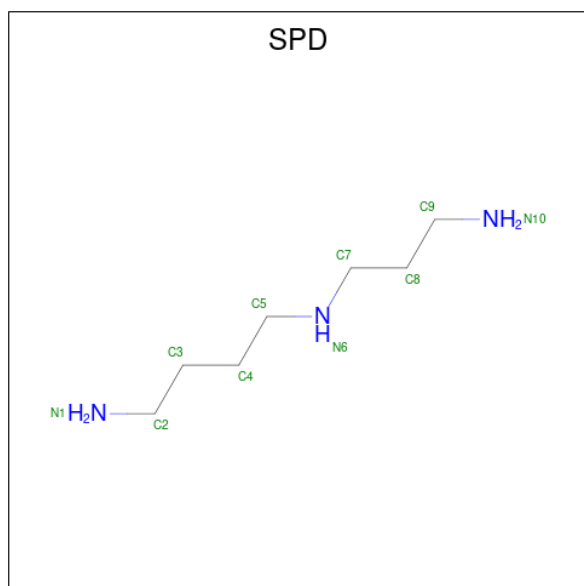
Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	
89	S2	1	Total	C	N	0
			14	10	4	

- Molecule 90 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			AltConf
90	L5	1	Total	C	N	0
			10	7	3	
90	L5	1	Total	C	N	0
			10	7	3	
90	L5	1	Total	C	N	0
			10	7	3	
90	L8	1	Total	C	N	0
			10	7	3	
90	LN	1	Total	C	N	0
			10	7	3	
90	S2	1	Total	C	N	0
			10	7	3	
90	S2	1	Total	C	N	0
			10	7	3	

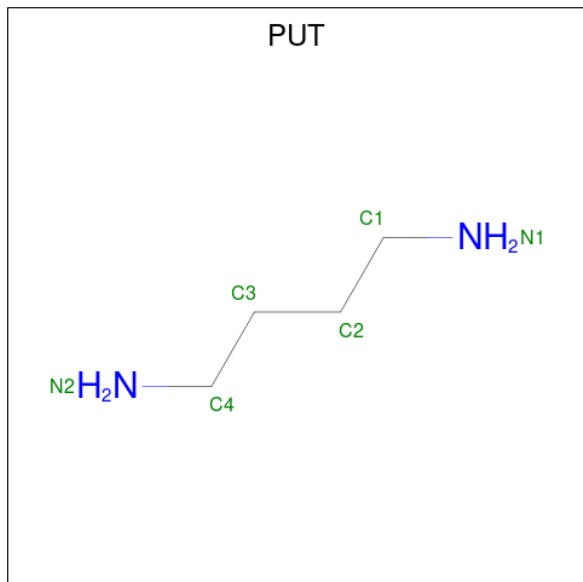
- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
91	L5	74	Total	K	0
			74	74	
91	Lg	1	Total	K	0
			1	1	

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 93 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	CF	1	Total	O	0
			1	1	
94	L5	3310	Total	O	0
			3310	3310	
94	L7	16	Total	O	0
			16	16	
94	L8	118	Total	O	0
			118	118	
94	LA	43	Total	O	0
			43	43	
94	LB	66	Total	O	0
			66	66	
94	LC	45	Total	O	0
			45	45	
94	LD	1	Total	O	0
			1	1	
94	LG	13	Total	O	0
			13	13	

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Mol	Chain	Residues	Atoms		AltConf
94	LH	1	Total 1	O 1	0
94	LI	7	Total 7	O 7	0
94	LL	33	Total 33	O 33	0
94	LN	99	Total 99	O 99	0
94	LO	58	Total 58	O 58	0
94	LP	38	Total 38	O 38	0
94	LQ	21	Total 21	O 21	0
94	LR	12	Total 12	O 12	0
94	LS	2	Total 2	O 2	0
94	LT	9	Total 9	O 9	0
94	LU	1	Total 1	O 1	0
94	LV	41	Total 41	O 41	0
94	LW	15	Total 15	O 15	0
94	LX	10	Total 10	O 10	0
94	La	38	Total 38	O 38	0
94	Lb	14	Total 14	O 14	0
94	Ld	1	Total 1	O 1	0
94	Le	50	Total 50	O 50	0
94	Lf	13	Total 13	O 13	0
94	Lg	2	Total 2	O 2	0
94	Lh	8	Total 8	O 8	0

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Mol	Chain	Residues	Atoms		AltConf
94	Li	10	Total 10	O 10	0
94	Lj	29	Total 29	O 29	0
94	Ll	5	Total 5	O 5	0
94	Ln	2	Total 2	O 2	0
94	Lo	37	Total 37	O 37	0
94	Lp	4	Total 4	O 4	0
94	Lr	3	Total 3	O 3	0
94	Pt	6	Total 6	O 6	0
94	S2	340	Total 340	O 340	0
94	SE	12	Total 12	O 12	0
94	SF	5	Total 5	O 5	0
94	SH	1	Total 1	O 1	0
94	SI	14	Total 14	O 14	0
94	SJ	1	Total 1	O 1	0
94	SL	22	Total 22	O 22	0
94	SP	1	Total 1	O 1	0
94	SQ	7	Total 7	O 7	0
94	SS	8	Total 8	O 8	0
94	ST	2	Total 2	O 2	0
94	SU	3	Total 3	O 3	0
94	SX	8	Total 8	O 8	0

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Mol	Chain	Residues	Atoms		AltConf
94	SZ	1	Total 1	O 1	0
94	Sc	1	Total 1	O 1	0
94	Sd	3	Total 3	O 3	0

3 Residue-property plots

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

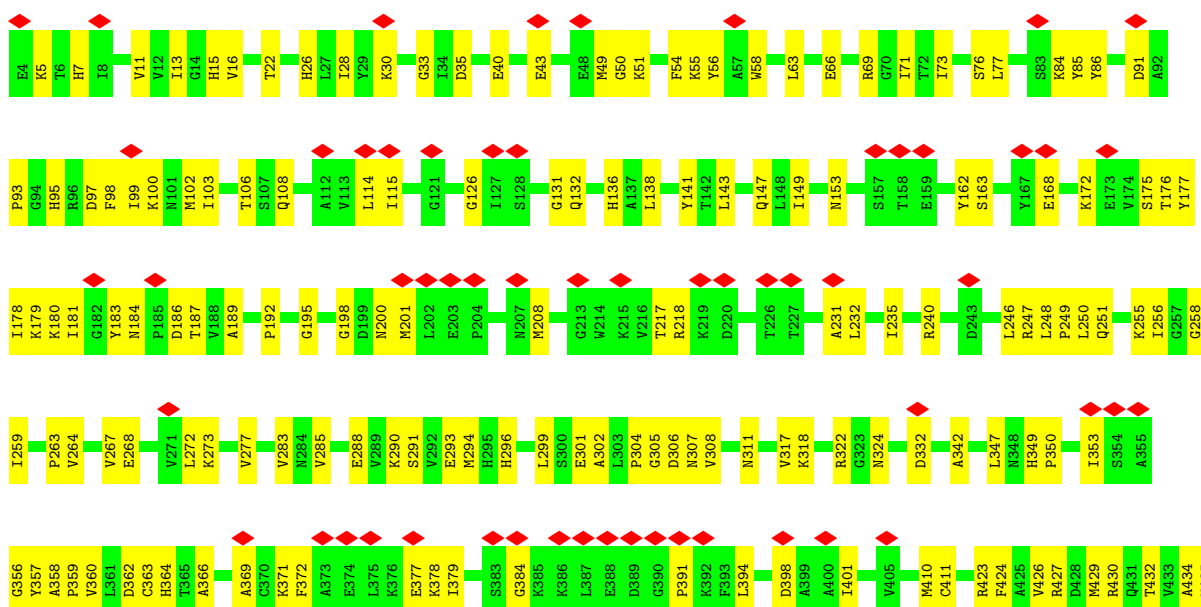
- Molecule 1: SERPINE1 mRNA-binding protein 1



- Molecule 2: Transcription factor BTF3



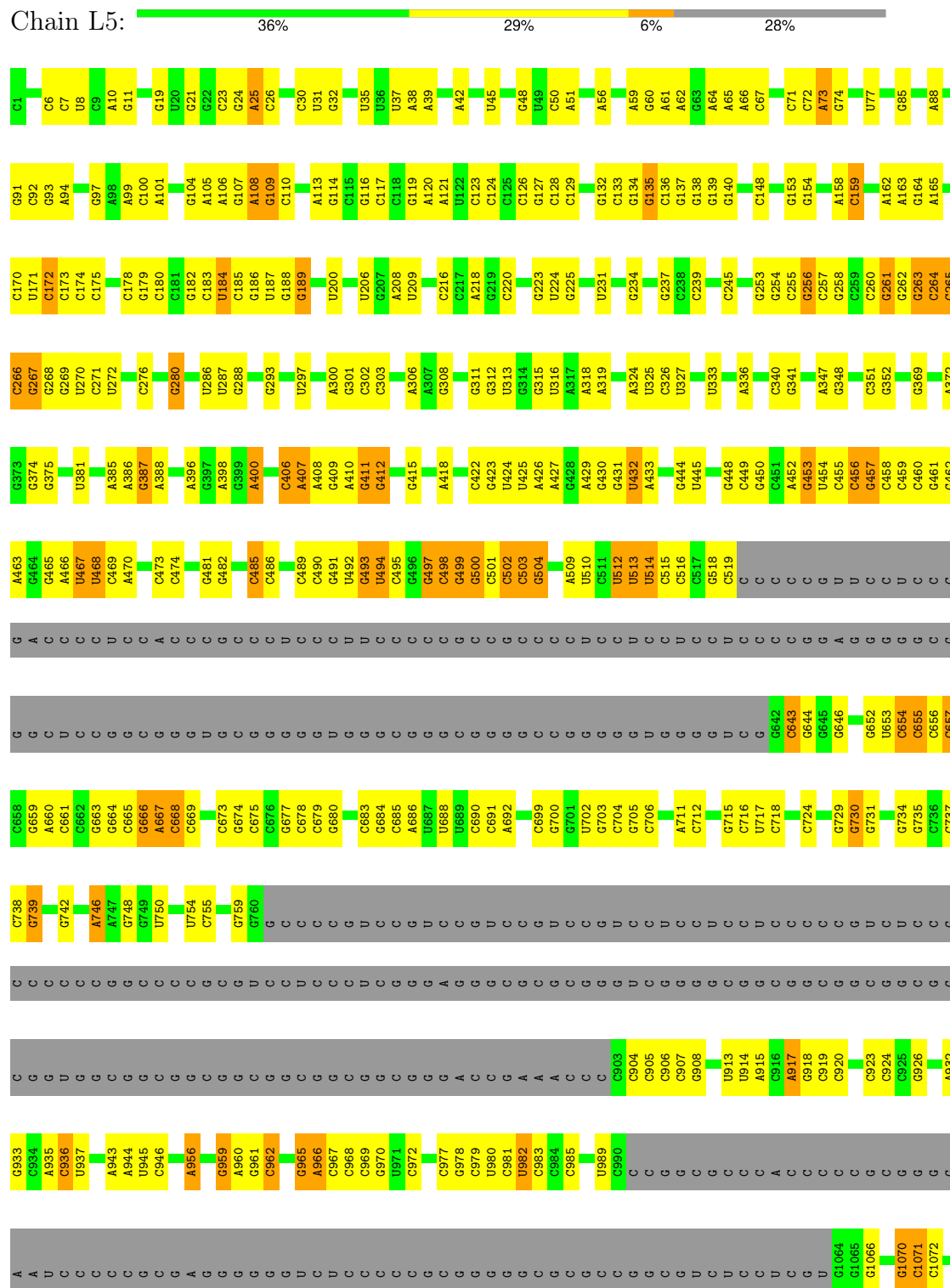
- Molecule 3: Elongation factor 1-alpha 1





● Molecule 4: 28S rRNA

Chain L5:



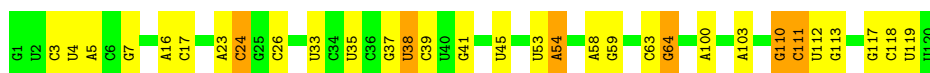
U	G2092	A1990	G1895	U1792	C	G1632	A1534	G1436	G1349	C1276	G1199	A	G1075
C	A2093	A1991	A1896	U1792	G1716	G1633	A1535	C1437	G1350	C1278	G1200	C	C1076
U	G2094	A1992	C1897	A1802	C1717	A1634	U1536	U1438	G1351	A1279	U1201	G	A1077
C	A2095	C1993	C1898	G1803	C1718	A1635	U1537	U1439	C1352	C1280	C1202	G	C1078
C	G2096	C1994	G1899	G1804	A1719	U1638	U1538	U1440	G1353	G1281	G1203	G	C1079
C	U2097	G1995	G1907	A1805	C1720	A1639	G1539	C1441	A1354	G1282	C1210	G	C1080
C	G2098	C1996	A1907	G1806	G1721	C1640	G1544	C1442	G1355	G1283	G1211	G	C1081
C	G2099	U1997	A1908	C1807	U1725	G1641	A1547	A1443	U1356	G1284	C1215	G	U1082
U	A2100	A1998	G1909	U1807	U1726	A1642	A1548	U1444	C1357	C1286	C1214	G	C1083
C	G2101	G2000	G1910	G1810	U1727	C1645	U1549	U1445	U1358	U1285	C1215	G	C1084
C	G2102	G2001	G1915	G1810	U1728	A1646	U1549	U1446	U1359	G1287	C1216	G	C1085
U	G2103	A2002	G1916	C1820	U1729	U1647	G1552	C1447	C1365	G1293	G1217	C	C1086
C	A2105	G2003	A1917	G1821	C1731	G1654	A1553	G1448	G1366	A1294	G1218	C	A1087
C	C2106	U1918	U1918	U1822	C1732	U1654	A1554	U1449	C1367	G1296	G1219	C	C1088
C	G2107	G1919	G1919	U1823	C1733	C1661	U1555	C1458	A1368	C1296	G1220	G	C1091
C	A2008	U2008	C1920	G1824	C1734	C1662	C1556	A1459	U1369	U1297	G1221	G	C1092
C	A2009	A2009	C1921	A1825	U1735	C1663	C1557	C1460	G1370	C1298	A1222	G	C1093
C	G2109	A2010	G1922	G1834	G1739	U1664	A1558	C1461	C1378	G1300	G	G	G1094
C	C2011	C2011	G1925	U1835	C1740	C1665	G1559	A1462	C1379	C1301	U	C	A1095
A	G2111	A2017	G1925	G1836	G1741	U1669	G1562	C1468	A1387	U1302	U	G	A1096
C	G2112	C2018	G1930	U1837	A1742	A1669	A1563	C1469	C1390	A1303	U	G	C1097
C	G	C2019	C1931	A1837	U1743	U1672	A1564	C1470	G1391	C1304	C	G	C1098
C	G	U2020	A1932	G1842	U1744	U1673	C1565	G1475	A1392	C1305	U	C	C1099
C	G	G2021	G1933	G1842	G1745	U1674	C1566	C1476	A1393	C1306	U	C	U1100
C	G	G2022	A1934	G1846	G1746	C1675	U1567	C1477	G1394	A1307	U	C	C
C	G	A2025	C1935	C1847	G1750	C1676	C1568	C1480	U1395	C1308	C	C	C
C	G	A2026	C1936	C1848	G1751	U1677	A1569	C1481	G1396	C1309	G	C	C
C	G	C2027	C1937	G1855	G1752	U1677	G1574	C1482	U1397	C1310	G	C	C
C	G	A2029	G1940	C1856	U1757	U1683	G1577	C1483	A1397	G1314	G1234	G	A
C	G	A2030	A1941	C1857	G1758	A1684	U1578	U1494	A1398	C1315	G1235	U	C
C	G	U2041	A1942	C1858	G1759	G1685	C1579	C1495	G1399	C1316	C1239	U	C
C	G	G2045	A1943	C1859	G1760	C1686	U1581	G1496	G1400	U1317	G1240	C	C
C	G	G2046	U1861	U1861	C1761	U1687	U1582	C1497	C1401	C1318	C1241	U	C
C	G	A2047	U1862	U1862	C1762	G1688	U1583	G1498	C1402	C1322	G1242	U	C
C	G	U2048	U1866	U1866	C1763	U1693	U1588	G1502	G1403	A1323	G1243	C	C
C	G	G2055	A1867	A1867	G1764	C1694	C1589	C1504	G1404	A1324	G1244	U	C
C	G	G2056	A1868	A1868	A1765	U1695	U1591	G1504	C1405	C1327	C1245	U	C
C	G	A2057	G1869	A1869	A1766	C1696	U1591	C1505	C1406	A1328	G1246	U	C
C	G	G2058	C1870	C1870	C1767	G1697	U1596	C1506	C1407	C1328	C1251	C	C
C	G	C2059	A1871	A1871	G1769	C1698	U1596	C1507	G1408	G1329	C1252	C	C
C	G	U2069	G1872	G1872	U1771	A1699	A1601	C1508	C1409	C1332	A1254	C	C
C	G	A2069	G1875	G1875	U1772	G1700	A1604	C1509	C1411	A1333	G1257	C	C
C	G	U2072	U1876	U1876	C1773	A1701	G1604	U1510	C1414	A1334	A1258	C	C
C	G	G2076	C1877	C1877	C1774	C1703	G1605	U1511	G1415	G1337	G1259	C	C
C	G	U2077	G1878	G1878	U1779	G1704	G1612	U1512	G1416	U1338	C	C	C
C	G	C2077	C1879	C1879	U1780	G1705	A1613	U1513	C1417	U1339	G1266	C	C
C	G	G2078	G1880	G1880	A1780	A1706	G1617	A1514	A1420	C1340	C1267	C	C
C	G	U2079	C1881	C1881	U1781	C	G	A1515	G1426	U1341	G1268	C	C
C	G	A2080	U1882	U1882	U1782	C	G	G1517	G1426	A1342	G1269	C	C
C	G	C2083	G1883	G1883	C1785	A	G1624	C	G1426	A1343	A1270	C	C
C	G	G2084	A1892	A1892	A1786	C	G1625	C	G1426	C1344	G1271	C	C
C	G	U2085	C1893	C1893	A1787	C	C1628	A1524	G1431	A1345	G1272	C	C
C	G	A2276	C1894	C1894	A1788	C	A1631	A1525	G1432	C1346	G1273	C	C
C	G				C1789	C			G1435	G1347	A1274	C	C







• Molecule 5: 5S rRNA



• Molecule 6: 5.8S rRNA

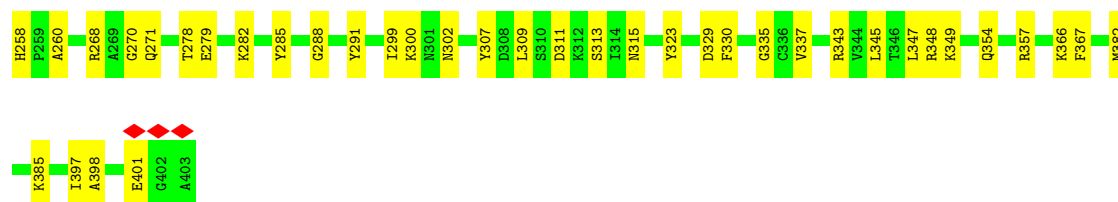


• Molecule 7: 60S ribosomal protein L8

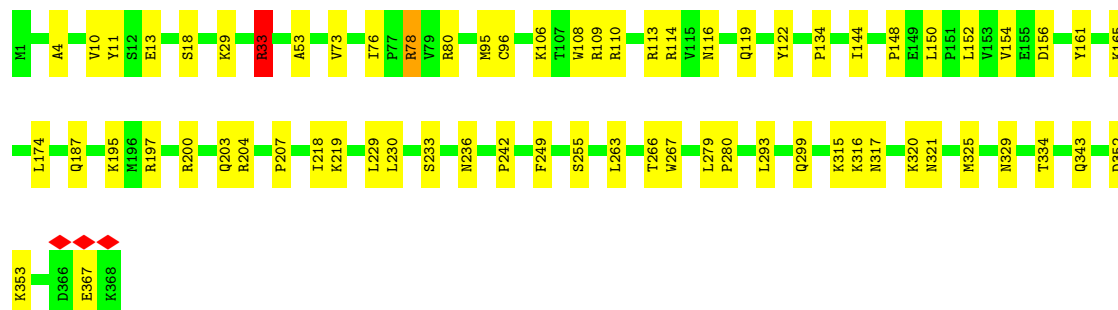
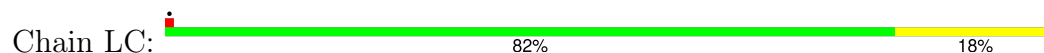


• Molecule 8: Large ribosomal subunit protein uL3

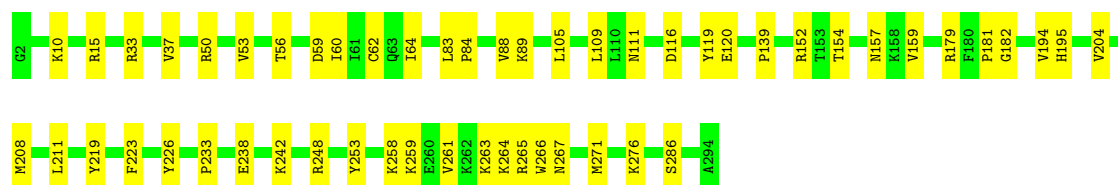
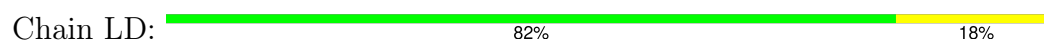




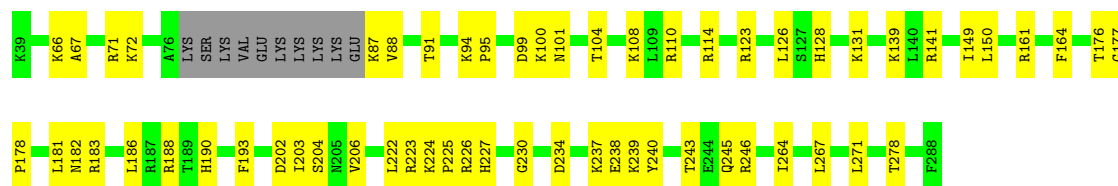
• Molecule 9: 60S ribosomal protein L4



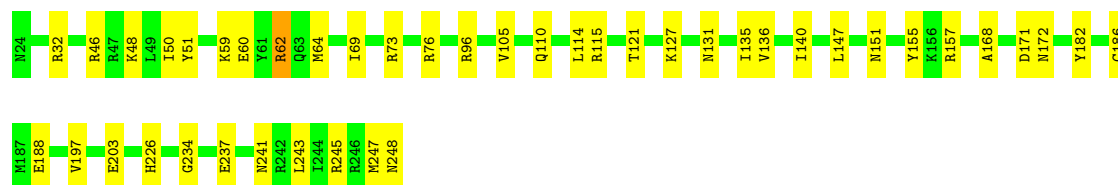
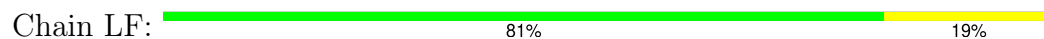
• Molecule 10: Large ribosomal subunit protein uL18



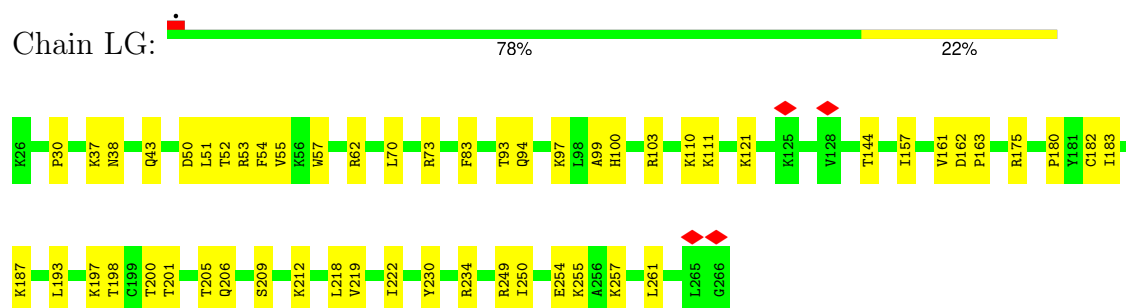
• Molecule 11: Large ribosomal subunit protein eL6



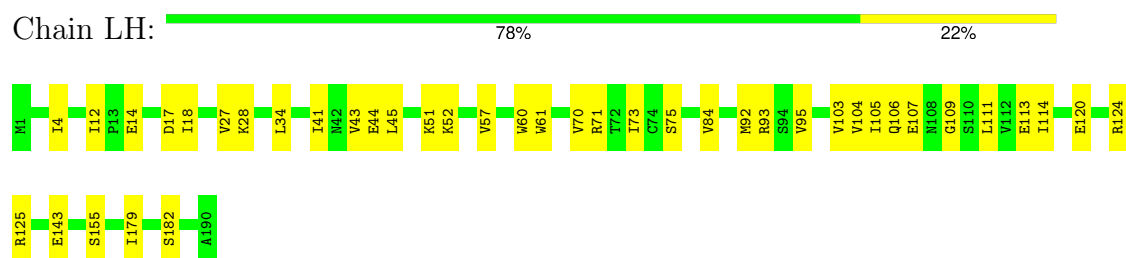
• Molecule 12: 60S ribosomal protein L7



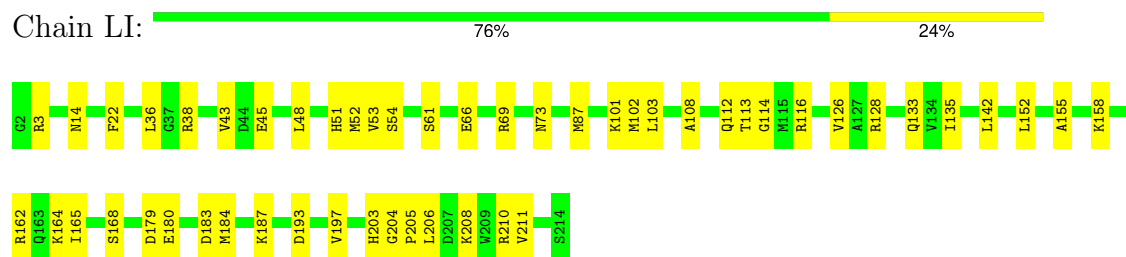
- Molecule 13: 60S ribosomal protein L7a



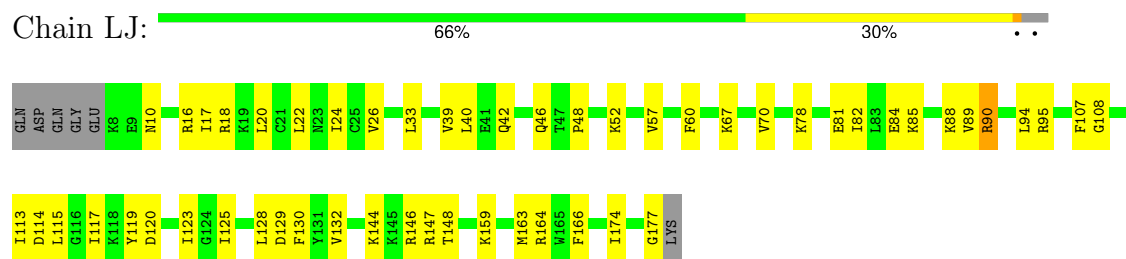
- Molecule 14: 60S ribosomal protein L9



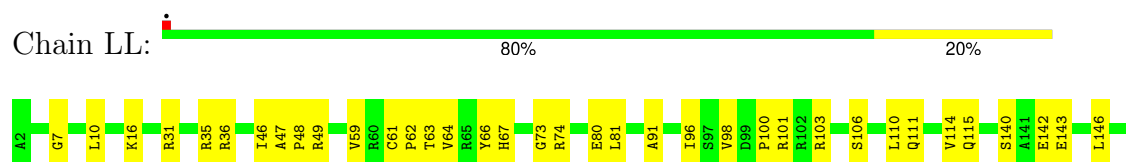
- Molecule 15: Ribosomal protein uL16-like



- Molecule 16: 60S ribosomal protein L11



- Molecule 17: Large ribosomal subunit protein eL13





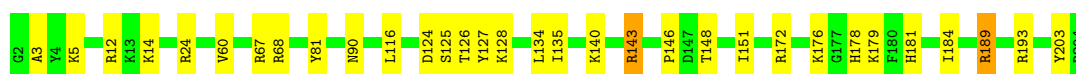
- Molecule 18: 60S ribosomal protein L14

Chain LM: 79% 21%



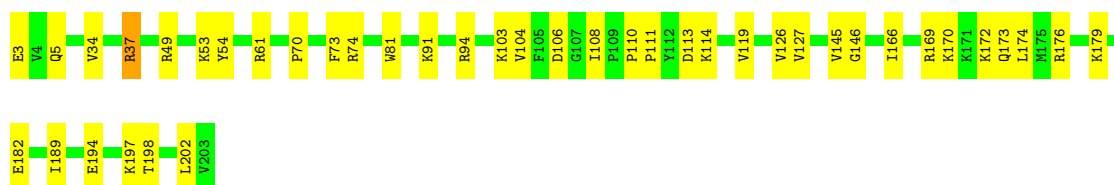
- Molecule 19: 60S ribosomal protein L15

Chain LN: 84% 15%



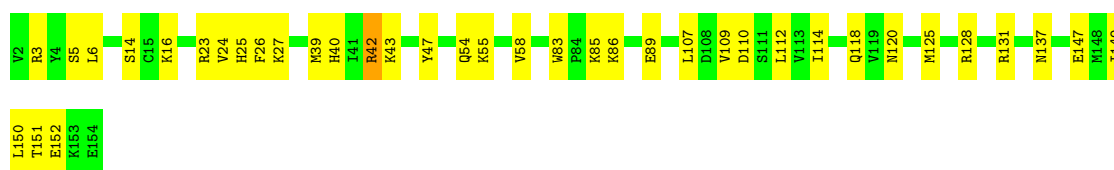
- Molecule 20: 60S ribosomal protein L13a

Chain LO: 80% 20%



- Molecule 21: 60S ribosomal protein L17

Chain LP: 75% 24%



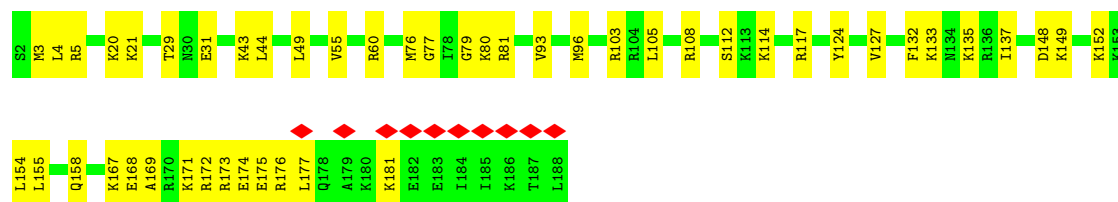
- Molecule 22: 60S ribosomal protein L18

Chain LQ: 88% 12%



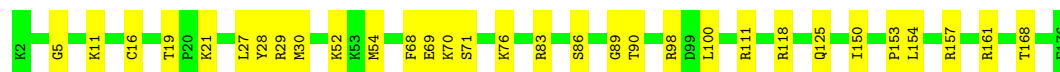
- Molecule 23: 60S ribosomal protein L19

Chain LR: 5% 74% 26%



- Molecule 24: 60S ribosomal protein L18a

Chain LS: 82% 18%



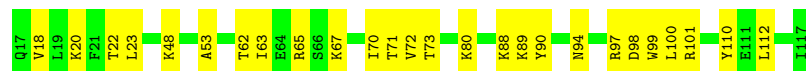
- Molecule 25: 60S ribosomal protein L21

Chain LT: 78% 22%



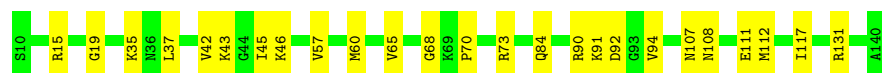
- Molecule 26: Heparin-binding protein HBp15

Chain LU: 74% 26%



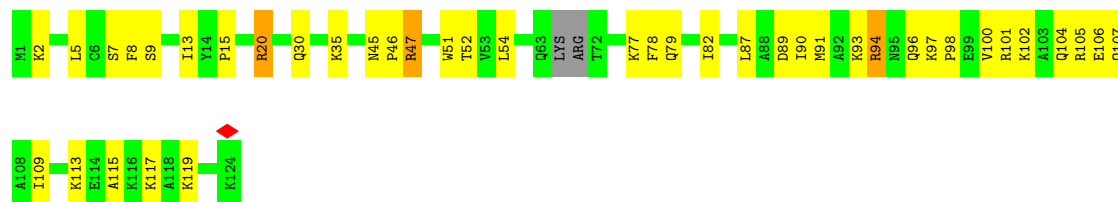
- Molecule 27: 60S ribosomal protein L23

Chain LV: 81% 19%



- Molecule 28: Ribosomal protein L24

Chain LW: 64% 32%



- Molecule 29: 60S ribosomal protein L23a

Chain LX:  88% 12%



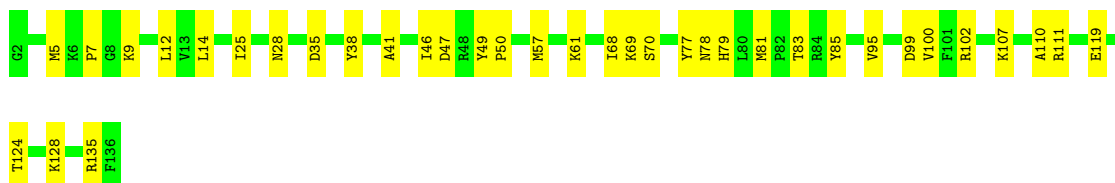
- Molecule 30: 60S ribosomal protein L26

Chain LY:  76% 23%



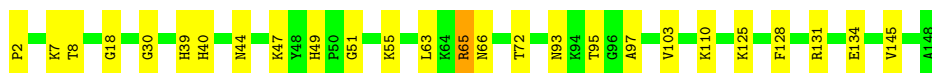
- Molecule 31: 60S ribosomal protein L27

Chain LZ:  73% 27%



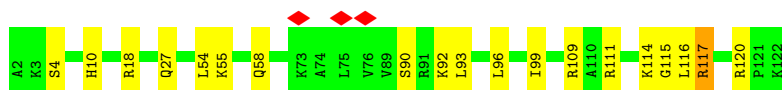
- Molecule 32: 60S ribosomal protein L27a

Chain La:  82% 17%



- Molecule 33: Large ribosomal subunit protein eL29

Chain Lb:  83% 17%



- Molecule 34: 60S ribosomal protein L30

Chain Lc:  76% 24%



- Molecule 35: 60S ribosomal protein L31

Chain Ld:  75% 25%



- Molecule 36: 60S ribosomal protein L32

Chain Le:  88% 12%



- Molecule 37: 60S ribosomal protein L35a

Chain Lf:  86% 14%



- Molecule 38: 60S ribosomal protein L34

Chain Lg:  87% 13%



- Molecule 39: 60S ribosomal protein L35

Chain Lh:  84% 16%



- Molecule 40: 60S ribosomal protein L36

Chain Li:  94% 6%



- Molecule 41: 60S ribosomal protein L37

Chain Lj:  77% 23%



- Molecule 42: 60S ribosomal protein L38

Chain Lk:  78% 22%



- Molecule 43: 60S ribosomal protein L39

Chain Ll:  70% 28% .



- Molecule 44: Large ribosomal subunit protein eL40

Chain Lm:  79% 21%



- Molecule 45: 60S ribosomal protein L41

Chain Ln:  75% 21% .



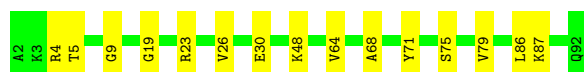
- Molecule 46: 60S ribosomal protein L36a

Chain Lo:  78% 22%



- Molecule 47: 60S ribosomal protein L37a

Chain Lp:  84% 16%



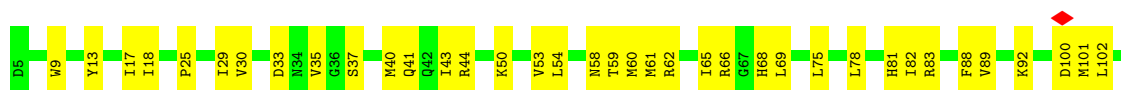
- Molecule 48: 60S ribosomal protein L28

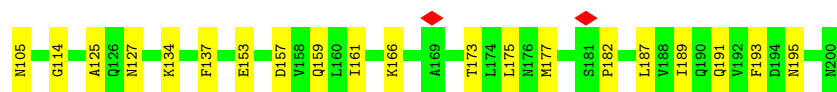
Chain Lr:  88% 12%



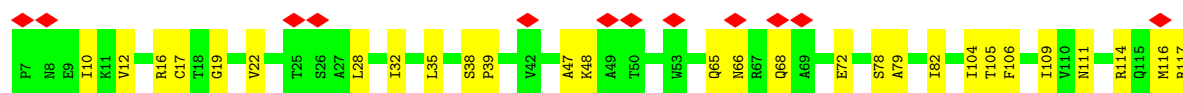
- Molecule 49: 60S acidic ribosomal protein P0

Chain Ls:  71% 29%





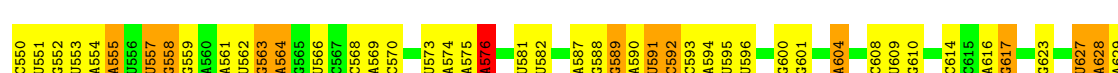
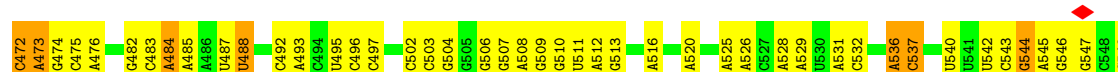
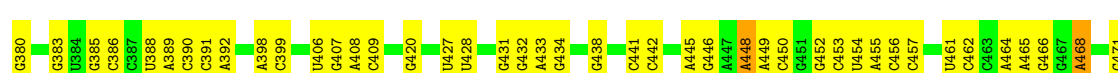
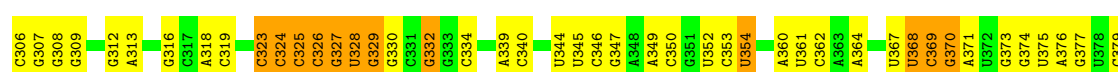
- Molecule 50: Large ribosomal subunit protein uL11



- Molecule 51: P site tRNA

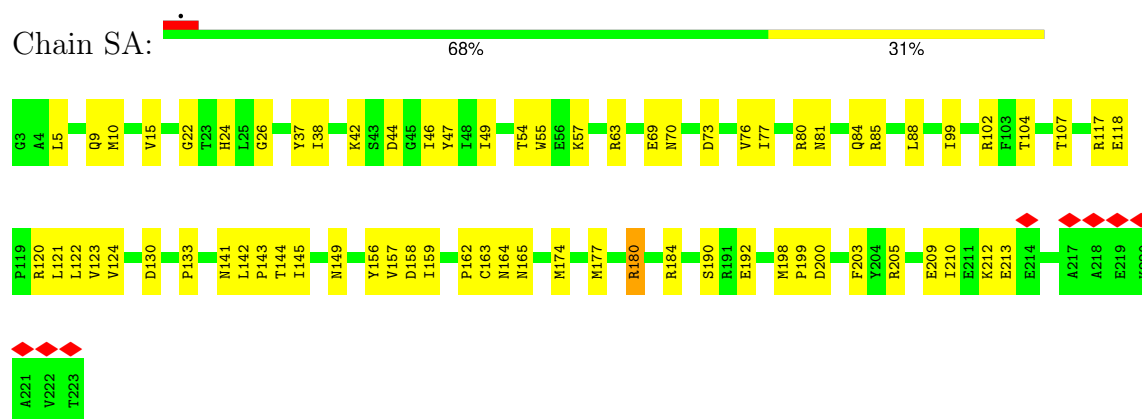


- Molecule 52: 18S rRNA

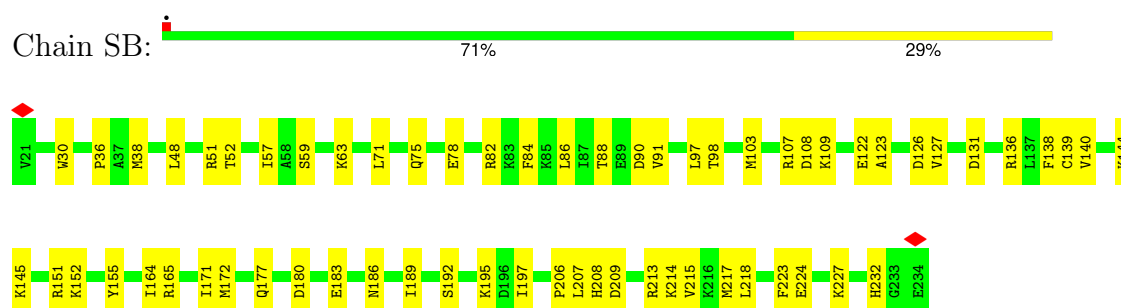




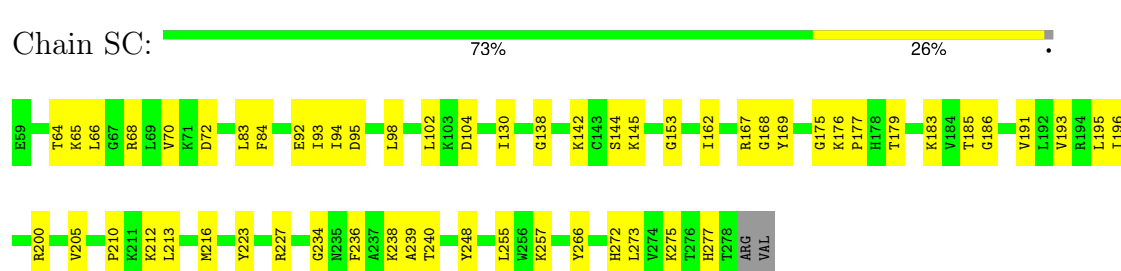
- Molecule 53: 40S ribosomal protein SA



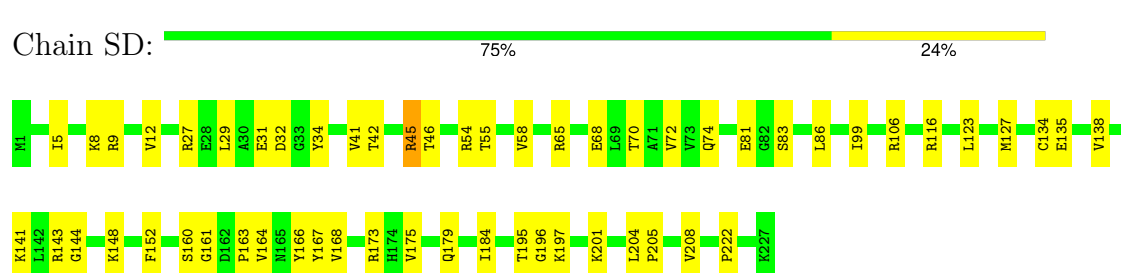
- Molecule 54: 40S ribosomal protein S3a



- Molecule 55: 40S ribosomal protein S2

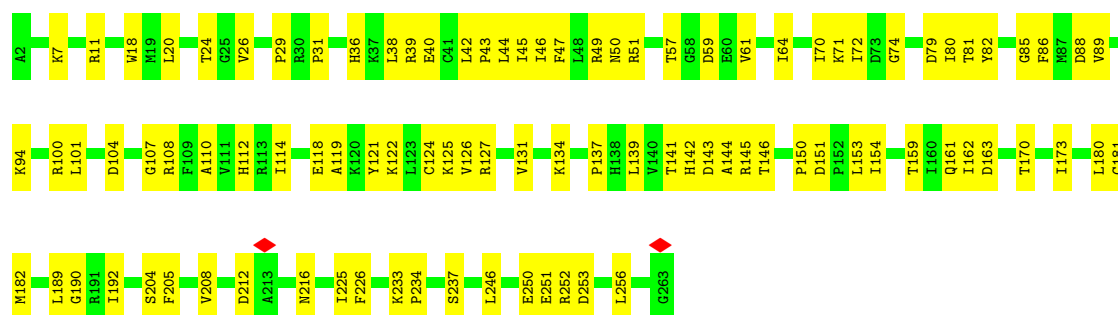


- Molecule 56: Small ribosomal subunit protein uS3

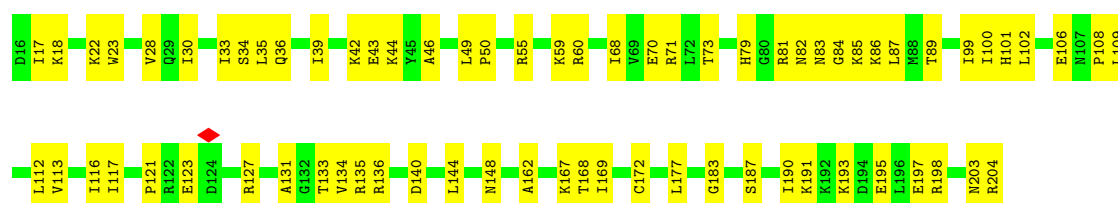


- Molecule 57: Small ribosomal subunit protein eS4, X isoform

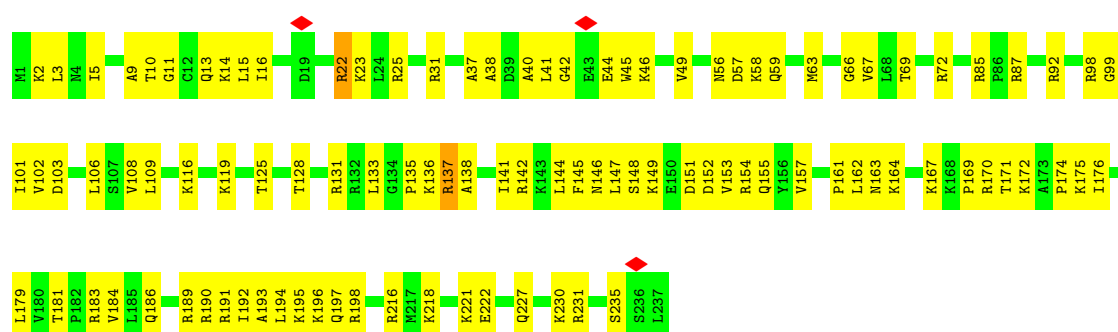




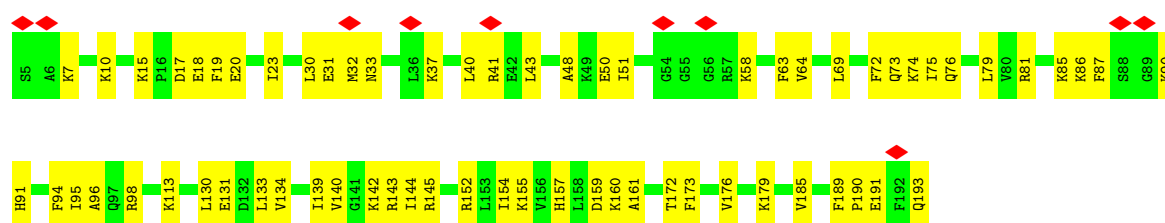
- Molecule 58: 40S ribosomal protein S5



- Molecule 59: 40S ribosomal protein S6

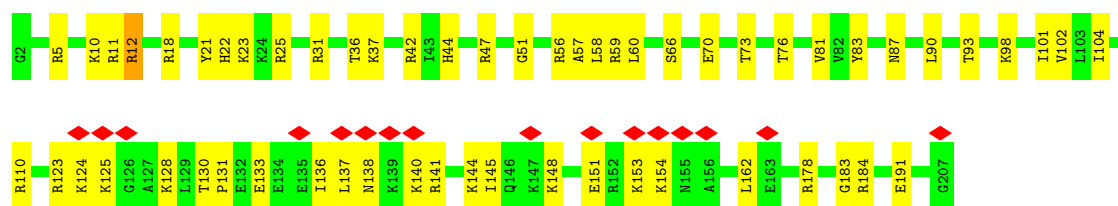


- Molecule 60: Small ribosomal subunit protein eS7

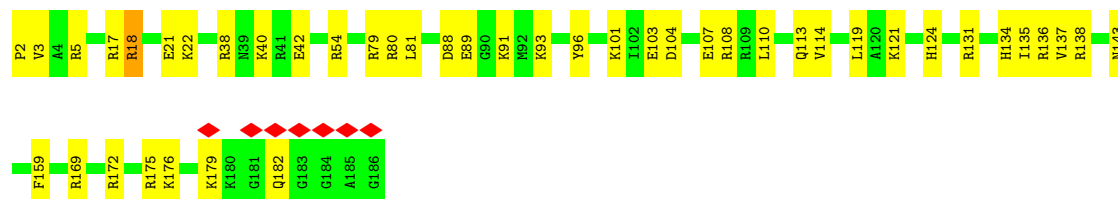
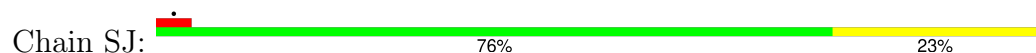


- Molecule 61: 40S ribosomal protein S8





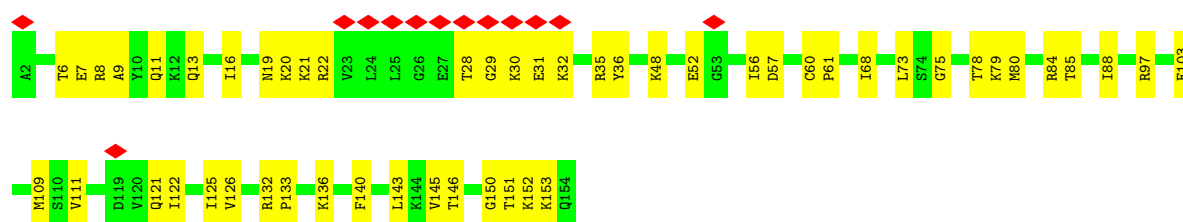
- Molecule 62: 40S ribosomal protein S9



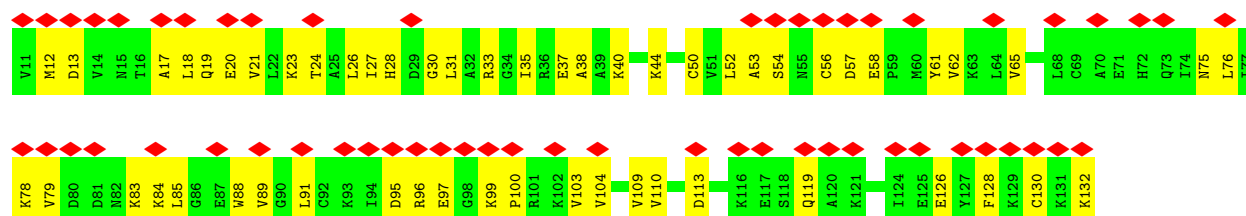
- Molecule 63: 40S ribosomal protein S10



- Molecule 64: 40S ribosomal protein S11



- Molecule 65: Small ribosomal subunit protein eS12



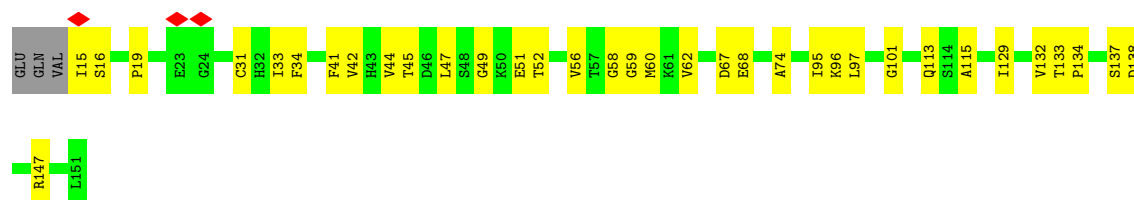
- Molecule 66: 40S ribosomal protein S13

Chain SN:  80% 19%



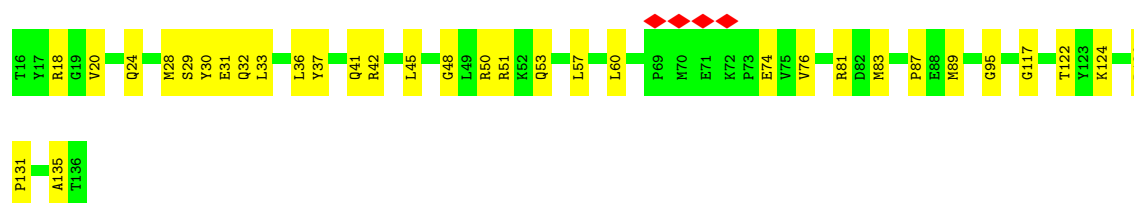
- Molecule 67: Small ribosomal subunit protein uS11

Chain SO:  73% 25%



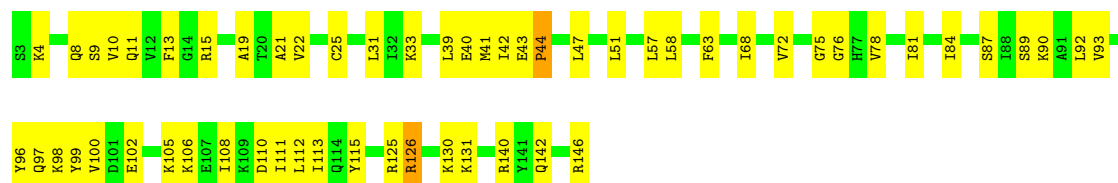
- Molecule 68: Small ribosomal subunit protein uS19

Chain SP:  73% 27%



- Molecule 69: Small ribosomal subunit protein uS9

Chain SQ:  60% 38%



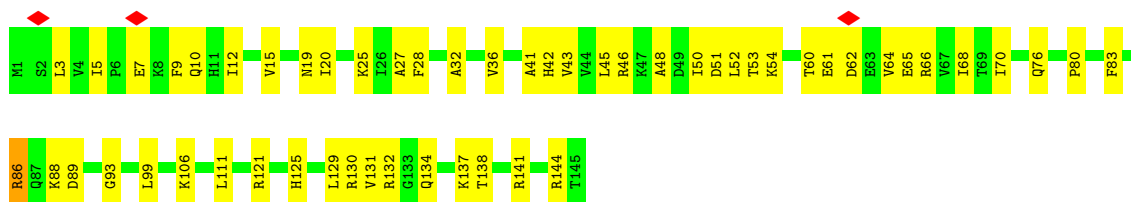
- Molecule 70: Small ribosomal subunit protein eS17

Chain SR:  61% 39%

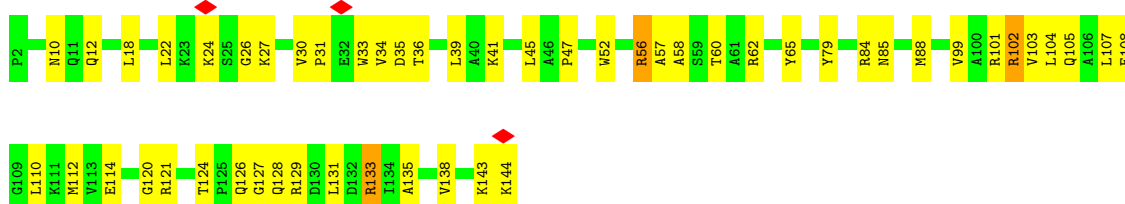


- Molecule 71: 40S ribosomal protein S18

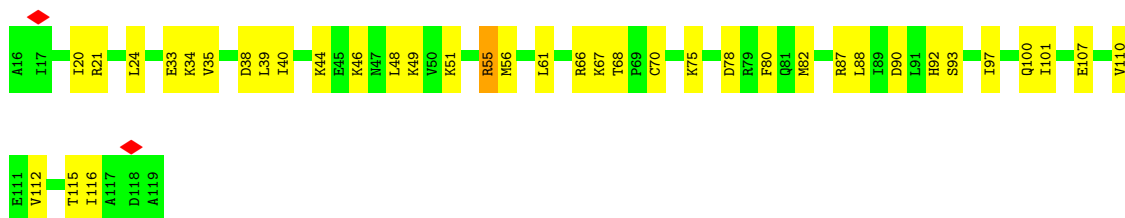
Chain SS:  63% 37%



- Molecule 72: 40S ribosomal protein S19



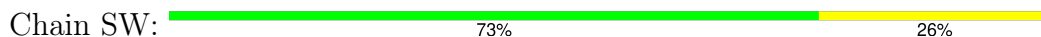
- Molecule 73: 40S ribosomal protein S20



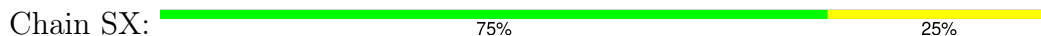
- Molecule 74: Small ribosomal subunit protein eS21



- Molecule 75: 40S ribosomal protein S15a



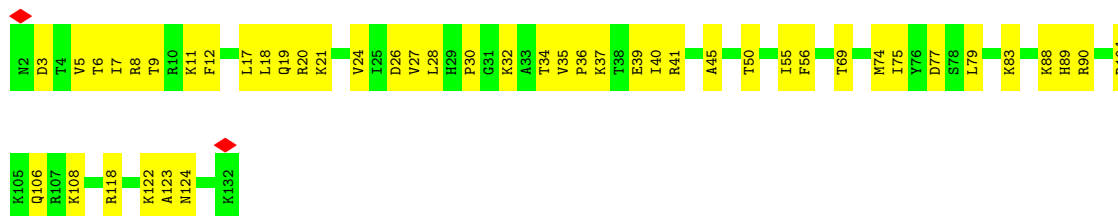
- Molecule 76: 40S ribosomal protein S23



R142

- Molecule 77: 40S ribosomal protein S24

Chain SY:  65% 35%



- Molecule 78: Small ribosomal subunit protein eS25

Chain SZ:  5% 67% 33%



- Molecule 79: 40S ribosomal protein S26

Chain Sa:  81% 19%



- Molecule 80: Small ribosomal subunit protein eS27

Chain Sb:  76% 24%



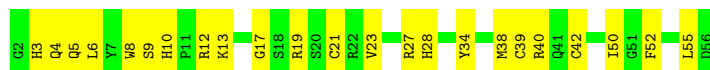
- Molecule 81: 40S ribosomal protein S28

Chain Sc:  73% 27%



- Molecule 82: 40S ribosomal protein S29

Chain Sd:  58% 42%



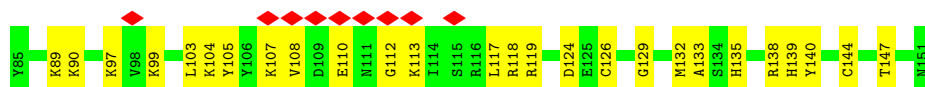
- Molecule 83: Small ribosomal subunit protein eS30

Chain Se:  88% 12%



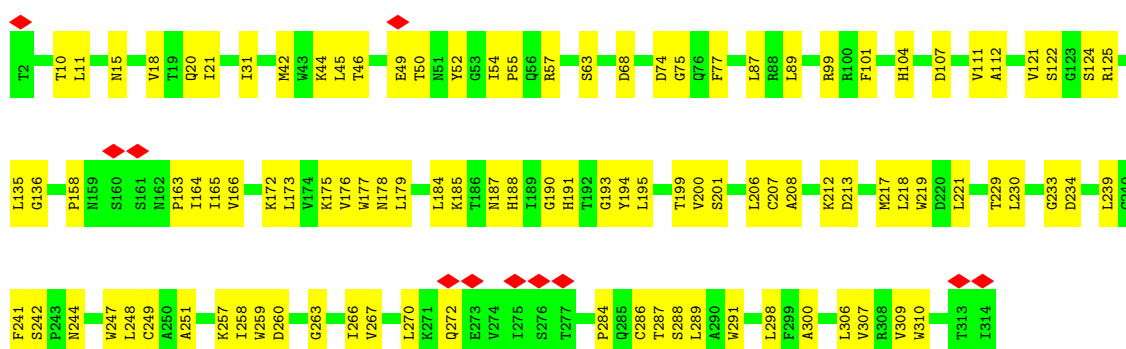
- Molecule 84: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  13% 61% 39%

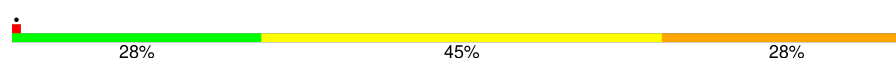


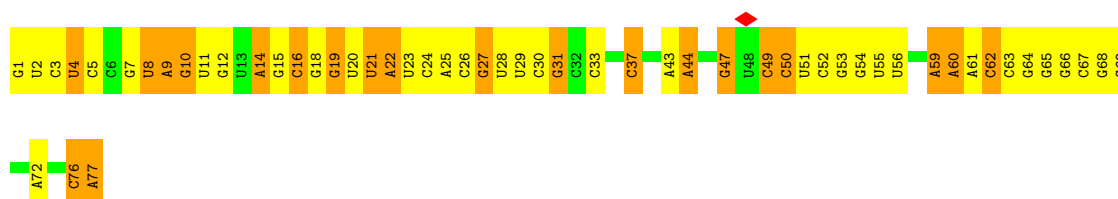
- Molecule 85: Receptor of activated protein C kinase 1

Chain Sg:  67% 33%



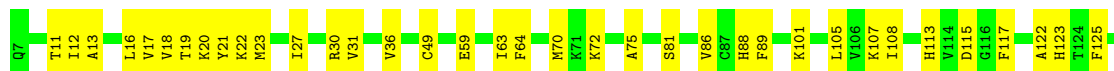
- Molecule 86: A/T site tRNA

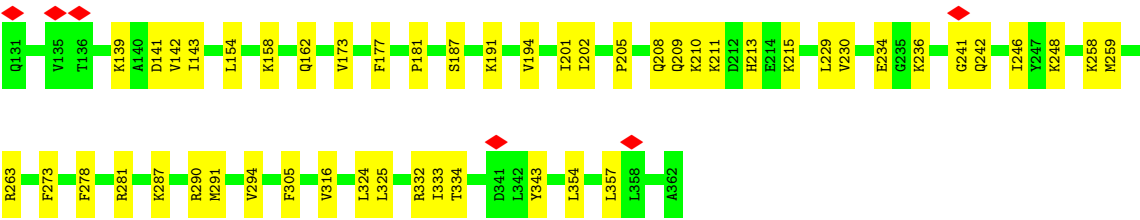
Chain AT:  28% 45% 28%



- Molecule 87: Proliferation-associated protein 2G4

Chain CA:  76% 24%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	221164	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.017	Depositor
Minimum map value	-0.302	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0575	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4AC, SPD, SPM, 5MC, 6MZ, 1MA, K, SEP, OMU, MA6, PSU, UY1, A2M, ZN, UR3, MG, B8N, G7M, OMC, OMG, PUT

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	CD	0.14	0/291	0.39	0/391
2	CI	0.16	0/247	0.44	0/323
3	CF	0.16	0/3442	0.40	0/4656
4	L5	0.16	0/85098	0.30	0/132762
5	L7	0.12	0/2861	0.23	0/4459
6	L8	0.13	0/3631	0.26	0/5657
7	LA	0.20	0/1936	0.39	0/2596
8	LB	0.18	0/3306	0.42	0/4424
9	LC	0.21	0/2981	0.45	1/4002 (0.0%)
10	LD	0.18	0/2428	0.36	0/3252
11	LE	0.19	0/1973	0.43	0/2645
12	LF	0.16	0/1905	0.31	0/2539
13	LG	0.21	0/1960	0.42	0/2637
14	LH	0.18	0/1537	0.39	0/2066
15	LI	0.16	0/1751	0.37	0/2340
16	LJ	0.19	0/1385	0.44	0/1852
17	LL	0.16	0/1732	0.36	0/2315
18	LM	0.18	0/1161	0.35	0/1554
19	LN	0.16	0/1746	0.37	1/2338 (0.0%)
20	LO	0.18	0/1682	0.36	0/2250
21	LP	0.19	0/1268	0.38	0/1701
22	LQ	0.16	0/1537	0.33	0/2052
23	LR	0.17	0/1582	0.38	0/2091
24	LS	0.14	0/1493	0.31	0/2003
25	LT	0.19	0/1326	0.43	0/1770
26	LU	0.21	0/839	0.53	0/1126
27	LV	0.21	0/993	0.40	0/1332
28	LW	0.18	0/959	0.48	1/1270 (0.1%)
29	LX	0.16	0/1002	0.33	0/1345
30	LY	0.19	0/1132	0.46	0/1504
31	LZ	0.18	0/1130	0.38	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	La	0.17	0/1191	0.38	0/1591
33	Lb	0.17	0/889	0.38	0/1175
34	Lc	0.17	0/774	0.39	0/1038
35	Ld	0.18	0/903	0.35	0/1216
36	Le	0.15	0/1071	0.35	0/1429
37	Lf	0.18	0/895	0.37	0/1198
38	Lg	0.15	0/916	0.36	0/1220
39	Lh	0.18	0/1023	0.34	0/1351
40	Li	0.17	0/843	0.40	0/1115
41	Lj	0.17	0/720	0.41	0/952
42	Lk	0.17	0/575	0.46	0/761
43	Ll	0.18	0/454	0.39	0/599
44	Lm	0.15	0/435	0.36	0/575
45	Ln	0.18	0/231	0.32	0/294
46	Lo	0.22	0/876	0.43	0/1156
47	Lp	0.16	0/718	0.39	0/953
48	Lr	0.19	0/1017	0.35	0/1364
49	Ls	0.20	0/1519	0.44	0/2052
50	Lt	0.20	0/1009	0.55	0/1363
51	Pt	0.10	0/1761	0.24	0/2741
52	S2	0.17	0/39755	0.28	0/61935
53	SA	0.18	0/1778	0.41	0/2416
54	SB	0.20	0/1765	0.45	0/2362
55	SC	0.18	0/1744	0.42	0/2357
56	SD	0.17	0/1793	0.40	0/2414
57	SE	0.19	0/2118	0.42	0/2849
58	SF	0.21	0/1516	0.43	0/2037
59	SG	0.19	0/1946	0.42	0/2590
60	SH	0.22	0/1519	0.46	0/2033
61	SI	0.18	0/1715	0.44	0/2287
62	SJ	0.16	0/1550	0.38	0/2069
63	SK	0.19	0/851	0.41	0/1147
64	SL	0.17	0/1268	0.40	0/1696
65	SM	0.20	0/950	0.52	0/1275
66	SN	0.16	0/1232	0.33	0/1656
67	SO	0.19	0/1037	0.41	0/1391
68	SP	0.23	0/1003	0.48	0/1342
69	SQ	0.22	0/1160	0.46	0/1553
70	SR	0.18	0/1105	0.48	0/1484
71	SS	0.20	0/1216	0.44	0/1628
72	ST	0.19	0/1131	0.53	0/1515
73	SU	0.21	0/831	0.48	0/1115
74	SV	0.21	0/643	0.46	0/860

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SW	0.22	0/1051	0.40	0/1406
76	SX	0.16	0/1116	0.39	0/1490
77	SY	0.19	0/1083	0.43	0/1438
78	SZ	0.22	0/604	0.47	0/810
79	Sa	0.21	0/836	0.47	0/1121
80	Sb	0.18	0/665	0.40	0/891
81	Sc	0.21	0/508	0.46	0/680
82	Sd	0.18	0/470	0.43	0/623
83	Se	0.19	0/465	0.40	0/612
84	Sf	0.34	0/560	0.60	0/745
85	Sg	0.17	0/2493	0.40	0/3394
86	AT	0.13	0/1805	0.28	0/2809
87	CA	0.18	0/2810	0.40	0/3780
All	All	0.17	0/238226	0.34	3/348712 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	LA	0	2
9	LC	0	2
12	LF	0	1
16	LJ	0	1
19	LN	0	1
20	LO	0	1
21	LP	0	1
28	LW	0	2
30	LY	0	1
31	LZ	0	1
32	La	0	1
33	Lb	0	1
36	Le	0	1
43	Ll	0	1
45	Ln	0	1
53	SA	0	1
54	SB	0	1
56	SD	0	1
59	SG	0	3
61	SI	0	2
62	SJ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	SK	0	1
66	SN	0	1
69	SQ	0	1
71	SS	0	1
72	ST	0	3
73	SU	0	1
74	SV	0	1
75	SW	0	1
83	Se	0	1
All	All	0	38

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	LN	143	ARG	CG-CD-NE	5.86	124.89	112.00
9	LC	33	ARG	CB-CA-C	5.44	118.43	110.87
28	LW	47	ARG	CB-CG-CD	5.18	123.22	111.30

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	LA	147	ARG	Sidechain
7	LA	245	ARG	Sidechain
9	LC	33	ARG	Sidechain
9	LC	78	ARG	Sidechain
12	LF	62	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CD	285	0	260	10	0
2	CI	247	0	283	8	0
3	CF	3383	0	3431	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L5	78445	0	39700	1215	0
5	L7	2561	0	1295	24	0
6	L8	3315	0	1685	49	0
7	LA	1898	0	1993	59	0
8	LB	3238	0	3375	101	0
9	LC	2927	0	3104	56	0
10	LD	2382	0	2410	36	0
11	LE	1935	0	2096	50	0
12	LF	1870	0	1996	33	0
13	LG	1927	0	2074	43	0
14	LH	1518	0	1601	30	0
15	LI	1711	0	1749	37	0
16	LJ	1362	0	1399	40	0
17	LL	1701	0	1818	35	0
18	LM	1138	0	1204	25	0
19	LN	1701	0	1749	28	0
20	LO	1650	0	1794	33	0
21	LP	1242	0	1269	30	0
22	LQ	1513	0	1628	20	0
23	LR	1566	0	1729	36	0
24	LS	1453	0	1490	21	0
25	LT	1298	0	1366	32	0
26	LU	825	0	850	24	0
27	LV	979	0	1039	23	0
28	LW	945	0	1003	34	0
29	LX	985	0	1066	27	0
30	LY	1115	0	1205	26	0
31	LZ	1107	0	1182	25	0
32	La	1162	0	1213	24	0
33	Lb	876	0	948	22	0
34	Lc	764	0	804	16	0
35	Ld	888	0	930	19	0
36	Le	1053	0	1147	12	0
37	Lf	876	0	912	11	0
38	Lg	906	0	998	15	0
39	Lh	1015	0	1148	21	0
40	Li	832	0	917	8	0
41	Lj	705	0	737	17	0
42	Lk	569	0	637	17	0
43	Ll	444	0	483	13	0
44	Lm	429	0	465	9	0
45	Ln	230	0	276	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Lo	862	0	929	16	0
47	Lp	708	0	756	13	0
48	Lr	1002	0	1068	11	0
49	Ls	1496	0	1540	41	0
50	Lt	998	0	1032	32	0
51	Pt	1576	0	802	20	0
52	S2	36953	0	18679	728	0
53	SA	1741	0	1746	66	0
54	SB	1738	0	1809	49	0
55	SC	1707	0	1791	43	0
56	SD	1765	0	1865	36	0
57	SE	2076	0	2177	76	0
58	SF	1495	0	1549	58	0
59	SG	1923	0	2089	94	0
60	SH	1497	0	1590	52	0
61	SI	1686	0	1772	54	0
62	SJ	1525	0	1640	37	0
63	SK	827	0	854	29	0
64	SL	1247	0	1323	44	0
65	SM	940	0	965	47	0
66	SN	1208	0	1294	24	0
67	SO	1024	0	1050	27	0
68	SP	985	0	1031	28	0
69	SQ	1142	0	1213	50	0
70	SR	1090	0	1149	48	0
71	SS	1198	0	1261	46	0
72	ST	1112	0	1146	42	0
73	SU	821	0	883	43	0
74	SV	636	0	637	28	0
75	SW	1034	0	1080	38	0
76	SX	1098	0	1167	26	0
77	SY	1065	0	1142	45	0
78	SZ	598	0	656	22	0
79	Sa	821	0	870	16	0
80	Sb	651	0	672	16	0
81	Sc	506	0	536	22	0
82	Sd	459	0	448	23	0
83	Se	459	0	503	7	0
84	Sf	548	0	551	27	0
85	Sg	2436	0	2393	77	0
86	AT	1616	0	823	94	0
87	CA	2764	0	2779	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	L5	185	0	0	0	0
88	L7	3	0	0	0	0
88	L8	5	0	0	0	0
88	LA	1	0	0	0	0
88	LP	1	0	0	0	0
88	LV	1	0	0	0	0
88	Le	1	0	0	0	0
88	S2	28	0	0	0	0
89	L5	98	0	182	10	0
89	S2	14	0	26	2	0
90	L5	80	0	151	3	0
90	L8	10	0	19	0	0
90	LN	10	0	19	0	0
90	S2	20	0	38	0	0
91	L5	74	0	0	0	0
91	Lg	1	0	0	0	0
92	Lg	1	0	0	0	0
92	Lj	1	0	0	0	0
92	Lm	1	0	0	0	0
92	Lo	1	0	0	0	0
92	Lp	1	0	0	0	0
92	Sa	1	0	0	0	0
92	Sd	1	0	0	0	0
93	S2	6	0	12	0	0
94	CF	1	0	0	0	0
94	L5	3310	0	0	17	0
94	L7	16	0	0	0	0
94	L8	118	0	0	0	0
94	LA	43	0	0	0	0
94	LB	66	0	0	1	0
94	LC	45	0	0	0	0
94	LD	1	0	0	0	0
94	LG	13	0	0	0	0
94	LH	1	0	0	0	0
94	LI	7	0	0	0	0
94	LL	33	0	0	0	0
94	LN	99	0	0	2	0
94	LO	58	0	0	1	0
94	LP	38	0	0	2	0
94	LQ	21	0	0	0	0
94	LR	12	0	0	0	0
94	LS	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	LT	9	0	0	0	0
94	LU	1	0	0	0	0
94	LV	41	0	0	3	0
94	LW	15	0	0	0	0
94	LX	10	0	0	0	0
94	La	38	0	0	0	0
94	Lb	14	0	0	0	0
94	Ld	1	0	0	0	0
94	Le	50	0	0	0	0
94	Lf	13	0	0	0	0
94	Lg	2	0	0	0	0
94	Lh	8	0	0	1	0
94	Li	10	0	0	1	0
94	Lj	29	0	0	0	0
94	Ll	5	0	0	0	0
94	Ln	2	0	0	0	0
94	Lo	37	0	0	1	0
94	Lp	4	0	0	0	0
94	Lr	3	0	0	0	0
94	Pt	6	0	0	1	0
94	S2	340	0	0	5	0
94	SE	12	0	0	2	0
94	SF	5	0	0	1	0
94	SH	1	0	0	0	0
94	SI	14	0	0	4	0
94	SJ	1	0	0	0	0
94	SL	22	0	0	0	0
94	SP	1	0	0	0	0
94	SQ	7	0	0	0	0
94	SS	8	0	0	0	0
94	ST	2	0	0	0	0
94	SU	3	0	0	0	0
94	SX	8	0	0	0	0
94	SZ	1	0	0	1	0
94	Sc	1	0	0	0	0
94	Sd	3	0	0	0	0
All	All	231160	0	170165	4176	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 11.

The worst 5 of 4176 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)
3:CF:358:ALA:CB	86:AT:52:C:H4'	1.43	1.47
3:CF:358:ALA:HB3	86:AT:52:C:C4'	1.59	1.30
3:CF:358:ALA:CB	86:AT:52:C:C4'	2.10	1.30
3:CF:358:ALA:H	86:AT:52:C:C3'	1.58	1.17
3:CF:358:ALA:HB3	86:AT:52:C:O4'	1.42	1.16

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	
1	CD	34/36 (94%)	34 (100%)	0	0	100	100
2	CI	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
3	CF	438/441 (99%)	410 (94%)	28 (6%)	0	100	100
7	LA	246/248 (99%)	223 (91%)	23 (9%)	0	100	100
8	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
9	LC	366/368 (100%)	347 (95%)	19 (5%)	0	100	100
10	LD	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
11	LE	236/250 (94%)	216 (92%)	20 (8%)	0	100	100
12	LF	223/225 (99%)	216 (97%)	6 (3%)	1 (0%)	30	51
13	LG	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
14	LH	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
15	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
16	LJ	168/176 (96%)	164 (98%)	4 (2%)	0	100	100
17	LL	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
18	LM	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
19	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
21	LP	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
22	LQ	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
23	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
24	LS	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
25	LT	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
26	LU	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
27	LV	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
28	LW	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
29	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
31	LZ	133/135 (98%)	124 (93%)	9 (7%)	0	100	100
32	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
33	Lb	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
34	Lc	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	12	28
35	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
36	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
37	Lf	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
38	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
39	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
40	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
41	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
42	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
43	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
44	Lm	50/52 (96%)	50 (100%)	0	0	100	100
45	Ln	22/24 (92%)	22 (100%)	0	0	100	100
46	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
47	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
48	Lr	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
49	Ls	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
50	Lt	128/141 (91%)	107 (84%)	21 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
54	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
55	SC	218/222 (98%)	204 (94%)	14 (6%)	0	100	100
56	SD	225/227 (99%)	213 (95%)	12 (5%)	0	100	100
57	SE	260/262 (99%)	244 (94%)	16 (6%)	0	100	100
58	SF	187/189 (99%)	173 (92%)	14 (8%)	0	100	100
59	SG	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
60	SH	182/186 (98%)	166 (91%)	15 (8%)	1 (0%)	24	45
61	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
62	SJ	183/185 (99%)	169 (92%)	14 (8%)	0	100	100
63	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
64	SL	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
65	SM	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
66	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
67	SO	135/140 (96%)	129 (96%)	6 (4%)	0	100	100
68	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
69	SQ	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	18	37
70	SR	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
71	SS	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
72	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
73	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
74	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
75	SW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
76	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
77	SY	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
78	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
79	Sa	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
80	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
81	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
82	Sd	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
83	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	Sf	65/67 (97%)	54 (83%)	11 (17%)	0	100	100
85	Sg	311/313 (99%)	286 (92%)	25 (8%)	0	100	100
87	CA	350/354 (99%)	334 (95%)	16 (5%)	0	100	100
All	All	12494/12701 (98%)	11820 (95%)	670 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	LF	197	VAL
34	Lc	99	PRO
69	SQ	44	PRO
60	SH	15	LYS

5.3.2 Protein sidechains [i](#)

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	
1	CD	31/31 (100%)	31 (100%)	0	100	100
2	CI	25/25 (100%)	25 (100%)	0	100	100
3	CF	365/366 (100%)	365 (100%)	0	100	100
7	LA	190/190 (100%)	190 (100%)	0	100	100
8	LB	348/348 (100%)	348 (100%)	0	100	100
9	LC	306/306 (100%)	306 (100%)	0	100	100
10	LD	246/247 (100%)	246 (100%)	0	100	100
11	LE	212/222 (96%)	212 (100%)	0	100	100
12	LF	194/194 (100%)	194 (100%)	0	100	100
13	LG	203/205 (99%)	203 (100%)	0	100	100
14	LH	169/169 (100%)	169 (100%)	0	100	100
15	LI	180/180 (100%)	180 (100%)	0	100	100
16	LJ	143/148 (97%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	LL	176/176 (100%)	176 (100%)	0	100	100
18	LM	118/118 (100%)	118 (100%)	0	100	100
19	LN	171/171 (100%)	171 (100%)	0	100	100
20	LO	173/173 (100%)	173 (100%)	0	100	100
21	LP	134/134 (100%)	134 (100%)	0	100	100
22	LQ	164/164 (100%)	164 (100%)	0	100	100
23	LR	166/166 (100%)	166 (100%)	0	100	100
24	LS	156/156 (100%)	156 (100%)	0	100	100
25	LT	139/139 (100%)	139 (100%)	0	100	100
26	LU	91/91 (100%)	91 (100%)	0	100	100
27	LV	101/101 (100%)	101 (100%)	0	100	100
28	LW	95/97 (98%)	95 (100%)	0	100	100
29	LX	108/108 (100%)	108 (100%)	0	100	100
30	LY	124/124 (100%)	124 (100%)	0	100	100
31	LZ	117/117 (100%)	117 (100%)	0	100	100
32	La	120/120 (100%)	120 (100%)	0	100	100
33	Lb	88/90 (98%)	88 (100%)	0	100	100
34	Lc	83/83 (100%)	83 (100%)	0	100	100
35	Ld	98/98 (100%)	98 (100%)	0	100	100
36	Le	114/114 (100%)	114 (100%)	0	100	100
37	Lf	88/88 (100%)	88 (100%)	0	100	100
38	Lg	98/98 (100%)	98 (100%)	0	100	100
39	Lh	109/109 (100%)	109 (100%)	0	100	100
40	Li	86/86 (100%)	86 (100%)	0	100	100
41	Lj	73/73 (100%)	73 (100%)	0	100	100
42	Lk	64/64 (100%)	64 (100%)	0	100	100
43	Ll	47/47 (100%)	47 (100%)	0	100	100
44	Lm	48/48 (100%)	48 (100%)	0	100	100
45	Ln	23/23 (100%)	23 (100%)	0	100	100
46	Lo	93/93 (100%)	93 (100%)	0	100	100
47	Lp	74/74 (100%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	Lr	109/109 (100%)	109 (100%)	0	100	100
49	Ls	162/164 (99%)	162 (100%)	0	100	100
50	Lt	107/115 (93%)	107 (100%)	0	100	100
53	SA	183/183 (100%)	183 (100%)	0	100	100
54	SB	195/195 (100%)	195 (100%)	0	100	100
55	SC	186/188 (99%)	186 (100%)	0	100	100
56	SD	190/190 (100%)	190 (100%)	0	100	100
57	SE	224/224 (100%)	224 (100%)	0	100	100
58	SF	159/159 (100%)	159 (100%)	0	100	100
59	SG	207/207 (100%)	207 (100%)	0	100	100
60	SH	166/166 (100%)	166 (100%)	0	100	100
61	SI	178/178 (100%)	178 (100%)	0	100	100
62	SJ	161/161 (100%)	161 (100%)	0	100	100
63	SK	89/89 (100%)	89 (100%)	0	100	100
64	SL	137/137 (100%)	137 (100%)	0	100	100
65	SM	102/104 (98%)	102 (100%)	0	100	100
66	SN	130/130 (100%)	130 (100%)	0	100	100
67	SO	107/110 (97%)	107 (100%)	0	100	100
68	SP	107/107 (100%)	107 (100%)	0	100	100
69	SQ	119/119 (100%)	119 (100%)	0	100	100
70	SR	122/122 (100%)	122 (100%)	0	100	100
71	SS	126/126 (100%)	126 (100%)	0	100	100
72	ST	113/113 (100%)	113 (100%)	0	100	100
73	SU	94/94 (100%)	94 (100%)	0	100	100
74	SV	67/67 (100%)	67 (100%)	0	100	100
75	SW	112/112 (100%)	112 (100%)	0	100	100
76	SX	113/113 (100%)	113 (100%)	0	100	100
77	SY	113/113 (100%)	113 (100%)	0	100	100
78	SZ	66/66 (100%)	66 (100%)	0	100	100
79	Sa	89/89 (100%)	89 (100%)	0	100	100
80	Sb	75/75 (100%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
81	Sc	57/57 (100%)	57 (100%)	0	100	100
82	Sd	48/48 (100%)	48 (100%)	0	100	100
83	Se	47/47 (100%)	47 (100%)	0	100	100
84	Sf	60/60 (100%)	60 (100%)	0	100	100
85	Sg	272/272 (100%)	272 (100%)	0	100	100
87	CA	303/303 (100%)	303 (100%)	0	100	100
All	All	10846/10886 (100%)	10846 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
59	SG	105	ASN
74	SV	33	GLN
60	SH	68	GLN
68	SP	79	HIS
80	Sb	65	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L5	3643/5070 (71%)	707 (19%)	24 (0%)
5	L7	119/120 (99%)	9 (7%)	0
51	Pt	72/74 (97%)	16 (22%)	0
52	S2	1715/1740 (98%)	379 (22%)	9 (0%)
6	L8	155/156 (99%)	24 (15%)	0
86	AT	74/76 (97%)	25 (33%)	1 (1%)
All	All	5778/7236 (79%)	1160 (20%)	34 (0%)

5 of 1160 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	L5	25	A
4	L5	30	C
4	L5	39	A
4	L5	42	A
4	L5	48	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	S2	688	U
52	S2	1418	C
52	S2	1556	A
4	L5	2587	A
4	L5	2485	U

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

179 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	$\# Z > 2$
4	PSU	L5	4673	4,88	18,21,22	1.12	1 (5%)	21,30,33	1.88	5 (23%)
52	OMU	S2	1288	52	19,22,23	3.34	7 (36%)	25,31,34	1.74	5 (20%)
4	OMG	L5	3744	4	23,26,27	0.45	0	32,38,41	0.50	0
52	PSU	S2	1367	52	18,21,22	1.13	1 (5%)	21,30,33	1.88	5 (23%)
4	OMG	L5	4370	4	23,26,27	0.47	0	32,38,41	0.52	0
52	PSU	S2	406	52	18,21,22	1.14	1 (5%)	21,30,33	1.94	5 (23%)
4	OMU	L5	4498	91,4	19,22,23	3.32	7 (36%)	25,31,34	1.77	5 (20%)
4	OMG	L5	3627	4	23,26,27	0.45	0	32,38,41	0.56	0
52	PSU	S2	93	52	18,21,22	1.13	1 (5%)	21,30,33	1.82	4 (19%)
52	PSU	S2	105	52	18,21,22	1.15	1 (5%)	21,30,33	1.79	4 (19%)
4	PSU	L5	4361	4	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
52	OMU	S2	627	52	19,22,23	3.40	7 (36%)	25,31,34	1.79	5 (20%)
52	A2M	S2	1383	52	22,25,26	1.24	1 (4%)	30,36,39	1.60	6 (20%)
4	OMC	L5	2422	4,88	19,22,23	0.50	0	25,31,34	0.64	0
4	PSU	L5	4353	4	18,21,22	1.14	1 (5%)	21,30,33	1.93	6 (28%)
52	A2M	S2	576	52	22,25,26	1.25	2 (9%)	30,36,39	1.53	5 (16%)
4	A2M	L5	398	4	22,25,26	1.26	2 (9%)	30,36,39	1.60	5 (16%)
52	A2M	S2	468	52	22,25,26	1.25	1 (4%)	30,36,39	1.57	6 (20%)
4	A2M	L5	2363	4,88	22,25,26	1.18	1 (4%)	30,36,39	1.48	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	A2M	S2	166	52	22,25,26	1.27	2 (9%)	30,36,39	1.48	4 (13%)
4	1MA	L5	1322	4,88	21,25,26	0.50	0	30,37,40	0.77	1 (3%)
4	PSU	L5	4973	4	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
4	OMC	L5	1340	4	19,22,23	0.52	0	25,31,34	0.76	0
52	A2M	S2	99	52,88	22,25,26	1.25	2 (9%)	30,36,39	1.41	4 (13%)
4	PSU	L5	3920	4,88	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
52	PSU	S2	801	52	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
6	PSU	L8	55	6	18,21,22	1.16	1 (5%)	21,30,33	1.84	4 (19%)
4	5MC	L5	4447	91,4	19,22,23	0.68	0	26,32,35	0.62	0
4	PSU	L5	4532	4	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
4	A2M	L5	1534	4,88	22,25,26	1.24	2 (9%)	30,36,39	1.46	6 (20%)
4	OMU	L5	2837	4	19,22,23	3.39	7 (36%)	25,31,34	1.83	5 (20%)
4	OMU	L5	4620	4	19,22,23	3.34	7 (36%)	25,31,34	1.66	4 (16%)
52	OMC	S2	462	52	19,22,23	0.49	0	25,31,34	0.68	0
4	6MZ	L5	4220	4	26,26,26	2.78	5 (19%)	36,39,39	2.83	17 (47%)
4	A2M	L5	400	4	22,25,26	1.27	1 (4%)	30,36,39	1.57	7 (23%)
4	OMC	L5	3869	4	19,22,23	0.50	0	25,31,34	0.70	0
4	PSU	L5	4628	4	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
52	B8N	S2	1248	52	25,29,30	3.27	6 (24%)	28,42,45	1.99	8 (28%)
4	OMG	L5	1625	91,4	23,26,27	0.47	0	32,38,41	0.48	0
4	OMG	L5	2424	4	23,26,27	0.46	0	32,38,41	0.45	0
52	OMG	S2	683	52	23,26,27	0.48	0	32,38,41	0.49	0
4	A2M	L5	3718	4	22,25,26	1.20	2 (9%)	30,36,39	1.48	4 (13%)
52	PSU	S2	866	52	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L5	3844	4	18,21,22	1.18	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	1677	4	18,21,22	1.21	2 (11%)	21,30,33	1.98	6 (28%)
4	A2M	L5	1871	4,88	22,25,26	1.23	1 (4%)	30,36,39	1.48	6 (20%)
52	A2M	S2	159	52	22,25,26	1.21	1 (4%)	30,36,39	1.52	5 (16%)
3	SEP	CF	163	3	8,9,10	1.61	1 (12%)	7,12,14	1.28	1 (14%)
4	5MC	L5	3782	4,88	19,22,23	0.51	0	26,32,35	0.67	0
4	PSU	L5	4442	4	18,21,22	1.13	1 (5%)	21,30,33	1.94	6 (28%)
4	OMG	L5	3792	4	23,26,27	0.45	0	32,38,41	0.51	0
4	A2M	L5	1323	4	22,25,26	1.24	2 (9%)	30,36,39	1.45	5 (16%)
52	PSU	S2	1244	52	18,21,22	1.12	1 (5%)	21,30,33	1.87	5 (23%)
4	PSU	L5	1862	4	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
52	4AC	S2	1842	52	21,24,25	0.35	0	28,34,37	0.40	0
4	PSU	L5	4972	4	18,21,22	1.15	1 (5%)	21,30,33	1.89	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L5	3822	4	18,21,22	1.14	1 (5%)	21,30,33	1.89	6 (28%)
4	PSU	L5	3851	4	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
52	OMG	S2	601	52	23,26,27	0.45	0	32,38,41	0.46	0
4	OMC	L5	3808	4	19,22,23	0.53	0	25,31,34	0.79	1 (4%)
4	PSU	L5	1792	4	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
52	OMU	S2	1326	52	19,22,23	3.36	7 (36%)	25,31,34	1.82	5 (20%)
4	PSU	L5	3637	91,4	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
4	OMG	L5	4228	4	23,26,27	0.48	0	32,38,41	0.62	0
52	4AC	S2	1337	52	21,24,25	0.37	0	28,34,37	0.56	0
4	PSU	L5	4403	91,4	18,21,22	1.15	1 (5%)	21,30,33	1.95	6 (28%)
4	OMG	L5	2364	4,88	23,26,27	0.47	0	32,38,41	0.46	0
52	PSU	S2	863	52	18,21,22	1.11	1 (5%)	21,30,33	1.80	4 (19%)
4	OMG	L5	4392	4	23,26,27	0.44	0	32,38,41	0.51	0
4	OMC	L5	4536	4	19,22,23	0.53	0	25,31,34	0.70	0
4	PSU	L5	4500	4	18,21,22	1.18	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	4521	91,4,88	18,21,22	1.14	1 (5%)	21,30,33	1.91	5 (23%)
52	MA6	S2	1850	52	23,26,27	1.28	2 (8%)	33,38,41	3.13	11 (33%)
4	OMC	L5	3701	91,4	19,22,23	0.57	0	25,31,34	1.51	4 (16%)
6	OMG	L8	75	6	23,26,27	0.45	0	32,38,41	0.47	0
52	PSU	S2	686	52	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
52	PSU	S2	1177	52	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
52	PSU	S2	1056	52	18,21,22	1.13	1 (5%)	21,30,33	1.93	6 (28%)
4	PSU	L5	3639	4	18,21,22	1.13	1 (5%)	21,30,33	1.94	5 (23%)
4	PSU	L5	4689	4	18,21,22	1.13	1 (5%)	21,30,33	1.99	4 (19%)
4	PSU	L5	4299	4	18,21,22	1.12	1 (5%)	21,30,33	1.86	5 (23%)
52	OMU	S2	1442	52	19,22,23	3.40	7 (36%)	25,31,34	1.78	4 (16%)
4	OMG	L5	1522	4	23,26,27	0.48	0	32,38,41	0.62	0
4	PSU	L5	1782	4	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	4576	4	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
52	OMU	S2	428	52	19,22,23	3.33	7 (36%)	25,31,34	1.76	5 (20%)
52	PSU	S2	651	52	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
4	A2M	L5	4523	4,88	22,25,26	1.26	1 (4%)	30,36,39	1.54	6 (20%)
52	OMU	S2	116	52	19,22,23	3.32	7 (36%)	25,31,34	1.67	5 (20%)
4	PSU	L5	1582	4	18,21,22	1.12	1 (5%)	21,30,33	1.79	4 (19%)
4	PSU	L5	4293	4	18,21,22	1.16	1 (5%)	21,30,33	1.95	5 (23%)
52	PSU	S2	1046	52	18,21,22	1.13	1 (5%)	21,30,33	1.80	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	A2M	S2	484	52	22,25,26	1.25	2 (9%)	30,36,39	1.51	7 (23%)
4	PSU	L5	4296	4	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
4	A2M	L5	3867	4	22,25,26	1.24	1 (4%)	30,36,39	1.50	8 (26%)
52	OMC	S2	174	52	19,22,23	0.49	0	25,31,34	0.65	0
4	PSU	L5	4636	4	18,21,22	1.12	1 (5%)	21,30,33	2.02	6 (28%)
52	PSU	S2	1081	52	18,21,22	1.14	1 (5%)	21,30,33	1.74	5 (23%)
52	PSU	S2	681	52	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	4552	4	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
52	OMU	S2	354	52	19,22,23	3.33	7 (36%)	25,31,34	1.79	5 (20%)
4	A2M	L5	1326	4	22,25,26	1.22	2 (9%)	30,36,39	1.36	5 (16%)
4	PSU	L5	1860	4	18,21,22	1.13	1 (5%)	21,30,33	1.83	4 (19%)
4	A2M	L5	4571	4	22,25,26	1.28	2 (9%)	30,36,39	1.59	7 (23%)
52	OMG	S2	644	52	23,26,27	0.45	0	32,38,41	0.51	0
52	OMU	S2	799	52	19,22,23	3.44	7 (36%)	25,31,34	1.79	5 (20%)
4	PSU	L5	2632	4	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
4	OMC	L5	3887	4	19,22,23	0.51	0	25,31,34	0.67	0
4	OMC	L5	2861	4	19,22,23	0.51	0	25,31,34	0.82	1 (4%)
52	PSU	S2	1174	52	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
52	OMC	S2	1391	52	19,22,23	0.51	0	25,31,34	0.71	0
4	A2M	L5	2787	4	22,25,26	1.25	1 (4%)	30,36,39	1.52	7 (23%)
4	OMG	L5	2876	4	23,26,27	0.47	0	32,38,41	0.51	0
52	G7M	S2	1639	52,51	23,26,27	2.68	8 (34%)	34,39,42	2.61	11 (32%)
4	PSU	L5	3695	91,4	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	5001	4	18,21,22	1.16	1 (5%)	21,30,33	1.79	4 (19%)
52	MA6	S2	1851	52	23,26,27	1.26	2 (8%)	33,38,41	3.23	12 (36%)
4	OMC	L5	3841	4	19,22,23	0.49	0	25,31,34	0.60	0
4	UY1	L5	3818	91,4	19,22,23	4.92	10 (52%)	21,31,34	2.01	5 (23%)
52	OMG	S2	1328	52	23,26,27	0.46	0	32,38,41	0.46	0
52	OMC	S2	517	52	19,22,23	0.50	0	25,31,34	0.71	0
4	PSU	L5	4431	4	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
4	A2M	L5	3785	4,88	22,25,26	1.18	1 (4%)	30,36,39	1.63	10 (33%)
4	A2M	L5	4590	4	22,25,26	1.22	1 (4%)	30,36,39	1.53	6 (20%)
4	OMG	L5	3899	4	23,26,27	0.51	0	32,38,41	0.54	0
52	A2M	S2	668	52,88	22,25,26	1.34	2 (9%)	30,36,39	1.59	6 (20%)
4	A2M	L5	1524	4	22,25,26	1.30	2 (9%)	30,36,39	1.53	5 (16%)
4	PSU	L5	4457	4	18,21,22	1.12	1 (5%)	21,30,33	1.84	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	S2	649	52	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L5	4493	91,4	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
4	OMG	L5	1316	4	23,26,27	0.49	0	32,38,41	0.56	0
4	OMG	L5	4499	4	23,26,27	0.44	0	32,38,41	0.47	0
4	A2M	L5	2815	4	22,25,26	1.24	2 (9%)	30,36,39	1.41	7 (23%)
4	OMG	L5	4637	91,4	23,26,27	0.47	0	32,38,41	0.49	0
4	PSU	L5	4579	4	18,21,22	1.10	1 (5%)	21,30,33	1.90	5 (23%)
4	OMC	L5	2365	4,88	19,22,23	0.49	0	25,31,34	0.59	0
52	PSU	S2	109	52	18,21,22	1.15	1 (5%)	21,30,33	1.90	6 (28%)
4	UR3	L5	4530	4	19,22,23	2.78	7 (36%)	26,32,35	1.56	3 (11%)
4	OMU	L5	4227	4	19,22,23	3.39	7 (36%)	25,31,34	1.79	4 (16%)
52	A2M	S2	27	52	22,25,26	1.25	2 (9%)	30,36,39	1.40	4 (13%)
4	OMG	L5	4494	4	23,26,27	0.47	0	32,38,41	0.50	0
4	OMC	L5	2824	4	19,22,23	0.50	0	25,31,34	0.68	0
4	A2M	L5	3825	4	22,25,26	1.24	1 (4%)	30,36,39	1.57	7 (23%)
4	OMC	L5	4456	4	19,22,23	0.55	0	25,31,34	0.63	0
52	A2M	S2	1031	52	22,25,26	1.21	2 (9%)	30,36,39	1.46	5 (16%)
52	OMC	S2	1703	52	19,22,23	0.50	0	25,31,34	0.51	0
4	PSU	L5	1744	4,88	18,21,22	1.14	1 (5%)	21,30,33	1.91	5 (23%)
52	PSU	S2	1004	52	18,21,22	1.13	1 (5%)	21,30,33	1.91	5 (23%)
52	OMG	S2	509	52	23,26,27	0.47	0	32,38,41	0.51	0
4	A2M	L5	2401	4	22,25,26	1.25	1 (4%)	30,36,39	1.61	6 (20%)
4	OMG	L5	4623	4	23,26,27	0.48	0	32,38,41	0.61	0
6	PSU	L8	69	6	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)
4	PSU	L5	2839	4	18,21,22	1.13	1 (5%)	21,30,33	1.93	5 (23%)
4	PSU	L5	3884	4	18,21,22	1.15	1 (5%)	21,30,33	1.93	5 (23%)
4	PSU	L5	4312	4	18,21,22	1.14	1 (5%)	21,30,33	1.89	4 (19%)
52	OMG	S2	436	52	23,26,27	0.47	0	32,38,41	0.54	0
52	PSU	S2	1045	52	18,21,22	1.10	1 (5%)	21,30,33	1.80	4 (19%)
52	OMC	S2	1272	52	19,22,23	0.55	0	25,31,34	0.91	2 (8%)
4	OMC	L5	2351	4	19,22,23	0.53	0	25,31,34	0.88	1 (4%)
4	OMU	L5	3925	4	19,22,23	3.38	7 (36%)	25,31,34	1.80	4 (16%)
52	6MZ	S2	1832	52,88	26,26,26	2.81	5 (19%)	36,39,39	2.47	13 (36%)
4	OMG	L5	4196	4,51	23,26,27	0.46	0	32,38,41	0.47	0
4	OMC	L5	2804	4	19,22,23	0.50	0	25,31,34	0.72	0
52	OMU	S2	121	52	19,22,23	3.33	7 (36%)	25,31,34	1.68	4 (16%)
4	A2M	L5	3830	4	22,25,26	1.25	1 (4%)	30,36,39	1.59	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L5	1781	4	18,21,22	1.09	1 (5%)	21,30,33	1.85	4 (19%)
4	PSU	L5	5010	4	18,21,22	1.13	1 (5%)	21,30,33	1.88	5 (23%)
52	PSU	S2	1232	52	18,21,22	1.15	1 (5%)	21,30,33	1.90	5 (23%)
4	PSU	L5	4471	4	18,21,22	1.10	1 (5%)	21,30,33	1.84	4 (19%)
4	OMG	L5	4618	4	23,26,27	0.48	0	32,38,41	0.53	0
52	PSU	S2	814	52	18,21,22	1.09	1 (5%)	21,30,33	1.76	4 (19%)
52	OMG	S2	867	52	23,26,27	0.51	0	32,38,41	0.48	0
52	PSU	S2	966	52,88	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
4	PSU	L5	1683	91,4	18,21,22	1.15	1 (5%)	21,30,33	1.83	4 (19%)
52	OMG	S2	1490	52	23,26,27	0.50	0	32,38,41	0.53	0
52	OMU	S2	172	52	19,22,23	3.40	7 (36%)	25,31,34	1.85	5 (20%)
4	PSU	L5	3853	91,4,88	18,21,22	1.09	1 (5%)	21,30,33	1.79	4 (19%)
4	PSU	L5	1536	4	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
4	OMU	L5	4306	4	19,22,23	3.33	7 (36%)	25,31,34	1.79	4 (16%)

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
4	PSU	L5	4673	4,88	-	0/7/25/26	0/2/2/2
52	OMU	S2	1288	52	-	2/9/27/28	0/2/2/2
4	OMG	L5	3744	4	-	0/9/27/28	0/3/3/3
52	PSU	S2	1367	52	-	0/7/25/26	0/2/2/2
4	OMG	L5	4370	4	-	0/9/27/28	0/3/3/3
52	PSU	S2	406	52	-	0/7/25/26	0/2/2/2
4	OMU	L5	4498	91,4	-	0/9/27/28	0/2/2/2
4	OMG	L5	3627	4	-	1/9/27/28	0/3/3/3
52	PSU	S2	93	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	105	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	4361	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	627	52	-	6/9/27/28	0/2/2/2
52	A2M	S2	1383	52	-	3/9/27/28	0/3/3/3
4	OMC	L5	2422	4,88	-	2/9/27/28	0/2/2/2
4	PSU	L5	4353	4	-	0/7/25/26	0/2/2/2
52	A2M	S2	576	52	-	3/9/27/28	0/3/3/3
4	A2M	L5	398	4	-	0/9/27/28	0/3/3/3
52	A2M	S2	468	52	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A2M	L5	2363	4,88	-	0/9/27/28	0/3/3/3
52	A2M	S2	166	52	-	0/9/27/28	0/3/3/3
4	1MA	L5	1322	4,88	-	0/7/25/26	0/3/3/3
4	PSU	L5	4973	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	1340	4	-	1/9/27/28	0/2/2/2
52	A2M	S2	99	52,88	-	1/9/27/28	0/3/3/3
4	PSU	L5	3920	4,88	-	0/7/25/26	0/2/2/2
52	PSU	S2	801	52	-	1/7/25/26	0/2/2/2
6	PSU	L8	55	6	-	0/7/25/26	0/2/2/2
4	5MC	L5	4447	91,4	-	4/7/25/26	0/2/2/2
4	PSU	L5	4532	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1534	4,88	-	1/9/27/28	0/3/3/3
4	OMU	L5	2837	4	-	0/9/27/28	0/2/2/2
4	OMU	L5	4620	4	-	1/9/27/28	0/2/2/2
52	OMC	S2	462	52	-	0/9/27/28	0/2/2/2
4	6MZ	L5	4220	4	-	1/12/28/28	0/3/3/3
4	A2M	L5	400	4	-	1/9/27/28	0/3/3/3
4	OMC	L5	3869	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	4628	4	-	0/7/25/26	0/2/2/2
52	B8N	S2	1248	52	-	4/16/34/35	0/2/2/2
4	OMG	L5	1625	91,4	-	2/9/27/28	0/3/3/3
4	OMG	L5	2424	4	-	1/9/27/28	0/3/3/3
52	OMG	S2	683	52	-	0/9/27/28	0/3/3/3
4	A2M	L5	3718	4	-	0/9/27/28	0/3/3/3
52	PSU	S2	866	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	3844	4	-	1/7/25/26	0/2/2/2
4	PSU	L5	1677	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1871	4,88	-	0/9/27/28	0/3/3/3
52	A2M	S2	159	52	-	1/9/27/28	0/3/3/3
3	SEP	CF	163	3	-	3/6/8/10	-
4	5MC	L5	3782	4,88	-	0/7/25/26	0/2/2/2
4	PSU	L5	4442	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	3792	4	-	2/9/27/28	0/3/3/3
4	A2M	L5	1323	4	-	1/9/27/28	0/3/3/3
52	PSU	S2	1244	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	1862	4	-	0/7/25/26	0/2/2/2
52	4AC	S2	1842	52	-	0/11/29/30	0/2/2/2
4	PSU	L5	4972	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3822	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3851	4	-	1/7/25/26	0/2/2/2
52	OMG	S2	601	52	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	L5	3808	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	1792	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	1326	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	3637	91,4	-	0/7/25/26	0/2/2/2
4	OMG	L5	4228	4	-	0/9/27/28	0/3/3/3
52	4AC	S2	1337	52	-	1/11/29/30	0/2/2/2
4	PSU	L5	4403	91,4	-	0/7/25/26	0/2/2/2
4	OMG	L5	2364	4,88	-	3/9/27/28	0/3/3/3
52	PSU	S2	863	52	-	2/7/25/26	0/2/2/2
4	OMG	L5	4392	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	4536	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	4500	4	-	4/7/25/26	0/2/2/2
4	PSU	L5	4521	91,4,88	-	0/7/25/26	0/2/2/2
52	MA6	S2	1850	52	-	1/11/29/30	0/3/3/3
4	OMC	L5	3701	91,4	-	6/9/27/28	0/2/2/2
6	OMG	L8	75	6	-	1/9/27/28	0/3/3/3
52	PSU	S2	686	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1177	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1056	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	3639	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4689	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4299	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	1442	52	-	2/9/27/28	0/2/2/2
4	OMG	L5	1522	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	1782	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4576	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	428	52	-	4/9/27/28	0/2/2/2
52	PSU	S2	651	52	-	0/7/25/26	0/2/2/2
4	A2M	L5	4523	4,88	-	0/9/27/28	0/3/3/3
52	OMU	S2	116	52	-	1/9/27/28	0/2/2/2
4	PSU	L5	1582	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4293	4	-	0/7/25/26	0/2/2/2
52	PSU	S2	1046	52	-	0/7/25/26	0/2/2/2
52	A2M	S2	484	52	-	0/9/27/28	0/3/3/3
4	PSU	L5	4296	4	-	1/7/25/26	0/2/2/2
4	A2M	L5	3867	4	-	3/9/27/28	0/3/3/3
52	OMC	S2	174	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	4636	4	-	2/7/25/26	0/2/2/2
52	PSU	S2	1081	52	-	1/7/25/26	0/2/2/2
52	PSU	S2	681	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L5	4552	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	354	52	-	1/9/27/28	0/2/2/2
4	A2M	L5	1326	4	-	3/9/27/28	0/3/3/3
4	PSU	L5	1860	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	4571	4	-	0/9/27/28	0/3/3/3
52	OMG	S2	644	52	-	4/9/27/28	0/3/3/3
52	OMU	S2	799	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	2632	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	3887	4	-	1/9/27/28	0/2/2/2
4	OMC	L5	2861	4	-	1/9/27/28	0/2/2/2
52	PSU	S2	1174	52	-	0/7/25/26	0/2/2/2
52	OMC	S2	1391	52	-	1/9/27/28	0/2/2/2
4	A2M	L5	2787	4	-	5/9/27/28	0/3/3/3
4	OMG	L5	2876	4	-	0/9/27/28	0/3/3/3
52	G7M	S2	1639	52,51	-	2/7/25/26	0/3/3/3
4	PSU	L5	3695	91,4	-	0/7/25/26	0/2/2/2
4	PSU	L5	5001	4	-	0/7/25/26	0/2/2/2
52	MA6	S2	1851	52	-	1/11/29/30	0/3/3/3
4	OMC	L5	3841	4	-	1/9/27/28	0/2/2/2
4	UY1	L5	3818	91,4	-	3/9/27/28	0/2/2/2
52	OMG	S2	1328	52	-	1/9/27/28	0/3/3/3
52	OMC	S2	517	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	4431	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	3785	4,88	-	0/9/27/28	0/3/3/3
4	A2M	L5	4590	4	-	3/9/27/28	0/3/3/3
4	OMG	L5	3899	4	-	2/9/27/28	0/3/3/3
52	A2M	S2	668	52,88	-	4/9/27/28	0/3/3/3
4	A2M	L5	1524	4	-	2/9/27/28	0/3/3/3
4	PSU	L5	4457	4	-	0/7/25/26	0/2/2/2
52	PSU	S2	649	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	4493	91,4	-	0/7/25/26	0/2/2/2
4	OMG	L5	1316	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	4499	4	-	0/9/27/28	0/3/3/3
4	A2M	L5	2815	4	-	1/9/27/28	0/3/3/3
4	OMG	L5	4637	91,4	-	2/9/27/28	0/3/3/3
4	PSU	L5	4579	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	2365	4,88	-	0/9/27/28	0/2/2/2
52	PSU	S2	109	52	-	0/7/25/26	0/2/2/2
4	UR3	L5	4530	4	-	0/7/25/26	0/2/2/2
4	OMU	L5	4227	4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	A2M	S2	27	52	-	1/9/27/28	0/3/3/3
4	OMG	L5	4494	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	2824	4	-	1/9/27/28	0/2/2/2
4	A2M	L5	3825	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	4456	4	-	0/9/27/28	0/2/2/2
52	A2M	S2	1031	52	-	0/9/27/28	0/3/3/3
52	OMC	S2	1703	52	-	2/9/27/28	0/2/2/2
4	PSU	L5	1744	4,88	-	0/7/25/26	0/2/2/2
52	PSU	S2	1004	52	-	0/7/25/26	0/2/2/2
52	OMG	S2	509	52	-	0/9/27/28	0/3/3/3
4	A2M	L5	2401	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	4623	4	-	0/9/27/28	0/3/3/3
6	PSU	L8	69	6	-	0/7/25/26	0/2/2/2
4	PSU	L5	2839	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3884	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4312	4	-	0/7/25/26	0/2/2/2
52	OMG	S2	436	52	-	0/9/27/28	0/3/3/3
52	PSU	S2	1045	52	-	0/7/25/26	0/2/2/2
52	OMC	S2	1272	52	-	4/9/27/28	0/2/2/2
4	OMC	L5	2351	4	-	3/9/27/28	0/2/2/2
4	OMU	L5	3925	4	-	0/9/27/28	0/2/2/2
52	6MZ	S2	1832	52,88	-	5/12/28/28	0/3/3/3
4	OMG	L5	4196	4,51	-	1/9/27/28	0/3/3/3
4	OMC	L5	2804	4	-	0/9/27/28	0/2/2/2
52	OMU	S2	121	52	-	0/9/27/28	0/2/2/2
4	A2M	L5	3830	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	1781	4	-	1/7/25/26	0/2/2/2
4	PSU	L5	5010	4	-	0/7/25/26	0/2/2/2
52	PSU	S2	1232	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	4471	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	4618	4	-	2/9/27/28	0/3/3/3
52	PSU	S2	814	52	-	0/7/25/26	0/2/2/2
52	OMG	S2	867	52	-	3/9/27/28	0/3/3/3
52	PSU	S2	966	52,88	-	0/7/25/26	0/2/2/2
4	PSU	L5	1683	91,4	-	0/7/25/26	0/2/2/2
52	OMG	S2	1490	52	-	2/9/27/28	0/3/3/3
52	OMU	S2	172	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	3853	91,4,88	-	0/7/25/26	0/2/2/2
4	PSU	L5	1536	4	-	2/7/25/26	0/2/2/2
4	OMU	L5	4306	4	-	0/9/27/28	0/2/2/2

The worst 5 of 275 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L5	3818	UY1	C6-C5	12.94	1.49	1.35
52	S2	1832	6MZ	C6-N6	12.64	1.48	1.34
4	L5	4220	6MZ	C6-N6	12.44	1.48	1.34
4	L5	3818	UY1	C2-N1	11.69	1.51	1.36
52	S2	799	OMU	C2-N1	8.66	1.52	1.38

The worst 5 of 671 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1851	MA6	N1-C6-N6	-11.20	103.22	116.86
52	S2	1850	MA6	N1-C6-N6	-10.69	103.83	116.86
52	S2	1832	6MZ	OP3-P-O5'	7.78	126.94	106.67
52	S2	1639	G7M	C1'-N9-C4	7.71	149.28	126.49
52	S2	1639	G7M	C1'-N9-C8	-7.66	100.89	126.74

There are no chirality outliers.

5 of 143 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	CF	163	SEP	N-CA-CB-OG
3	CF	163	SEP	C-CA-CB-OG
3	CF	163	SEP	CA-CB-OG-P
6	L8	75	OMG	C1'-C2'-O2'-CM2
4	L5	400	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

82 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	S2	1288	OMU	1	0
52	S2	1367	PSU	1	0
52	S2	1383	A2M	1	0
52	S2	576	A2M	2	0
52	S2	468	A2M	1	0
4	L5	2363	A2M	1	0
52	S2	166	A2M	1	0
4	L5	1340	OMC	2	0
52	S2	99	A2M	3	0
4	L5	3920	PSU	1	0
4	L5	4447	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	1534	A2M	2	0
4	L5	4620	OMU	4	0
52	S2	462	OMC	3	0
4	L5	4220	6MZ	4	0
4	L5	400	A2M	1	0
4	L5	3869	OMC	1	0
4	L5	1625	OMG	1	0
4	L5	2424	OMG	1	0
4	L5	3718	A2M	5	0
4	L5	1871	A2M	1	0
52	S2	159	A2M	2	0
4	L5	4442	PSU	1	0
52	S2	601	OMG	2	0
4	L5	3637	PSU	1	0
52	S2	1337	4AC	3	0
4	L5	4536	OMC	1	0
4	L5	4500	PSU	1	0
4	L5	4521	PSU	1	0
52	S2	1850	MA6	3	0
4	L5	3701	OMC	1	0
6	L8	75	OMG	1	0
52	S2	1177	PSU	1	0
4	L5	4689	PSU	1	0
4	L5	4523	A2M	1	0
52	S2	116	OMU	4	0
4	L5	4293	PSU	1	0
52	S2	484	A2M	2	0
4	L5	3867	A2M	4	0
4	L5	4636	PSU	1	0
52	S2	681	PSU	1	0
52	S2	354	OMU	1	0
4	L5	1326	A2M	3	0
4	L5	4571	A2M	2	0
52	S2	644	OMG	1	0
4	L5	2632	PSU	1	0
4	L5	2861	OMC	1	0
52	S2	1391	OMC	4	0
4	L5	2876	OMG	1	0
4	L5	5001	PSU	1	0
4	L5	3841	OMC	1	0
4	L5	3818	UY1	1	0
52	S2	1328	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	4431	PSU	1	0
4	L5	3785	A2M	1	0
4	L5	4590	A2M	1	0
4	L5	4457	PSU	1	0
52	S2	649	PSU	1	0
4	L5	2815	A2M	3	0
4	L5	4637	OMG	1	0
4	L5	4579	PSU	2	0
4	L5	4227	OMU	1	0
52	S2	27	A2M	2	0
4	L5	3825	A2M	1	0
4	L5	4456	OMC	1	0
52	S2	1031	A2M	2	0
52	S2	1703	OMC	1	0
52	S2	509	OMG	6	0
52	S2	1272	OMC	1	0
4	L5	2351	OMC	2	0
4	L5	3925	OMU	1	0
52	S2	1832	6MZ	2	0
4	L5	4196	OMG	1	0
4	L5	2804	OMC	1	0
52	S2	121	OMU	4	0
4	L5	1781	PSU	1	0
52	S2	1232	PSU	2	0
4	L5	4618	OMG	1	0
52	S2	867	OMG	1	0
4	L5	1683	PSU	3	0
52	S2	1490	OMG	1	0
4	L5	4306	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 328 ligands modelled in this entry, 307 are monoatomic - leaving 21 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	$\# Z > 2$
89	SPM	L5	5264	-	13,13,13	0.34	0	12,12,12	0.98	0
89	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.83	0
90	SPD	S2	1931	-	9,9,9	0.32	0	8,8,8	0.77	0
89	SPM	L5	5263	-	13,13,13	0.34	0	12,12,12	0.95	0
89	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.95	0
89	SPM	S2	1929	-	13,13,13	0.36	0	12,12,12	1.01	0
90	SPD	S2	1930	-	9,9,9	0.31	0	8,8,8	0.83	0
89	SPM	L5	5291	-	13,13,13	0.35	0	12,12,12	0.74	0
90	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.86	0
89	SPM	L5	5288	-	13,13,13	0.35	0	12,12,12	1.02	0
90	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.68	0
90	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.85	0
93	PUT	S2	1932	-	5,5,5	0.24	0	4,4,4	0.52	0
90	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.91	0
89	SPM	L5	5267	-	13,13,13	0.34	0	12,12,12	0.97	0
90	SPD	L5	5283	88	9,9,9	0.33	0	8,8,8	0.84	0
90	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.94	0
90	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.75	0
90	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.85	0
90	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.85	0
90	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.77	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
89	SPM	L5	5264	-	-	3/11/11/11	-
89	SPM	L5	5292	-	-	3/11/11/11	-
90	SPD	S2	1931	-	-	4/7/7/7	-
89	SPM	L5	5263	-	-	4/11/11/11	-
89	SPM	L5	5259	-	-	1/11/11/11	-
89	SPM	S2	1929	-	-	5/11/11/11	-
90	SPD	S2	1930	-	-	2/7/7/7	-
89	SPM	L5	5291	-	-	2/11/11/11	-
90	SPD	L8	202	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPM	L5	5288	-	-	6/11/11/11	-
90	SPD	L5	5290	-	-	3/7/7/7	-
90	SPD	L5	5289	-	-	1/7/7/7	-
93	PUT	S2	1932	-	-	0/3/3/3	-
90	SPD	L5	5285	-	-	4/7/7/7	-
89	SPM	L5	5267	-	-	4/11/11/11	-
90	SPD	L5	5283	88	-	1/7/7/7	-
90	SPD	L5	5261	-	-	0/7/7/7	-
90	SPD	LN	301	-	-	1/7/7/7	-
90	SPD	L5	5287	-	-	1/7/7/7	-
90	SPD	L5	5286	-	-	2/7/7/7	-
90	SPD	L5	5284	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

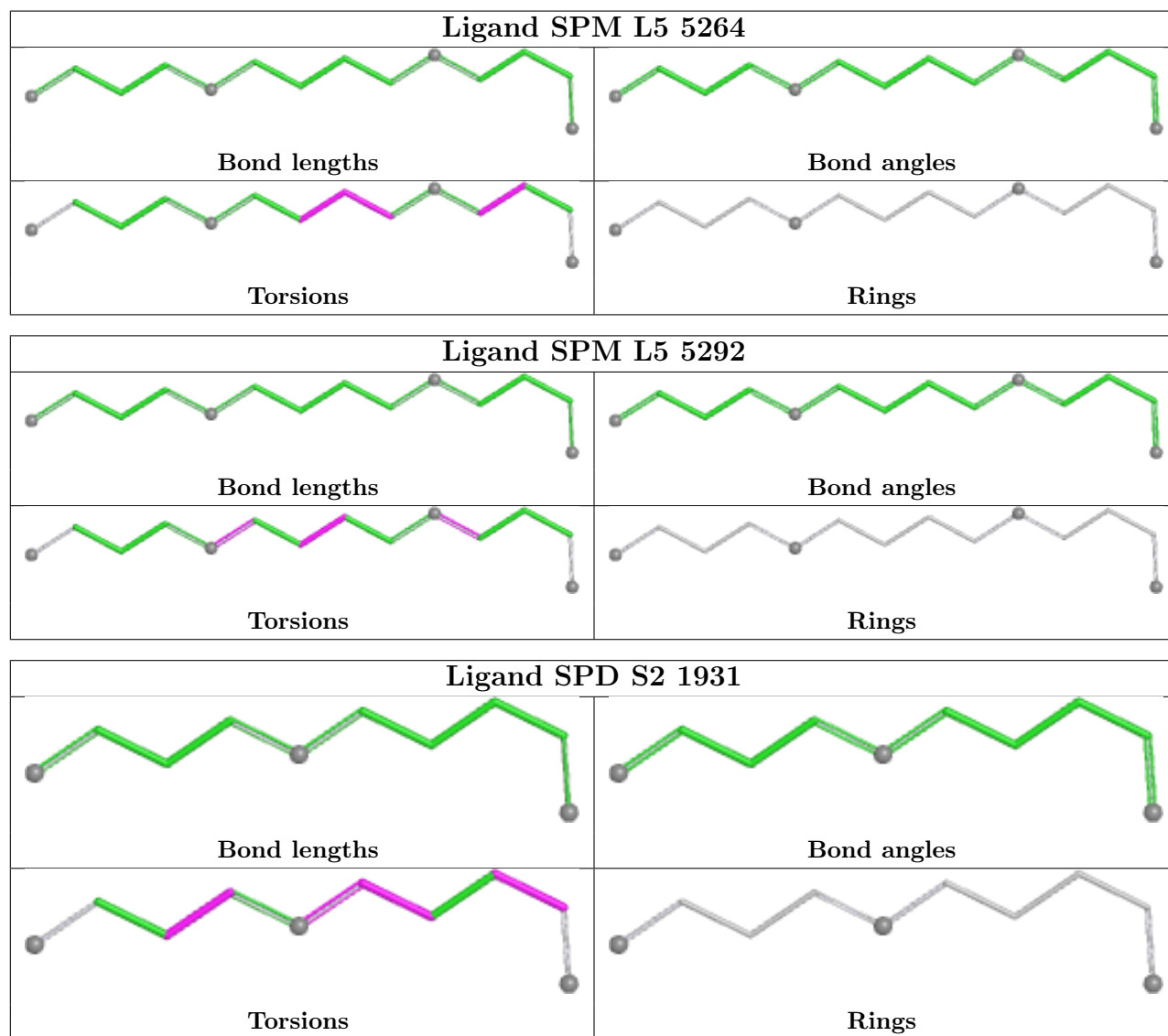
Mol	Chain	Res	Type	Atoms
89	L5	5263	SPM	N10-C11-C12-C13
89	L5	5267	SPM	C7-C8-C9-N10
89	S2	1929	SPM	C7-C8-C9-N10
90	L5	5285	SPD	C3-C4-C5-N6
90	L8	202	SPD	C3-C4-C5-N6

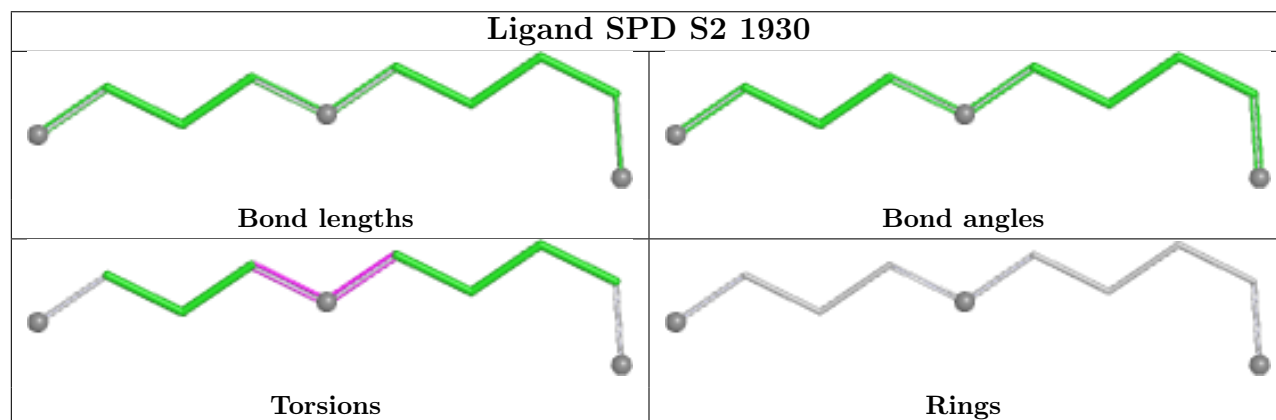
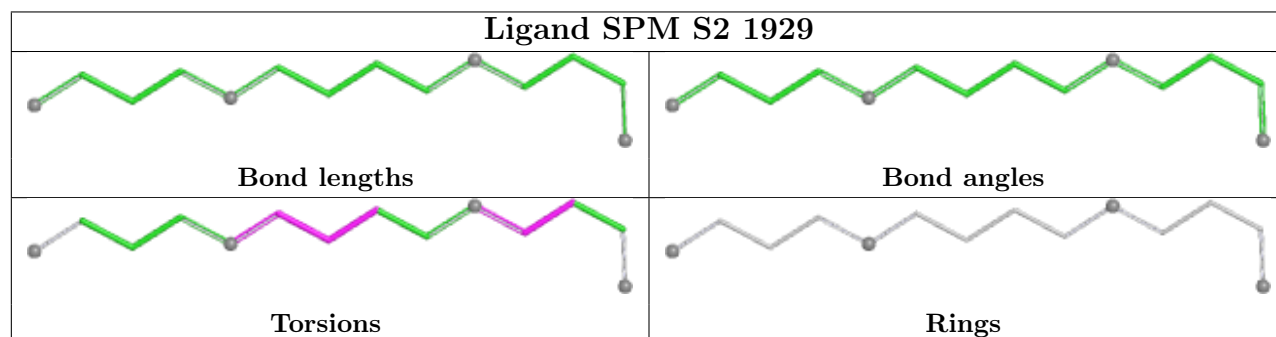
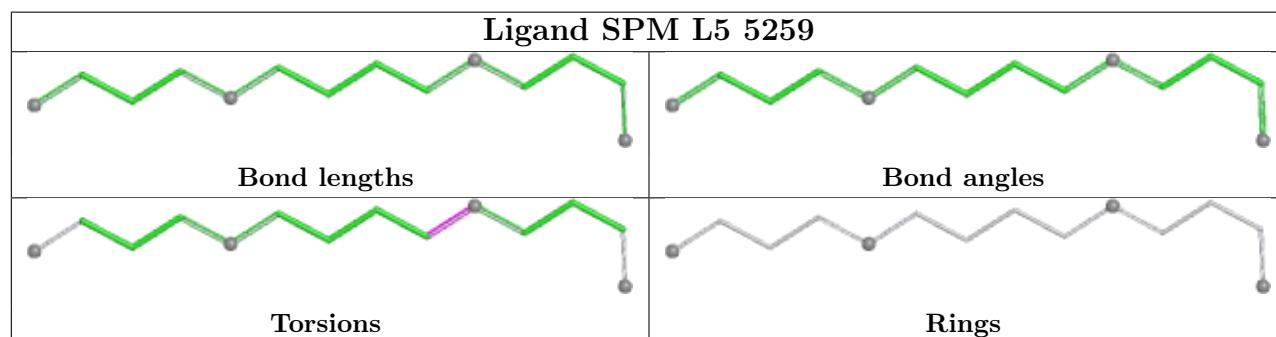
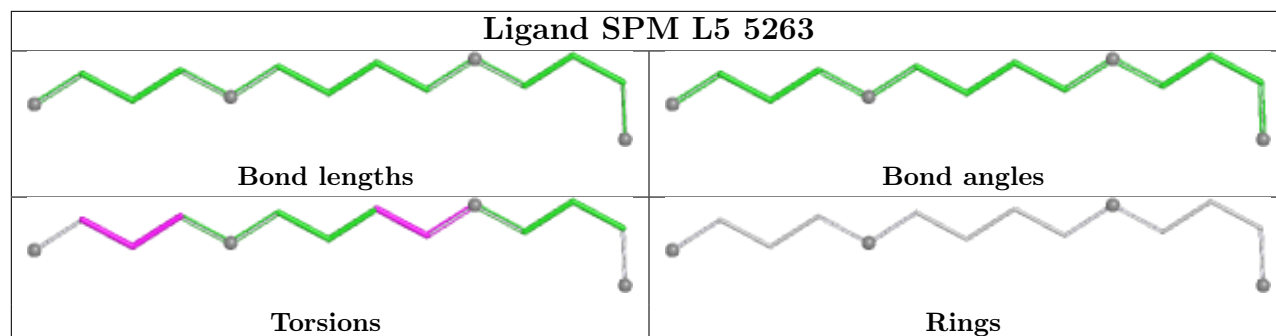
There are no ring outliers.

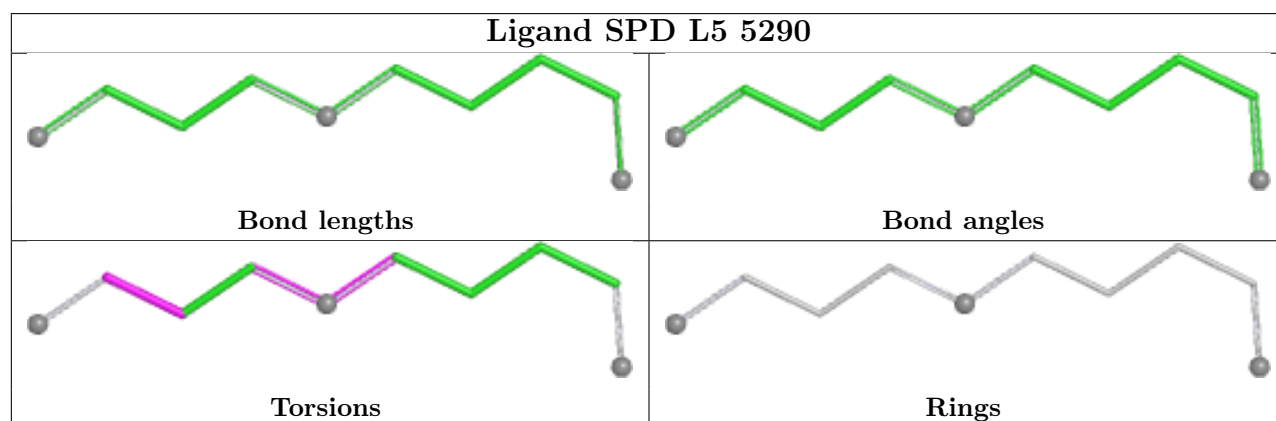
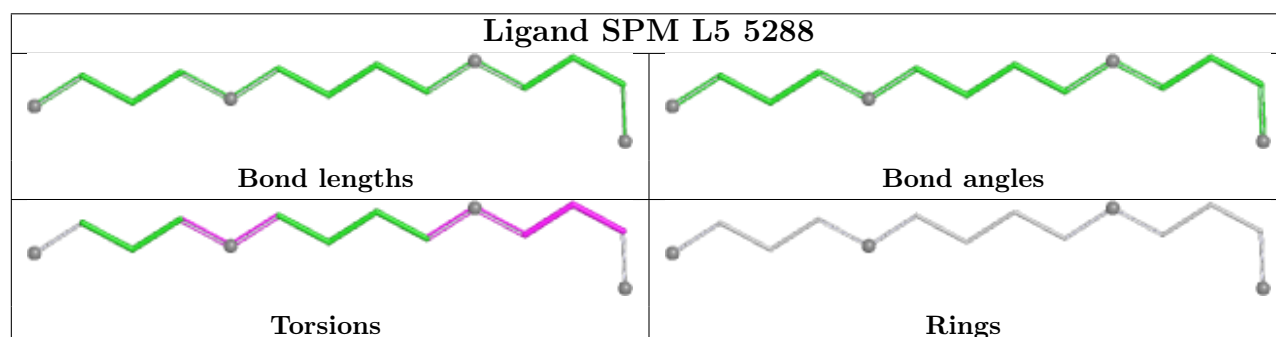
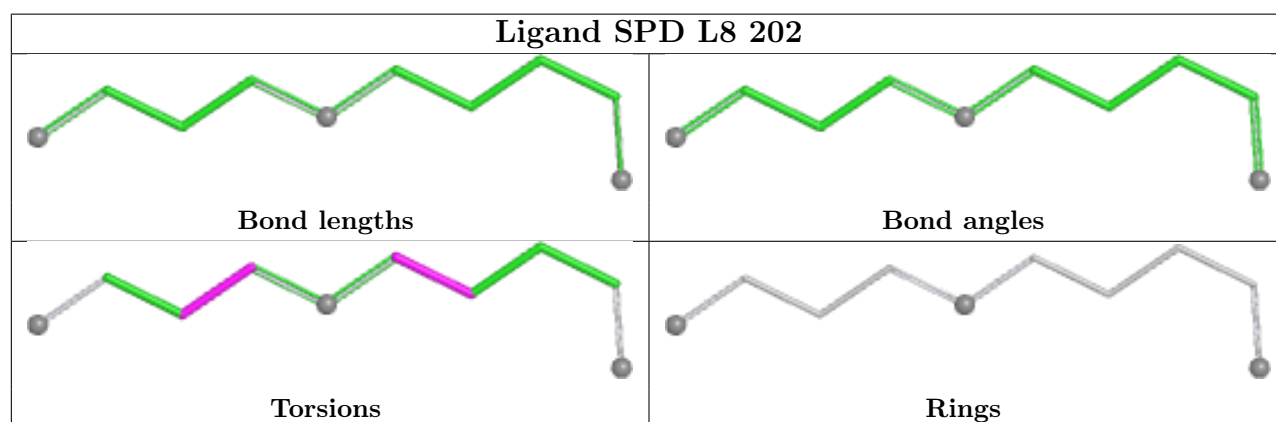
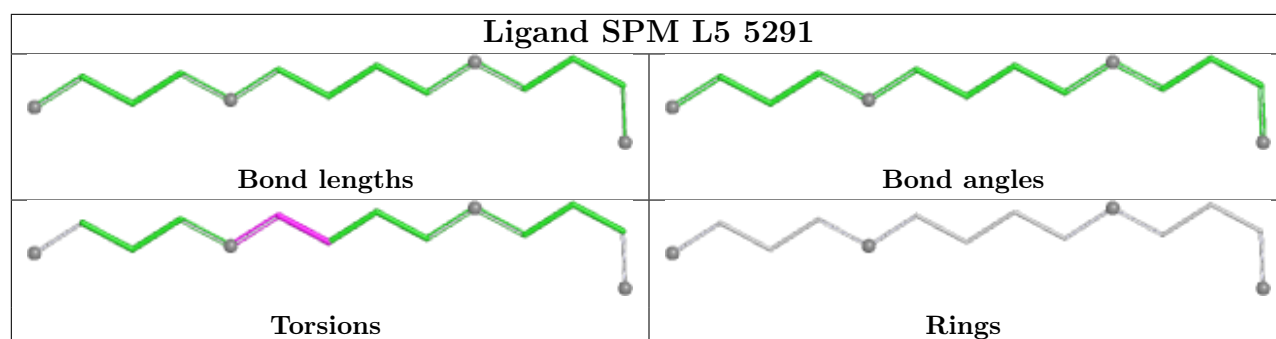
9 monomers are involved in 15 short contacts:

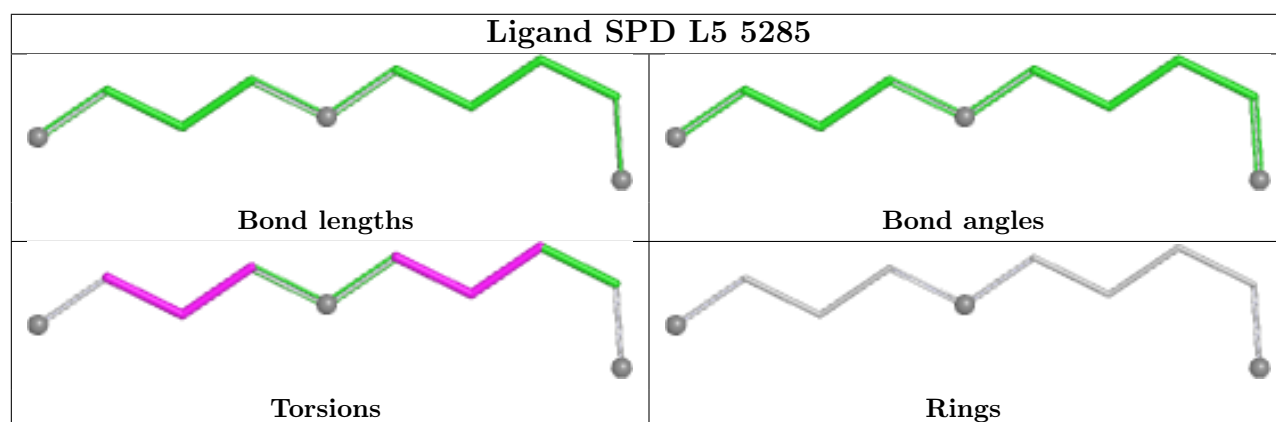
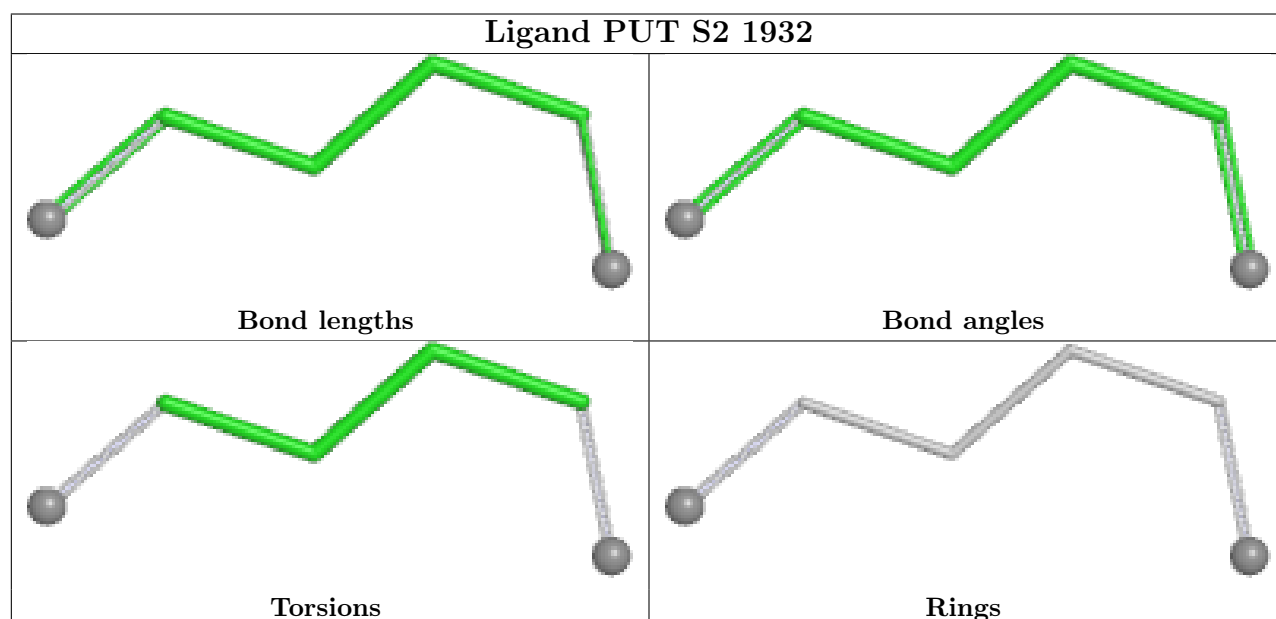
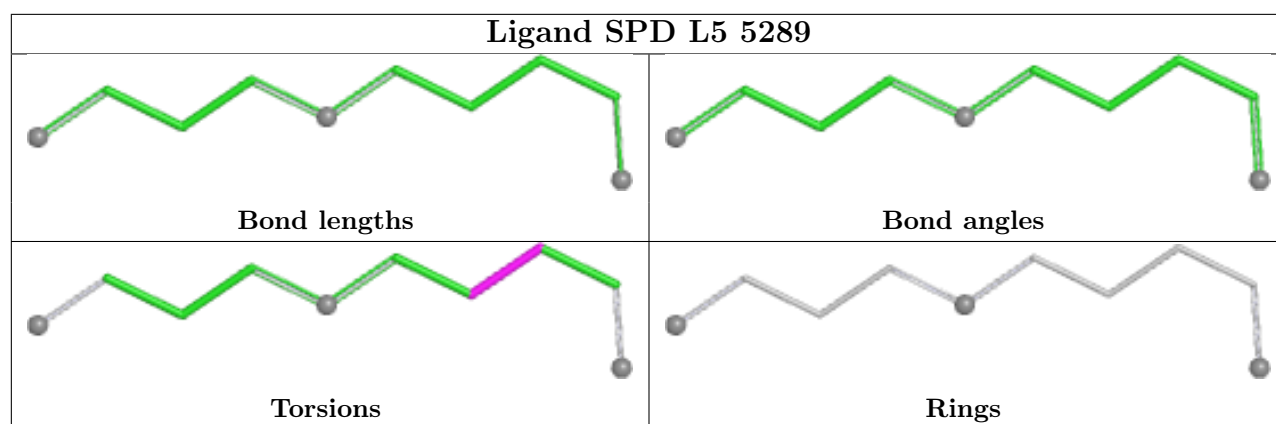
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5264	SPM	2	0
89	L5	5292	SPM	4	0
89	L5	5259	SPM	2	0
89	S2	1929	SPM	2	0
89	L5	5291	SPM	1	0
89	L5	5288	SPM	1	0
90	L5	5290	SPD	1	0
90	L5	5261	SPD	1	0
90	L5	5284	SPD	1	0

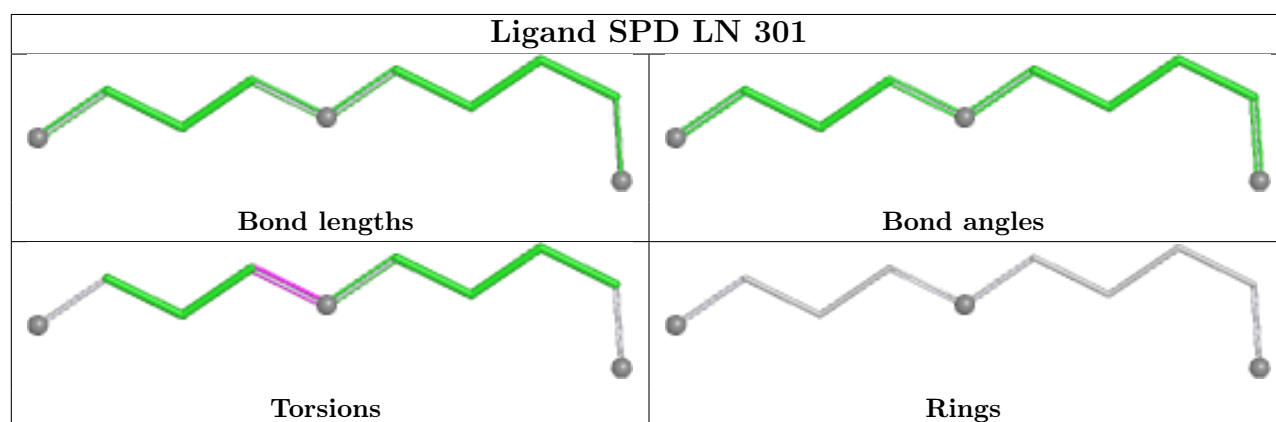
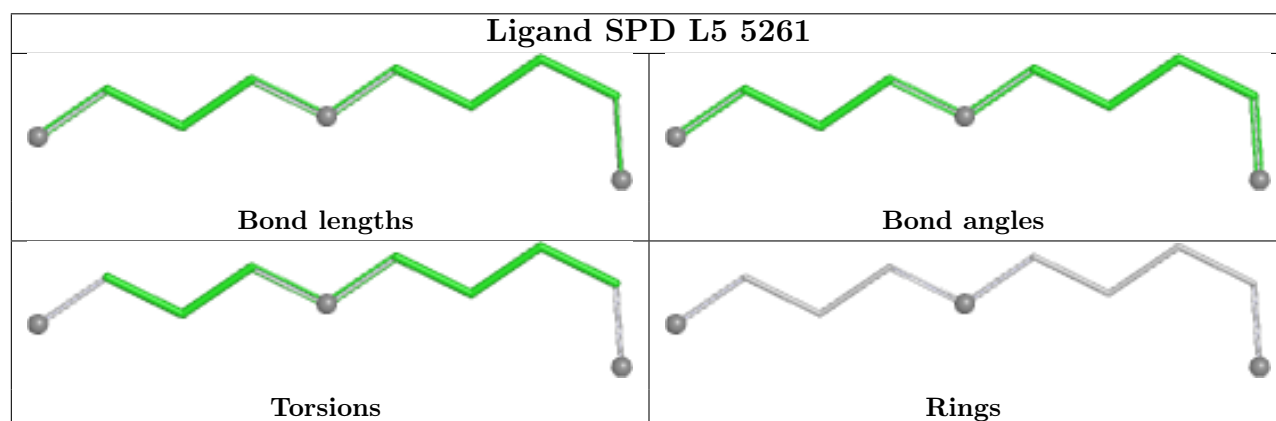
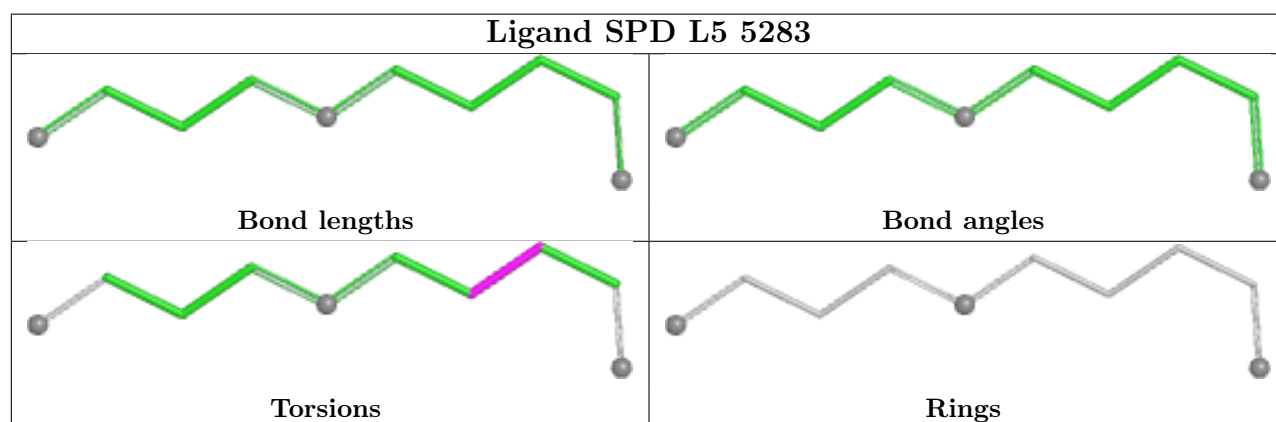
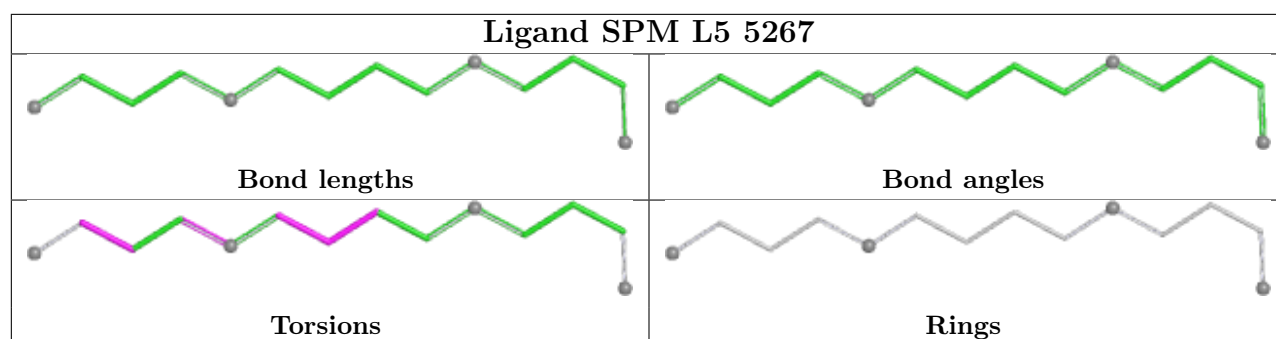
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

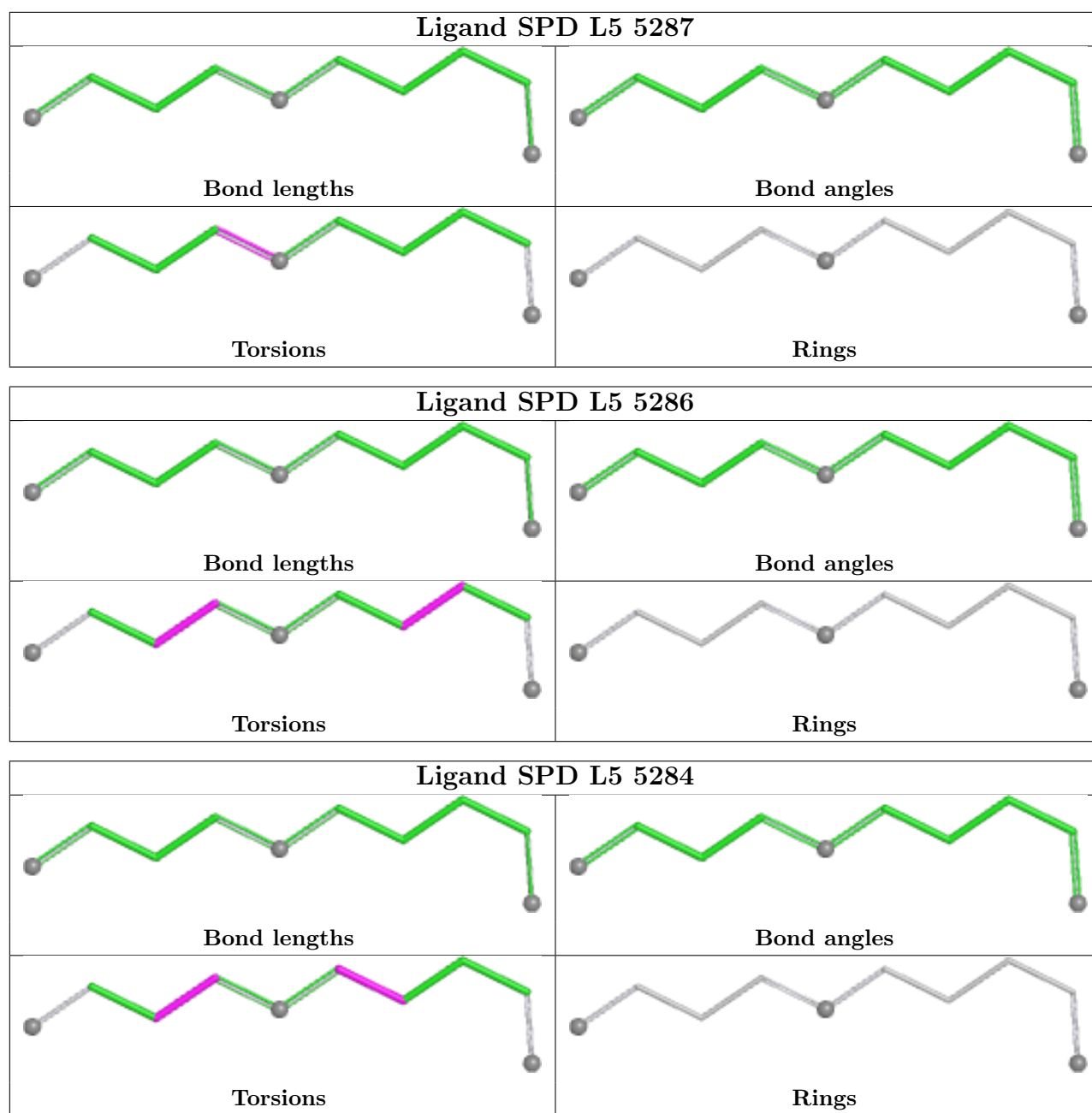












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	S2	5

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Mol	Chain	Number of breaks
33	Lb	1
50	Lt	1
60	SH	1
51	Pt	1
86	AT	1
87	CA	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	35.22
1	S2	753:C	O3'	785:C	P	28.37
1	S2	739:C	O3'	746:C	P	13.09
1	S2	698:G	O3'	730:C	P	12.71
1	Lt	87:GLU	C	104:ILE	N	12.55

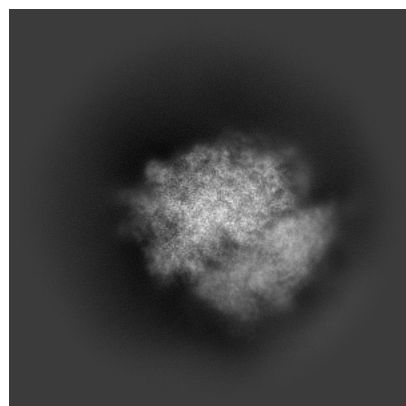
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71435. These allow visual inspection of the internal detail of the map and identification of artifacts.

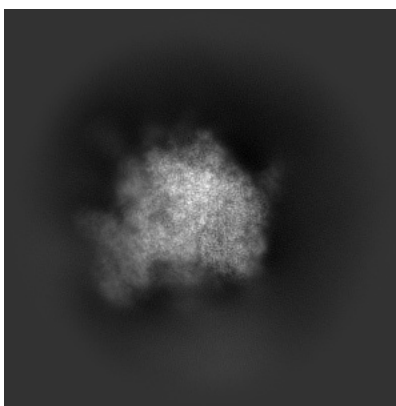
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

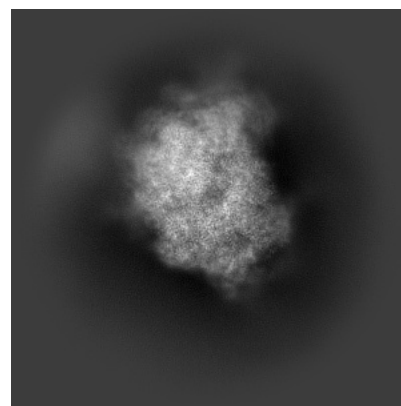
6.1.1 Primary map



X

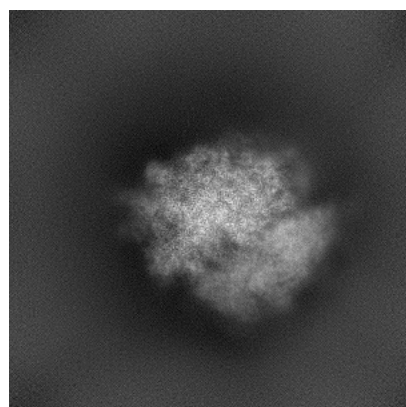


Y

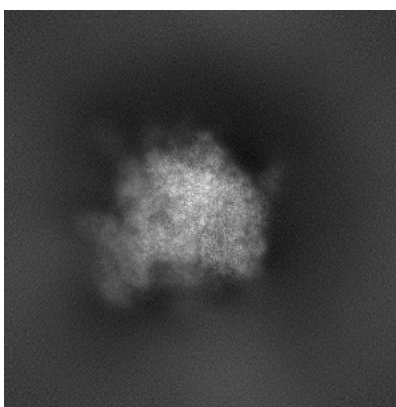


Z

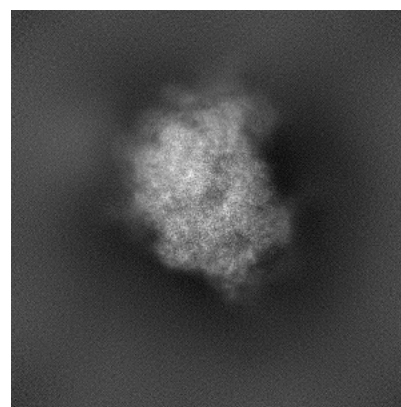
6.1.2 Raw map



X



Y

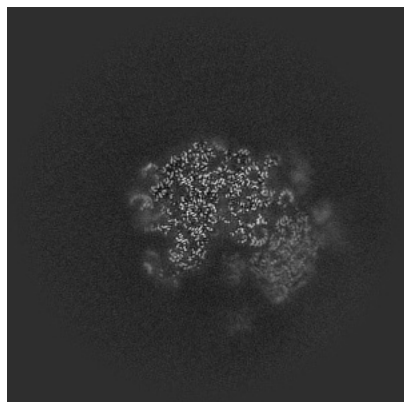


Z

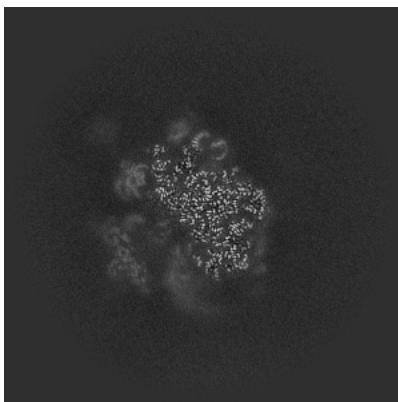
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

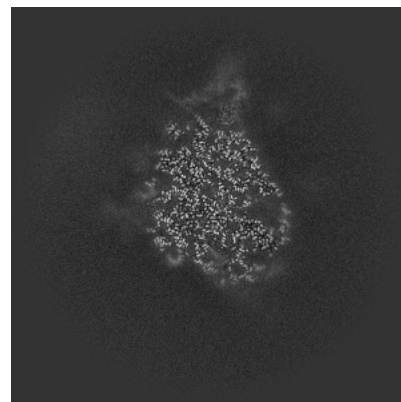
6.2.1 Primary map



X Index: 256

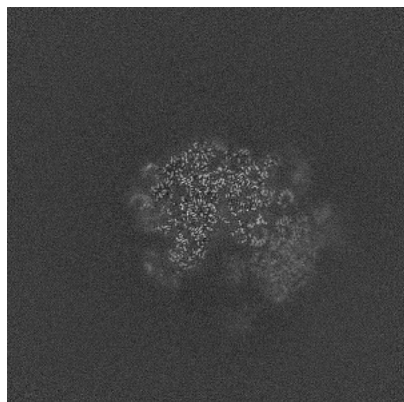


Y Index: 256

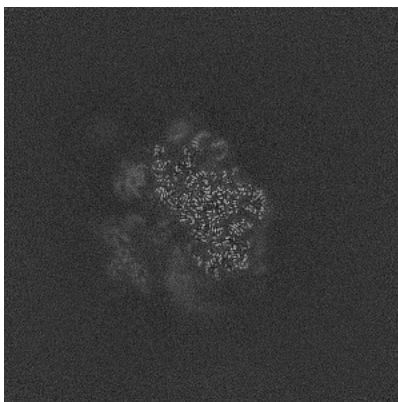


Z Index: 256

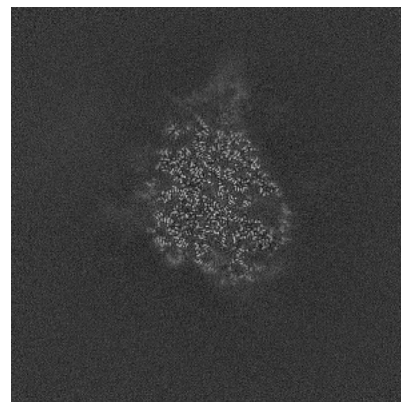
6.2.2 Raw map



X Index: 256



Y Index: 256

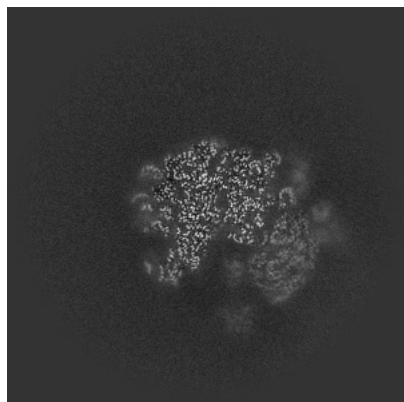


Z Index: 256

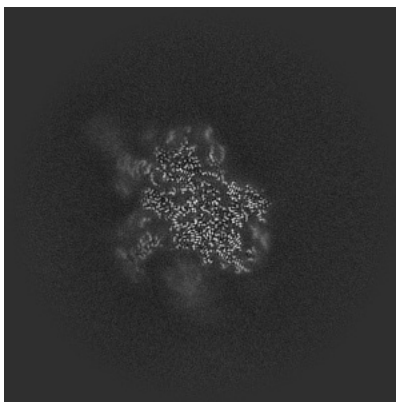
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

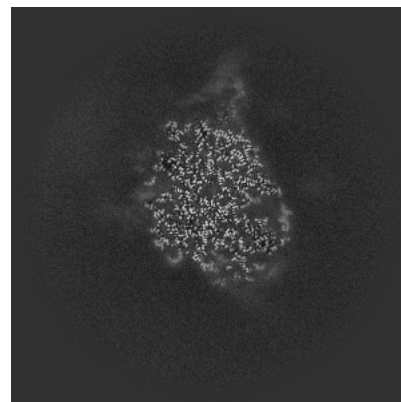
6.3.1 Primary map



X Index: 253

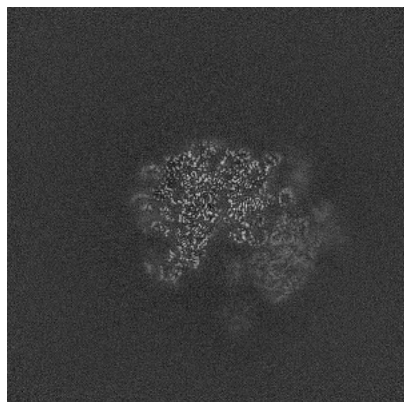


Y Index: 243

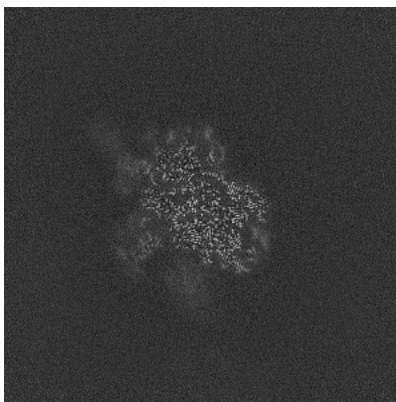


Z Index: 258

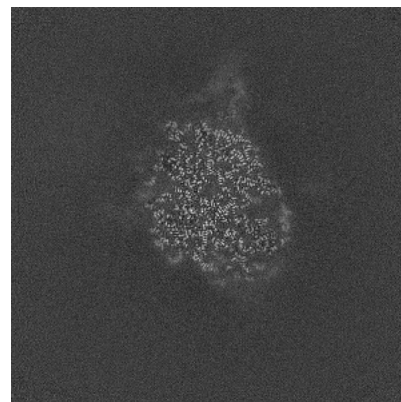
6.3.2 Raw map



X Index: 254



Y Index: 243

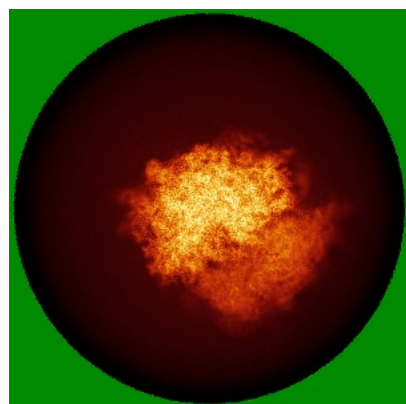


Z Index: 258

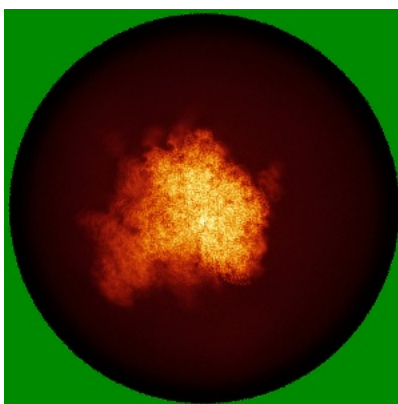
The images above show the largest variance slices of the map in three orthogonal directions.

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

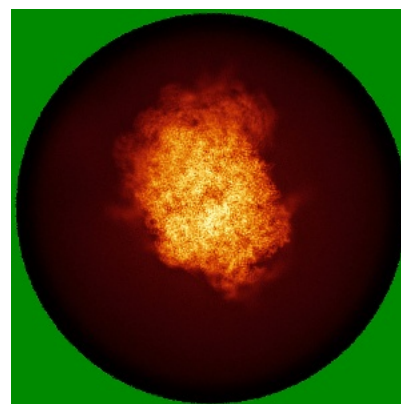
6.4.1 Primary map



X

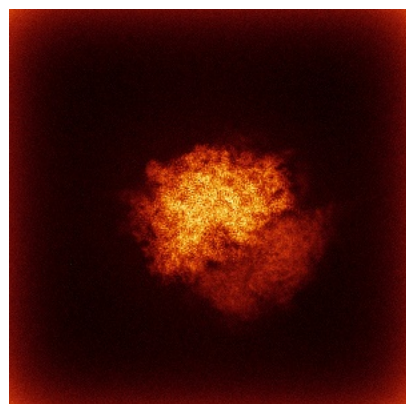


Y

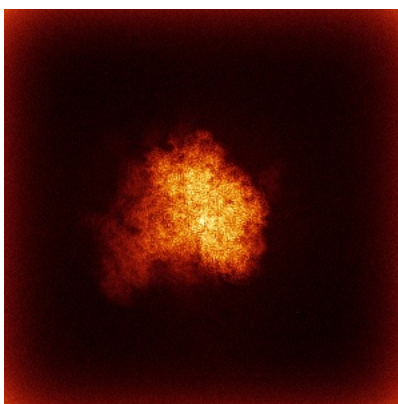


Z

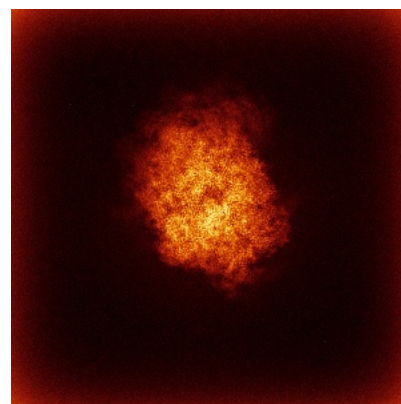
6.4.2 Raw map



X



Y

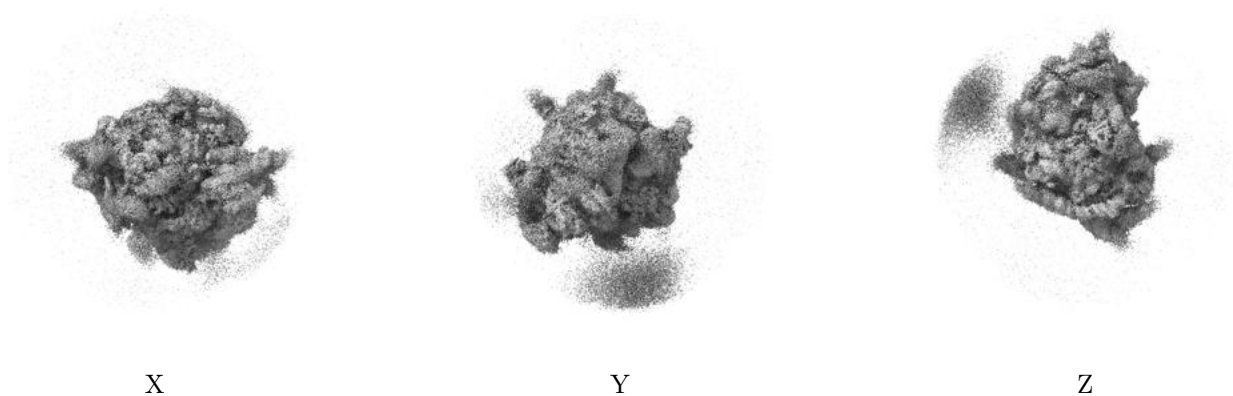


Z

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

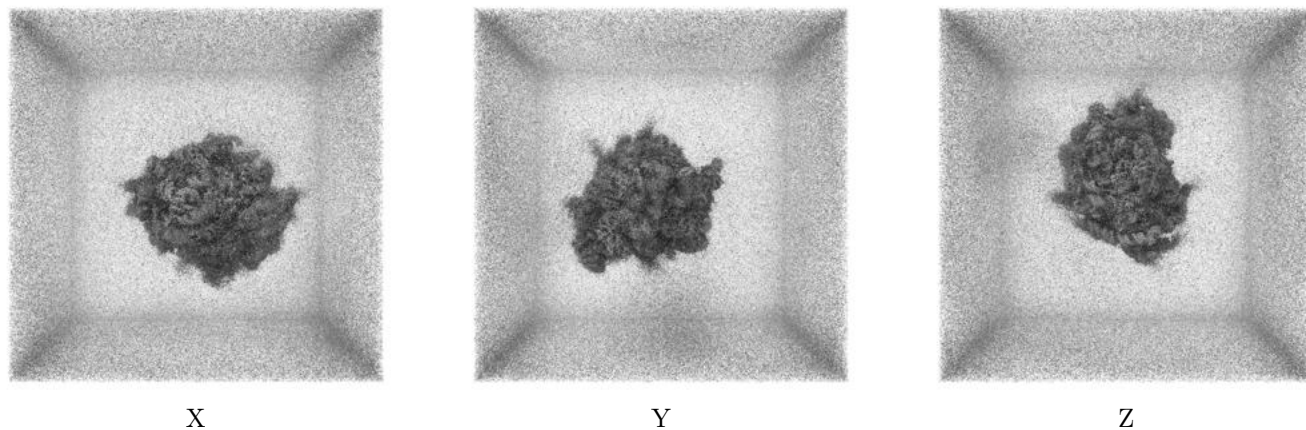
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0575. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

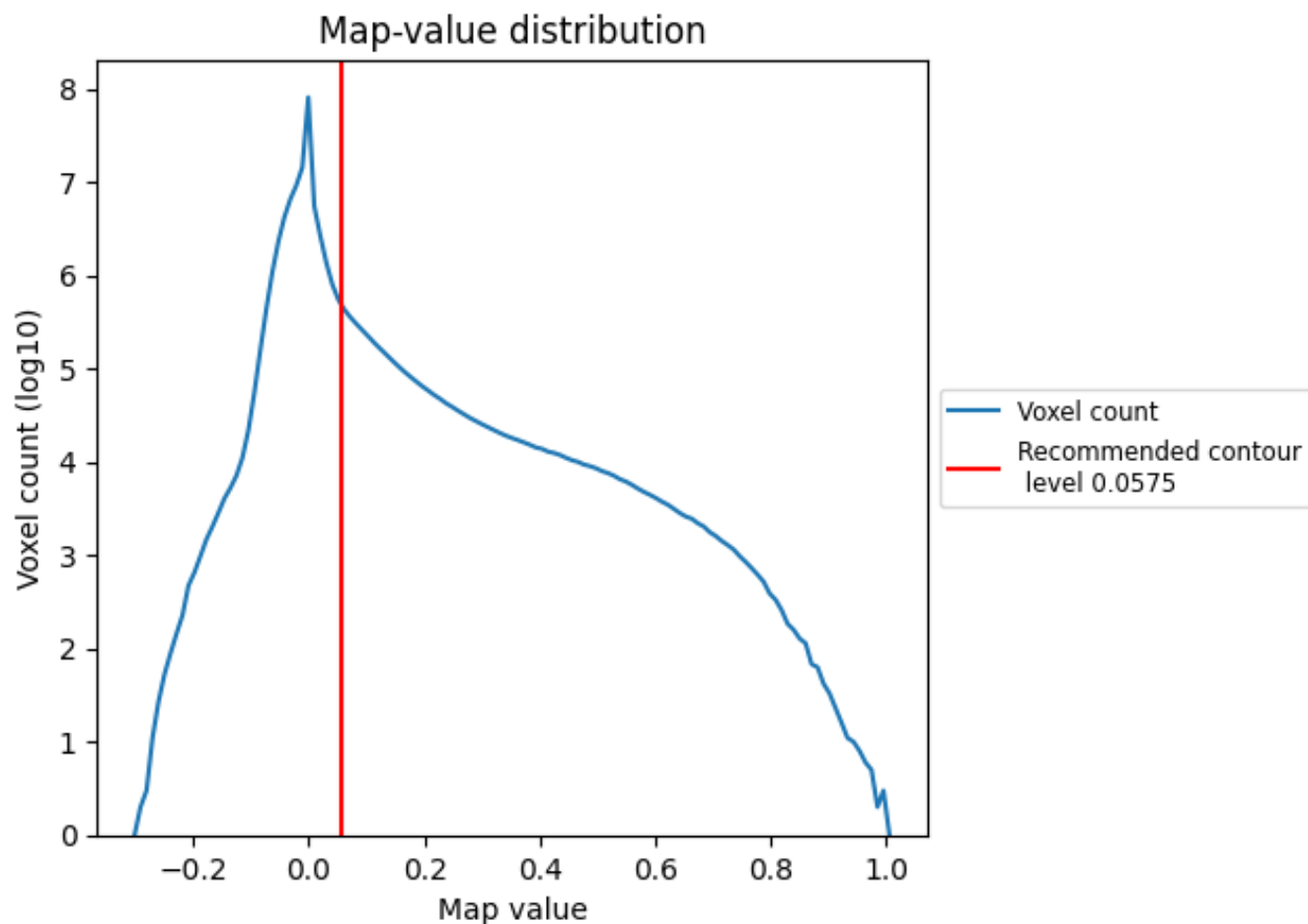
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

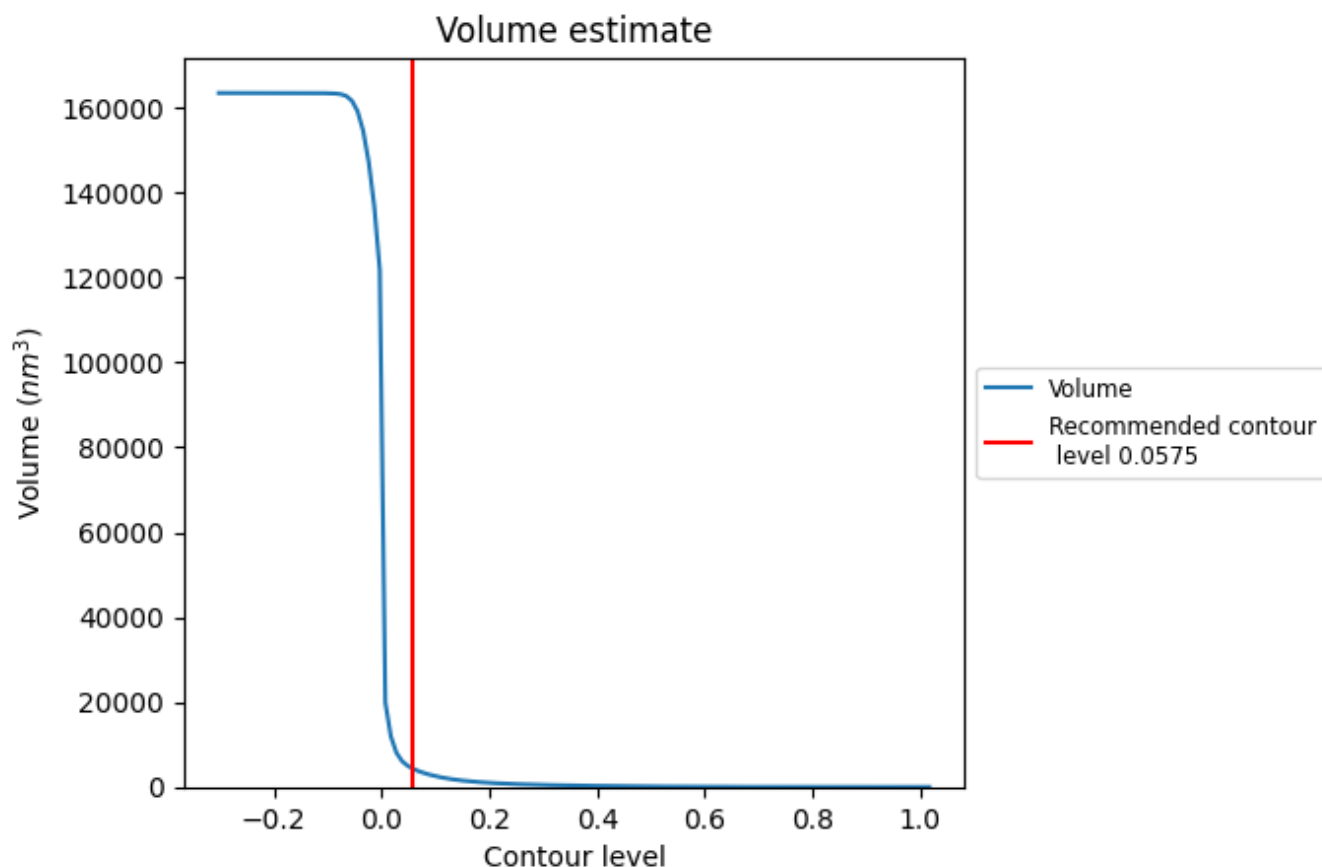
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

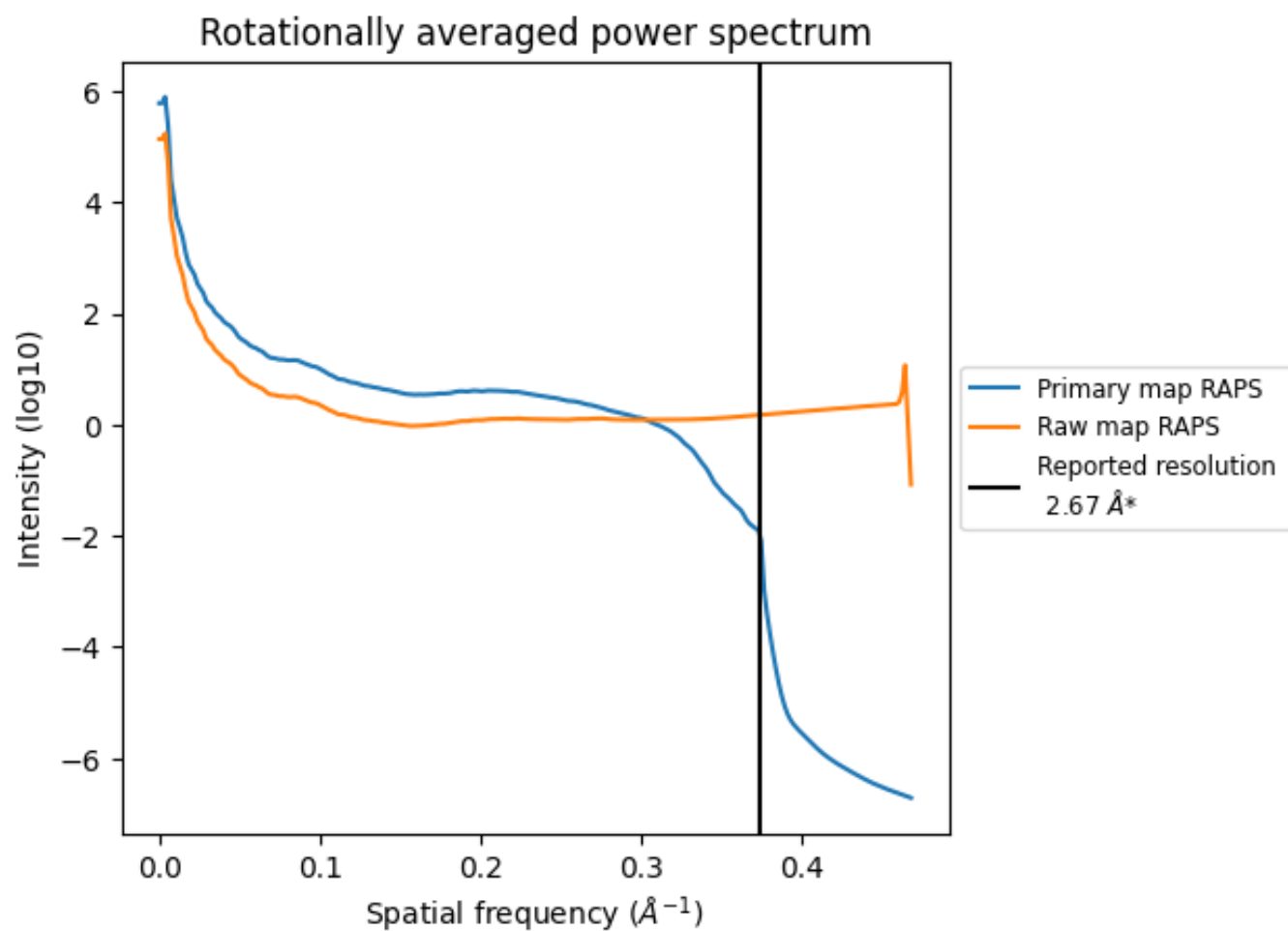
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4349 nm^3 ; this corresponds to an approximate mass of 3929 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 ⓘ

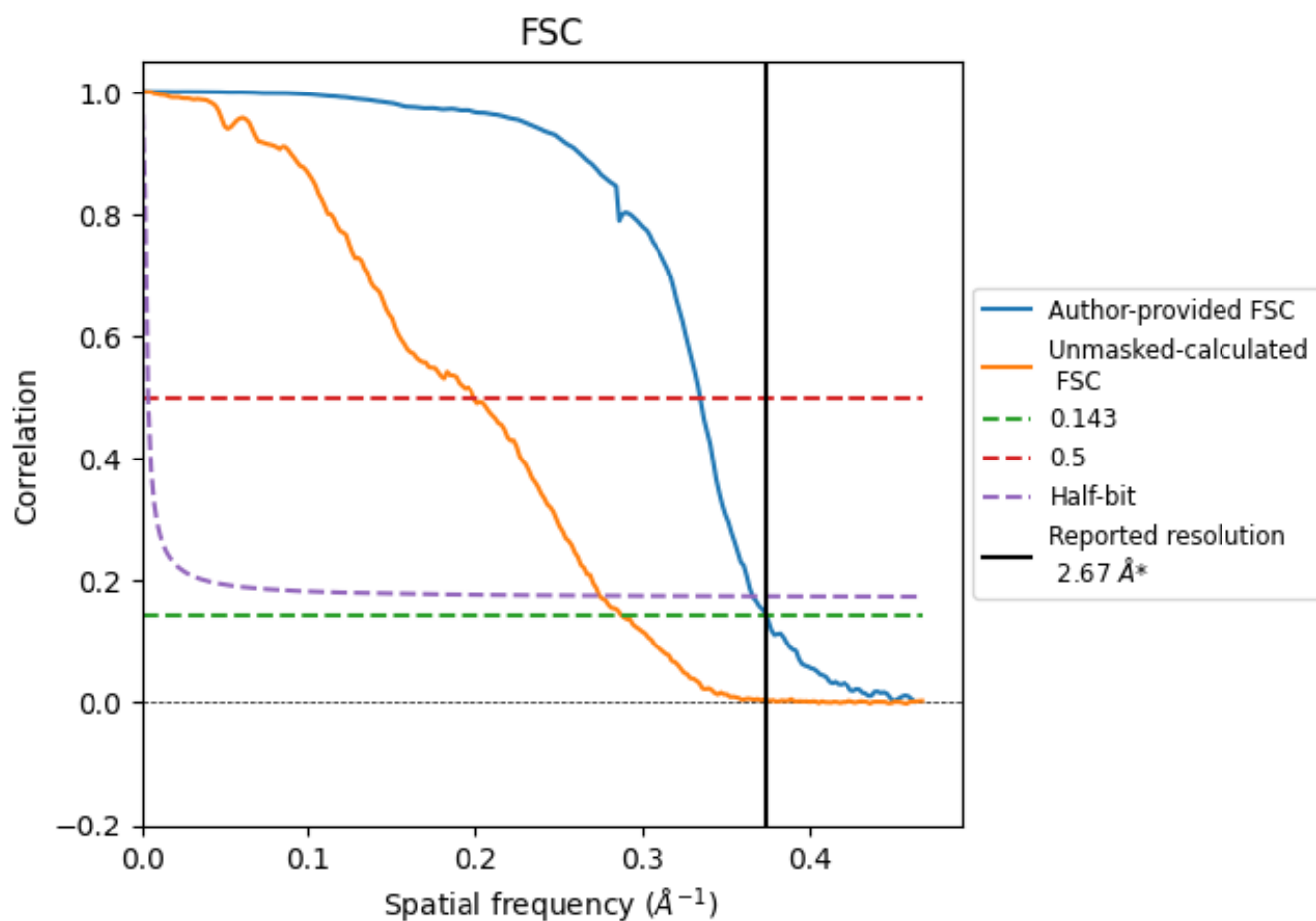


*Reported resolution corresponds to spatial frequency of 0.375 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.375 Å⁻¹

8.2 Resolution estimates [i](#)

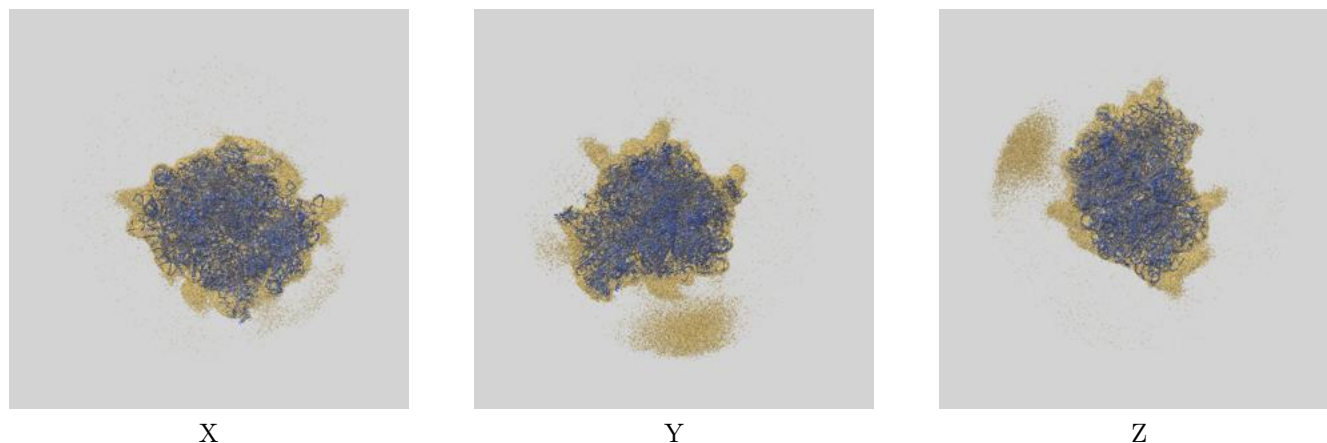
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	2.99	2.73
Unmasked-calculated*	3.48	5.03	3.65

*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 3.48 differs from the reported value 2.67 by more than 10 %

9 Map-model fit [i](#)

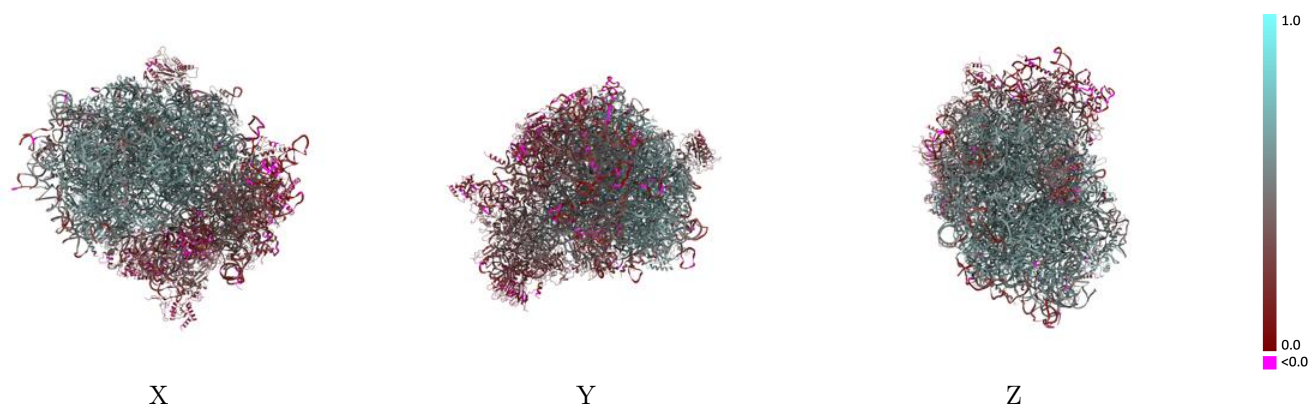
This section contains information regarding the fit between EMDB map EMD-71435 and PDB model 9PA7. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

9.1 Map-model overlay [i](#)



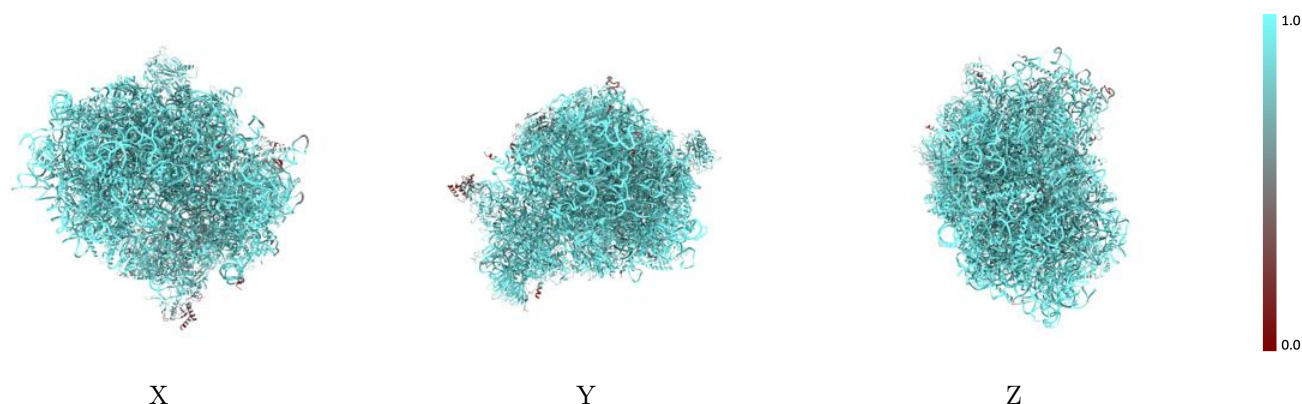
The images above show the 3D surface view of the map at the recommended contour level 0.0575 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



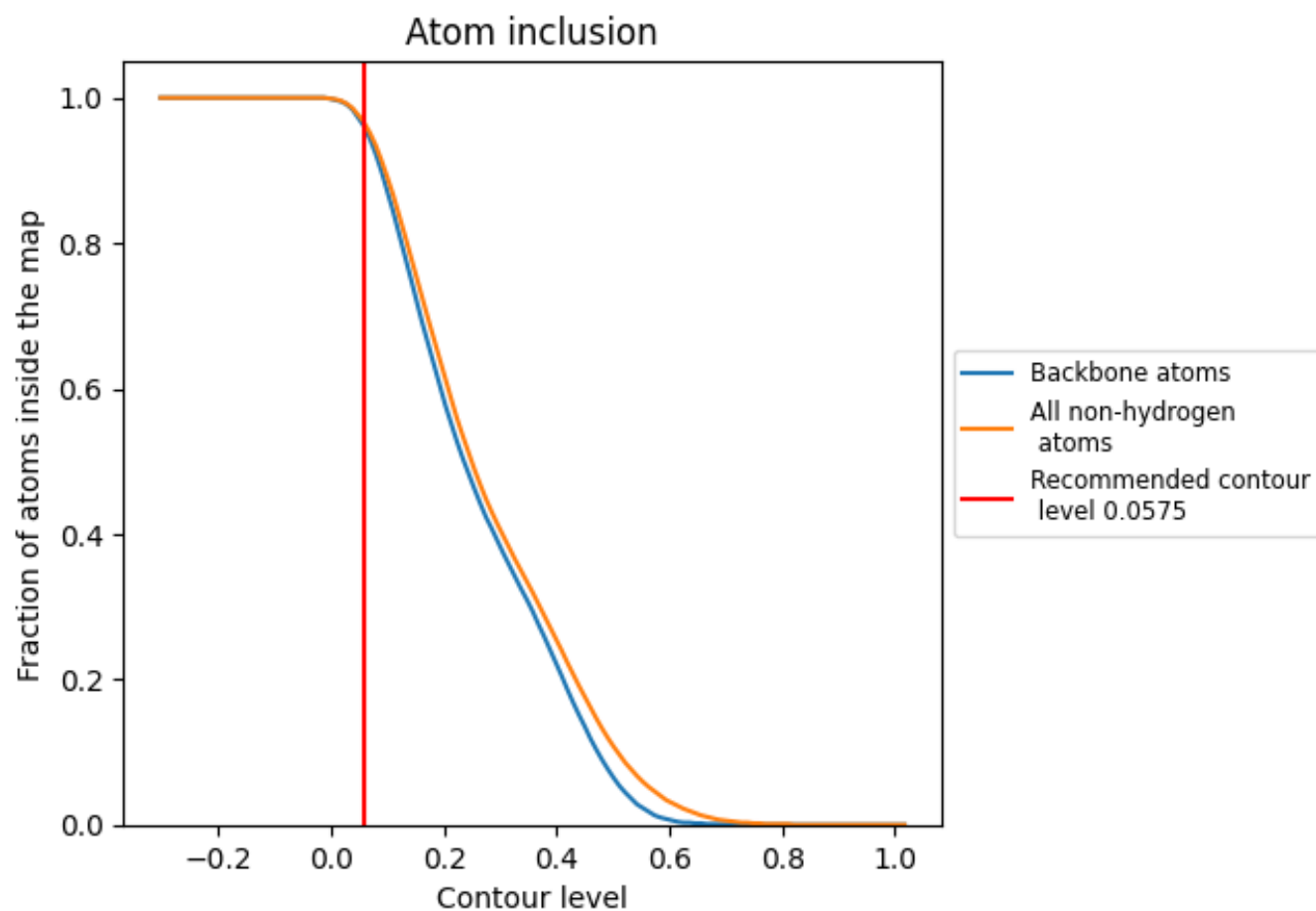
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0575).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (0.0575) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.4530
AT	 0.9150	 0.1400
CA	 0.8400	 0.2860
CD	 0.8660	 0.4180
CF	 0.7510	 0.1490
CI	 0.8790	 0.4240
L5	 0.9950	 0.5320
L7	 1.0000	 0.5760
L8	 0.9960	 0.5550
LA	 0.9980	 0.5920
LB	 0.9830	 0.5790
LC	 0.9850	 0.5750
LD	 0.9830	 0.5410
LE	 0.9800	 0.5170
LF	 0.9920	 0.5790
LG	 0.9620	 0.5210
LH	 0.9910	 0.5700
LI	 0.9900	 0.5780
LJ	 0.9600	 0.4900
LL	 0.9680	 0.5510
LM	 0.9890	 0.5640
LN	 1.0000	 0.6050
LO	 0.9910	 0.5840
LP	 0.9950	 0.5920
LQ	 0.9980	 0.6020
LR	 0.9230	 0.5160
LS	 0.9990	 0.6020
LT	 0.9830	 0.5630
LU	 0.9700	 0.4910
LV	 0.9950	 0.5790
LW	 0.9310	 0.3790
LX	 0.9850	 0.5650
LY	 0.9900	 0.5690
LZ	 0.9960	 0.5640
La	 0.9960	 0.6030



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Chain	Atom inclusion	Q-score
Lb	 0.9590	 0.5150
Lc	 0.9720	 0.5320
Ld	 0.9840	 0.5640
Le	 0.9920	 0.5970
Lf	 0.9960	 0.6040
Lg	 0.9870	 0.5670
Lh	 0.9850	 0.5620
Li	 0.9900	 0.5590
Lj	 0.9960	 0.5980
Lk	 0.9700	 0.5080
Ll	 0.9950	 0.5790
Lm	 0.9830	 0.5860
Ln	 0.9860	 0.5510
Lo	 0.9870	 0.5770
Lp	 0.9860	 0.5690
Lr	 0.9900	 0.5850
Ls	 0.9040	 0.2910
Lt	 0.8120	 0.1510
Pt	 0.9400	 0.3930
S2	 0.9840	 0.3550
SA	 0.9290	 0.3820
SB	 0.9480	 0.3720
SC	 0.9810	 0.4300
SD	 0.9440	 0.3210
SE	 0.9450	 0.2820
SF	 0.9340	 0.2290
SG	 0.9190	 0.2510
SH	 0.8670	 0.2620
SI	 0.8580	 0.3570
SJ	 0.9350	 0.3140
SK	 0.8830	 0.2750
SL	 0.8590	 0.3580
SM	 0.4280	 0.1080
SN	 0.9660	 0.4090
SO	 0.9290	 0.4010
SP	 0.8800	 0.1820
SQ	 0.9610	 0.2370
SR	 0.9020	 0.2720
SS	 0.8660	 0.1650
ST	 0.9140	 0.2040
SU	 0.9150	 0.2810
SV	 0.9730	 0.3960

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Chain	Atom inclusion	Q-score
SW	 0.9800	 0.4060
SX	 0.9600	 0.3740
SY	 0.9290	 0.2080
SZ	 0.8410	 0.1190
Sa	 0.9630	 0.4210
Sb	 0.9300	 0.3390
Sc	 0.9220	 0.2370
Sd	 0.9910	 0.3520
Se	 0.9300	 0.2630
Sf	 0.7950	 0.1290
Sg	 0.8980	 0.1680