



wwPDB EM Validation Summary Report ⓘ

Jun 27, 2026 – 03:44 PM EDT

PDB ID : 9P7Y / pdb_00009p7y
EMDB ID : EMD-71357
Title : In situ human A-P-E state 80S ribosome
Authors : Zheng, W.; Xiong, Y.
Deposited on : 2025-06-22
Resolution : 2.75 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:

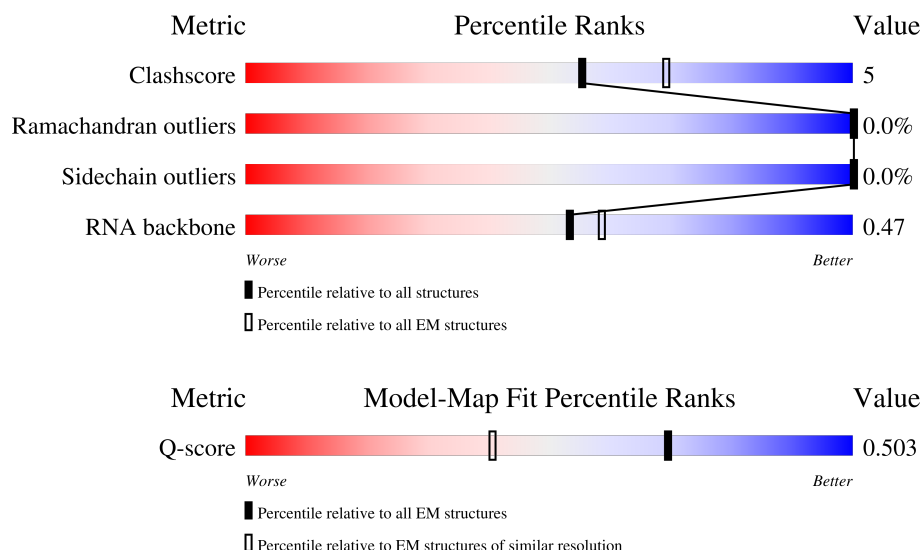
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.75 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.



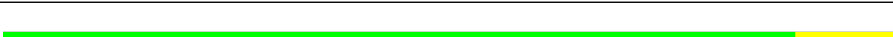
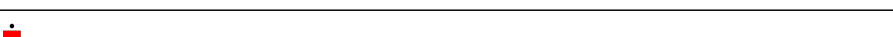
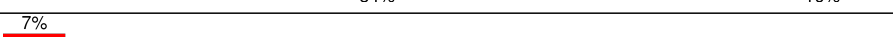
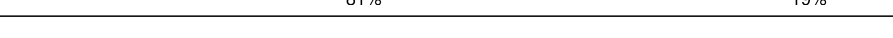
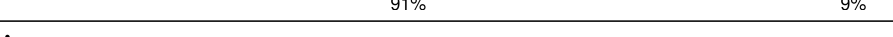
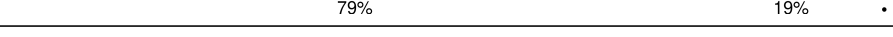
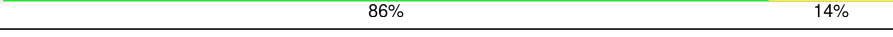
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10570 (2.25 - 3.25)

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	SA	221	 83% 16%
2	SB	214	 79% 21%
3	SC	222	 82% 18%

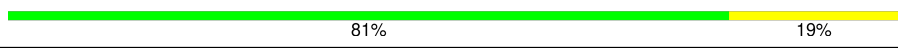
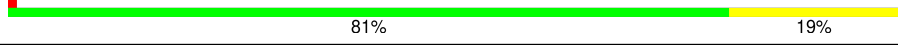
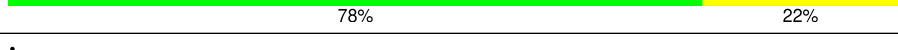
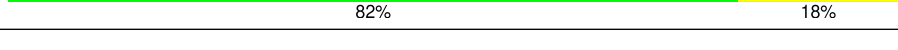
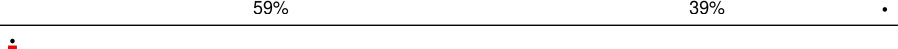
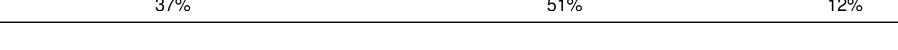
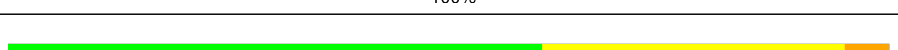
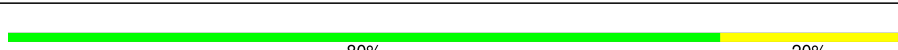
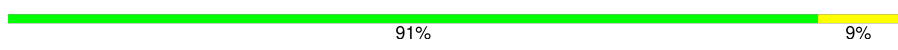
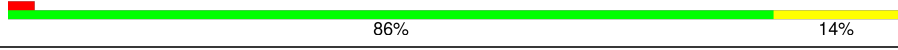
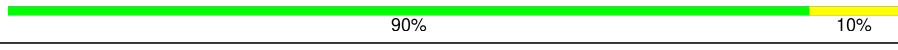
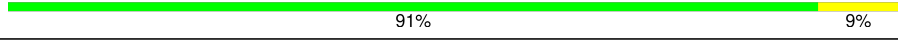
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Mol	Chain	Length	Quality of chain
4	SE	262	
5	SG	237	
6	SH	186	
7	SI	206	
8	SJ	185	
9	SL	153	
10	SN	150	
11	SO	140	
12	SV	83	
13	SW	129	
14	SX	141	
15	SY	131	
16	Sa	102	
17	Sb	83	
18	Se	58	
19	S2	1740	
20	LR	187	
21	LW	118	
22	SR	135	
23	SD	227	
24	SF	189	
25	SK	98	
26	SM	122	
27	SP	121	
28	SQ	144	

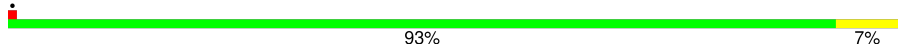
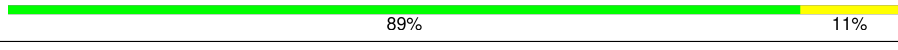
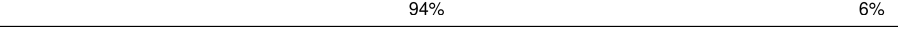
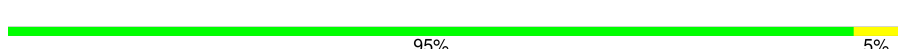
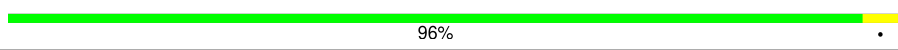
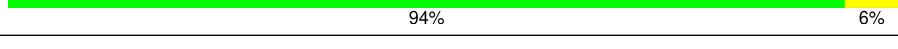
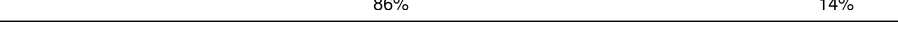
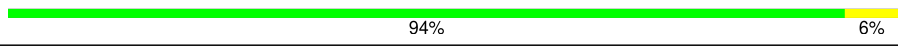
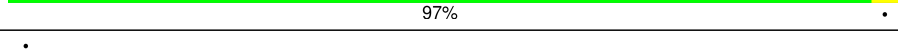
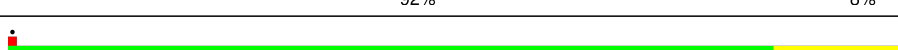
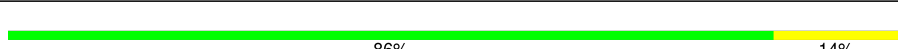
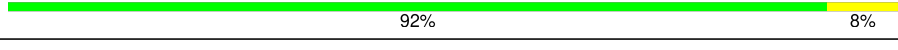
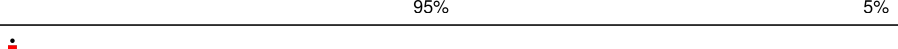
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Mol	Chain	Length	Quality of chain
29	SS	145	
30	ST	143	
31	SU	104	
32	SZ	75	
33	Sc	64	
34	Sd	55	
35	Sf	67	
36	Sg	313	
37	At	71	
38	Et	75	
39	Pt	74	
40	CI	31	
41	L5	3655	
42	L7	120	
43	L8	156	
44	LA	248	
45	LB	402	
46	LC	368	
47	LD	293	
48	LE	250	
49	LF	225	
50	LG	241	
51	LH	190	
52	LI	213	
53	LJ	176	

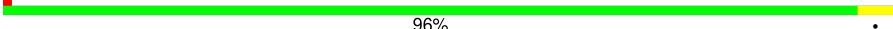
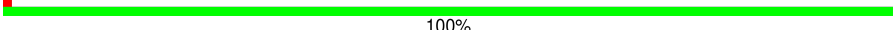
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Mol	Chain	Length	Quality of chain
54	LL	210	
55	LM	139	
56	LN	203	
57	LO	201	
58	LP	153	
59	LQ	187	
60	LS	175	
61	LT	159	
62	LU	101	
63	LV	131	
64	LX	120	
65	LY	134	
66	LZ	135	
67	La	147	
68	Lb	109	
69	Lc	98	
70	Ld	107	
71	Le	128	
72	Lf	109	
73	Lg	114	
74	Lh	122	
75	Li	102	
76	Lj	86	
77	Lk	69	
78	Ll	50	

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Mol	Chain	Length	Quality of chain
79	Lm	52	 90%10%
80	Ln	24	 88%12%
81	Lo	105	 90%10%
82	Lp	91	 96%.
83	Lr	125	 100%
84	Ls	196	 36%87%13%
85	Lt	141	 30%84%11%5%

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 221484 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 40S ribosomal protein SA.

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

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

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

- Molecule 4 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 5 is a protein called 40S ribosomal protein S6.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	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 7 is a protein called 40S ribosomal protein S8.

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

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

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

- Molecule 9 is a protein called 40S ribosomal protein S11.

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

- Molecule 10 is a protein called 40S ribosomal protein S13.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 12 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 13 is a protein called 40S ribosomal protein S15a.

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

- Molecule 14 is a protein called 40S ribosomal protein S23.

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

- Molecule 15 is a protein called 40S ribosomal protein S24.

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

- Molecule 16 is a protein called 40S ribosomal protein S26.

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

- Molecule 17 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 18 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 19 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S2	1740	Total	C	N	O	P	0	0
			36952	16508	6600	12105	1739		

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	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 22 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 24 is a protein called 40S ribosomal protein S5.

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

- Molecule 25 is a protein called 40S ribosomal protein S10.

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

- Molecule 26 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 29 is a protein called 40S ribosomal protein S18.

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

- Molecule 30 is a protein called 40S ribosomal protein S19.

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

- Molecule 31 is a protein called 40S ribosomal protein S20.

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

- Molecule 32 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 33 is a protein called 40S ribosomal protein S28.

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

- Molecule 34 is a protein called 40S ribosomal protein S29.

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

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 37 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	At	71	Total	C	N	O	P	0	0
			1514	677	275	492	70		

- Molecule 38 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Et	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 39 is a RNA chain called P site tRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Pt	74	Total	C	N	O	P	0	0
			1576	705	286	512	73		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Pt	3	C	U	conflict	GB X64278
Pt	?	-	U	deletion	GB X64278
Pt	?	-	G	deletion	GB X64278
Pt	19	G	U	conflict	GB X64278
Pt	50	U	-	insertion	GB X64278
Pt	74	C	-	insertion	GB X64278

- Molecule 40 is a protein called Transcription factor BTF3.

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

- Molecule 41 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	L5	3655	Total	C	N	O	P	1	0
			78444	34968	14346	25475	3655		

- Molecule 42 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 43 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

- Molecule 44 is a protein called 60S ribosomal protein L8.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 46 is a protein called 60S ribosomal protein L4.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 48 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 49 is a protein called 60S ribosomal protein L7.

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

- Molecule 50 is a protein called 60S ribosomal protein L7a.

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

- Molecule 51 is a protein called 60S ribosomal protein L9.

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

- Molecule 52 is a protein called Ribosomal protein uL16-like.

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

- Molecule 53 is a protein called 60S ribosomal protein L11.

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

- Molecule 54 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 55 is a protein called 60S ribosomal protein L14.

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

- Molecule 56 is a protein called 60S ribosomal protein L15.

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

- Molecule 57 is a protein called 60S ribosomal protein L13a.

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

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

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

- Molecule 59 is a protein called 60S ribosomal protein L18.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L21.

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

- Molecule 62 is a protein called Heparin-binding protein HBp15.

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

- Molecule 63 is a protein called 60S ribosomal protein L23.

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

- Molecule 64 is a protein called 60S ribosomal protein L23a.

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

- Molecule 65 is a protein called 60S ribosomal protein L26.

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

- Molecule 66 is a protein called 60S ribosomal protein L27.

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

- Molecule 67 is a protein called 60S ribosomal protein L27a.

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

- Molecule 68 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	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 69 is a protein called 60S ribosomal protein L30.

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

- Molecule 70 is a protein called 60S ribosomal protein L31.

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

- Molecule 71 is a protein called 60S ribosomal protein L32.

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

- Molecule 72 is a protein called 60S ribosomal protein L35a.

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

- Molecule 73 is a protein called 60S ribosomal protein L34.

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

- Molecule 74 is a protein called 60S ribosomal protein L35.

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

- Molecule 75 is a protein called 60S ribosomal protein L36.

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

- Molecule 76 is a protein called 60S ribosomal protein L37.

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

- Molecule 77 is a protein called 60S ribosomal protein L38.

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

- Molecule 78 is a protein called 60S ribosomal protein L39.

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

- Molecule 79 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 80 is a protein called 60S ribosomal protein L41.

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

- Molecule 81 is a protein called 60S ribosomal protein L36a.

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

- Molecule 82 is a protein called 60S ribosomal protein L37a.

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

- Molecule 83 is a protein called 60S ribosomal protein L28.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	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
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

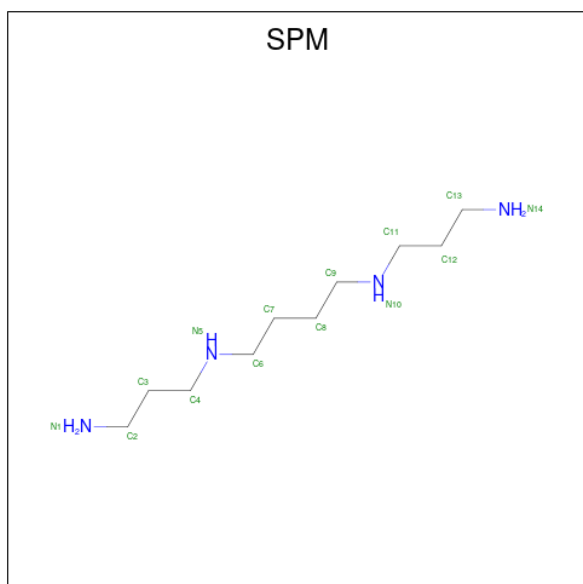
- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
86	SO	1	Total 1	Mg 1	0
86	S2	26	Total 26	Mg 26	0
86	SS	1	Total 1	Mg 1	0
86	L5	179	Total 179	Mg 179	0
86	L7	3	Total 3	Mg 3	0
86	L8	5	Total 5	Mg 5	0
86	LA	1	Total 1	Mg 1	0
86	LP	1	Total 1	Mg 1	0
86	LV	1	Total 1	Mg 1	0
86	Le	1	Total 1	Mg 1	0

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 88 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



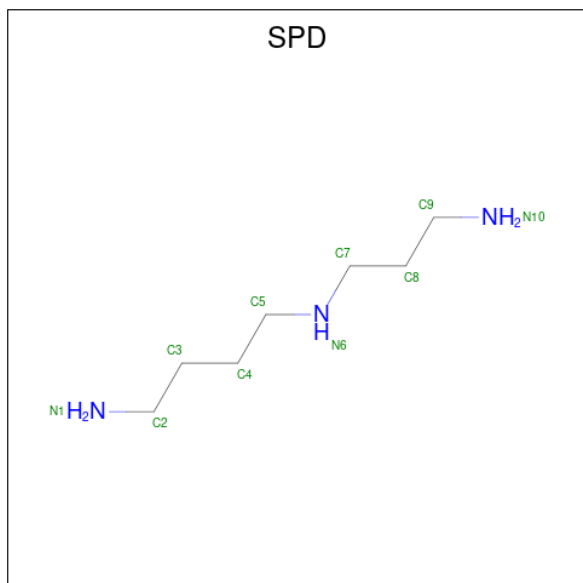
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	

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

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

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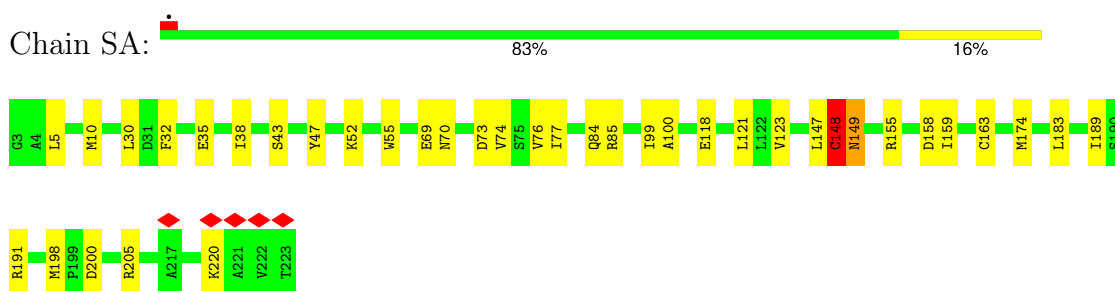
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
89	LN	1	10	7	3	0

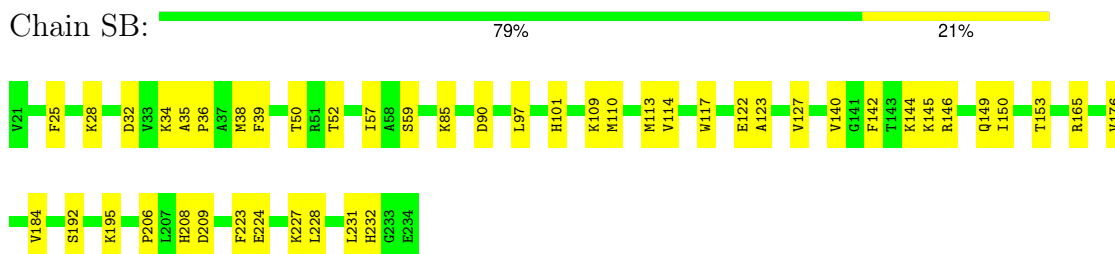
3 Residue-property plots [i](#)

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.

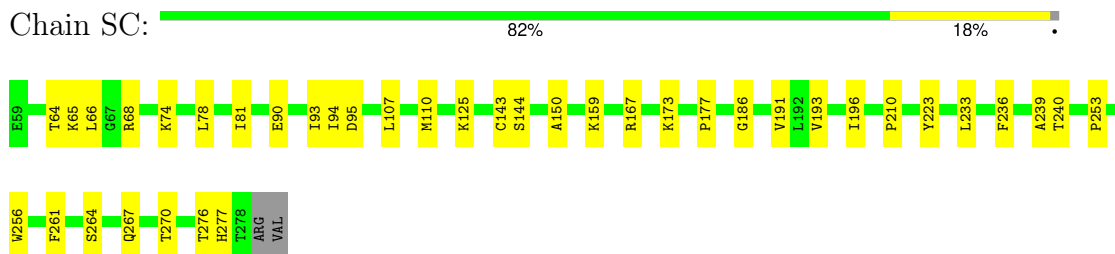
- Molecule 1: 40S ribosomal protein SA



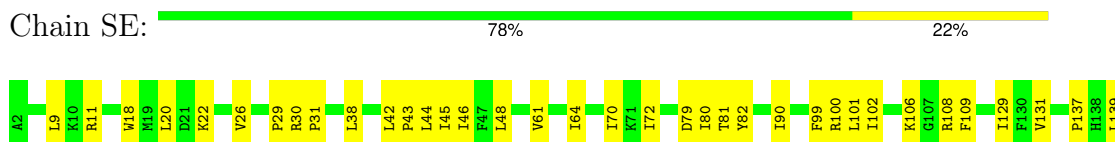
- Molecule 2: 40S ribosomal protein S3a



- Molecule 3: 40S ribosomal protein S2

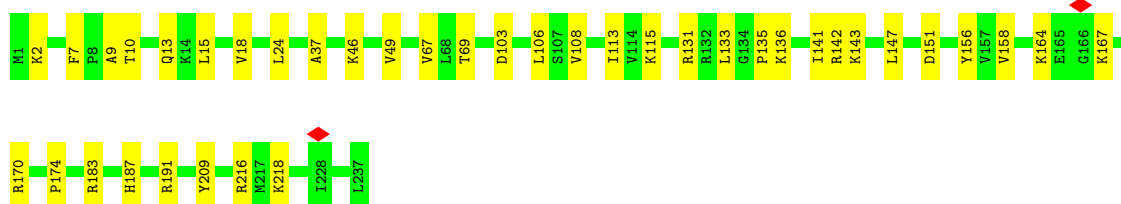
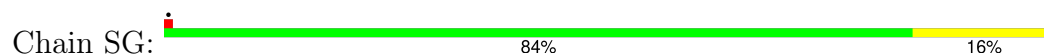


- Molecule 4: Small ribosomal subunit protein eS4, X isoform

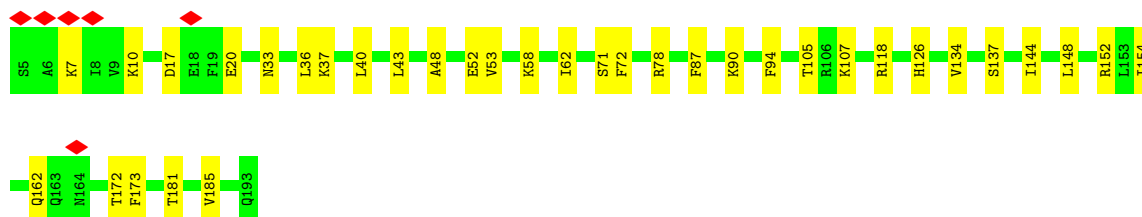
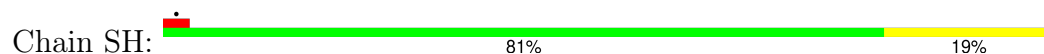




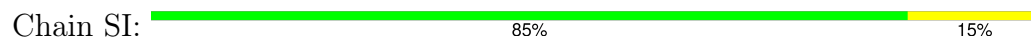
- Molecule 5: 40S ribosomal protein S6



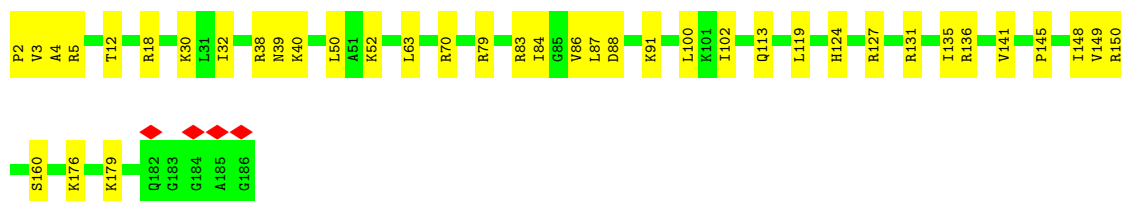
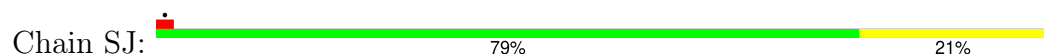
- Molecule 6: Small ribosomal subunit protein eS7



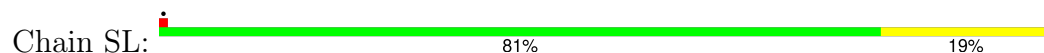
- Molecule 7: 40S ribosomal protein S8

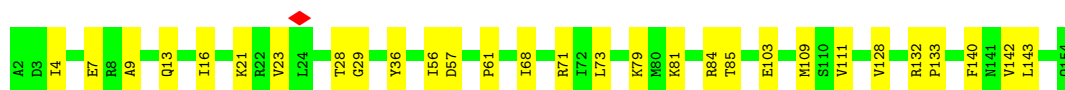


- Molecule 8: 40S ribosomal protein S9



- Molecule 9: 40S ribosomal protein S11

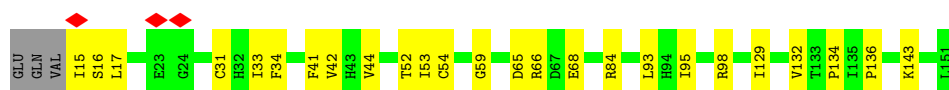
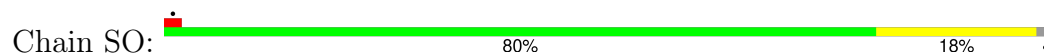




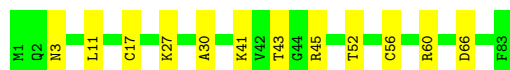
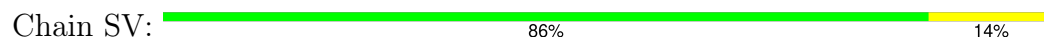
- Molecule 10: 40S ribosomal protein S13



- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein eS21



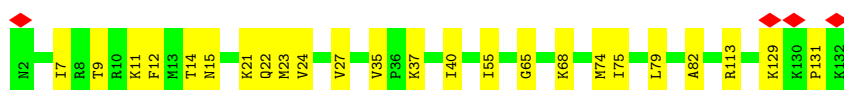
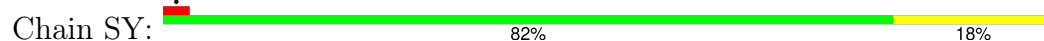
- Molecule 13: 40S ribosomal protein S15a



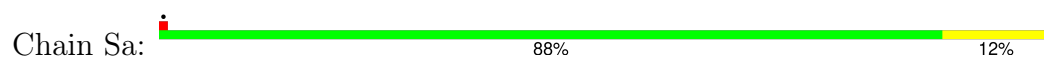
- Molecule 14: 40S ribosomal protein S23



- Molecule 15: 40S ribosomal protein S24

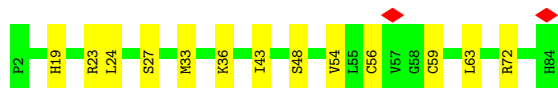
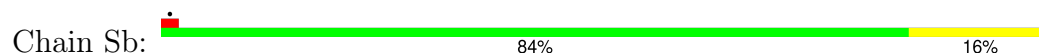


- Molecule 16: 40S ribosomal protein S26

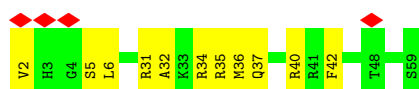
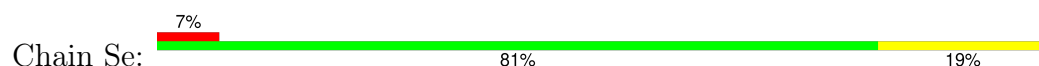




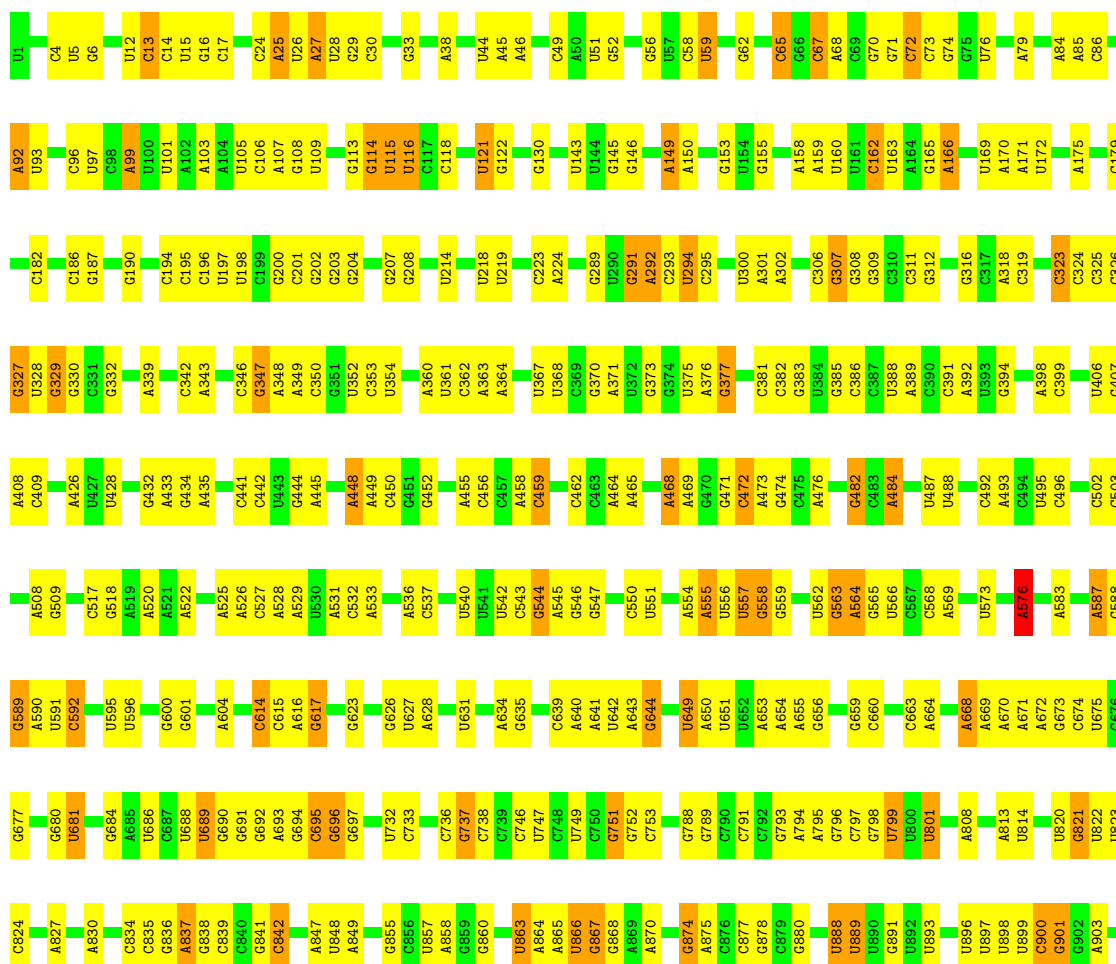
- Molecule 17: Small ribosomal subunit protein eS27



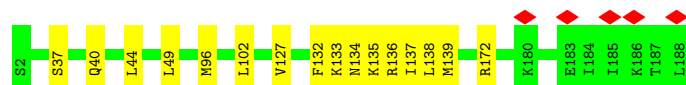
- Molecule 18: Small ribosomal subunit protein eS30



- Molecule 19: 18S rRNA



- Molecule 20: 60S ribosomal protein L19

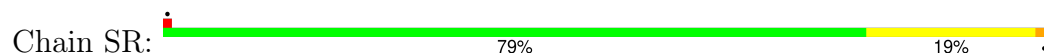


- Molecule 21: Ribosomal protein L24

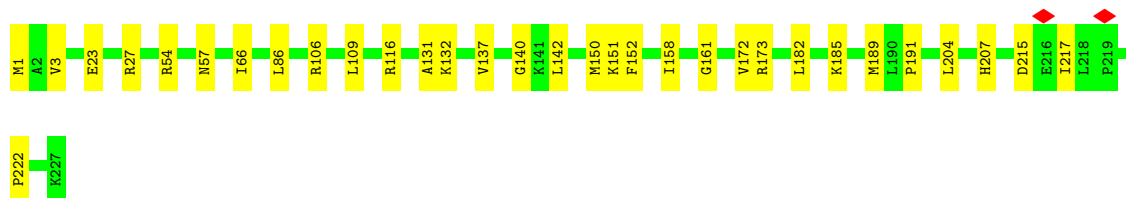




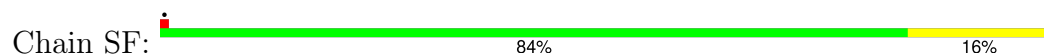
- Molecule 22: Small ribosomal subunit protein eS17



- Molecule 23: Small ribosomal subunit protein uS3



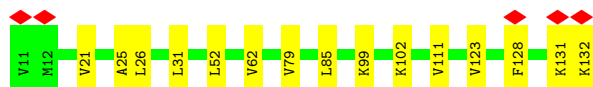
- Molecule 24: 40S ribosomal protein S5



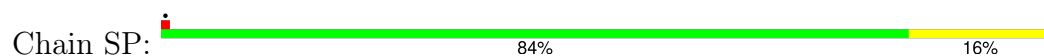
- Molecule 25: 40S ribosomal protein S10



- Molecule 26: Small ribosomal subunit protein eS12

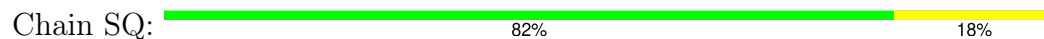


- Molecule 27: Small ribosomal subunit protein uS19

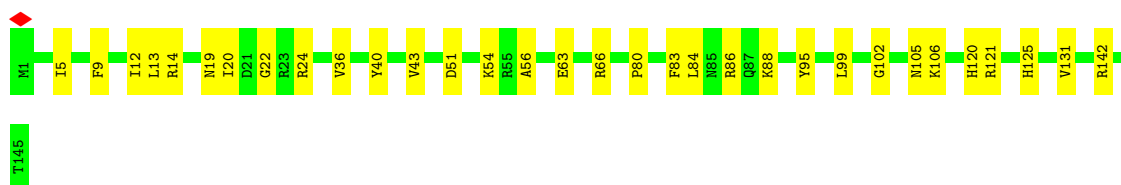
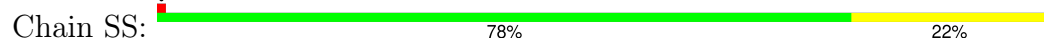




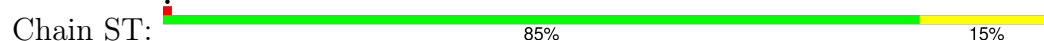
- Molecule 28: Small ribosomal subunit protein uS9



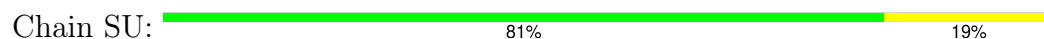
- Molecule 29: 40S ribosomal protein S18



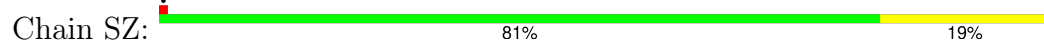
- Molecule 30: 40S ribosomal protein S19



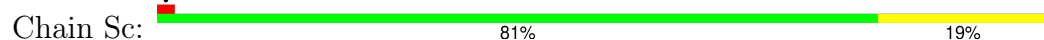
- Molecule 31: 40S ribosomal protein S20



- Molecule 32: Small ribosomal subunit protein eS25



- Molecule 33: 40S ribosomal protein S28



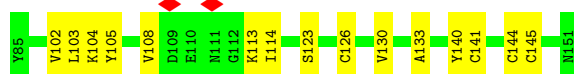
- Molecule 34: 40S ribosomal protein S29

Chain Sd:  82% 18%



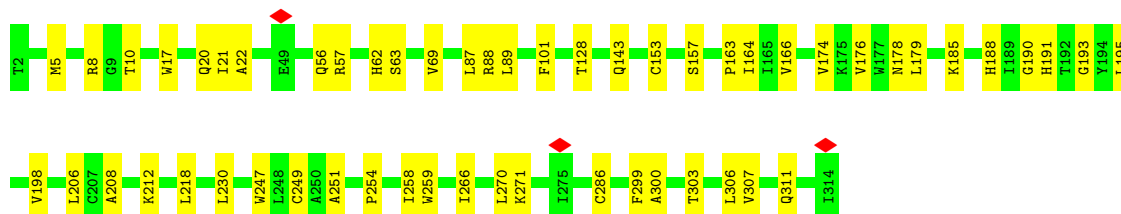
- Molecule 35: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  78% 22%



- Molecule 36: Receptor of activated protein C kinase 1

Chain Sg:  82% 18%

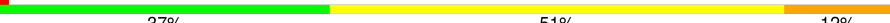


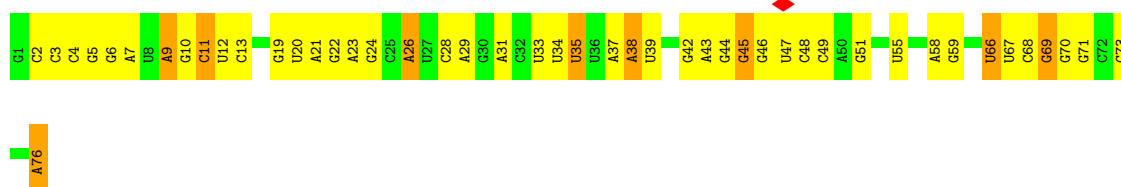
- Molecule 37: A site tRNA

Chain At:  59% 39%



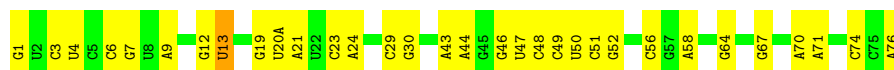
- Molecule 38: E site tRNA

Chain Et:  37% 51% 12%



- Molecule 39: P site tRNA [Homo sapiens]

Chain Pt:  57% 42%



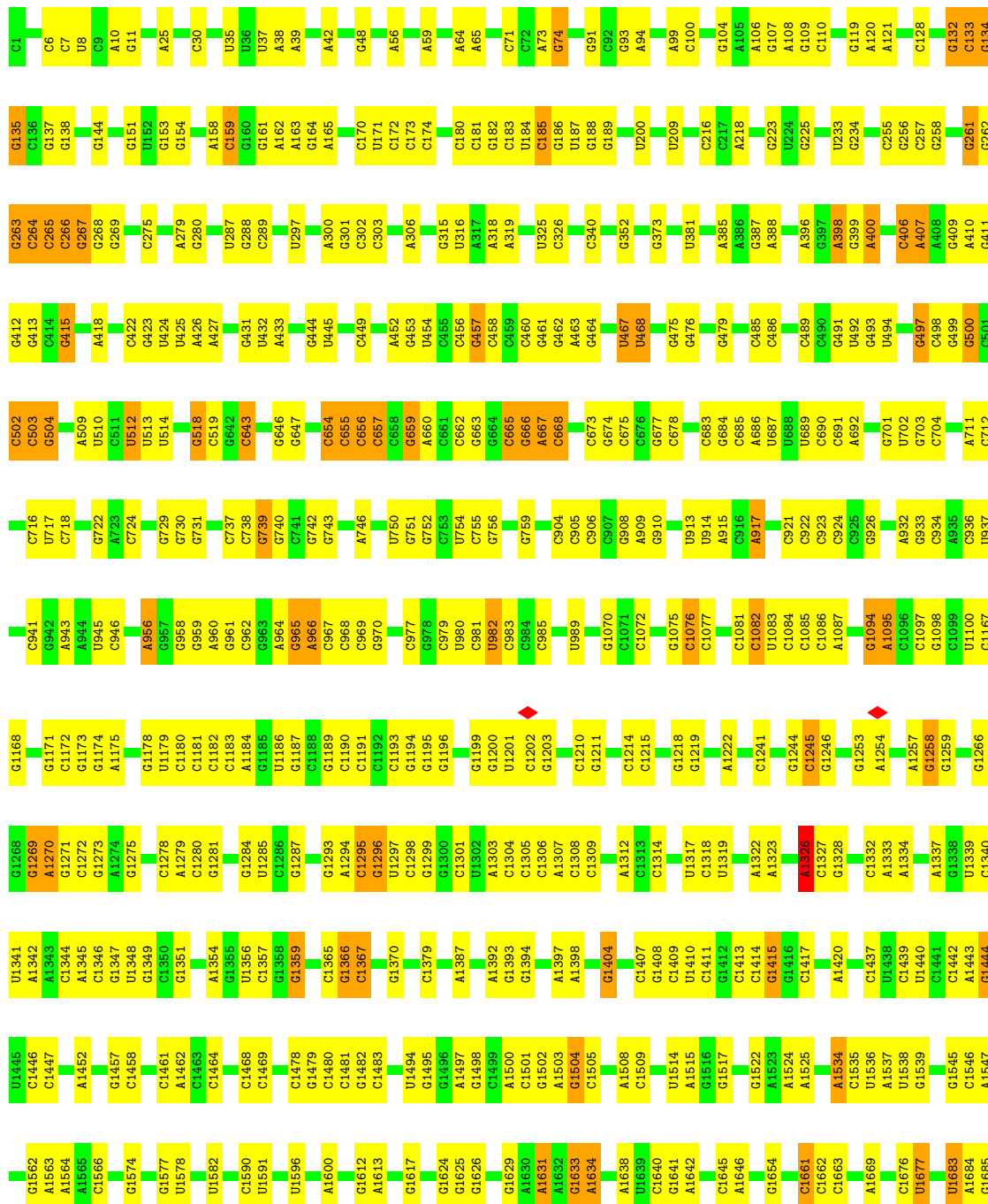
- Molecule 40: Transcription factor BTF3

Chain CI:  100%

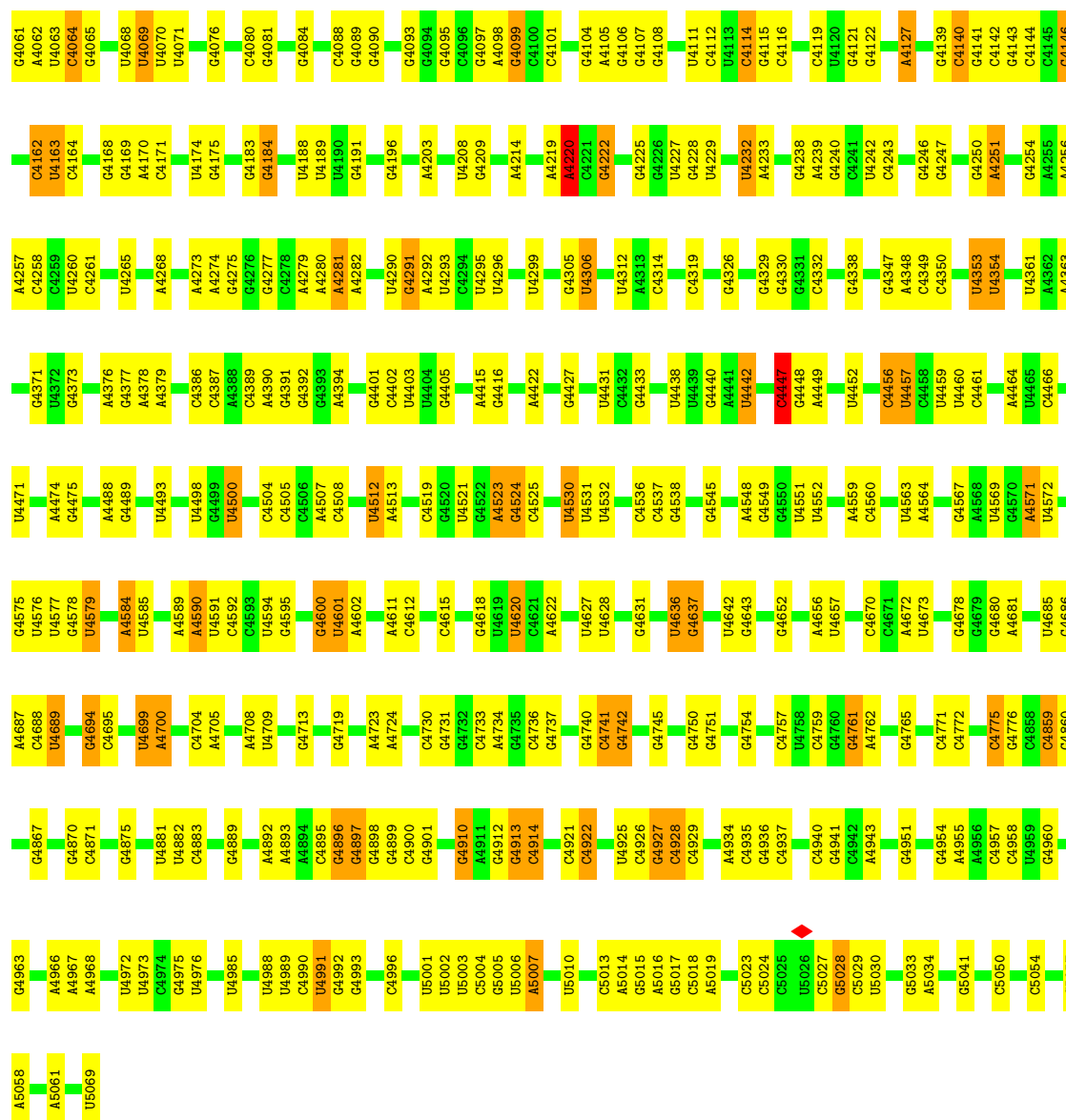


- Molecule 41: 28S rRNA

Chain L5:  60% 34% 5%







- Molecule 42: 5S rRNA [Homo sapiens]

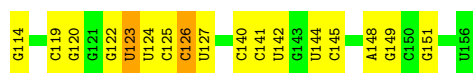
Chain L7: 80% 17%



- Molecule 43: 5.8S rRNA [Homo sapiens]

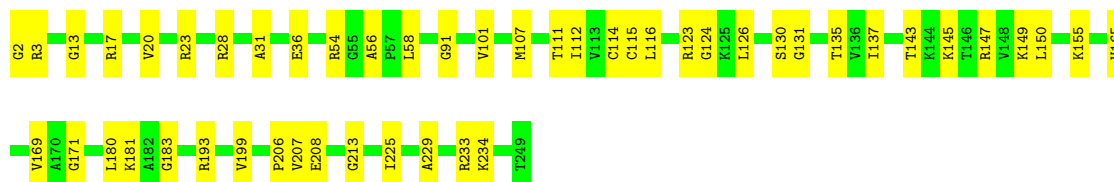
Chain L8: 65% 33%





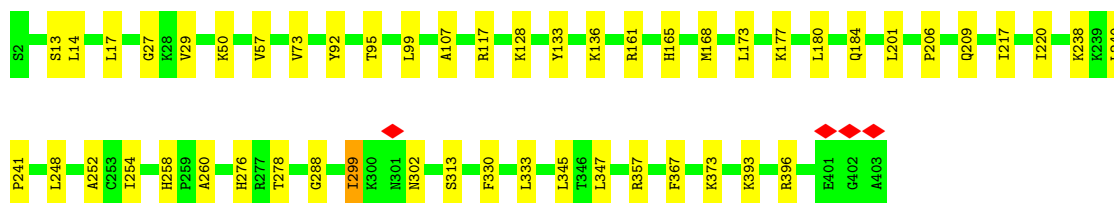
- Molecule 44: 60S ribosomal protein L8

Chain LA: 80% 20%



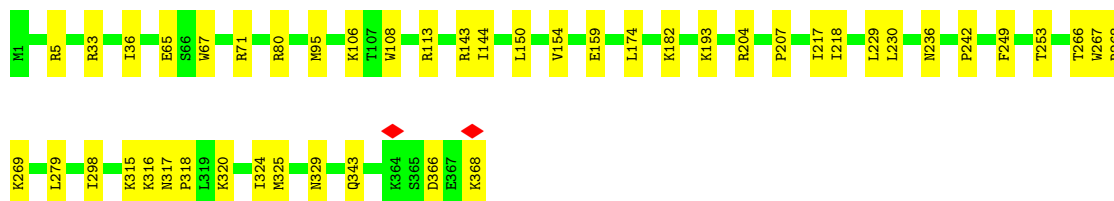
- Molecule 45: Large ribosomal subunit protein uL3

Chain LB: 87% 12%



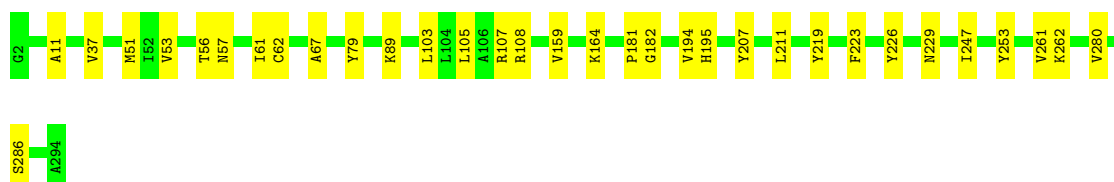
- Molecule 46: 60S ribosomal protein L4

Chain LC: 88% 12%



- Molecule 47: Large ribosomal subunit protein uL18

Chain LD: 89% 11%

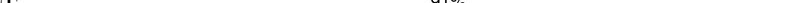


- Molecule 48: Large ribosomal subunit protein eL6

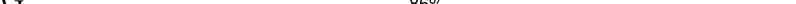
Chain LE: 84% 12%

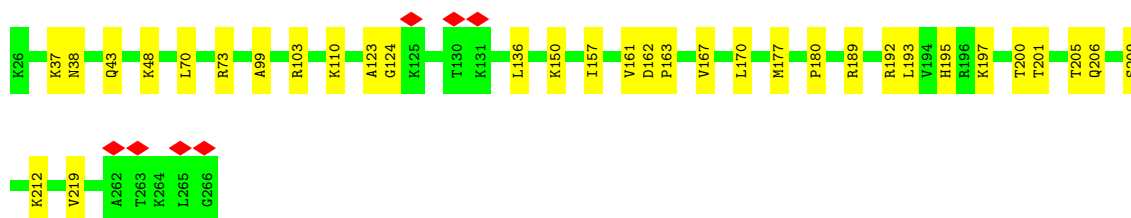




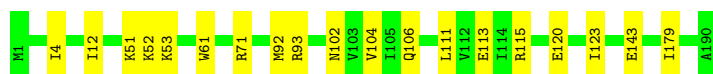
- Chain LF:  91% 9%

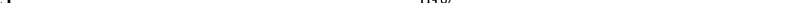


- Chain LG:  86% 14%

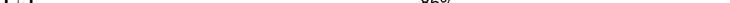


- Chain LH: 90% 10%



- Chain LI:  91% 9%



- Chain LJ:  86% 11% .



- Chain LL: 93% 7%



- Molecule 55: 60S ribosomal protein L14

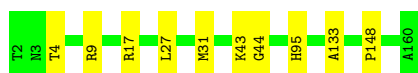
Chain LM: 89% 11%



- Molecule 56: 60S ribosomal protein L15

Chain LN: 94% 6%





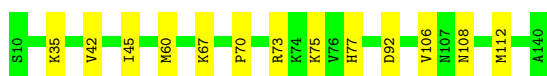
- Molecule 62: Heparin-binding protein HBp15

Chain LU: 86% 14%



- Molecule 63: 60S ribosomal protein L23

Chain LV: 90% 10%



- Molecule 64: 60S ribosomal protein L23a

Chain LX: 95% 5%



- Molecule 65: 60S ribosomal protein L26

Chain LY: 84% 16%



- Molecule 66: 60S ribosomal protein L27

Chain LZ: 94% 6%



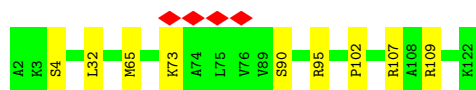
- Molecule 67: 60S ribosomal protein L27a

Chain La: 97% 3%

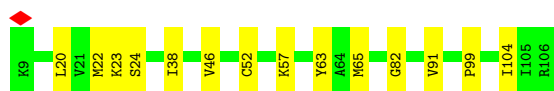
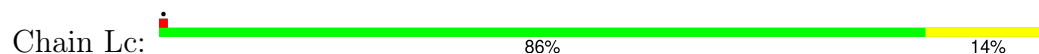


- Molecule 68: Large ribosomal subunit protein eL29

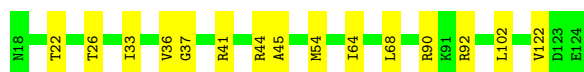
Chain Lb: 92% 8%



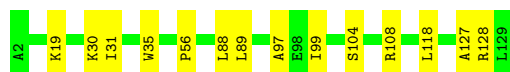
- Molecule 69: 60S ribosomal protein L30



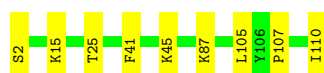
- Molecule 70: 60S ribosomal protein L31



- Molecule 71: 60S ribosomal protein L32



- Molecule 72: 60S ribosomal protein L35a



- Molecule 73: 60S ribosomal protein L34



- Molecule 74: 60S ribosomal protein L35



- Molecule 75: 60S ribosomal protein L36





- Molecule 76: 60S ribosomal protein L37

Chain Lj: 100%

There are no outlier residues recorded for this chain.

- Molecule 77: 60S ribosomal protein L38

Chain Lk: 87% 13%



- Molecule 78: 60S ribosomal protein L39

Chain Ll: 80% 20%



- Molecule 79: Large ribosomal subunit protein eL40

Chain Lm: 90% 10%



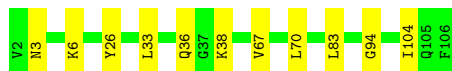
- Molecule 80: 60S ribosomal protein L41

Chain Ln: 88% 12%



- Molecule 81: 60S ribosomal protein L36a

Chain Lo: 90% 10%



- Molecule 82: 60S ribosomal protein L37a

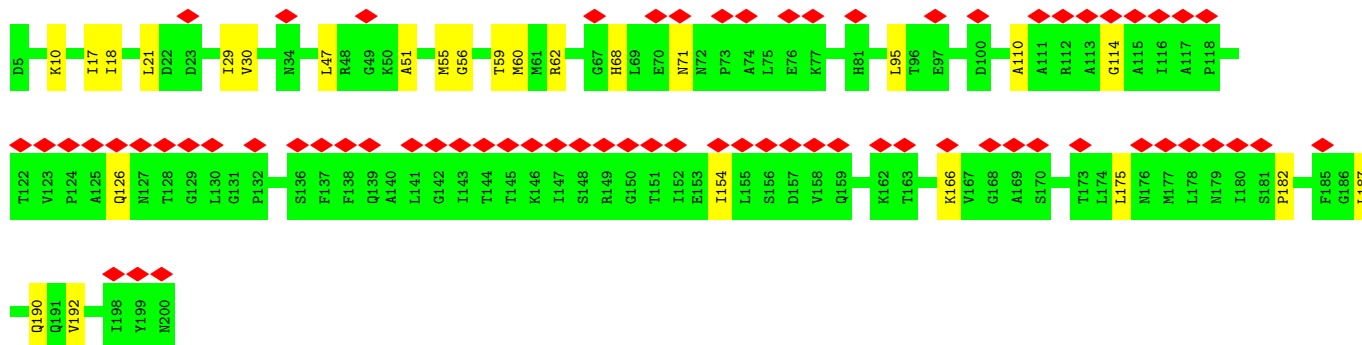
Chain Lp: 96% .



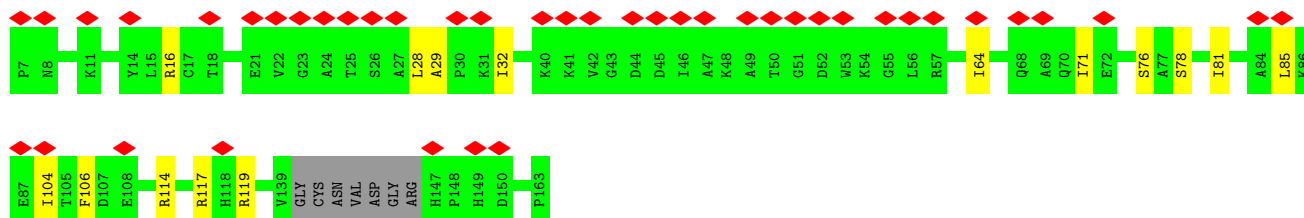
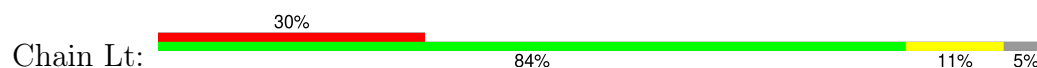
- Molecule 83: 60S ribosomal protein L28



- Molecule 84: 60S acidic ribosomal protein P0



- Molecule 85: Large ribosomal subunit protein uL11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86538	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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	0.186	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0121	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: OMG, UY1, MA6, 1MA, OMU, 4AC, A2M, 6MZ, MG, UR3, OMC, 5MC, B8N, PSU, SPD, SPM, G7M, ZN

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	SA	0.48	3/1778 (0.2%)	0.55	3/2416 (0.1%)
2	SB	0.12	0/1765	0.31	0/2362
3	SC	0.13	0/1744	0.29	0/2357
4	SE	0.14	0/2118	0.32	0/2849
5	SG	0.12	0/1946	0.30	0/2590
6	SH	0.13	0/1519	0.37	0/2033
7	SI	0.14	0/1715	0.34	0/2287
8	SJ	0.12	0/1550	0.30	0/2069
9	SL	0.14	0/1268	0.27	0/1696
10	SN	0.11	0/1232	0.24	0/1656
11	SO	0.13	0/1037	0.32	0/1391
12	SV	0.12	0/643	0.29	0/860
13	SW	0.13	0/1051	0.28	0/1406
14	SX	0.15	0/1116	0.33	0/1490
15	SY	0.15	0/1083	0.35	0/1438
16	Sa	0.14	0/836	0.32	0/1121
17	Sb	0.13	0/665	0.31	0/891
18	Se	0.11	0/465	0.32	0/612
19	S2	0.18	0/39756	0.28	0/61939
20	LR	0.23	0/1582	0.42	0/2091
21	LW	0.16	0/959	0.30	0/1270
22	SR	0.22	0/1105	0.47	0/1484
23	SD	0.11	0/1793	0.27	0/2414
24	SF	0.11	0/1516	0.30	0/2037
25	SK	0.12	0/851	0.31	0/1147
26	SM	0.10	0/950	0.31	0/1275
27	SP	0.12	0/1003	0.32	0/1342
28	SQ	0.12	0/1160	0.32	0/1553
29	SS	0.11	0/1216	0.30	0/1628
30	ST	0.11	0/1131	0.26	0/1515
31	SU	0.12	0/831	0.33	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SZ	0.14	0/604	0.37	0/810
33	Sc	0.12	0/508	0.33	0/680
34	Sd	0.16	0/470	0.34	0/623
35	Sf	0.16	0/560	0.46	0/745
36	Sg	0.13	0/2493	0.34	0/3394
37	At	0.12	0/1692	0.25	0/2634
38	Et	0.13	0/1778	0.31	0/2767
39	Pt	0.12	0/1761	0.27	0/2741
40	CI	0.12	0/247	0.25	0/323
41	L5	0.22	0/85098	0.31	0/132762
42	L7	0.19	0/2861	0.27	0/4459
43	L8	0.20	0/3631	0.29	0/5657
44	LA	0.22	0/1936	0.40	0/2596
45	LB	0.20	0/3306	0.36	1/4424 (0.0%)
46	LC	0.21	0/2981	0.35	0/4002
47	LD	0.17	0/2428	0.30	0/3252
48	LE	0.18	0/1973	0.37	0/2645
49	LF	0.19	0/1905	0.29	0/2539
50	LG	0.18	0/1960	0.36	0/2637
51	LH	0.18	0/1537	0.31	0/2066
52	LI	0.17	0/1751	0.28	0/2340
53	LJ	0.14	0/1385	0.31	0/1852
54	LL	0.18	0/1732	0.29	0/2315
55	LM	0.19	0/1161	0.32	0/1554
56	LN	0.21	0/1746	0.31	0/2338
57	LO	0.23	0/1682	0.32	0/2250
58	LP	0.21	0/1268	0.33	0/1701
59	LQ	0.21	0/1537	0.31	0/2052
60	LS	0.19	0/1493	0.28	0/2003
61	LT	0.18	0/1326	0.30	0/1770
62	LU	0.16	0/839	0.36	0/1126
63	LV	0.19	0/993	0.31	0/1332
64	LX	0.17	0/1002	0.29	0/1345
65	LY	0.20	0/1132	0.32	0/1504
66	LZ	0.17	0/1130	0.31	0/1507
67	La	0.19	0/1191	0.29	0/1591
68	Lb	0.16	0/889	0.31	0/1175
69	Lc	0.18	0/774	0.37	0/1038
70	Ld	0.19	0/903	0.33	0/1216
71	Le	0.20	0/1071	0.30	0/1429
72	Lf	0.20	0/895	0.32	0/1198
73	Lg	0.17	0/916	0.29	0/1220
74	Lh	0.16	0/1023	0.29	0/1351

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Li	0.15	0/843	0.28	0/1115
76	Lj	0.21	0/720	0.34	0/952
77	Lk	0.17	0/575	0.31	0/761
78	Ll	0.19	0/454	0.24	0/599
79	Lm	0.17	0/435	0.32	0/575
80	Ln	0.16	0/231	0.23	0/294
81	Lo	0.19	0/876	0.31	0/1156
82	Lp	0.18	0/718	0.30	0/953
83	Lr	0.19	0/1017	0.31	0/1364
84	Ls	0.11	0/1519	0.32	0/2052
85	Lt	0.16	0/1009	0.46	0/1363
All	All	0.19	3/233349 (0.0%)	0.31	4/342481 (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
1	SA	0	2
20	LR	0	1
22	SR	0	3
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	149	ASN	CA-CB	-12.65	1.33	1.53
1	SA	148	CYS	CA-CB	9.79	1.70	1.53
1	SA	149	ASN	CA-C	8.75	1.63	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	SA	149	ASN	N-CA-CB	16.35	137.24	111.24
1	SA	149	ASN	N-CA-C	-7.60	96.96	108.52
1	SA	148	CYS	CB-CA-C	-7.32	95.85	110.42
45	LB	299	ILE	N-CA-C	-5.02	108.40	113.47

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	LR	136	ARG	Sidechain
1	SA	205	ARG	Sidechain
1	SA	85	ARG	Sidechain
22	SR	78	ARG	Sidechain
22	SR	80	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	SA	1741	0	1744	24	0
2	SB	1738	0	1809	29	0
3	SC	1707	0	1791	26	0
4	SE	2076	0	2177	39	0
5	SG	1923	0	2089	32	0
6	SH	1497	0	1590	22	0
7	SI	1686	0	1772	20	0
8	SJ	1525	0	1640	27	0
9	SL	1247	0	1323	20	0
10	SN	1208	0	1294	9	0
11	SO	1024	0	1050	18	0
12	SV	636	0	637	9	0
13	SW	1034	0	1080	14	0
14	SX	1098	0	1167	12	0
15	SY	1065	0	1142	15	0
16	Sa	821	0	870	8	0
17	Sb	651	0	670	8	0
18	Se	459	0	503	10	0
19	S2	36952	0	18678	412	0
20	LR	1566	0	1729	11	0
21	LW	945	0	1003	9	0
22	SR	1090	0	1149	18	0
23	SD	1765	0	1865	21	0
24	SF	1495	0	1549	21	0
25	SK	827	0	854	6	0
26	SM	940	0	965	9	0
27	SP	985	0	1031	13	0
28	SQ	1142	0	1213	18	0
29	SS	1198	0	1261	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	ST	1112	0	1146	17	0
31	SU	821	0	883	15	0
32	SZ	598	0	656	9	0
33	Sc	506	0	536	9	0
34	Sd	459	0	449	8	0
35	Sf	548	0	551	11	0
36	Sg	2436	0	2391	34	0
37	At	1514	0	770	15	0
38	Et	1593	0	810	22	0
39	Pt	1576	0	803	14	0
40	CI	247	0	283	0	0
41	L5	78444	0	39718	593	0
42	L7	2561	0	1295	14	0
43	L8	3315	0	1685	25	0
44	LA	1898	0	1993	34	0
45	LB	3238	0	3376	34	0
46	LC	2927	0	3104	32	0
47	LD	2382	0	2410	21	0
48	LE	1935	0	2096	19	0
49	LF	1870	0	1996	15	0
50	LG	1927	0	2074	21	0
51	LH	1518	0	1601	12	0
52	LI	1711	0	1749	14	0
53	LJ	1362	0	1399	11	0
54	LL	1701	0	1818	12	0
55	LM	1138	0	1204	11	0
56	LN	1701	0	1749	11	0
57	LO	1650	0	1794	19	0
58	LP	1242	0	1269	14	0
59	LQ	1513	0	1628	6	0
60	LS	1453	0	1490	5	0
61	LT	1298	0	1366	7	0
62	LU	825	0	850	9	0
63	LV	979	0	1039	7	0
64	LX	985	0	1066	4	0
65	LY	1115	0	1205	13	0
66	LZ	1107	0	1182	5	0
67	La	1162	0	1213	3	0
68	Lb	876	0	948	7	0
69	Lc	764	0	804	9	0
70	Ld	888	0	930	10	0
71	Le	1053	0	1147	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	Lf	876	0	912	6	0
73	Lg	906	0	998	5	0
74	Lh	1015	0	1148	12	0
75	Li	832	0	917	3	0
76	Lj	705	0	737	0	0
77	Lk	569	0	637	6	0
78	Ll	444	0	483	8	0
79	Lm	429	0	465	3	0
80	Ln	230	0	276	4	0
81	Lo	862	0	929	9	0
82	Lp	708	0	756	3	0
83	Lr	1002	0	1068	0	0
84	Ls	1496	0	1540	16	0
85	Lt	998	0	1032	9	0
86	L5	179	0	0	0	0
86	L7	3	0	0	0	0
86	L8	5	0	0	0	0
86	LA	1	0	0	0	0
86	LP	1	0	0	0	0
86	LV	1	0	0	0	0
86	Le	1	0	0	0	0
86	S2	26	0	0	0	0
86	SO	1	0	0	0	0
86	SS	1	0	0	0	0
87	Lg	1	0	0	0	0
87	Lj	1	0	0	0	0
87	Lm	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Sa	1	0	0	0	0
88	L5	98	0	182	4	0
89	L5	80	0	152	3	0
89	L8	10	0	19	0	0
89	LN	10	0	19	0	0
All	All	221484	0	164391	1911	0

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

The worst 5 of 1911 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)
41:L5:1100:U:H3	41:L5:1194:G:H1	1.09	0.98
41:L5:2557:G:H1	41:L5:2570:U:H3	1.04	0.96
19:S2:1652:G:H1	19:S2:1672:U:H3	1.00	0.95
19:S2:1533:A:N6	19:S2:1602:U:H3	1.64	0.94
19:S2:1417:C:N4	19:S2:1422:G:H22	1.66	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SA	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	14	28
2	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	SC	218/222 (98%)	209 (96%)	9 (4%)	0	100	100
4	SE	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
5	SG	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
6	SH	182/186 (98%)	171 (94%)	11 (6%)	0	100	100
7	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
8	SJ	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
9	SL	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
10	SN	148/150 (99%)	144 (97%)	4 (3%)	0	100	100
11	SO	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
12	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
13	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
14	SX	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
15	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
16	Sa	100/102 (98%)	96 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Sb	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
18	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
20	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
21	LW	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
22	SR	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	30
23	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
24	SF	187/189 (99%)	179 (96%)	8 (4%)	0	100	100
25	SK	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
26	SM	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
27	SP	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
28	SQ	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
29	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
30	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
31	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
32	SZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
33	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
34	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
35	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
36	Sg	311/313 (99%)	299 (96%)	12 (4%)	0	100	100
40	CI	29/31 (94%)	29 (100%)	0	0	100	100
44	LA	246/248 (99%)	232 (94%)	14 (6%)	0	100	100
45	LB	400/402 (100%)	384 (96%)	16 (4%)	0	100	100
46	LC	366/368 (100%)	354 (97%)	12 (3%)	0	100	100
47	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
48	LE	236/250 (94%)	220 (93%)	16 (7%)	0	100	100
49	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
50	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
51	LH	188/190 (99%)	180 (96%)	8 (4%)	0	100	100
52	LI	211/213 (99%)	208 (99%)	3 (1%)	0	100	100
53	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
54	LL	208/210 (99%)	202 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	LM	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
56	LN	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
57	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
58	LP	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
59	LQ	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
60	LS	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
61	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
62	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
63	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
64	LX	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
65	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
66	LZ	133/135 (98%)	124 (93%)	9 (7%)	0	100	100
67	La	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
68	Lb	105/109 (96%)	101 (96%)	4 (4%)	0	100	100
69	Lc	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
70	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
71	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
72	Lf	107/109 (98%)	107 (100%)	0	0	100	100
73	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
74	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
75	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
76	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
77	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
78	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
79	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
80	Ln	22/24 (92%)	22 (100%)	0	0	100	100
81	Lo	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
82	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
83	Lr	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
84	Ls	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
85	Lt	128/141 (91%)	108 (84%)	20 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11672/11870 (98%)	11211 (96%)	458 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	SA	148	CYS
1	SA	147	LEU
22	SR	129	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	SA	183/183 (100%)	183 (100%)	0	100	100
2	SB	195/195 (100%)	195 (100%)	0	100	100
3	SC	186/188 (99%)	186 (100%)	0	100	100
4	SE	224/224 (100%)	224 (100%)	0	100	100
5	SG	207/207 (100%)	207 (100%)	0	100	100
6	SH	166/166 (100%)	166 (100%)	0	100	100
7	SI	178/178 (100%)	178 (100%)	0	100	100
8	SJ	161/161 (100%)	161 (100%)	0	100	100
9	SL	137/137 (100%)	137 (100%)	0	100	100
10	SN	130/130 (100%)	130 (100%)	0	100	100
11	SO	107/110 (97%)	107 (100%)	0	100	100
12	SV	67/67 (100%)	67 (100%)	0	100	100
13	SW	112/112 (100%)	112 (100%)	0	100	100
14	SX	113/113 (100%)	113 (100%)	0	100	100
15	SY	113/113 (100%)	112 (99%)	1 (1%)	70	82
16	Sa	89/89 (100%)	89 (100%)	0	100	100
17	Sb	75/75 (100%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Se	47/47 (100%)	47 (100%)	0	100	100
20	LR	166/166 (100%)	166 (100%)	0	100	100
21	LW	95/97 (98%)	95 (100%)	0	100	100
22	SR	122/122 (100%)	121 (99%)	1 (1%)	73	84
23	SD	190/190 (100%)	190 (100%)	0	100	100
24	SF	159/159 (100%)	159 (100%)	0	100	100
25	SK	89/89 (100%)	89 (100%)	0	100	100
26	SM	102/104 (98%)	102 (100%)	0	100	100
27	SP	107/107 (100%)	107 (100%)	0	100	100
28	SQ	119/119 (100%)	119 (100%)	0	100	100
29	SS	126/126 (100%)	126 (100%)	0	100	100
30	ST	113/113 (100%)	113 (100%)	0	100	100
31	SU	94/94 (100%)	94 (100%)	0	100	100
32	SZ	66/66 (100%)	66 (100%)	0	100	100
33	Sc	57/57 (100%)	57 (100%)	0	100	100
34	Sd	48/48 (100%)	48 (100%)	0	100	100
35	Sf	60/60 (100%)	60 (100%)	0	100	100
36	Sg	272/272 (100%)	272 (100%)	0	100	100
40	CI	25/25 (100%)	25 (100%)	0	100	100
44	LA	190/190 (100%)	190 (100%)	0	100	100
45	LB	348/348 (100%)	348 (100%)	0	100	100
46	LC	306/306 (100%)	306 (100%)	0	100	100
47	LD	246/247 (100%)	246 (100%)	0	100	100
48	LE	212/222 (96%)	212 (100%)	0	100	100
49	LF	194/194 (100%)	194 (100%)	0	100	100
50	LG	203/205 (99%)	203 (100%)	0	100	100
51	LH	169/169 (100%)	169 (100%)	0	100	100
52	LI	180/180 (100%)	180 (100%)	0	100	100
53	LJ	143/148 (97%)	143 (100%)	0	100	100
54	LL	176/176 (100%)	176 (100%)	0	100	100
55	LM	118/118 (100%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	LN	171/171 (100%)	171 (100%)	0	100	100
57	LO	173/173 (100%)	173 (100%)	0	100	100
58	LP	134/134 (100%)	134 (100%)	0	100	100
59	LQ	164/164 (100%)	164 (100%)	0	100	100
60	LS	156/156 (100%)	156 (100%)	0	100	100
61	LT	139/139 (100%)	139 (100%)	0	100	100
62	LU	91/91 (100%)	91 (100%)	0	100	100
63	LV	101/101 (100%)	101 (100%)	0	100	100
64	LX	108/108 (100%)	108 (100%)	0	100	100
65	LY	124/124 (100%)	124 (100%)	0	100	100
66	LZ	117/117 (100%)	117 (100%)	0	100	100
67	La	120/120 (100%)	120 (100%)	0	100	100
68	Lb	88/90 (98%)	88 (100%)	0	100	100
69	Lc	83/83 (100%)	83 (100%)	0	100	100
70	Ld	98/98 (100%)	98 (100%)	0	100	100
71	Le	114/114 (100%)	114 (100%)	0	100	100
72	Lf	88/88 (100%)	88 (100%)	0	100	100
73	Lg	98/98 (100%)	98 (100%)	0	100	100
74	Lh	109/109 (100%)	109 (100%)	0	100	100
75	Li	86/86 (100%)	86 (100%)	0	100	100
76	Lj	73/73 (100%)	73 (100%)	0	100	100
77	Lk	64/64 (100%)	64 (100%)	0	100	100
78	Ll	47/47 (100%)	47 (100%)	0	100	100
79	Lm	48/48 (100%)	48 (100%)	0	100	100
80	Ln	23/23 (100%)	23 (100%)	0	100	100
81	Lo	93/93 (100%)	93 (100%)	0	100	100
82	Lp	74/74 (100%)	74 (100%)	0	100	100
83	Lr	109/109 (100%)	109 (100%)	0	100	100
84	Ls	162/164 (99%)	162 (100%)	0	100	100
85	Lt	107/115 (93%)	107 (100%)	0	100	100
All	All	10147/10186 (100%)	10145 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	SY	15	ASN
22	SR	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
50	LG	94	GLN
57	LO	199	HIS
84	Ls	190	GLN
51	LH	102	ASN
55	LM	48	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S2	1715/1740 (98%)	390 (22%)	5 (0%)
37	At	69/71 (97%)	11 (15%)	0
38	Et	73/75 (97%)	29 (39%)	0
39	Pt	72/74 (97%)	14 (19%)	0
41	L5	3643/3655 (99%)	786 (21%)	15 (0%)
42	L7	119/120 (99%)	10 (8%)	0
43	L8	155/156 (99%)	25 (16%)	0
All	All	5846/5891 (99%)	1265 (21%)	20 (0%)

5 of 1265 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	S2	13	C
19	S2	14	C
19	S2	17	C
19	S2	25	A
19	S2	33	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	L5	2760	G
41	L5	4600	G
41	L5	4913	G

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Mol	Chain	Res	Type
41	L5	4699	U
41	L5	914	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

178 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$
41	PSU	L5	4579	41	18,21,22	1.07	1 (5%)	21,30,33	1.85	4 (19%)
41	PSU	L5	4673	41,86	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
19	OMC	S2	517	19	19,22,23	0.54	0	25,31,34	0.73	0
19	PSU	S2	686	19	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
19	PSU	S2	651	19	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
19	A2M	S2	668	86,19	22,25,26	1.30	2 (9%)	30,36,39	1.57	6 (20%)
41	PSU	L5	4403	41	18,21,22	1.08	1 (5%)	21,30,33	1.90	6 (28%)
41	PSU	L5	4532	41	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)
41	OMC	L5	3808	41	19,22,23	0.62	0	25,31,34	0.84	1 (4%)
19	OMU	S2	354	19	19,22,23	3.32	7 (36%)	25,31,34	1.77	5 (20%)
19	A2M	S2	468	19	22,25,26	1.24	1 (4%)	30,36,39	1.56	7 (23%)
19	OMU	S2	627	19	19,22,23	3.36	7 (36%)	25,31,34	1.82	5 (20%)
41	UR3	L5	4530	41	19,22,23	2.73	7 (36%)	26,32,35	1.59	3 (11%)
19	PSU	S2	1174	19	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
41	PSU	L5	3920	41,86	18,21,22	1.06	1 (5%)	21,30,33	1.92	5 (23%)
41	PSU	L5	1860	41	18,21,22	1.14	1 (5%)	21,30,33	1.86	4 (19%)
19	OMU	S2	121	19	19,22,23	3.34	7 (36%)	25,31,34	1.75	4 (16%)
41	PSU	L5	4552	41	18,21,22	1.12	2 (11%)	21,30,33	1.95	4 (19%)
41	PSU	L5	4493	41	18,21,22	1.07	1 (5%)	21,30,33	1.87	4 (19%)
41	OMG	L5	1316	41	23,26,27	0.56	0	32,38,41	0.56	0
19	OMU	S2	116	19	19,22,23	3.32	7 (36%)	25,31,34	1.67	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	A2M	S2	1031	19	22,25,26	1.20	1 (4%)	30,36,39	1.52	7 (23%)
41	OMC	L5	2861	41	19,22,23	0.57	0	25,31,34	0.82	1 (4%)
19	OMC	S2	1272	19	19,22,23	0.54	0	25,31,34	0.69	0
41	OMG	L5	1625	41	23,26,27	0.52	0	32,38,41	0.47	0
41	A2M	L5	3718	41	22,25,26	1.18	1 (4%)	30,36,39	1.53	6 (20%)
19	OMC	S2	1391	19	19,22,23	0.51	0	25,31,34	0.70	0
41	PSU	L5	1744	41,86	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
41	OMG	L5	4637	41	23,26,27	0.51	0	32,38,41	0.50	0
41	OMG	L5	4618	41	23,26,27	0.55	0	32,38,41	0.49	0
41	OMG	L5	3627	41	23,26,27	0.53	0	32,38,41	0.59	0
19	PSU	S2	681	19	18,21,22	1.04	1 (5%)	21,30,33	1.83	4 (19%)
41	PSU	L5	1782	41	18,21,22	1.10	1 (5%)	21,30,33	1.82	4 (19%)
41	PSU	L5	2632	41	18,21,22	1.05	1 (5%)	21,30,33	1.94	5 (23%)
19	OMC	S2	1703	19	19,22,23	0.53	0	25,31,34	0.66	0
41	OMG	L5	4228	41	23,26,27	0.55	0	32,38,41	0.71	0
19	OMG	S2	509	19	23,26,27	0.49	0	32,38,41	0.49	0
41	PSU	L5	4312	41	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)
41	OMC	L5	2365	41	19,22,23	0.55	0	25,31,34	0.56	0
41	OMU	L5	2837	41	19,22,23	3.31	7 (36%)	25,31,34	1.89	5 (20%)
19	PSU	S2	966	19	18,21,22	1.13	1 (5%)	21,30,33	1.93	4 (19%)
19	OMU	S2	428	19	19,22,23	3.36	7 (36%)	25,31,34	1.83	5 (20%)
41	PSU	L5	4296	41	18,21,22	1.08	1 (5%)	21,30,33	1.92	4 (19%)
41	PSU	L5	2839	41	18,21,22	1.09	2 (11%)	21,30,33	1.86	4 (19%)
41	A2M	L5	4590	41	22,25,26	1.20	1 (4%)	30,36,39	1.57	6 (20%)
41	PSU	L5	4293	41	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
41	OMC	L5	4456	41	19,22,23	0.64	0	25,31,34	0.79	1 (4%)
19	PSU	S2	649	19	18,21,22	1.10	1 (5%)	21,30,33	1.83	4 (19%)
19	PSU	S2	406	19	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
19	OMG	S2	1328	19	23,26,27	0.47	0	32,38,41	0.47	0
19	PSU	S2	1244	19	18,21,22	1.10	1 (5%)	21,30,33	1.92	5 (23%)
19	6MZ	S2	1832	86,19	22,25,26	4.02	11 (50%)	29,36,39	2.33	10 (34%)
41	PSU	L5	4972	41	18,21,22	1.08	1 (5%)	21,30,33	1.86	4 (19%)
41	OMG	L5	3744	41	23,26,27	0.51	0	32,38,41	0.51	0
41	PSU	L5	4521	41,86	18,21,22	1.10	1 (5%)	21,30,33	1.95	5 (23%)
41	PSU	L5	1536	41	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
19	OMC	S2	462	19	19,22,23	0.54	0	25,31,34	0.73	1 (4%)
41	PSU	L5	3695	41	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	OMG	L8	75	43	23,26,27	0.54	0	32,38,41	0.48	0
19	OMU	S2	1442	19	19,22,23	3.40	7 (36%)	25,31,34	1.81	4 (16%)
41	OMC	L5	2422	41,86	19,22,23	0.57	0	25,31,34	0.73	1 (4%)
19	OMG	S2	867	19	23,26,27	0.49	0	32,38,41	0.48	0
19	OMU	S2	799	19	19,22,23	3.40	7 (36%)	25,31,34	1.81	5 (20%)
41	OMC	L5	2351	41,86	19,22,23	0.59	0	25,31,34	0.76	1 (4%)
41	PSU	L5	4636	41	18,21,22	1.11	2 (11%)	21,30,33	2.09	6 (28%)
41	A2M	L5	3825	41	22,25,26	1.19	1 (4%)	30,36,39	1.55	8 (26%)
19	PSU	S2	1056	19	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
41	PSU	L5	4299	41	18,21,22	1.10	1 (5%)	21,30,33	1.81	4 (19%)
41	OMG	L5	4623	41	23,26,27	0.51	0	32,38,41	0.55	0
19	MA6	S2	1850	19	23,26,27	2.65	8 (34%)	33,38,41	3.36	13 (39%)
41	OMG	L5	2364	41,86	23,26,27	0.53	0	32,38,41	0.43	0
19	A2M	S2	27	19	22,25,26	1.21	1 (4%)	30,36,39	1.51	6 (20%)
41	PSU	L5	3844	41	18,21,22	1.11	1 (5%)	21,30,33	1.77	4 (19%)
41	OMG	L5	2424	41	23,26,27	0.52	0	32,38,41	0.45	0
41	OMC	L5	1340	41	19,22,23	0.55	0	25,31,34	0.74	0
41	OMC	L5	2804	41	19,22,23	0.55	0	25,31,34	0.64	0
19	PSU	S2	1045	19	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
41	A2M	L5	4523	41,86	22,25,26	1.23	1 (4%)	30,36,39	1.51	7 (23%)
41	A2M	L5	4571	41	22,25,26	1.28	2 (9%)	30,36,39	1.54	7 (23%)
41	A2M	L5	3830	41	22,25,26	1.20	1 (4%)	30,36,39	1.55	5 (16%)
41	OMC	L5	3869	41	19,22,23	0.58	0	25,31,34	0.60	0
19	OMG	S2	1490	19	23,26,27	0.50	0	32,38,41	0.47	0
41	OMG	L5	3792	41	23,26,27	0.51	0	32,38,41	0.53	0
41	PSU	L5	1582	41	18,21,22	1.07	1 (5%)	21,30,33	1.73	4 (19%)
41	A2M	L5	1524	41	22,25,26	1.27	2 (9%)	30,36,39	1.52	6 (20%)
41	OMC	L5	2824	41	19,22,23	0.56	0	25,31,34	0.71	1 (4%)
41	PSU	L5	1677	41	18,21,22	1.09	2 (11%)	21,30,33	2.01	6 (28%)
41	PSU	L5	4361	41	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
19	PSU	S2	801	19	18,21,22	1.14	1 (5%)	21,30,33	1.81	4 (19%)
41	OMG	L5	4392	41	23,26,27	0.53	0	32,38,41	0.52	0
41	OMU	L5	3925	41	19,22,23	3.28	7 (36%)	25,31,34	1.80	5 (20%)
19	4AC	S2	1842	19	21,24,25	0.38	0	28,34,37	0.47	0
19	PSU	S2	1046	19	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
19	PSU	S2	1232	19	18,21,22	1.15	1 (5%)	21,30,33	1.91	4 (19%)
41	PSU	L5	1862	41	18,21,22	1.08	1 (5%)	21,30,33	1.92	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	OMG	L5	4370	41	23,26,27	0.52	0	32,38,41	0.51	0
41	5MC	L5	4447	41	19,22,23	0.74	0	26,32,35	0.69	1 (3%)
41	OMG	L5	2876	41	23,26,27	0.52	0	32,38,41	0.47	0
41	OMC	L5	3887	41	19,22,23	0.56	0	25,31,34	0.65	0
19	G7M	S2	1639	19,39	23,26,27	2.66	9 (39%)	34,39,42	2.65	11 (32%)
19	PSU	S2	1177	19	18,21,22	1.13	1 (5%)	21,30,33	1.89	4 (19%)
41	1MA	L5	1322	41,86	21,25,26	0.55	0	30,37,40	0.79	2 (6%)
41	PSU	L5	3851	41	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
41	PSU	L5	4628	41	18,21,22	1.05	1 (5%)	21,30,33	1.82	4 (19%)
43	PSU	L8	69	43	18,21,22	1.09	1 (5%)	21,30,33	1.92	5 (23%)
41	A2M	L5	1534	41,86	22,25,26	1.16	1 (4%)	30,36,39	1.44	7 (23%)
41	A2M	L5	2401	41	22,25,26	1.20	1 (4%)	30,36,39	1.55	7 (23%)
19	A2M	S2	576	19	22,25,26	1.21	1 (4%)	30,36,39	1.50	4 (13%)
41	OMC	L5	4536	41	19,22,23	0.58	0	25,31,34	0.65	0
41	PSU	L5	4576	41	18,21,22	1.11	1 (5%)	21,30,33	1.89	6 (28%)
19	OMU	S2	172	19	19,22,23	3.35	7 (36%)	25,31,34	1.86	5 (20%)
41	PSU	L5	3853	41,86	18,21,22	1.05	1 (5%)	21,30,33	1.84	4 (19%)
41	5MC	L5	3782	41,86	19,22,23	0.59	0	26,32,35	0.76	0
41	PSU	L5	3884	41	18,21,22	1.11	2 (11%)	21,30,33	1.90	4 (19%)
19	A2M	S2	484	19	22,25,26	1.19	1 (4%)	30,36,39	1.46	5 (16%)
41	PSU	L5	4431	41	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
41	OMU	L5	4498	41	19,22,23	3.31	7 (36%)	25,31,34	1.84	5 (20%)
19	PSU	S2	863	19	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
19	B8N	S2	1248	19	25,29,30	3.27	6 (24%)	28,42,45	2.04	7 (25%)
41	OMU	L5	4306	41	19,22,23	3.27	7 (36%)	25,31,34	1.74	4 (16%)
41	A2M	L5	2787	41	22,25,26	1.17	1 (4%)	30,36,39	1.49	8 (26%)
41	OMG	L5	3899	41	23,26,27	0.56	0	32,38,41	0.51	0
19	A2M	S2	166	19	22,25,26	1.26	1 (4%)	30,36,39	1.55	7 (23%)
19	A2M	S2	1383	19	22,25,26	1.21	1 (4%)	30,36,39	1.66	7 (23%)
41	A2M	L5	3867	41	22,25,26	1.21	1 (4%)	30,36,39	1.48	9 (30%)
19	OMG	S2	601	19	23,26,27	0.50	0	32,38,41	0.45	0
41	OMC	L5	3841	41	19,22,23	0.56	0	25,31,34	0.60	0
41	A2M	L5	400	41	22,25,26	1.24	2 (9%)	30,36,39	1.55	8 (26%)
19	4AC	S2	1337	19	21,24,25	0.38	0	28,34,37	0.72	1 (3%)
19	OMC	S2	174	19	19,22,23	0.52	0	25,31,34	0.61	0
19	PSU	S2	109	19	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PSU	S2	1367	19	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
41	PSU	L5	3637	41	18,21,22	1.10	1 (5%)	21,30,33	2.01	5 (23%)
19	OMU	S2	1326	19	19,22,23	3.36	7 (36%)	25,31,34	1.81	5 (20%)
19	OMG	S2	436	19	23,26,27	0.48	0	32,38,41	0.56	0
19	PSU	S2	1004	19	18,21,22	1.10	1 (5%)	21,30,33	1.82	4 (19%)
41	PSU	L5	1683	41	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
41	PSU	L5	3639	41	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
41	OMG	L5	4196	41,39	23,26,27	0.50	0	32,38,41	0.47	0
41	PSU	L5	1792	41	18,21,22	1.04	1 (5%)	21,30,33	1.82	4 (19%)
41	PSU	L5	4973	41	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
41	PSU	L5	4457	41	18,21,22	1.08	1 (5%)	21,30,33	1.97	6 (28%)
41	A2M	L5	2363	41,86	22,25,26	1.20	2 (9%)	30,36,39	1.54	8 (26%)
19	MA6	S2	1851	19	23,26,27	1.28	2 (8%)	33,38,41	3.41	13 (39%)
19	OMG	S2	644	19	23,26,27	0.47	0	32,38,41	0.48	0
41	OMG	L5	1522	41	23,26,27	0.53	0	32,38,41	0.66	1 (3%)
19	PSU	S2	105	19	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
41	PSU	L5	3822	41	18,21,22	1.10	1 (5%)	21,30,33	1.90	5 (23%)
41	PSU	L5	4442	41	18,21,22	1.06	1 (5%)	21,30,33	1.95	6 (28%)
41	UY1	L5	3818	41	19,22,23	4.90	9 (47%)	21,31,34	2.02	5 (23%)
41	PSU	L5	4471	41	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
41	A2M	L5	1326	41	22,25,26	1.21	1 (4%)	30,36,39	1.45	6 (20%)
41	PSU	L5	4353	41	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
41	OMC	L5	3701	41	19,22,23	0.64	0	25,31,34	1.71	4 (16%)
19	A2M	S2	159	19	22,25,26	1.22	1 (4%)	30,36,39	1.53	6 (20%)
41	A2M	L5	1871	41,86	22,25,26	1.21	1 (4%)	30,36,39	1.57	5 (16%)
19	OMG	S2	683	19	23,26,27	0.48	0	32,38,41	0.52	0
41	PSU	L5	5001	41	18,21,22	1.10	1 (5%)	21,30,33	1.82	4 (19%)
19	A2M	S2	99	86,19	22,25,26	1.21	1 (4%)	30,36,39	1.58	7 (23%)
41	A2M	L5	1323	41	22,25,26	1.27	3 (13%)	30,36,39	1.58	8 (26%)
41	PSU	L5	1781	41	18,21,22	1.06	1 (5%)	21,30,33	1.85	4 (19%)
19	OMU	S2	1288	19	19,22,23	3.41	7 (36%)	25,31,34	1.78	4 (16%)
19	PSU	S2	93	19	18,21,22	1.11	1 (5%)	21,30,33	1.79	4 (19%)
41	6MZ	L5	4220	41	22,25,26	2.98	5 (22%)	29,36,39	2.35	10 (34%)
41	OMG	L5	4494	41	23,26,27	0.52	0	32,38,41	0.53	0
41	PSU	L5	5010	41	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
41	PSU	L5	4689	41	18,21,22	1.11	2 (11%)	21,30,33	1.80	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	PSU	L5	4500	41	18,21,22	1.14	1 (5%)	21,30,33	2.00	5 (23%)
41	A2M	L5	398	41	22,25,26	1.20	1 (4%)	30,36,39	1.60	7 (23%)
41	A2M	L5	2815	41	22,25,26	1.18	1 (4%)	30,36,39	1.49	8 (26%)
41	OMG	L5	4499	41	23,26,27	0.49	0	32,38,41	0.47	0
19	PSU	S2	866	19	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
41	OMU	L5	4620	41	19,22,23	3.28	7 (36%)	25,31,34	1.71	4 (16%)
19	PSU	S2	814	19	18,21,22	1.10	1 (5%)	21,30,33	1.83	4 (19%)
43	PSU	L8	55	43	18,21,22	1.09	1 (5%)	21,30,33	1.81	4 (19%)
41	OMU	L5	4227	41	19,22,23	3.31	7 (36%)	25,31,34	1.77	4 (16%)
41	A2M	L5	3785	41,86	22,25,26	1.12	1 (4%)	30,36,39	1.56	9 (30%)
19	PSU	S2	1081	19	18,21,22	1.11	1 (5%)	21,30,33	1.93	6 (28%)

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
41	PSU	L5	4579	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4673	41,86	-	0/7/25/26	0/2/2/2
19	OMC	S2	517	19	-	0/9/27/28	0/2/2/2
19	PSU	S2	686	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	651	19	-	0/7/25/26	0/2/2/2
19	A2M	S2	668	86,19	-	2/9/27/28	0/3/3/3
41	PSU	L5	4403	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4532	41	-	0/7/25/26	0/2/2/2
41	OMC	L5	3808	41	-	0/9/27/28	0/2/2/2
19	OMU	S2	354	19	-	0/9/27/28	0/2/2/2
19	A2M	S2	468	19	-	1/9/27/28	0/3/3/3
19	OMU	S2	627	19	-	0/9/27/28	0/2/2/2
41	UR3	L5	4530	41	-	0/7/25/26	0/2/2/2
19	PSU	S2	1174	19	-	0/7/25/26	0/2/2/2
41	PSU	L5	3920	41,86	-	0/7/25/26	0/2/2/2
41	PSU	L5	1860	41	-	0/7/25/26	0/2/2/2
19	OMU	S2	121	19	-	0/9/27/28	0/2/2/2
41	PSU	L5	4552	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4493	41	-	0/7/25/26	0/2/2/2
41	OMG	L5	1316	41	-	0/9/27/28	0/3/3/3
19	OMU	S2	116	19	-	0/9/27/28	0/2/2/2
19	A2M	S2	1031	19	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	OMC	L5	2861	41	-	1/9/27/28	0/2/2/2
19	OMC	S2	1272	19	-	3/9/27/28	0/2/2/2
41	OMG	L5	1625	41	-	2/9/27/28	0/3/3/3
41	A2M	L5	3718	41	-	0/9/27/28	0/3/3/3
19	OMC	S2	1391	19	-	0/9/27/28	0/2/2/2
41	PSU	L5	1744	41,86	-	0/7/25/26	0/2/2/2
41	OMG	L5	4637	41	-	3/9/27/28	0/3/3/3
41	OMG	L5	4618	41	-	2/9/27/28	0/3/3/3
41	OMG	L5	3627	41	-	0/9/27/28	0/3/3/3
19	PSU	S2	681	19	-	0/7/25/26	0/2/2/2
41	PSU	L5	1782	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	2632	41	-	2/7/25/26	0/2/2/2
19	OMC	S2	1703	19	-	1/9/27/28	0/2/2/2
41	OMG	L5	4228	41	-	0/9/27/28	0/3/3/3
19	OMG	S2	509	19	-	0/9/27/28	0/3/3/3
41	PSU	L5	4312	41	-	0/7/25/26	0/2/2/2
41	OMC	L5	2365	41	-	0/9/27/28	0/2/2/2
41	OMU	L5	2837	41	-	0/9/27/28	0/2/2/2
19	PSU	S2	966	19	-	1/7/25/26	0/2/2/2
19	OMU	S2	428	19	-	6/9/27/28	0/2/2/2
41	PSU	L5	4296	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	2839	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	4590	41	-	3/9/27/28	0/3/3/3
41	PSU	L5	4293	41	-	0/7/25/26	0/2/2/2
41	OMC	L5	4456	41	-	0/9/27/28	0/2/2/2
19	PSU	S2	649	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	406	19	-	0/7/25/26	0/2/2/2
19	OMG	S2	1328	19	-	0/9/27/28	0/3/3/3
19	PSU	S2	1244	19	-	2/7/25/26	0/2/2/2
19	6MZ	S2	1832	86,19	-	2/9/27/28	0/3/3/3
41	PSU	L5	4972	41	-	0/7/25/26	0/2/2/2
41	OMG	L5	3744	41	-	0/9/27/28	0/3/3/3
41	PSU	L5	4521	41,86	-	0/7/25/26	0/2/2/2
41	PSU	L5	1536	41	-	2/7/25/26	0/2/2/2
19	OMC	S2	462	19	-	1/9/27/28	0/2/2/2
41	PSU	L5	3695	41	-	0/7/25/26	0/2/2/2
43	OMG	L8	75	43	-	2/9/27/28	0/3/3/3
19	OMU	S2	1442	19	-	2/9/27/28	0/2/2/2
41	OMC	L5	2422	41,86	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	OMG	S2	867	19	-	2/9/27/28	0/3/3/3
19	OMU	S2	799	19	-	2/9/27/28	0/2/2/2
41	OMC	L5	2351	41,86	-	1/9/27/28	0/2/2/2
41	PSU	L5	4636	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	3825	41	-	0/9/27/28	0/3/3/3
19	PSU	S2	1056	19	-	1/7/25/26	0/2/2/2
41	PSU	L5	4299	41	-	0/7/25/26	0/2/2/2
41	OMG	L5	4623	41	-	0/9/27/28	0/3/3/3
19	MA6	S2	1850	19	-	0/11/29/30	0/3/3/3
41	OMG	L5	2364	41,86	-	2/9/27/28	0/3/3/3
19	A2M	S2	27	19	-	0/9/27/28	0/3/3/3
41	PSU	L5	3844	41	-	1/7/25/26	0/2/2/2
41	OMG	L5	2424	41	-	0/9/27/28	0/3/3/3
41	OMC	L5	1340	41	-	0/9/27/28	0/2/2/2
41	OMC	L5	2804	41	-	0/9/27/28	0/2/2/2
19	PSU	S2	1045	19	-	2/7/25/26	0/2/2/2
41	A2M	L5	4523	41,86	-	1/9/27/28	0/3/3/3
41	A2M	L5	4571	41	-	0/9/27/28	0/3/3/3
41	A2M	L5	3830	41	-	0/9/27/28	0/3/3/3
41	OMC	L5	3869	41	-	0/9/27/28	0/2/2/2
19	OMG	S2	1490	19	-	1/9/27/28	0/3/3/3
41	OMG	L5	3792	41	-	2/9/27/28	0/3/3/3
41	PSU	L5	1582	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	1524	41	-	4/9/27/28	0/3/3/3
41	OMC	L5	2824	41	-	1/9/27/28	0/2/2/2
41	PSU	L5	1677	41	-	2/7/25/26	0/2/2/2
41	PSU	L5	4361	41	-	0/7/25/26	0/2/2/2
19	PSU	S2	801	19	-	2/7/25/26	0/2/2/2
41	OMG	L5	4392	41	-	0/9/27/28	0/3/3/3
41	OMU	L5	3925	41	-	0/9/27/28	0/2/2/2
19	4AC	S2	1842	19	-	0/11/29/30	0/2/2/2
19	PSU	S2	1046	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	1232	19	-	0/7/25/26	0/2/2/2
41	PSU	L5	1862	41	-	0/7/25/26	0/2/2/2
41	OMG	L5	4370	41	-	0/9/27/28	0/3/3/3
41	5MC	L5	4447	41	-	4/7/25/26	0/2/2/2
41	OMG	L5	2876	41	-	0/9/27/28	0/3/3/3
41	OMC	L5	3887	41	-	1/9/27/28	0/2/2/2
19	G7M	S2	1639	19,39	-	0/7/25/26	0/3/3/3
19	PSU	S2	1177	19	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	1MA	L5	1322	41,86	-	2/7/25/26	0/3/3/3
41	PSU	L5	3851	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4628	41	-	0/7/25/26	0/2/2/2
43	PSU	L8	69	43	-	0/7/25/26	0/2/2/2
41	A2M	L5	1534	41,86	-	1/9/27/28	0/3/3/3
41	A2M	L5	2401	41	-	0/9/27/28	0/3/3/3
19	A2M	S2	576	19	-	4/9/27/28	0/3/3/3
41	OMC	L5	4536	41	-	0/9/27/28	0/2/2/2
41	PSU	L5	4576	41	-	0/7/25/26	0/2/2/2
19	OMU	S2	172	19	-	0/9/27/28	0/2/2/2
41	PSU	L5	3853	41,86	-	0/7/25/26	0/2/2/2
41	5MC	L5	3782	41,86	-	2/7/25/26	0/2/2/2
41	PSU	L5	3884	41	-	0/7/25/26	0/2/2/2
19	A2M	S2	484	19	-	0/9/27/28	0/3/3/3
41	PSU	L5	4431	41	-	0/7/25/26	0/2/2/2
41	OMU	L5	4498	41	-	0/9/27/28	0/2/2/2
19	PSU	S2	863	19	-	2/7/25/26	0/2/2/2
19	B8N	S2	1248	19	-	4/16/34/35	0/2/2/2
41	OMU	L5	4306	41	-	0/9/27/28	0/2/2/2
41	A2M	L5	2787	41	-	5/9/27/28	0/3/3/3
41	OMG	L5	3899	41	-	2/9/27/28	0/3/3/3
19	A2M	S2	166	19	-	1/9/27/28	0/3/3/3
19	A2M	S2	1383	19	-	3/9/27/28	0/3/3/3
41	A2M	L5	3867	41	-	3/9/27/28	0/3/3/3
19	OMG	S2	601	19	-	0/9/27/28	0/3/3/3
41	OMC	L5	3841	41	-	0/9/27/28	0/2/2/2
41	A2M	L5	400	41	-	1/9/27/28	0/3/3/3
19	4AC	S2	1337	19	-	1/11/29/30	0/2/2/2
19	OMC	S2	174	19	-	0/9/27/28	0/2/2/2
19	PSU	S2	109	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	1367	19	-	0/7/25/26	0/2/2/2
41	PSU	L5	3637	41	-	0/7/25/26	0/2/2/2
19	OMU	S2	1326	19	-	0/9/27/28	0/2/2/2
19	OMG	S2	436	19	-	0/9/27/28	0/3/3/3
19	PSU	S2	1004	19	-	0/7/25/26	0/2/2/2
41	PSU	L5	1683	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	3639	41	-	0/7/25/26	0/2/2/2
41	OMG	L5	4196	41,39	-	1/9/27/28	0/3/3/3
41	PSU	L5	1792	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4973	41	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	L5	4457	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	2363	41,86	-	0/9/27/28	0/3/3/3
19	MA6	S2	1851	19	-	1/11/29/30	0/3/3/3
19	OMG	S2	644	19	-	4/9/27/28	0/3/3/3
41	OMG	L5	1522	41	-	0/9/27/28	0/3/3/3
19	PSU	S2	105	19	-	0/7/25/26	0/2/2/2
41	PSU	L5	3822	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4442	41	-	0/7/25/26	0/2/2/2
41	UY1	L5	3818	41	-	2/9/27/28	0/2/2/2
41	PSU	L5	4471	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	1326	41	-	3/9/27/28	0/3/3/3
41	PSU	L5	4353	41	-	0/7/25/26	0/2/2/2
41	OMC	L5	3701	41	-	6/9/27/28	0/2/2/2
19	A2M	S2	159	19	-	0/9/27/28	0/3/3/3
41	A2M	L5	1871	41,86	-	0/9/27/28	0/3/3/3
19	OMG	S2	683	19	-	0/9/27/28	0/3/3/3
41	PSU	L5	5001	41	-	0/7/25/26	0/2/2/2
19	A2M	S2	99	86,19	-	2/9/27/28	0/3/3/3
41	A2M	L5	1323	41	-	2/9/27/28	0/3/3/3
41	PSU	L5	1781	41	-	0/7/25/26	0/2/2/2
19	OMU	S2	1288	19	-	2/9/27/28	0/2/2/2
19	PSU	S2	93	19	-	0/7/25/26	0/2/2/2
41	6MZ	L5	4220	41	-	2/9/27/28	0/3/3/3
41	OMG	L5	4494	41	-	0/9/27/28	0/3/3/3
41	PSU	L5	5010	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4689	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4500	41	-	3/7/25/26	0/2/2/2
41	A2M	L5	398	41	-	1/9/27/28	0/3/3/3
41	A2M	L5	2815	41	-	2/9/27/28	0/3/3/3
41	OMG	L5	4499	41	-	0/9/27/28	0/3/3/3
19	PSU	S2	866	19	-	0/7/25/26	0/2/2/2
41	OMU	L5	4620	41	-	0/9/27/28	0/2/2/2
19	PSU	S2	814	19	-	0/7/25/26	0/2/2/2
43	PSU	L8	55	43	-	0/7/25/26	0/2/2/2
41	OMU	L5	4227	41	-	0/9/27/28	0/2/2/2
41	A2M	L5	3785	41,86	-	2/9/27/28	0/3/3/3
19	PSU	S2	1081	19	-	1/7/25/26	0/2/2/2

The worst 5 of 283 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	L5	3818	UY1	C6-C5	12.82	1.49	1.35
19	S2	1832	6MZ	C6-N6	12.77	1.48	1.34
41	L5	4220	6MZ	C6-N6	12.21	1.48	1.34
41	L5	3818	UY1	C2-N1	11.77	1.52	1.36
19	S2	799	OMU	C2-N1	8.58	1.51	1.38

The worst 5 of 670 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1851	MA6	N1-C6-N6	-12.21	101.98	116.86
19	S2	1850	MA6	N1-C6-N6	-11.39	102.97	116.86
19	S2	1851	MA6	C5-C6-N6	8.12	138.18	125.33
19	S2	1639	G7M	C1'-N9-C4	7.71	149.25	126.49
19	S2	1639	G7M	C1'-N9-C8	-7.69	100.76	126.74

There are no chirality outliers.

5 of 135 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	L8	75	OMG	C1'-C2'-O2'-CM2
19	S2	166	A2M	C1'-C2'-O2'-CM'
19	S2	462	OMC	C1'-C2'-O2'-CM2
19	S2	468	A2M	C1'-C2'-O2'-CM'
19	S2	576	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

62 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	L5	4579	PSU	2	0
19	S2	517	OMC	1	0
19	S2	468	A2M	2	0
41	L5	4530	UR3	1	0
41	L5	3920	PSU	1	0
19	S2	121	OMU	1	0
19	S2	116	OMU	4	0
19	S2	1031	A2M	3	0
41	L5	3718	A2M	4	0
41	L5	4637	OMG	1	0
41	L5	3627	OMG	1	0
19	S2	681	PSU	3	0
41	L5	2632	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S2	1703	OMC	1	0
19	S2	509	OMG	3	0
41	L5	2839	PSU	1	0
41	L5	4456	OMC	1	0
19	S2	649	PSU	1	0
43	L8	75	OMG	2	0
41	L5	2422	OMC	1	0
19	S2	867	OMG	2	0
41	L5	2351	OMC	2	0
41	L5	3825	A2M	1	0
19	S2	1850	MA6	2	0
41	L5	2364	OMG	1	0
19	S2	27	A2M	2	0
41	L5	2424	OMG	1	0
41	L5	1340	OMC	2	0
41	L5	4523	A2M	3	0
41	L5	4571	A2M	1	0
41	L5	3830	A2M	1	0
41	L5	4392	OMG	1	0
41	L5	4447	5MC	1	0
41	L5	3851	PSU	1	0
19	S2	576	A2M	2	0
41	L5	4536	OMC	1	0
19	S2	484	A2M	2	0
19	S2	166	A2M	2	0
19	S2	1383	A2M	2	0
41	L5	3867	A2M	3	0
19	S2	601	OMG	2	0
41	L5	3841	OMC	1	0
41	L5	400	A2M	1	0
19	S2	1337	4AC	3	0
19	S2	1004	PSU	1	0
41	L5	1683	PSU	1	0
41	L5	4196	OMG	1	0
41	L5	4457	PSU	1	0
41	L5	2363	A2M	1	0
19	S2	644	OMG	1	0
41	L5	1326	A2M	1	0
41	L5	4353	PSU	1	0
41	L5	3701	OMC	1	0
41	L5	1871	A2M	1	0
19	S2	1288	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	L5	4220	6MZ	2	0
41	L5	4689	PSU	1	0
41	L5	398	A2M	1	0
41	L5	2815	A2M	1	0
19	S2	866	PSU	1	0
41	L5	4620	OMU	1	0
41	L5	3785	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 225 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.85	0
89	SPD	L5	5290	-	9,9,9	0.33	0	8,8,8	0.80	0
89	SPD	L5	5261	-	9,9,9	0.31	0	8,8,8	1.02	0
89	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.90	0
88	SPM	L5	5288	-	13,13,13	0.36	0	12,12,12	0.97	0
88	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPM	L5	5267	-	13,13,13	0.34	0	12,12,12	0.97	0
88	SPM	L5	5291	-	13,13,13	0.35	0	12,12,12	0.80	0
89	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.85	0
89	SPD	L5	5286	-	9,9,9	0.34	0	8,8,8	0.87	0
89	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.93	0
89	SPD	L8	202	-	9,9,9	0.32	0	8,8,8	0.87	0
89	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.90	0
89	SPD	L5	5287	-	9,9,9	0.31	0	8,8,8	0.87	0
89	SPD	L5	5283	-	9,9,9	0.34	0	8,8,8	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPM	L5	5264	-	13,13,13	0.35	0	12,12,12	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPM	L5	5292	-	-	2/11/11/11	-
89	SPD	L5	5290	-	-	2/7/7/7	-
89	SPD	L5	5261	-	-	2/7/7/7	-
89	SPD	LN	301	-	-	2/7/7/7	-
88	SPM	L5	5288	-	-	4/11/11/11	-
88	SPM	L5	5259	-	-	4/11/11/11	-
88	SPM	L5	5263	-	-	3/11/11/11	-
88	SPM	L5	5267	-	-	3/11/11/11	-
88	SPM	L5	5291	-	-	7/11/11/11	-
89	SPD	L5	5284	-	-	1/7/7/7	-
89	SPD	L5	5286	-	-	3/7/7/7	-
89	SPD	L5	5289	-	-	3/7/7/7	-
89	SPD	L8	202	-	-	2/7/7/7	-
89	SPD	L5	5285	-	-	2/7/7/7	-
89	SPD	L5	5287	-	-	4/7/7/7	-
89	SPD	L5	5283	-	-	1/7/7/7	-
88	SPM	L5	5264	-	-	5/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

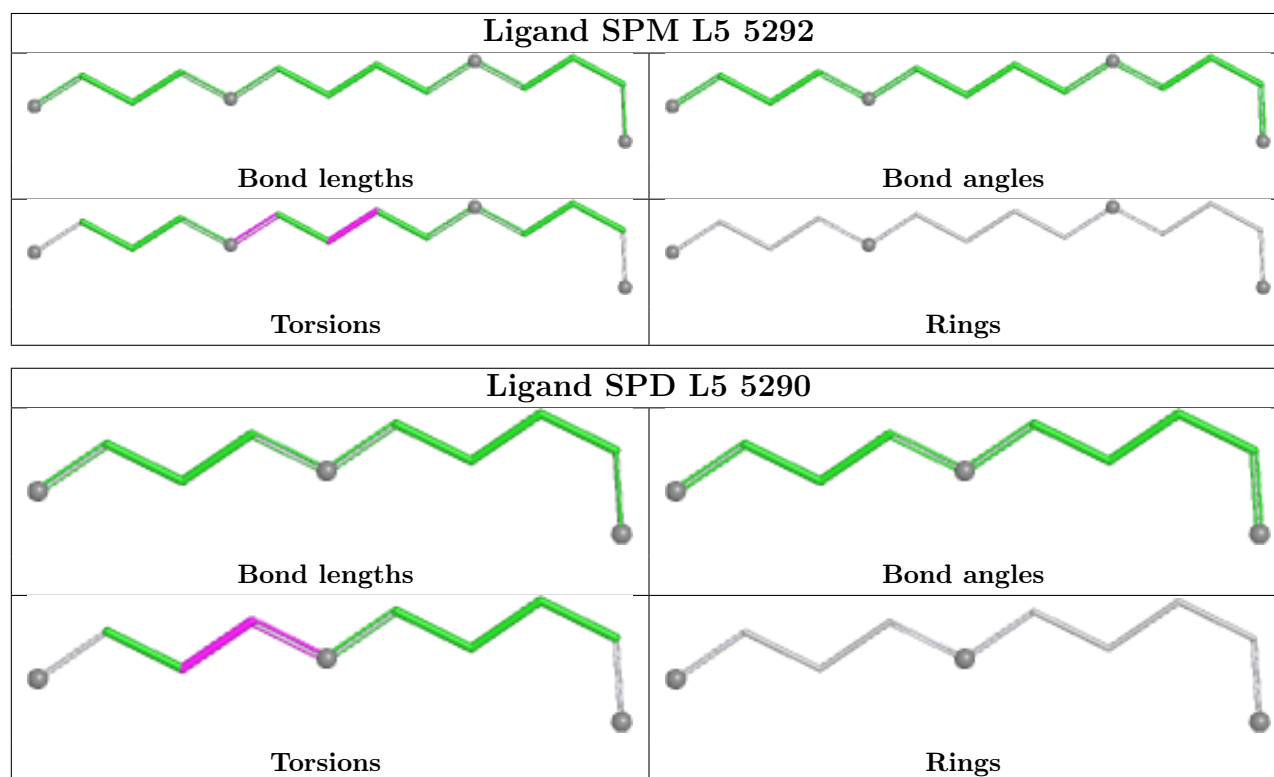
Mol	Chain	Res	Type	Atoms
89	L5	5287	SPD	N6-C7-C8-C9
88	L5	5264	SPM	N5-C6-C7-C8
89	L5	5286	SPD	C3-C4-C5-N6
89	L5	5289	SPD	C3-C4-C5-N6
89	L8	202	SPD	N6-C7-C8-C9

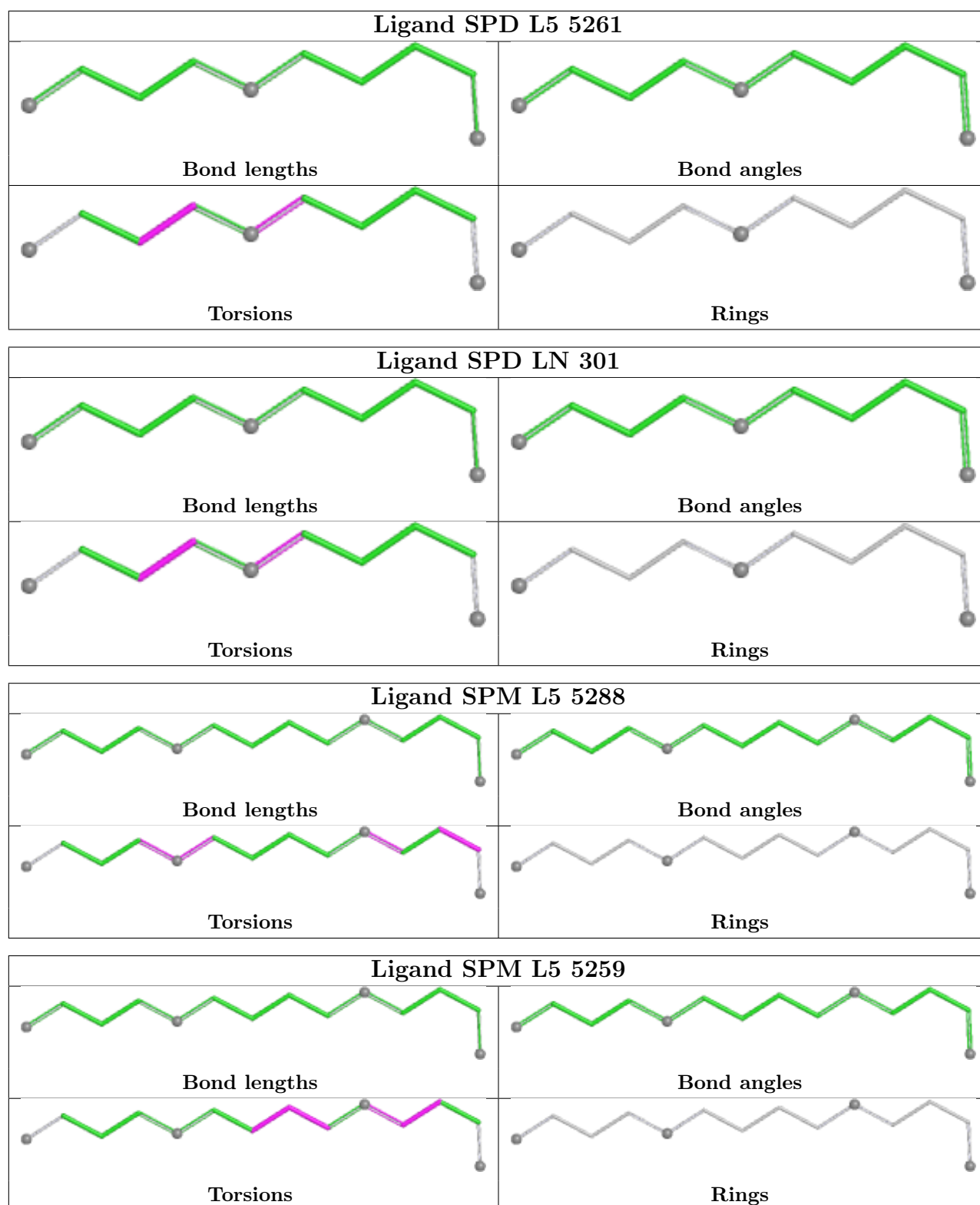
There are no ring outliers.

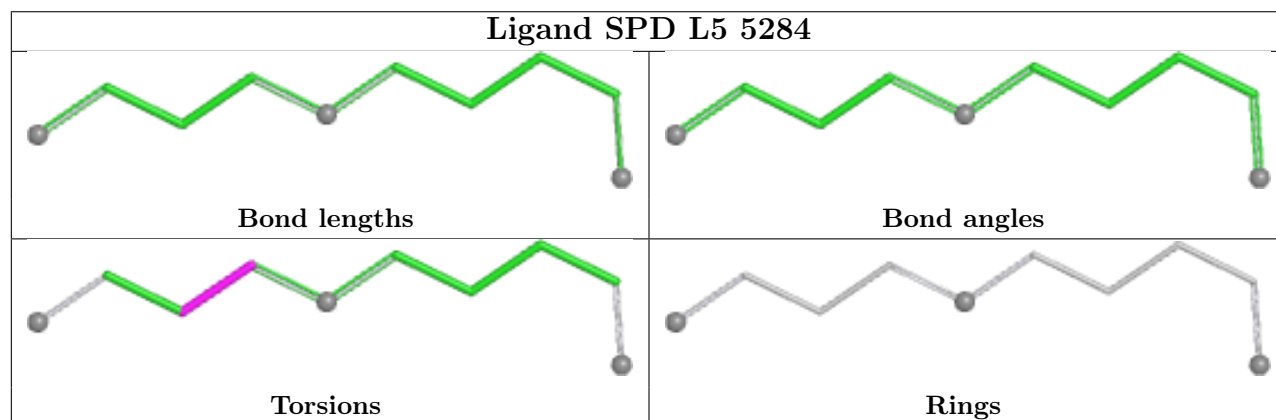
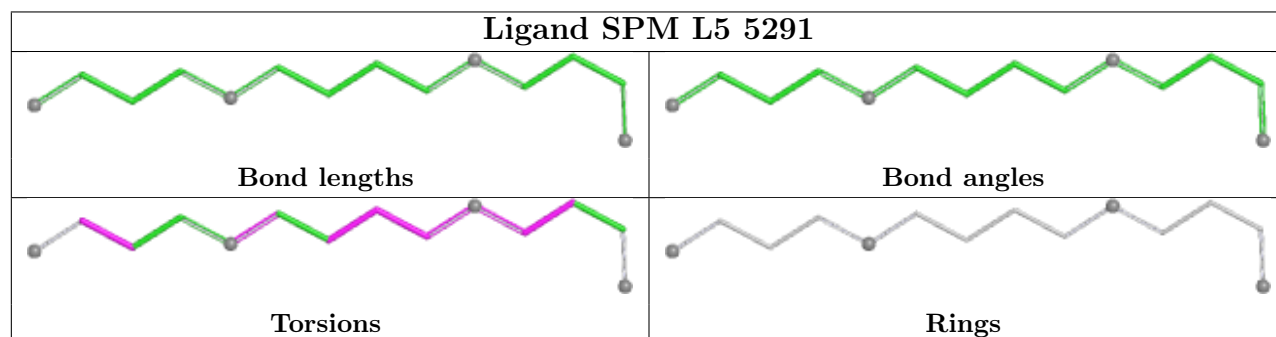
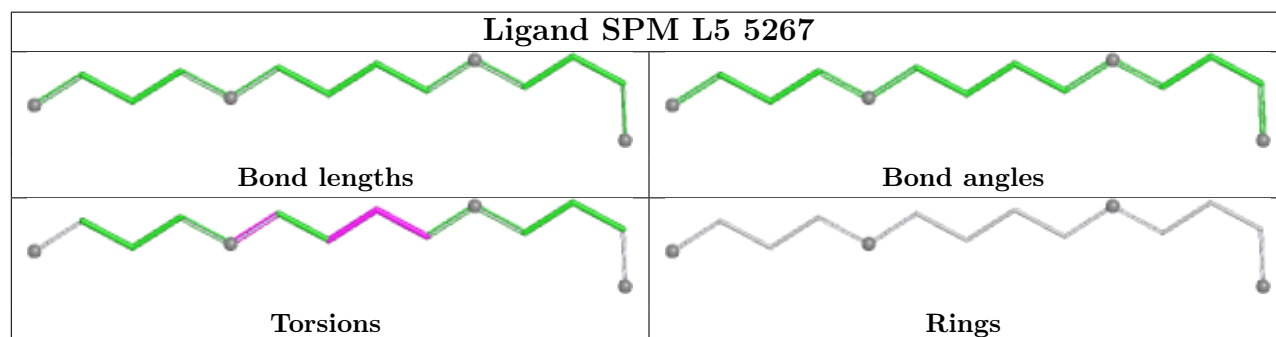
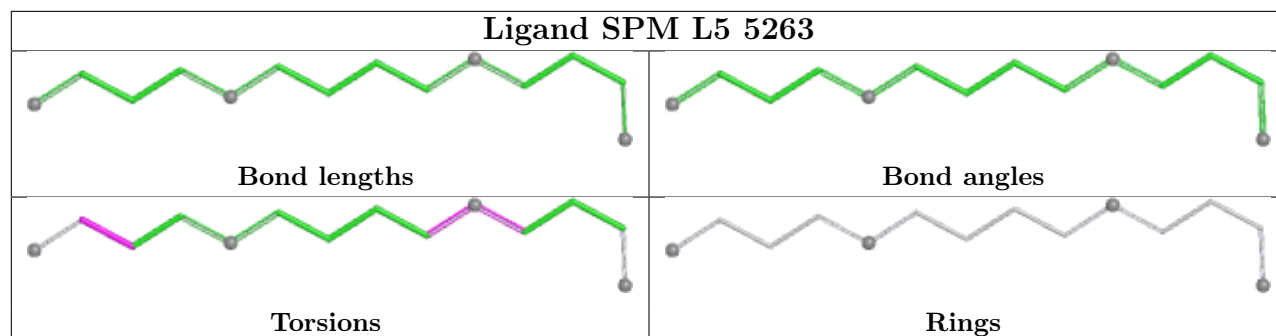
4 monomers are involved in 6 short contacts:

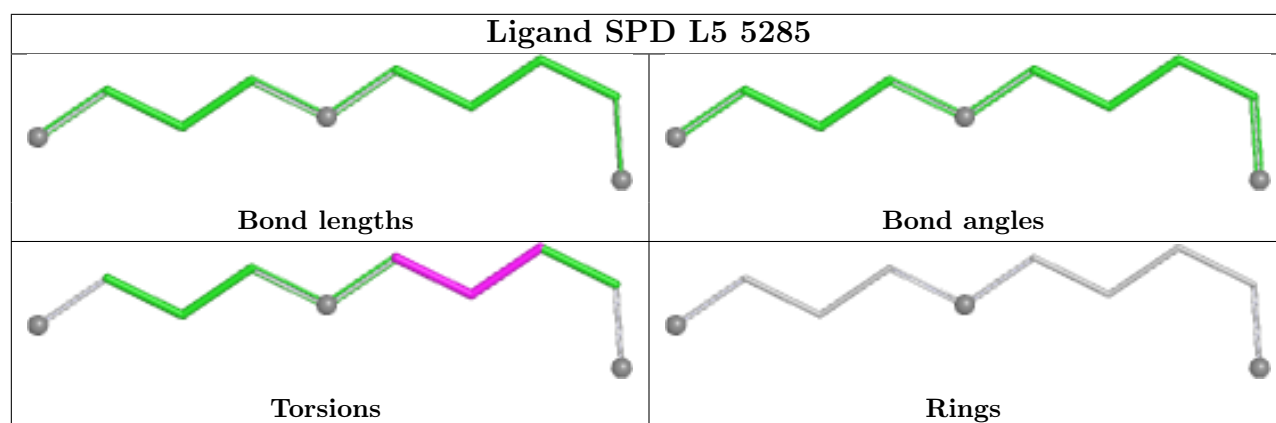
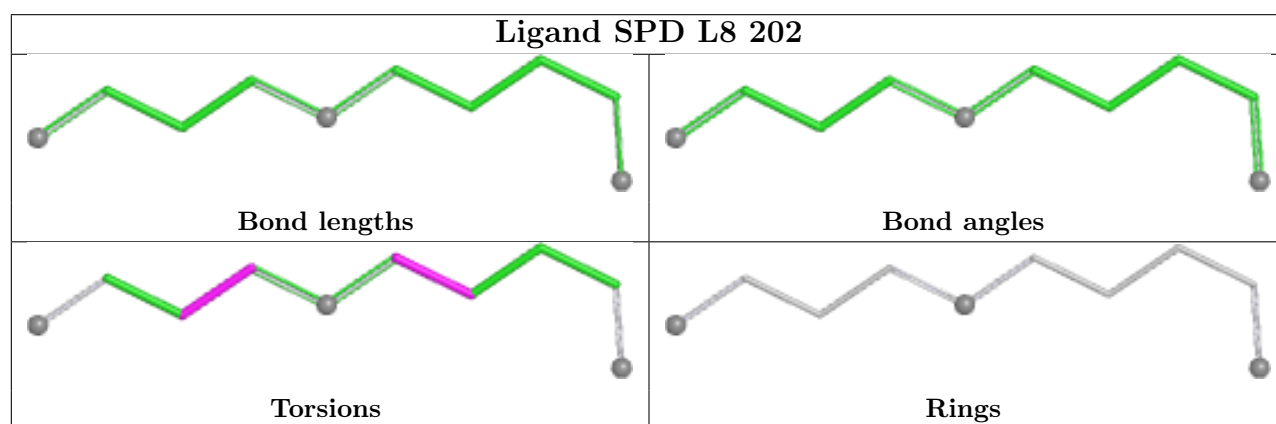
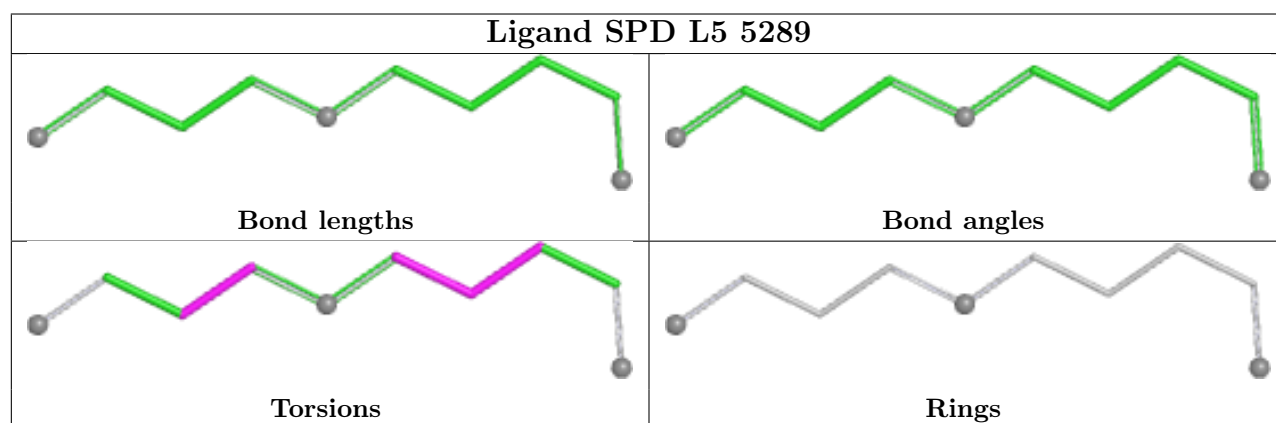
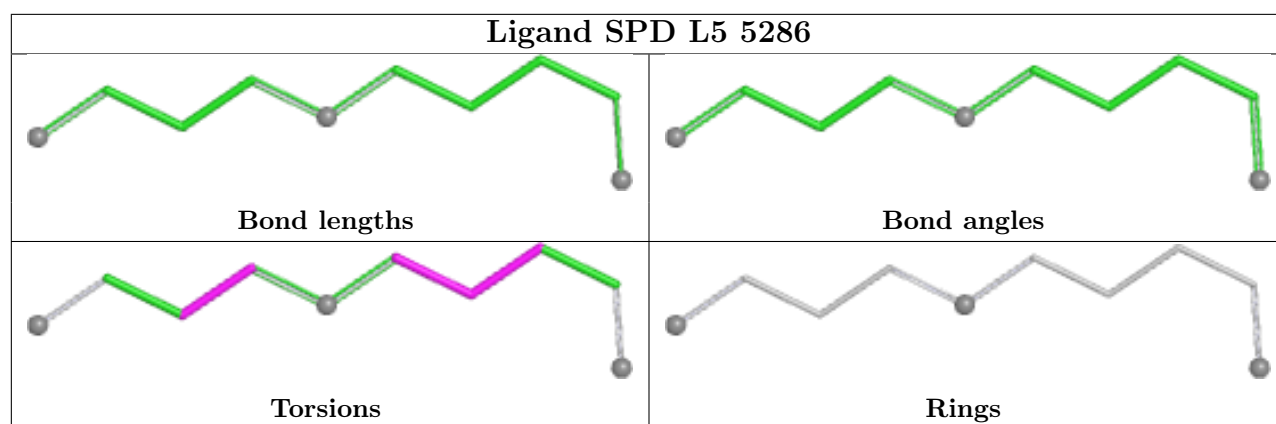
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5292	SPM	3	0
88	L5	5288	SPM	1	0
89	L5	5284	SPD	1	0
89	L5	5289	SPD	2	0

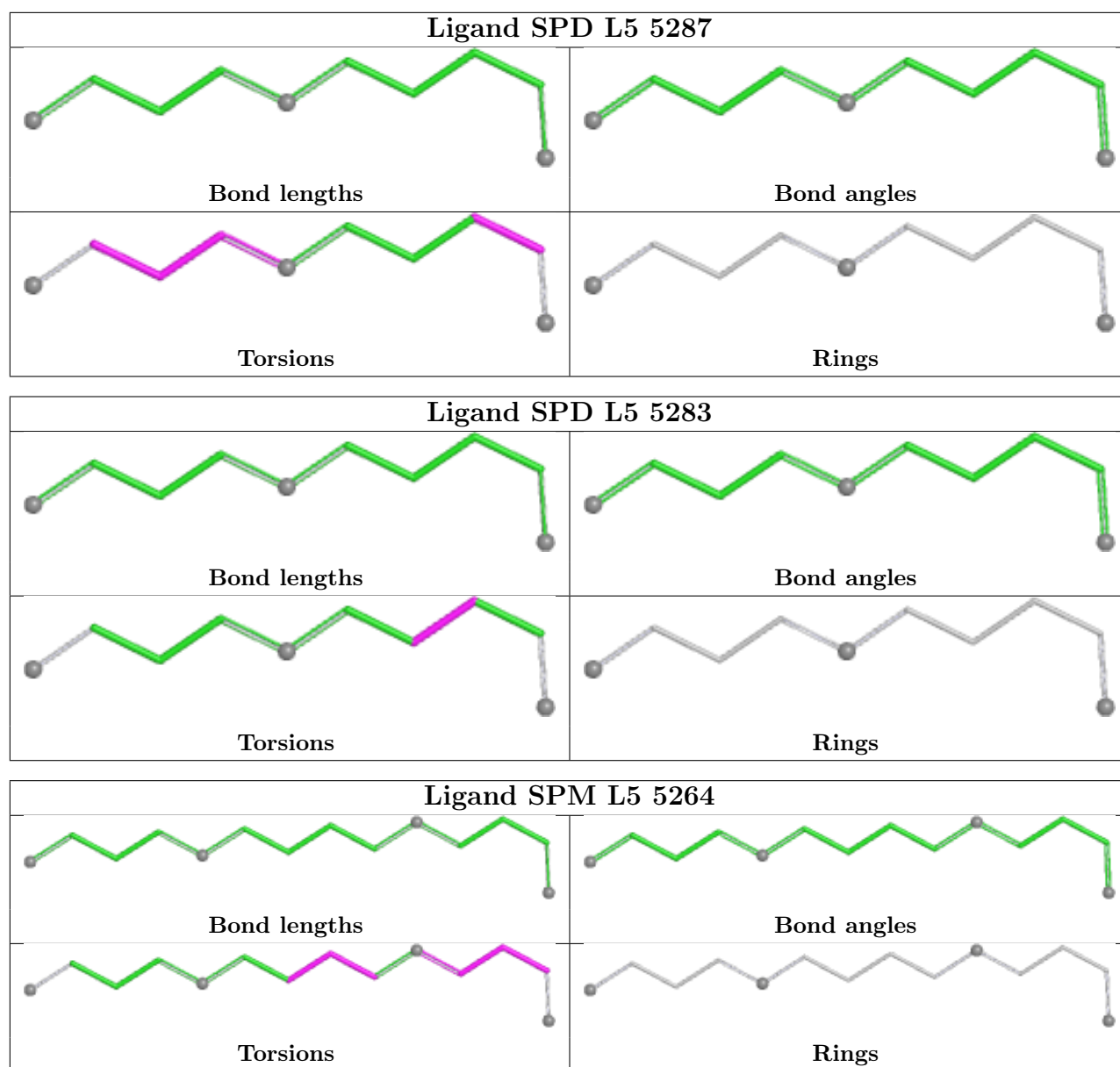
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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
41	L5	10
19	S2	4
68	Lb	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
85	Lt	1
37	At	1
6	SH	1
39	Pt	1
38	Et	1

The worst 5 of 20 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	34.91
1	S2	753:C	O3'	785:C	P	28.49
1	L5	2910:G	O3'	3584:C	P	21.09
1	L5	1706:A	O3'	1716:G	P	20.80
1	L5	760:G	O3'	903:C	P	16.70

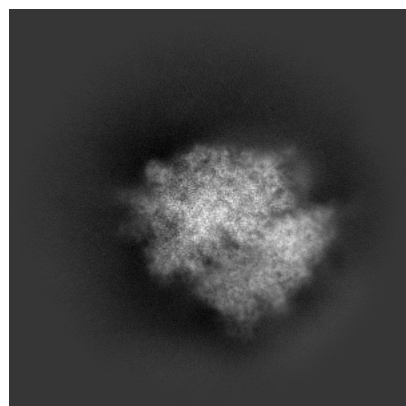
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71357. These allow visual inspection of the internal detail of the map and identification of artifacts.

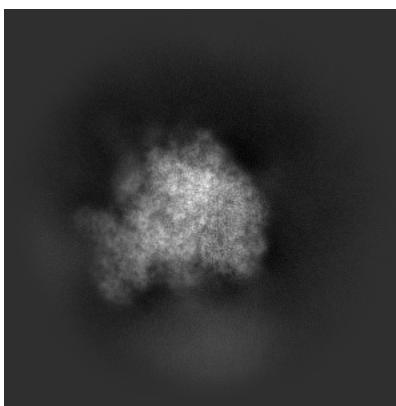
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

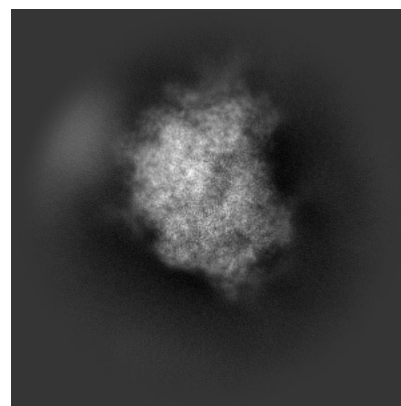
6.1.1 Primary map



X

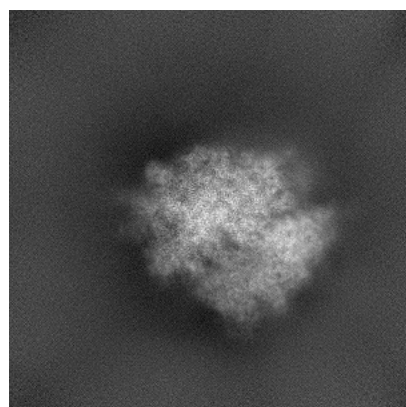


Y

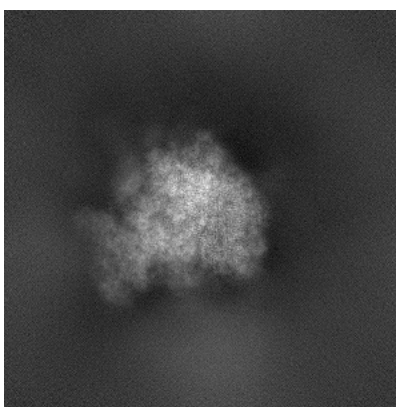


Z

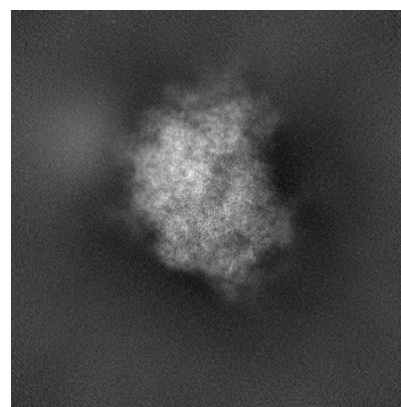
6.1.2 Raw map



X



Y

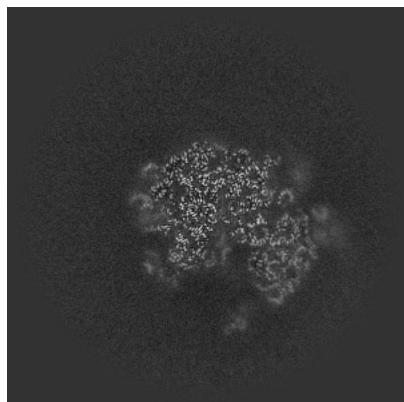


Z

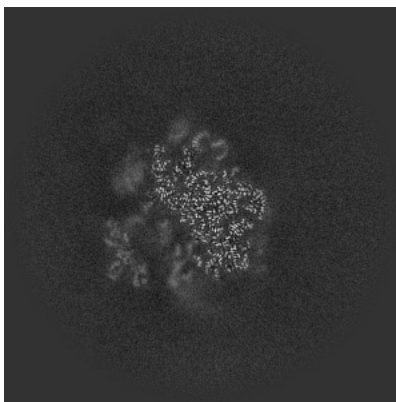
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

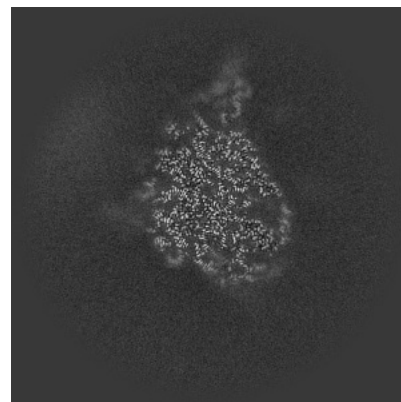
6.2.1 Primary map



X Index: 256

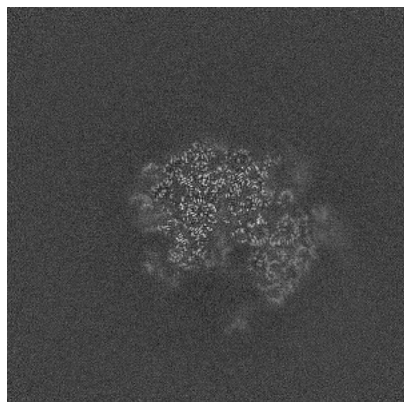


Y Index: 256

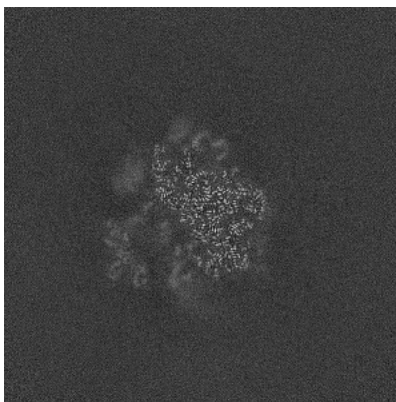


Z Index: 256

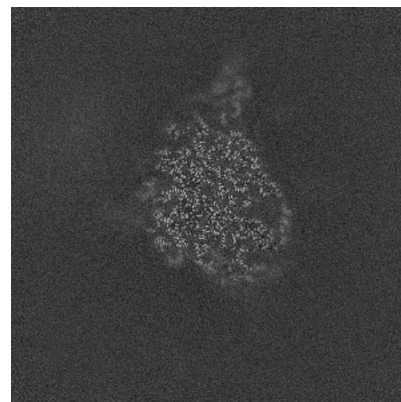
6.2.2 Raw map



X Index: 256



Y Index: 256

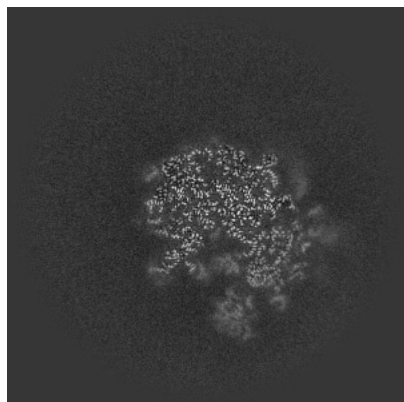


Z Index: 256

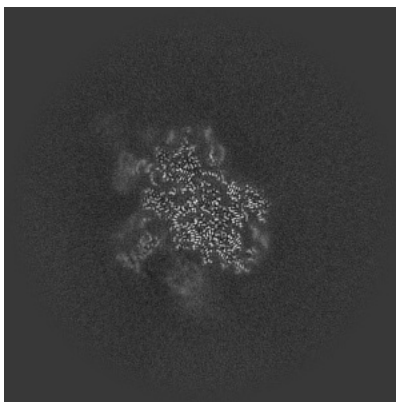
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

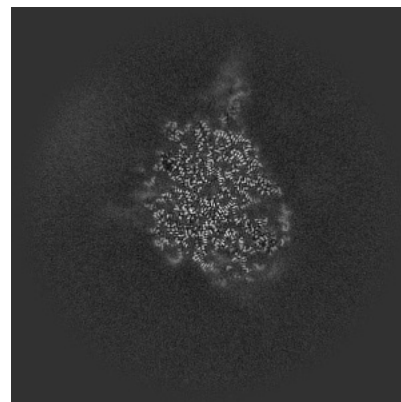
6.3.1 Primary map



X Index: 243

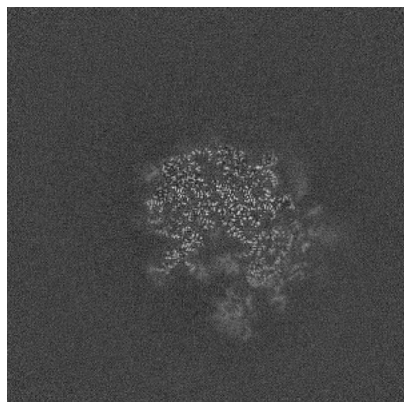


Y Index: 243

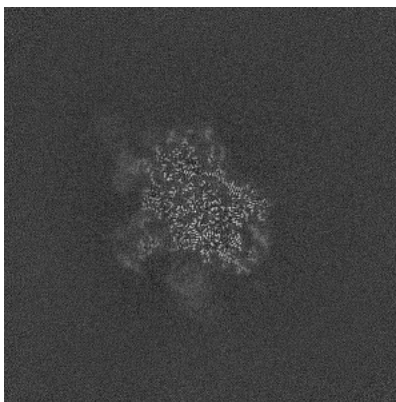


Z Index: 258

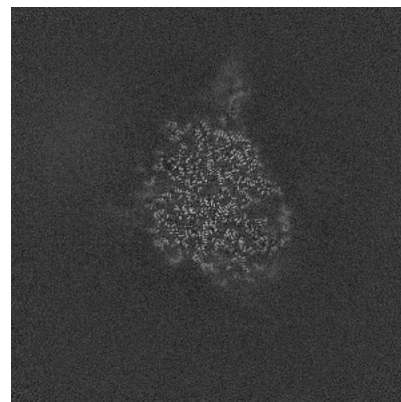
6.3.2 Raw map



X Index: 243



Y Index: 242

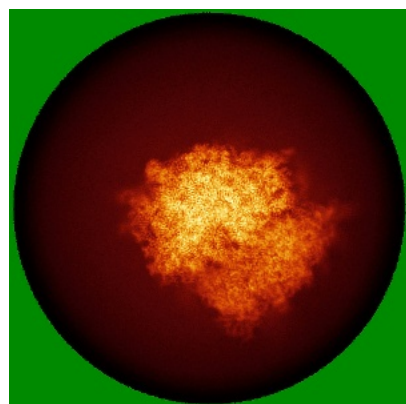


Z Index: 258

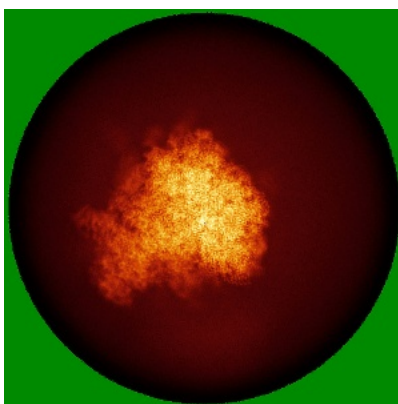
The images above show the largest variance slices of the map in three orthogonal directions.

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

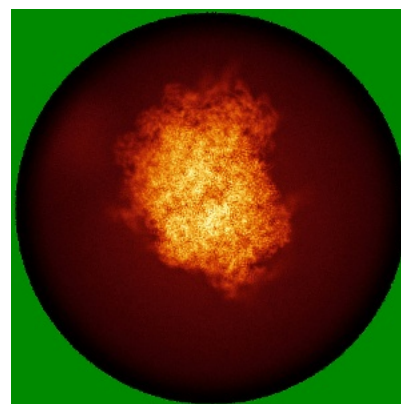
6.4.1 Primary map



X

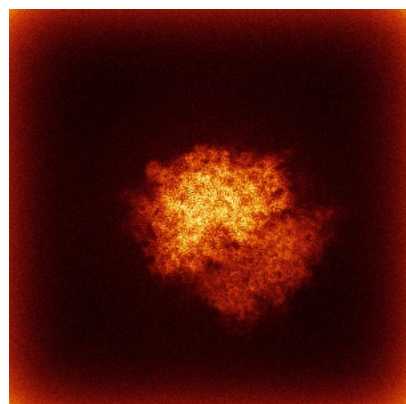


Y

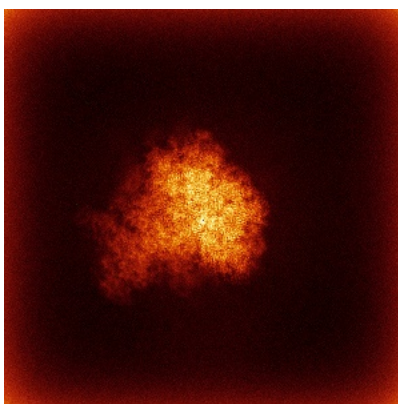


Z

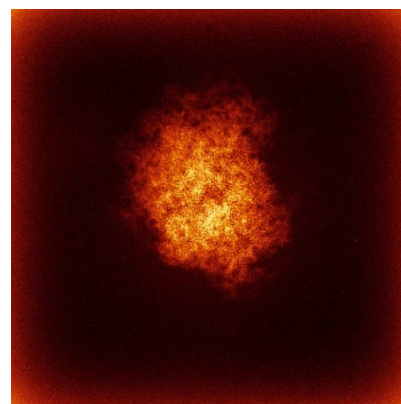
6.4.2 Raw map



X



Y

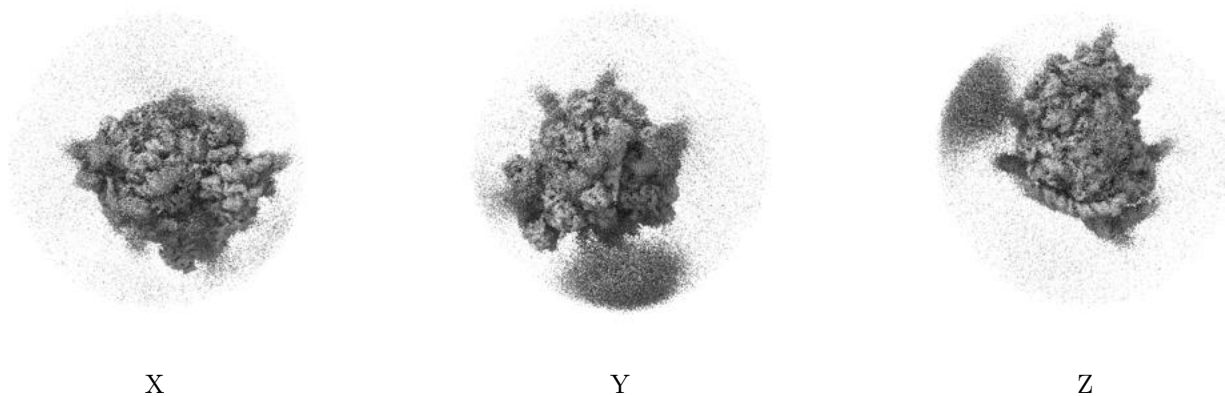


Z

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.

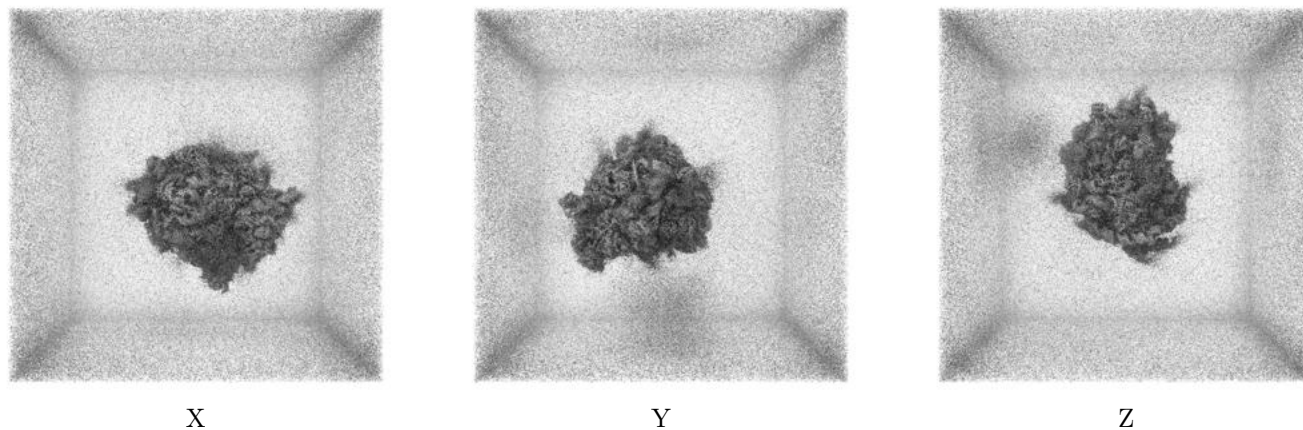
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0121. 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.

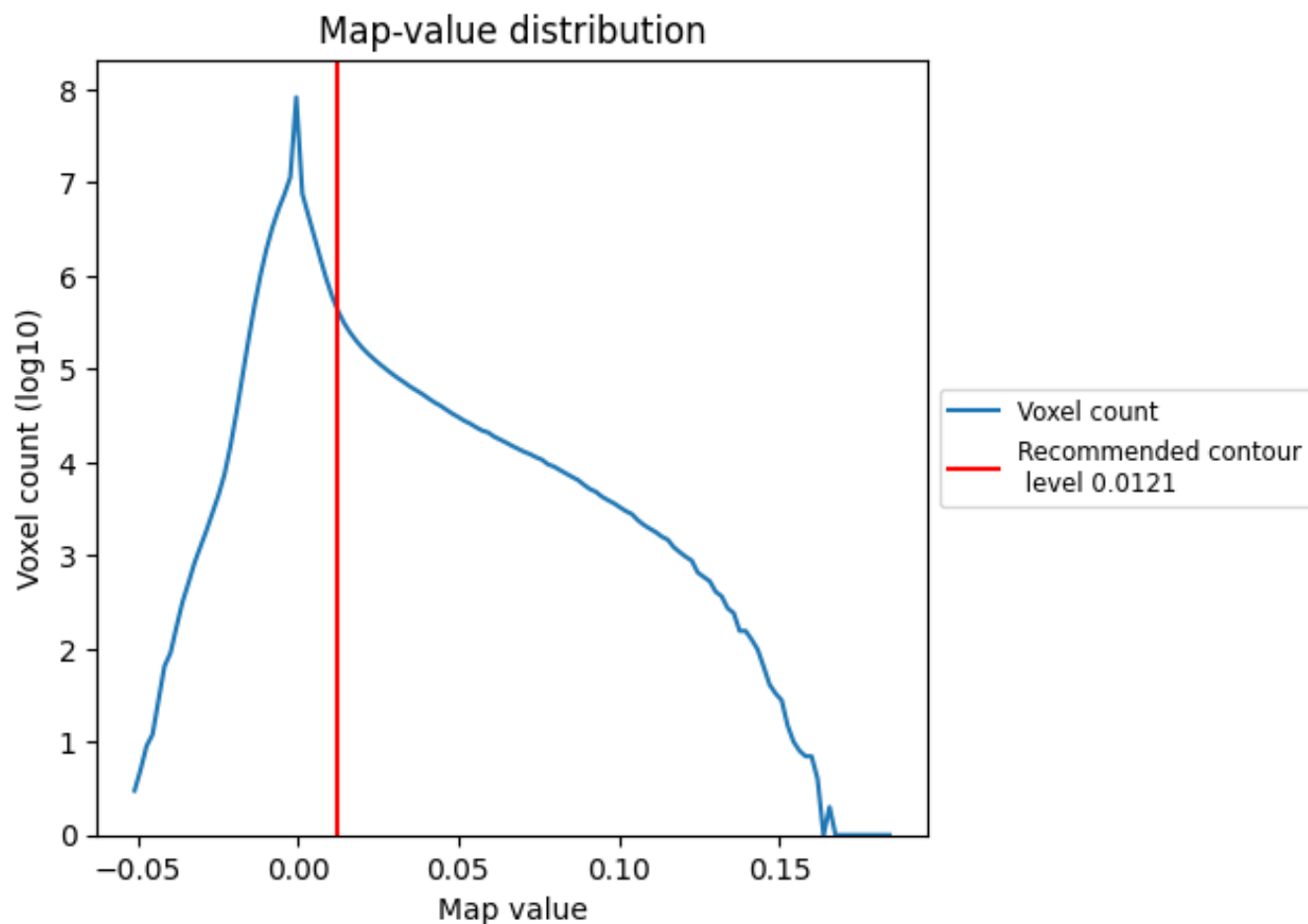
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

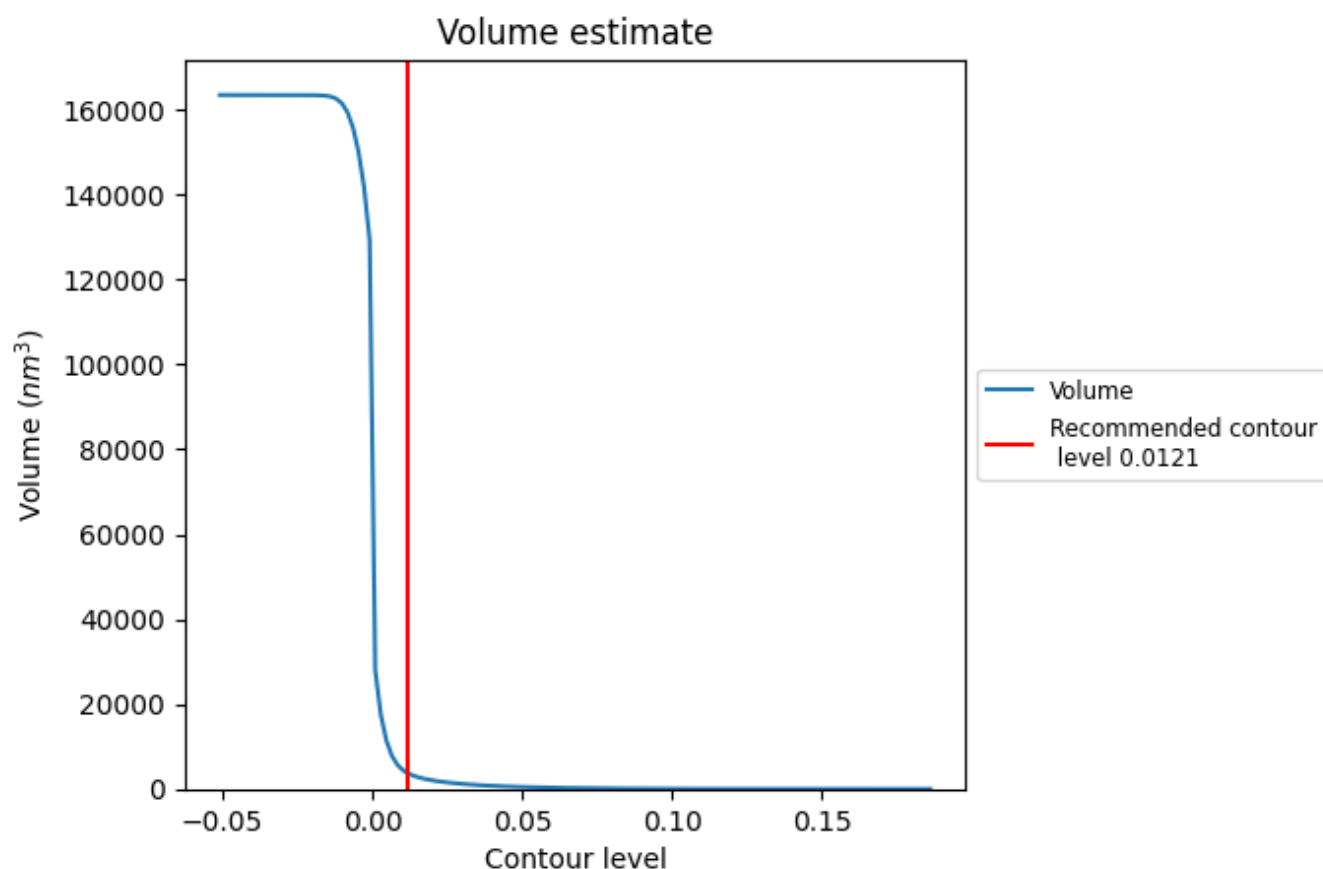
This section contains the results of statistical analysis of the map.

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.

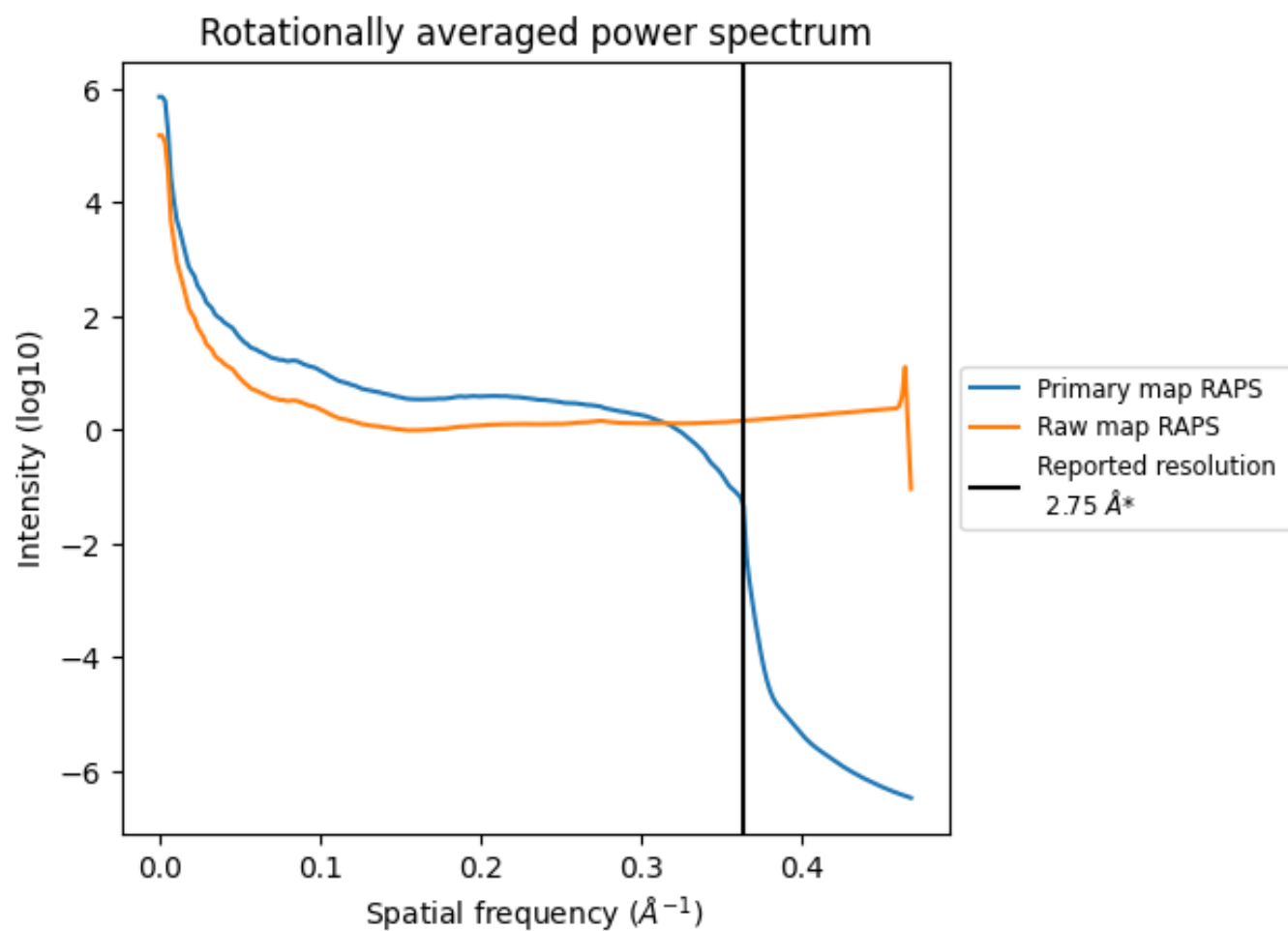
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3611 nm^3 ; this corresponds to an approximate mass of 3262 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 ⓘ

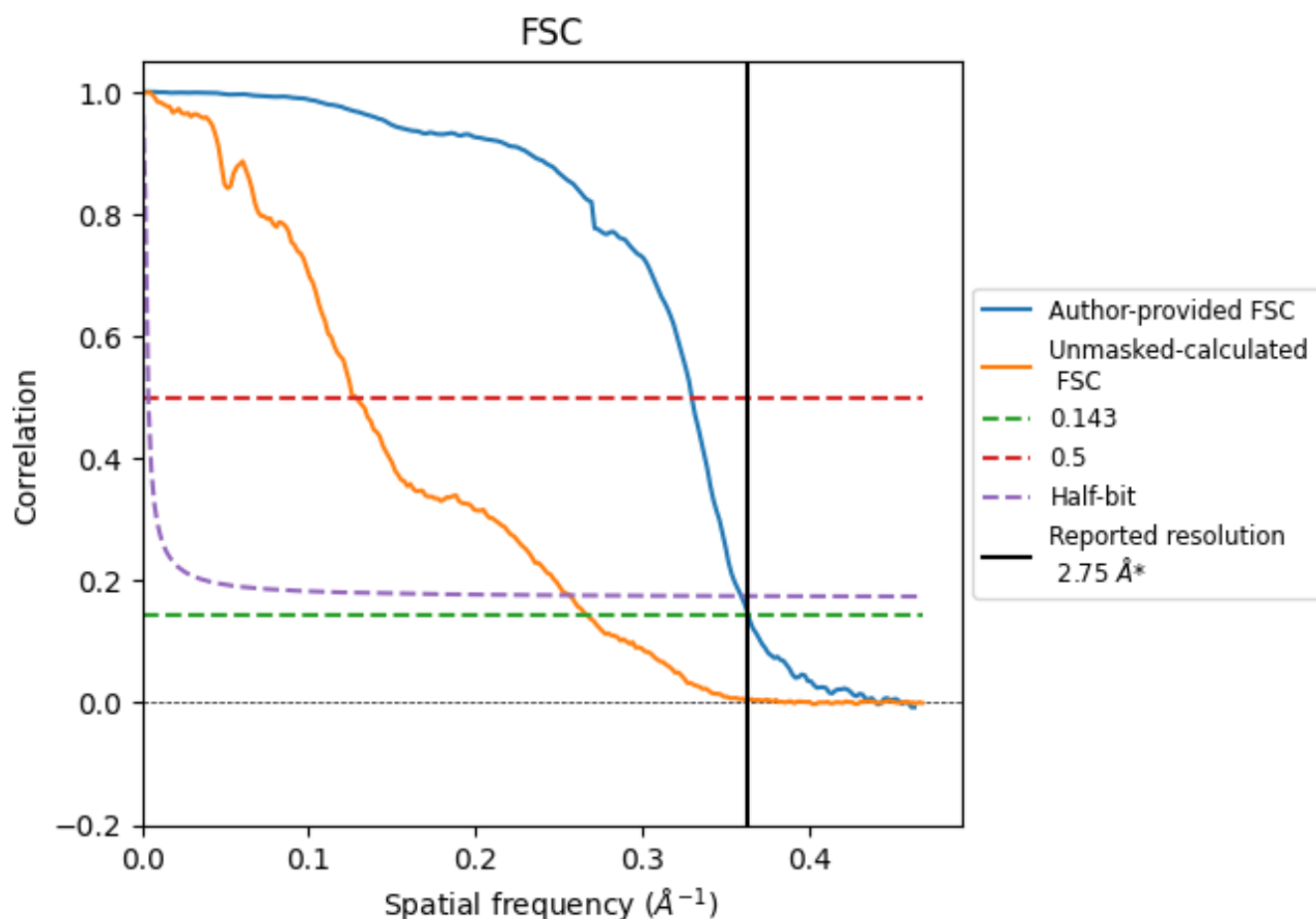


*Reported resolution corresponds to spatial frequency of 0.364 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.364 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

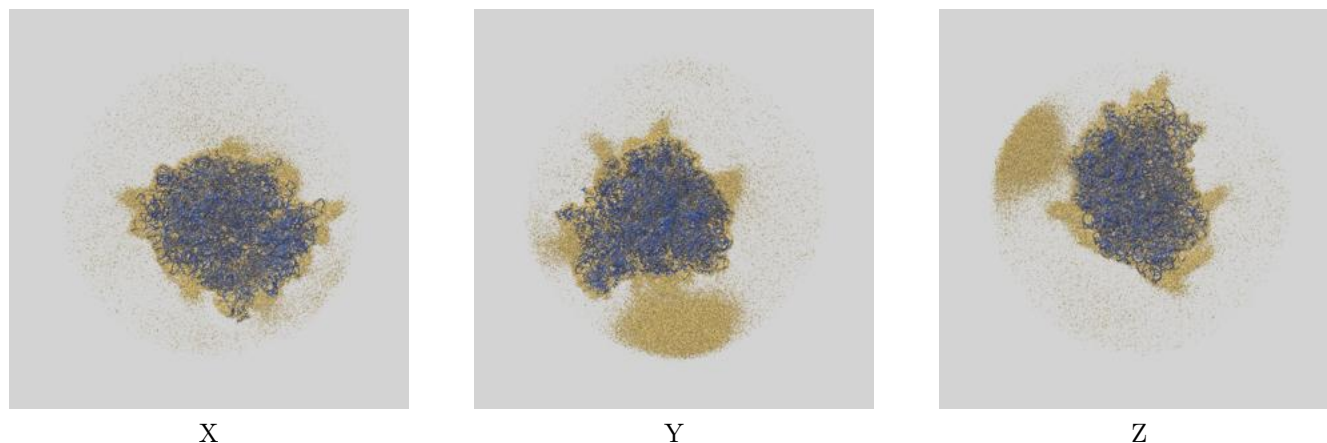
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.75	3.03	2.78
Unmasked-calculated*	3.74	7.93	3.90

*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 3.74 differs from the reported value 2.75 by more than 10 %

9 Map-model fit [i](#)

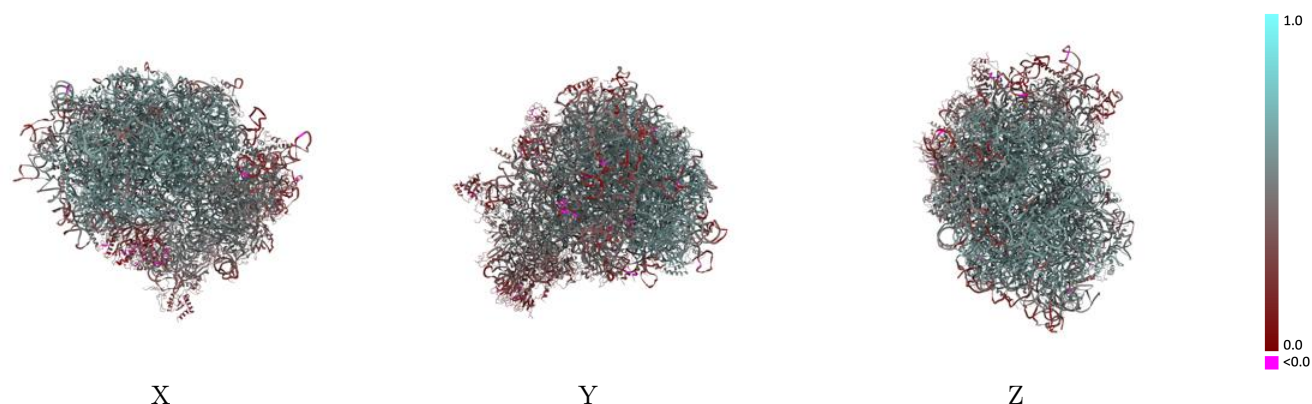
This section contains information regarding the fit between EMDB map EMD-71357 and PDB model 9P7Y. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



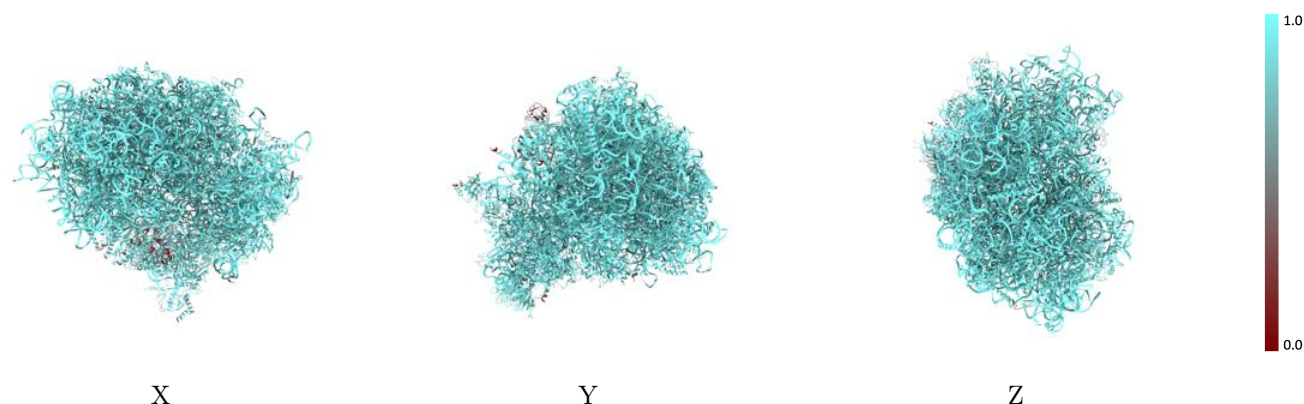
The images above show the 3D surface view of the map at the recommended contour level 0.0121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



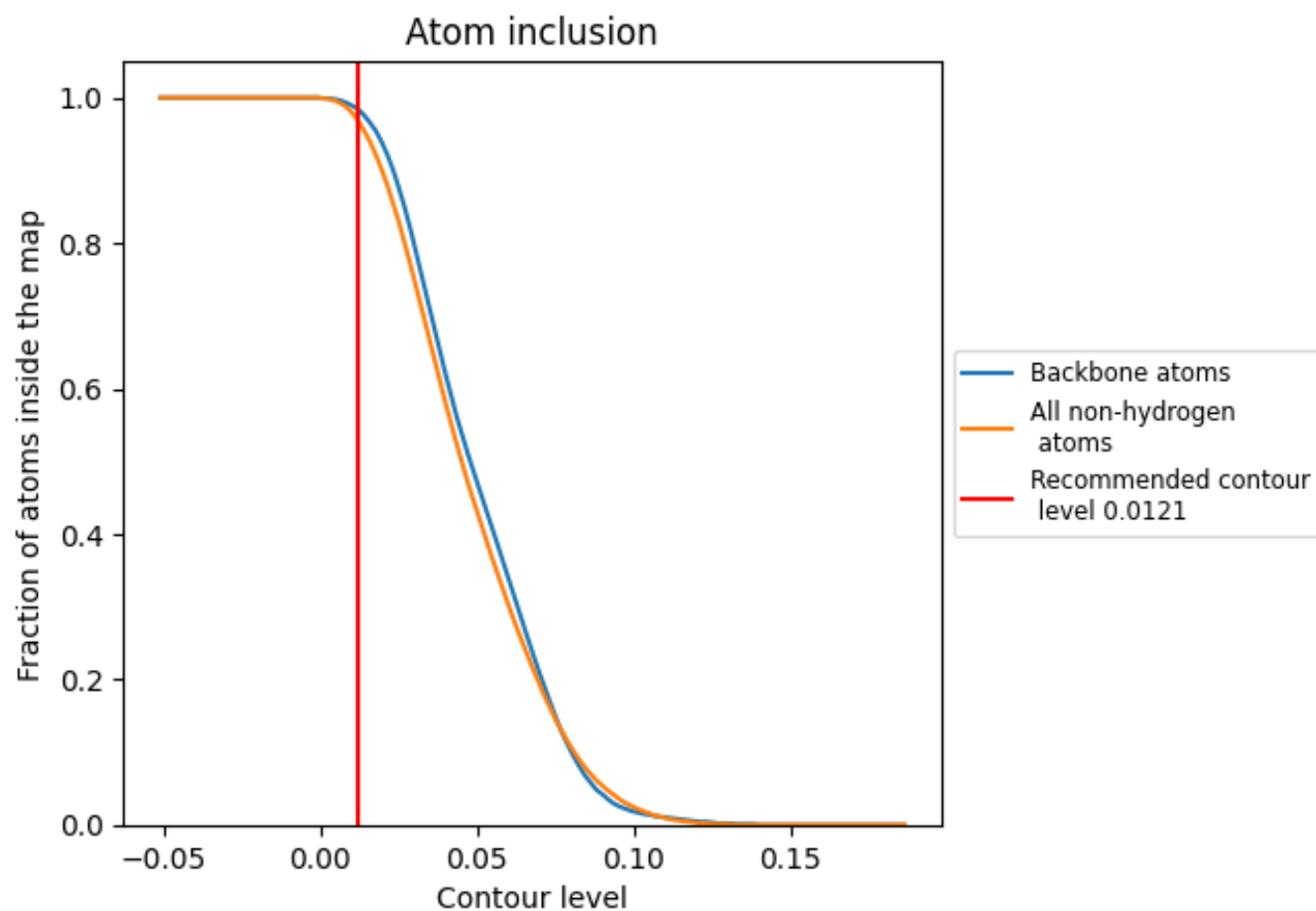
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0121).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (0.0121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.5030
At	 0.9640	 0.4070
CI	 0.8830	 0.4810
Et	 0.9320	 0.2110
L5	 0.9870	 0.5420
L7	 0.9980	 0.5830
L8	 0.9930	 0.5670
LA	 0.9910	 0.6000
LB	 0.9700	 0.5890
LC	 0.9720	 0.5830
LD	 0.9690	 0.5450
LE	 0.9510	 0.5250
LF	 0.9900	 0.5920
LG	 0.9390	 0.5320
LH	 0.9780	 0.5740
LI	 0.9740	 0.5800
LJ	 0.9450	 0.5010
LL	 0.9520	 0.5700
LM	 0.9770	 0.5700
LN	 0.9990	 0.6190
LO	 0.9840	 0.5940
LP	 0.9810	 0.5990
LQ	 0.9900	 0.6080
LR	 0.9520	 0.5370
LS	 0.9960	 0.6060
LT	 0.9720	 0.5740
LU	 0.9420	 0.5060
LV	 0.9830	 0.5900
LW	 0.9140	 0.4340
LX	 0.9790	 0.5790
LY	 0.9750	 0.5740
LZ	 0.9850	 0.5650
La	 0.9920	 0.6150
Lb	 0.9400	 0.5310
Lc	 0.9570	 0.5450



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Chain	Atom inclusion	Q-score
Ld	 0.9760	 0.5750
Le	 0.9910	 0.6060
Lf	 0.9930	 0.6160
Lg	 0.9780	 0.5820
Lh	 0.9720	 0.5730
Li	 0.9750	 0.5690
Lj	 0.9900	 0.6050
Lk	 0.9350	 0.5200
Ll	 0.9860	 0.5880
Lm	 0.9780	 0.5930
Ln	 0.9900	 0.5840
Lo	 0.9810	 0.5800
Lp	 0.9720	 0.5820
Lr	 0.9860	 0.5920
Ls	 0.6000	 0.1910
Lt	 0.5670	 0.1720
Pt	 0.9730	 0.4320
S2	 0.9920	 0.4610
SA	 0.9210	 0.3970
SB	 0.9190	 0.3960
SC	 0.9600	 0.4650
SD	 0.9240	 0.4040
SE	 0.9610	 0.4600
SF	 0.9080	 0.3520
SG	 0.9270	 0.4090
SH	 0.8910	 0.3420
SI	 0.9400	 0.4630
SJ	 0.9360	 0.4220
SK	 0.9230	 0.3850
SL	 0.9430	 0.4880
SM	 0.8090	 0.2460
SN	 0.9620	 0.4590
SO	 0.9240	 0.4330
SP	 0.9140	 0.4100
SQ	 0.9130	 0.3600
SR	 0.9040	 0.3500
SS	 0.9040	 0.3730
ST	 0.9320	 0.3650
SU	 0.9270	 0.3870
SV	 0.9410	 0.4190
SW	 0.9730	 0.4860
SX	 0.9640	 0.5240

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Chain	Atom inclusion	Q-score
SY	 0.8990	 0.3910
SZ	 0.8700	 0.3240
Sa	 0.9470	 0.4530
Sb	 0.9360	 0.4050
Sc	 0.8830	 0.3570
Sd	 0.9710	 0.4660
Se	 0.8720	 0.3980
Sf	 0.8670	 0.3040
Sg	 0.9030	 0.2570