



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2026 – 12:33 AM EDT

PDB ID : 9P72 / pdb_00009p72
EMDB ID : EMD-71331
Title : In situ human P-E state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

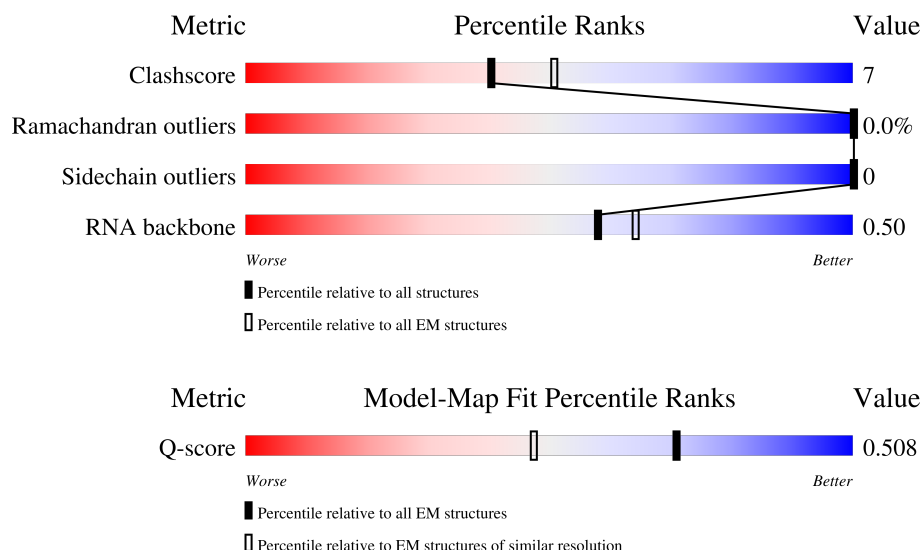
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



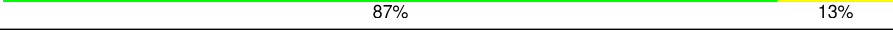
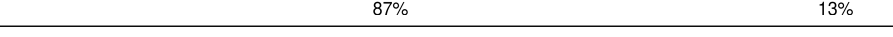
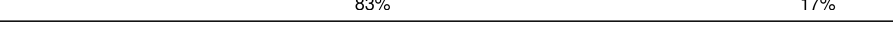
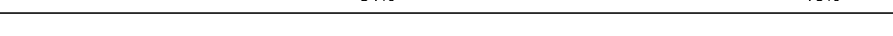
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	Pt	74	53% 45% .
2	Et	75	24% 63% 13%
3	L5	3655	56% 37% 7%

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	240	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	
24	LT	159	
25	LU	101	
26	LV	131	
27	LW	118	
28	LX	120	

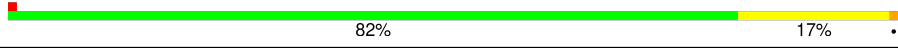
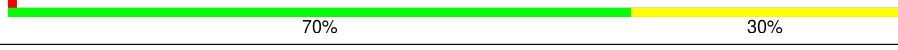
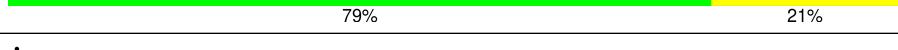
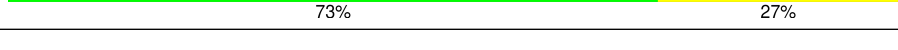
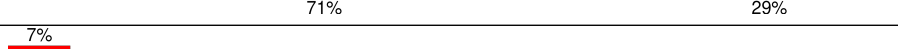
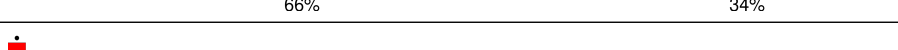
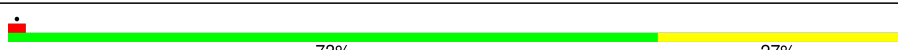
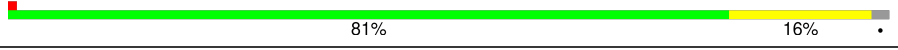
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	109	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	141	
50	SD	227	
51	SF	189	
52	SK	98	
53	SM	122	

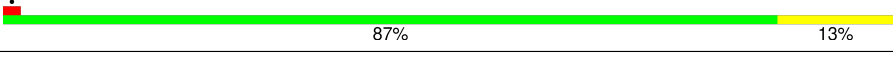
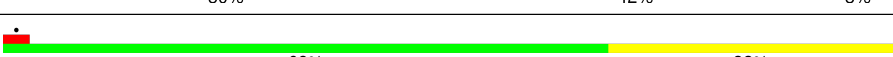
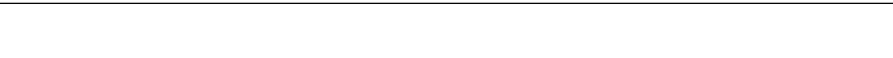
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Mol	Chain	Length	Quality of chain
54	SP	121	
55	SQ	144	
56	SR	135	
57	SS	145	
58	ST	143	
59	SU	104	
60	SZ	75	
61	Sc	64	
62	Sd	55	
63	Sf	67	
64	Sg	313	
65	SA	221	
66	SB	214	
67	SC	222	
68	SE	262	
69	SG	237	
70	SH	186	
71	SI	206	
72	SJ	185	
73	SL	153	
74	SN	150	
75	SO	140	
76	SV	83	
77	SW	129	
78	SX	141	

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Mol	Chain	Length	Quality of chain
79	SY	131	
80	Sa	102	
81	Sb	83	
82	Se	58	
83	S2	1740	
84	CI	31	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 219971 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called P site tRNA.

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

- Molecule 2 is a RNA chain called E site tRNA.

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

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

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

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

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

- Molecule 5 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

- Molecule 6 is a protein called 60S ribosomal protein L8.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 8 is a protein called 60S ribosomal protein L4.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LE	?	-	SER	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	VAL	deletion	UNP Q02878
LE	?	-	GLU	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	GLU	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878

- Molecule 11 is a protein called 60S ribosomal protein L7.

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

- Molecule 12 is a protein called 60S ribosomal protein L7a.

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

- Molecule 13 is a protein called 60S ribosomal protein L9.

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

- Molecule 14 is a protein called Ribosomal protein uL16-like.

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

- Molecule 15 is a protein called 60S ribosomal protein L11.

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

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 17 is a protein called 60S ribosomal protein L14.

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

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

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

- Molecule 20 is a protein called 60S ribosomal protein L17.

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

- Molecule 21 is a protein called 60S ribosomal protein L18.

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

- Molecule 22 is a protein called 60S ribosomal protein L19.

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

- Molecule 23 is a protein called 60S ribosomal protein L18a.

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

- Molecule 24 is a protein called 60S ribosomal protein L21.

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

- Molecule 25 is a protein called Heparin-binding protein HBp15.

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

- Molecule 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	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 28 is a protein called 60S ribosomal protein L23a.

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

- Molecule 29 is a protein called 60S ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	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 33 is a protein called 60S ribosomal protein L30.

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

- Molecule 34 is a protein called 60S ribosomal protein L31.

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

- Molecule 35 is a protein called 60S ribosomal protein L32.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

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

- Molecule 37 is a protein called 60S ribosomal protein L34.

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

- Molecule 38 is a protein called 60S ribosomal protein L35.

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

- Molecule 39 is a protein called 60S ribosomal protein L36.

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

- Molecule 40 is a protein called 60S ribosomal protein L37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 44 is a protein called 60S ribosomal protein L41.

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

- Molecule 45 is a protein called 60S ribosomal protein L36a.

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

- Molecule 46 is a protein called 60S ribosomal protein L37a.

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

- Molecule 47 is a protein called 60S ribosomal protein L28.

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

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	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 50 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S10.

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

- Molecule 53 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 55 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 57 is a protein called 40S ribosomal protein S18.

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

- Molecule 58 is a protein called 40S ribosomal protein S19.

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

- Molecule 59 is a protein called 40S ribosomal protein S20.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 61 is a protein called 40S ribosomal protein S28.

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

- Molecule 62 is a protein called 40S ribosomal protein S29.

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

- Molecule 63 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 64 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 65 is a protein called 40S ribosomal protein SA.

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

- Molecule 66 is a protein called 40S ribosomal protein S3a.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

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

- Molecule 68 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 69 is a protein called 40S ribosomal protein S6.

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

- Molecule 70 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	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 71 is a protein called 40S ribosomal protein S8.

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

- Molecule 72 is a protein called 40S ribosomal protein S9.

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

- Molecule 73 is a protein called 40S ribosomal protein S11.

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

- Molecule 74 is a protein called 40S ribosomal protein S13.

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

- Molecule 75 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 77 is a protein called 40S ribosomal protein S15a.

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

- Molecule 78 is a protein called 40S ribosomal protein S23.

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

- Molecule 79 is a protein called 40S ribosomal protein S24.

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

- Molecule 80 is a protein called 40S ribosomal protein S26.

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

- Molecule 81 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 83 is a RNA chain called 18S rRNA.

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

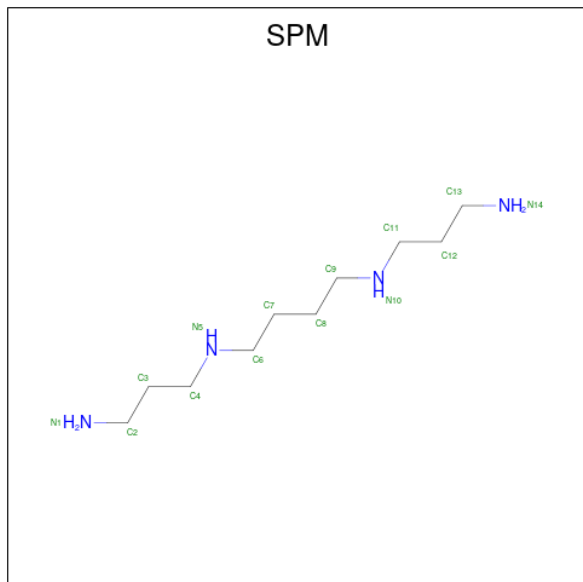
- Molecule 84 is a protein called Transcription factor BTF3.

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

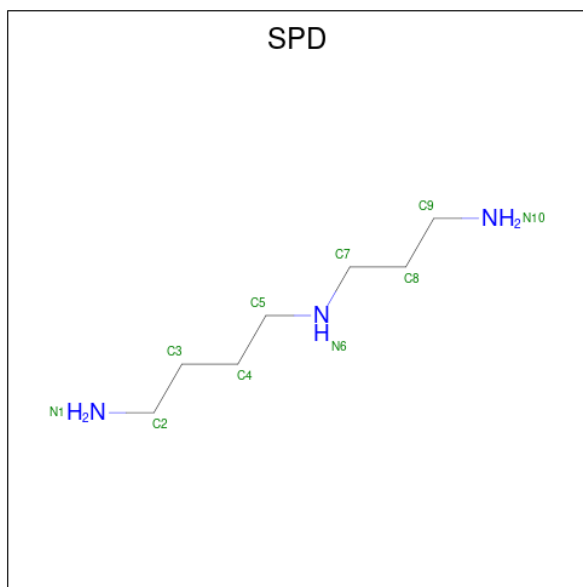
Mol	Chain	Residues	Atoms		AltConf
85	L5	179	Total	Mg	0
			179	179	
85	L7	3	Total	Mg	0
			3	3	
85	L8	5	Total	Mg	0
			5	5	
85	LA	1	Total	Mg	0
			1	1	
85	LP	1	Total	Mg	0
			1	1	
85	LV	1	Total	Mg	0
			1	1	
85	Le	1	Total	Mg	0
			1	1	
85	SS	1	Total	Mg	0
			1	1	
85	S2	27	Total	Mg	0
			27	27	

- Molecule 86 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
88	Lg	1	Total	Zn	0
			1	1	

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

3 Residue-property plots

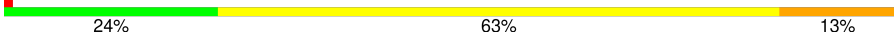
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

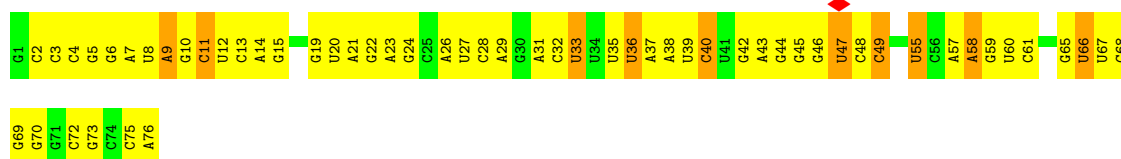
• Molecule 1: P site tRNA

Chain Pt: 



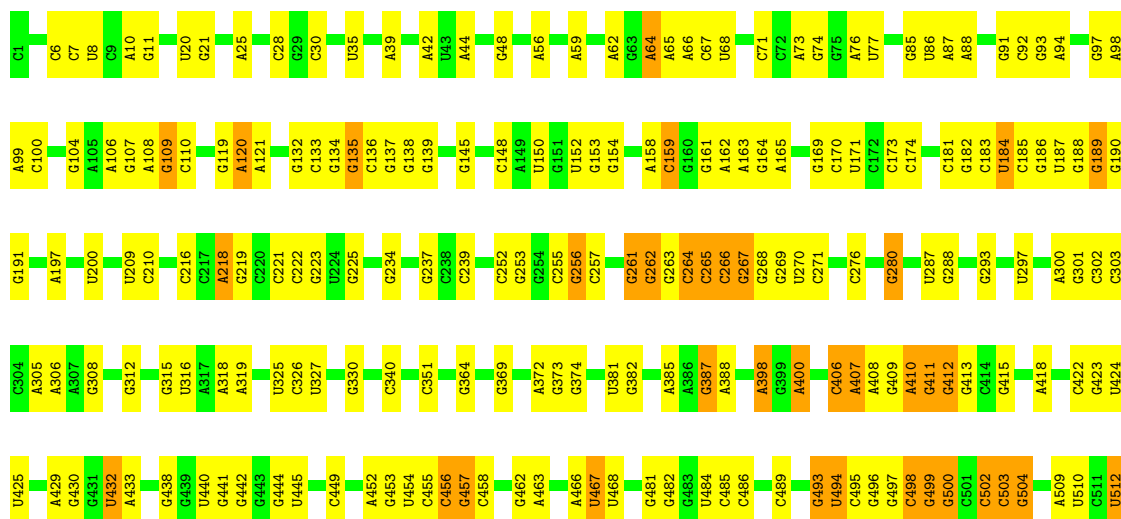
• Molecule 2: E site tRNA

Chain Et: 



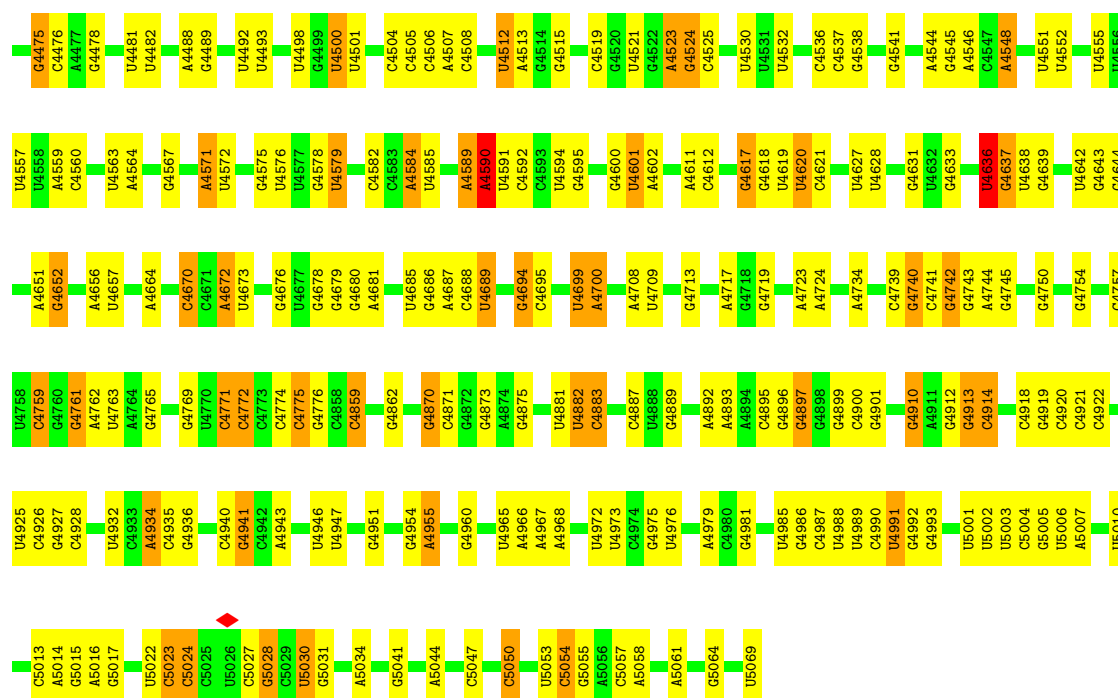
• Molecule 3: 28S rRNA

Chain L5: 



C2256	G2021	C1857	A1558	G1457	G1281	C1181	G957	G724	U513
C2257	G2024	A1858	G1559	C1457	G1282	C1182	G958	G728	U514
C2258	A2025	C1859	A1563	C1458	G1283	C1183	G959	U729	C515
G2262	A2026	U1860	A1564	C1459	G1284	C1184	A960	G730	C516
A2263	A2029	U1861	A1565	C1460	G1287	C1185	G961	G731	C517
C2264	A2030	U1862	C1566	A1462	G1290	U1186	G962	G735	G518
G2265	A2041	U1866	G1574	C1468	G1291	C1187	G965	G736	C519
G2275	G2045	A1867	G1577	C1478	G1292	C1188	A966	G737	G643
A2276	G2046	A1868	U1578	C1479	G1293	G1194	C967	G738	G646
G2279	G2047	C1870	U1582	C1480	A1294	G1195	G969	G739	G647
G2280	U2048	G1871	U1586	G1481	G1296	G1196	G970	G742	C654
U2281	G2049	U1876	U1591	C1483	U1297	G1200	C979	A746	C655
G2284	G2055	U1877	C1596	U1494	C1301	C1202	U980	A747	C656
C2289	G2056	C1878	U1596	G1496	U1302	G1203	C981	G748	C657
C2295	A2069	U1881	U1600	A1497	C1306	C1210	C982	G755	G659
G2296	C2072	U1882	C1702	C1498	C1307	G1211	C983	G756	C662
G2297	G2076	U1887	C1703	G1498	C1308	C1214	C984	G759	G663
U2298	G2077	C1888	C1704	C1499	C1309	C1215	C985	G765	G664
G2299	G2078	U1889	G1705	A1500	C1310	C1219	C986	G904	C665
A2300	U2080	C1890	A1706	A1501	C1314	A1222	C987	C905	G666
C2301	G2083	C1891	G1716	G1502	C1317	G1070	C988	C906	A667
C2302	C2084	C1892	C1718	G1504	U1318	C1071	C989	C907	C668
C2303	G2085	U1893	G1719	G1506	U1319	C1072	C990	G908	C672
G2306	U2090	C1894	U1725	C1509	U1320	C1075	C991	G910	C673
A2313	C2091	U1895	U1726	G1510	G1321	C1081	C992	U913	G677
C2323	A2092	C1896	U1727	U1511	A1322	C1082	C993	U914	C678
C2324	G2093	U1897	U1728	U1514	C1323	U1247	C994	A915	C679
C2325	G2094	G1912	C1731	A1515	A1324	C1248	C995	C916	G680
G2326	A2095	C1913	G1732	G1516	C1325	C1250	C996	C917	G684
G2331	U2097	C1914	G1733	G1517	C1326	C1251	C997	C918	C685
A2332	G2098	G1917	G1734	C1523	C1327	C1252	C998	C919	A686
C2333	C2101	U1918	U1735	A1524	G1328	G1253	C999	C920	U687
C2334	G2102	C1919	U1736	A1525	C1332	A1254	C923	C924	U688
C2335	G2103	U1920	A1631	C1536	A1333	A1255	C925	A932	U689
G2336	G2104	C1921	G1632	U1537	A1334	G1256	C926	C932	C690
G2345	A2105	G1922	A1633	U1538	C1337	G1257	C927	C933	A692
G2346	G2106	U1925	A1634	U1539	G1338	G1258	C928	A935	G700
A2347	C2107	G1926	U1638	G1545	U1339	G1259	C929	C936	U701
G2348	G2108	U1927	U1639	C1546	C1340	G1260	C930	C941	U702
A2349	C2109	C1931	G1640	A1547	C1344	G1266	C931	G942	G703
U2350	G2110	U1932	G1641	C1548	A1345	G1267	C943	G943	C704
C2351	G2111	C1933	A1642	G1549	C1346	G1268	A944	A944	A711
G2352	G2112	U1934	C1645	G1552	C1347	G1269	U945	U945	C712
C2353	C2249	C1935	U1646	A1553	U1348	G1270	C950	G950	C716
G2354	G2250	G1936	C1665	A1554	G1349	G1271	G951	G951	C717
A2355	G2251	A1942	A1669	A1555	C1350	G1272	C956	C956	C718
C2356	A2253	A1943	G1760	C1446	G1351	G1273	C957	A956	
G2364				C1447		C1280			

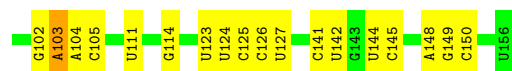
C4365	C4377	A4376	C4377	A4378	A4379	C4387	A4388	C4389	A4390	G4391	C4392	A4404	U4403	U4405	C4413	U4419	U4420	U4421	U4422	U4431	C4432	A4435	C4436	U4438	U4439	U4442	U4445	U4448	U4449	U4450	U4451	U4452	C4456	U4457	U4458	U4459	U4460	C4461	A4464	U4465	U4466	U4471	C4472								
U4190	G4191	G4196	A4203	U4208	U4209	U4210	A4212	A4213	A4214	A4219	A4220	A4221	G4222	G4225	U4312	A4313	C4314	C4318	C4319	A4320	U4321	C4322	A4325	G4326	C4327	U4328	C4329	C4330	C4331	C4332	C4333	C4334	U4340	C4341	U4344	U4346	C4347	U4348	C4349	C4350	U4353	U4354	U4361	A4362	A4363	U4471	C4472				
G4097	A4098	C4099	C4100	C4101	C4104	G4107	G4108	U4111	C4112	U4113	C4114	C4115	C4116	U4117	C4122	C4126	A4127	C4139	C4140	C4141	C4142	C4143	C4144	C4145	C4146	C4149	C4150	C4153	C4154	C4162	U4163	C4164	C4168	G4169	C4170	C4171	C4177	A4178	C4179	C4180	C4183	C4184	C4185	A4186	A4187	U4188	U4189				
A3917	G3918	C3919	U3920	A3923	C3924	U3925	U3930	C3931	U3932	C3933	G3934	C3937	G3938	G3939	A3942	A3943	G3944	A3945	G3946	A3947	C3948	C3949	U3950	G3953	A3954	C4056	C4057	U4058	C4059	U4060	G4061	A4062	U4063	C4064	U4067	U4068	U4069	U4070	U4071	G4076	A4077	C4084	C4088	G4089	G4092	C4093	G4094	G4095	C4096		
C3841	C3842	C3843	U3844	U3848	A3849	C3850	A3851	C3852	C3853	C3854	C3855	A3856	A3861	A3862	A3865	C3866	A3867	C3868	C3869	C3870	A3871	A3872	G3873	G3874	A3877	C3878	A3879	C3880	G3881	U3884	C3885	G3886	U3892	C3893	A3894	U4068	C3895	U4069	G3897	C3898	G3899	A3901	A3906	G3907	A3908	C3909	C3910	U3912	U3915	C3916	C3917
U3639	U3640	U3641	U3644	U3645	A3646	A3647	A3648	G3654	G3659	C3660	G3661	A3662	C3663	G3664	G3665	C3670	C3673	C3674	A3687	U3688	G3689	U3690	C3691	A3692	U3693	U3694	C3695	C3696	U3697	C3698	C3701	U3707	C3708	U3709	G3710	A3711	C3712	U3713	A3717	A3718	A3719	G3720	U3721	G3722	C3723	A3724	C3725	A3726	U3727	A3728	
C2875	G2876	C2877	C2890	U2891	A2894	A2895	C2899	U2900	G2901	C2902	U2903	U2904	C2905	G2906	C2907	U2908	C2909	G2910	C3584	G3585	G3590	C3591	C3594	U3595	A3596	C3597	C3598	A3599	C3600	C3601	A3604	C3605	U3606	U3607	A3608	C3609	A3610	A3611	G3615	G3619	A3624	G3625	G3626	C3633	G3634	A3635	C3636	G3638			
U2767	C2768	U2769	C2770	G2773	G2777	G2778	A2787	U2788	U2789	U2803	C2804	C2805	U2806	A2807	G2808	U2811	U2810	G2811	A2812	U2813	C2814	A2815	C2824	U2825	U2826	G2827	G2831	A2832	U2837	C2838	U2839	A2844	C2845	C2846	G2847	G2848	C2855	C2856	C2861	A2864	U2865	C2866	C2867	U2870	A2871						
C2683	C2684	U2687	G2688	U2691	U2692	G2693	A2694	A2695	A2696	C2702	G2706	U2707	U2708	C2709	C2710	G2711	U2718	C2719	U2720	G2721	G2724	A2725	U2726	C2727	U2730	C2731	G2732	C2733	C2738	C2739	G2742	A2743	A2744	A2745	A2746	C2749	G2750	G2756	U2757	C2759	C2760	U2761	C2762	U2763	A2764	A2765	A2766				
C2572	A2573	C2577	G2578	G2579	U2580	A2581	C2582	C2583	A2587	C2588	G2601	G2608	C2609	G2610	A2611	C2612	C2613	C2614	G2622	A2623	U2625	U2626	C2627	U2632	U2633	C2634	U2635	G2638	U2639	A2641	C2653	U2656	G2657	C2658	G2662	C2667	G2668	C2669	C2670	C2671	C2672	G2675	A2676								
G2481	C2482	G2483	A2484	U2485	G2486	G2487	C2488	U2489	A2491	C2492	A2493	U2494	C2504	C2505	G2506	A2513	G2516	A2517	U2518	C2520	G2521	A2529	U2537	U2538	C2539	G2540	C2541	A2542	A2543	G2544	U2545	G2546	G2547	G2550	U2554	G2555	G2556	C2557	C2558	U2559	C2560	C2561	G2562	A2565	C2568	U2570	C2571				



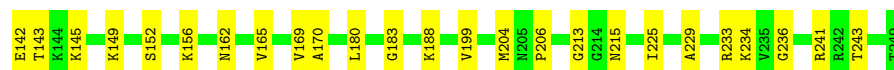
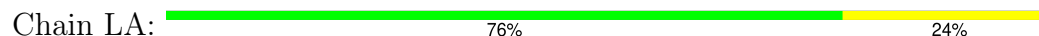
- Molecule 4: 5S rRNA



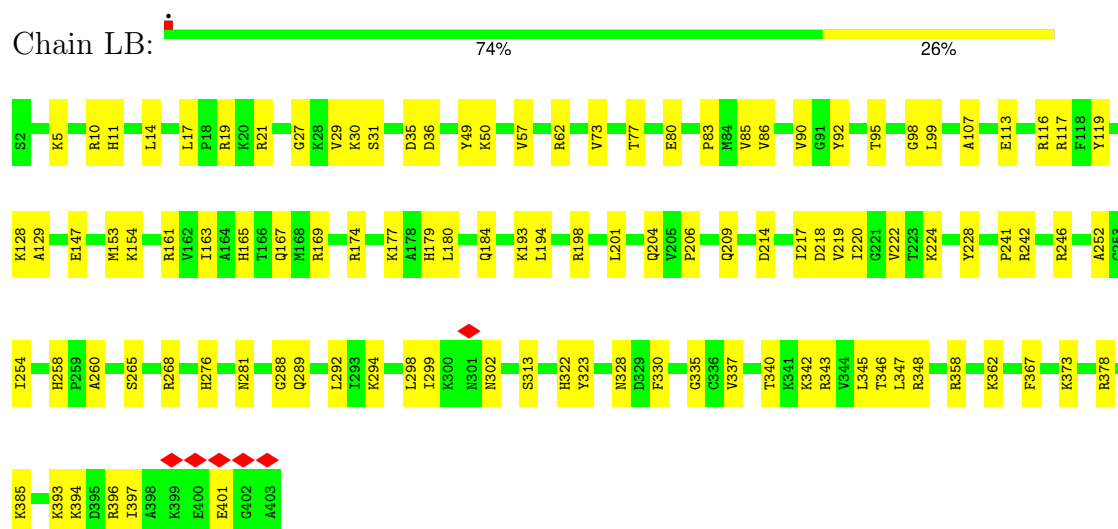
- Molecule 5: 5.8S rRNA [Homo sapiens]



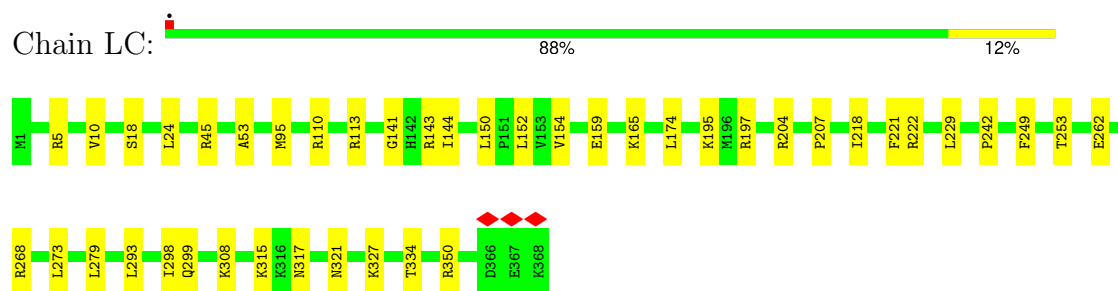
- Molecule 6: 60S ribosomal protein L8



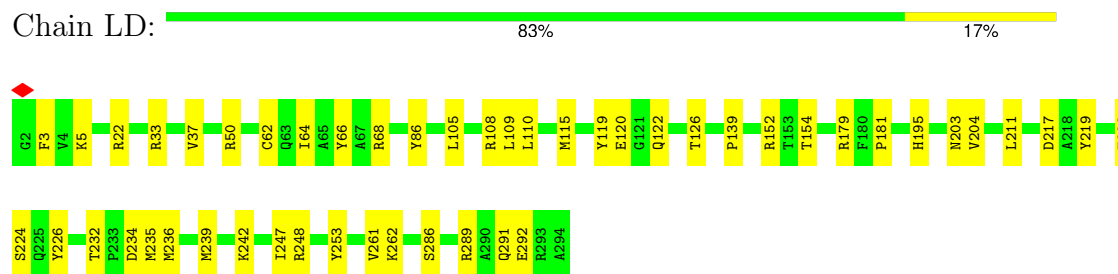
- Molecule 7: Large ribosomal subunit protein uL3



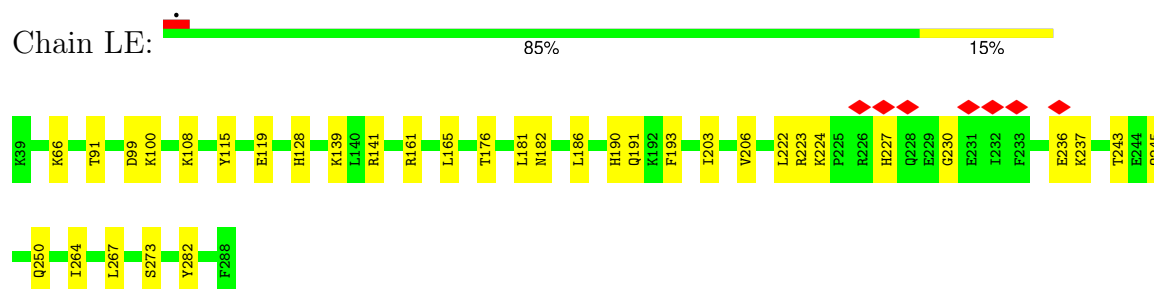
- Molecule 8: 60S ribosomal protein L4



- Molecule 9: Large ribosomal subunit protein uL18



- Molecule 10: Large ribosomal subunit protein eL6



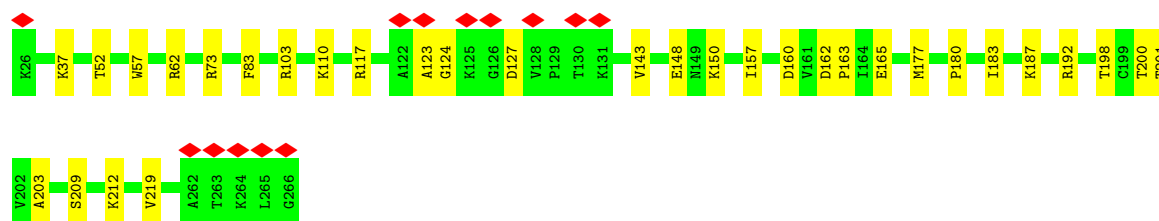
- Molecule 11: 60S ribosomal protein L7

Chain LF:  83% 17%



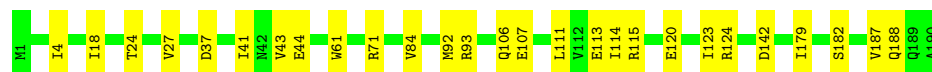
- Molecule 12: 60S ribosomal protein L7a

Chain LG:  5% 87% 13%



- Molecule 13: 60S ribosomal protein L9

Chain LH:  86% 14%



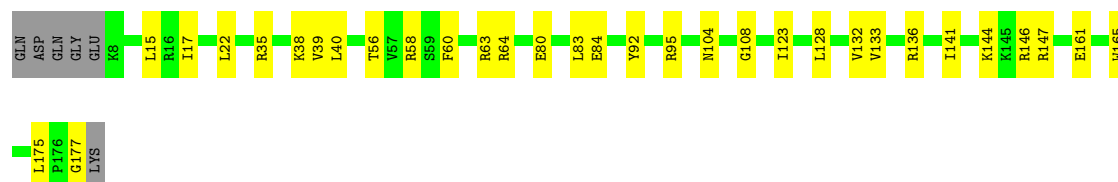
- Molecule 14: Ribosomal protein uL16-like

Chain LI:  87% 13%



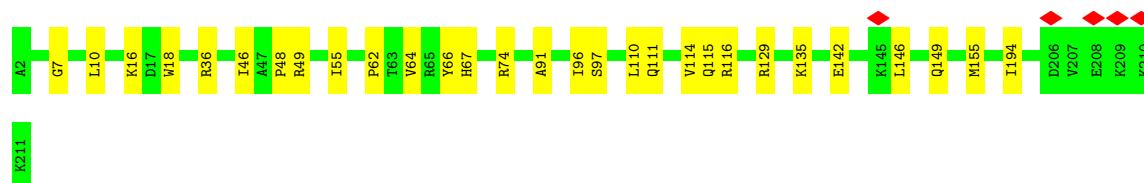
- Molecule 15: 60S ribosomal protein L11

Chain LJ:  78% 18% .



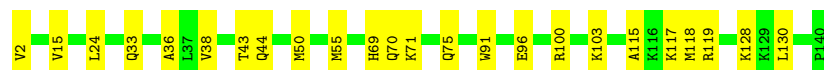
- Molecule 16: Large ribosomal subunit protein eL13

Chain LL:  86% 14%



- Molecule 17: 60S ribosomal protein L14

Chain LM: 83% 17%



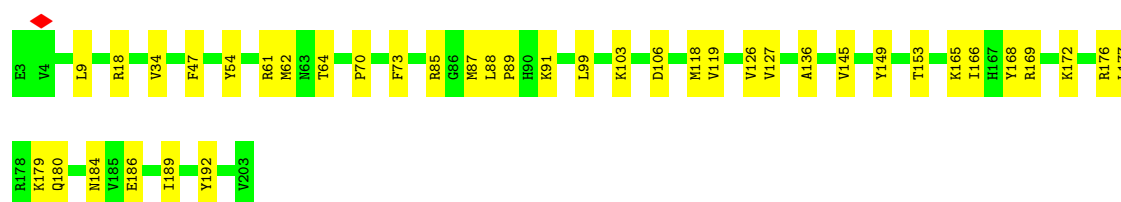
- Molecule 18: 60S ribosomal protein L15

Chain LN: 87% 13%



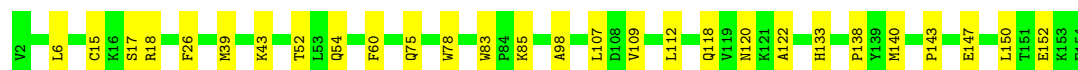
- Molecule 19: 60S ribosomal protein L13a

Chain LO: 81% 19%



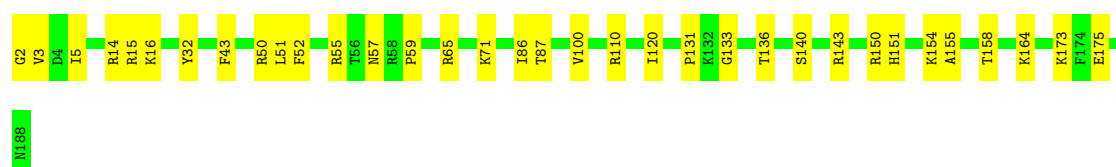
- Molecule 20: 60S ribosomal protein L17

Chain LP: 82% 18%



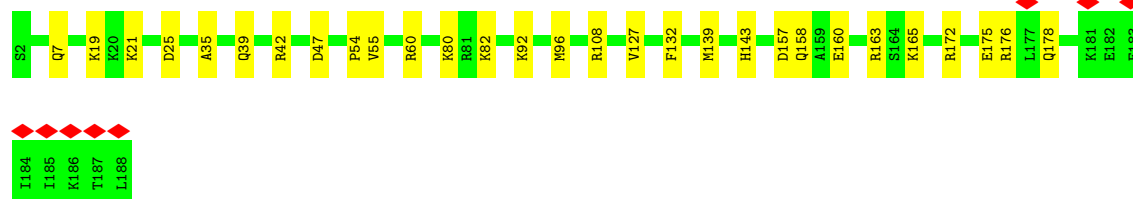
- Molecule 21: 60S ribosomal protein L18

Chain LQ: 82% 18%



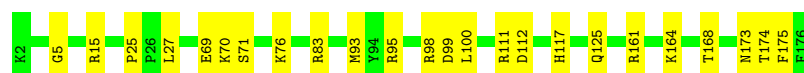
- Molecule 22: 60S ribosomal protein L19

Chain LR:  84% 16%



- Molecule 23: 60S ribosomal protein L18a

Chain LS:  86% 14%



- Molecule 24: 60S ribosomal protein L21

Chain LT:  85% 15%



- Molecule 25: Heparin-binding protein HBp15

Chain LU:  82% 18%



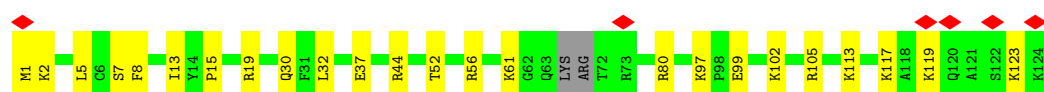
- Molecule 26: 60S ribosomal protein L23

Chain LV:  89% 11%

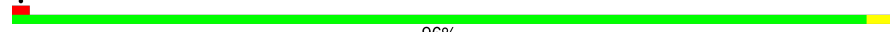


- Molecule 27: Ribosomal protein L24

Chain LW:  5% 78% 20%



- Molecule 28: 60S ribosomal protein L23a

Chain LX:  96%



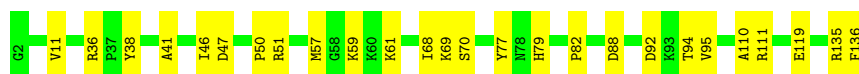
- Molecule 29: 60S ribosomal protein L26

Chain LY: 85% 15%



- Molecule 30: 60S ribosomal protein L27

Chain LZ: 81% 19%



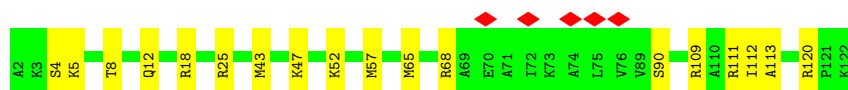
- Molecule 31: 60S ribosomal protein L27a

Chain La: 90% 10%



- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb: 5% 83% 17%



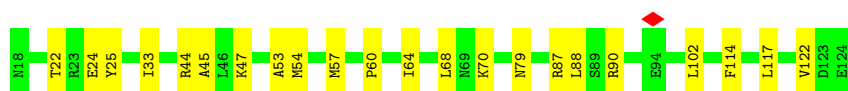
- Molecule 33: 60S ribosomal protein L30

Chain Lc: 77% 23%



- Molecule 34: 60S ribosomal protein L31

Chain Ld: 79% 21%



- Molecule 35: 60S ribosomal protein L32

Chain Le:  91% 9%



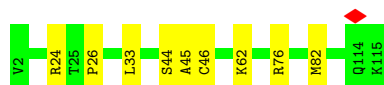
- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  89% 11%



- Molecule 37: 60S ribosomal protein L34

Chain Lg:  92% 8%



- Molecule 38: 60S ribosomal protein L35

Chain Lh:  84% 16%



- Molecule 39: 60S ribosomal protein L36

Chain Li:  91% 9%



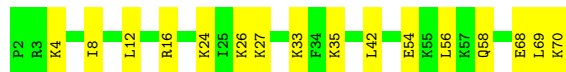
- Molecule 40: 60S ribosomal protein L37

Chain Lj:  80% 20%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  77% 23%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  88% 12%



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  90% 10%



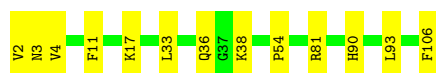
- Molecule 44: 60S ribosomal protein L41

Chain Ln:  92% 8%



- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  88% 12%



- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  91% 9%



- Molecule 47: 60S ribosomal protein L28

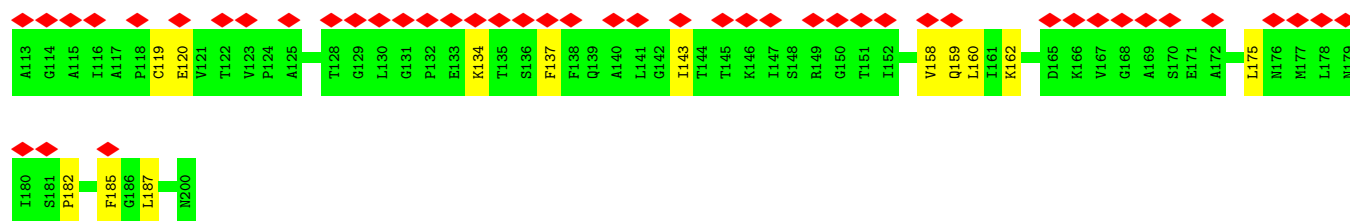
Chain Lr:  88% 12%



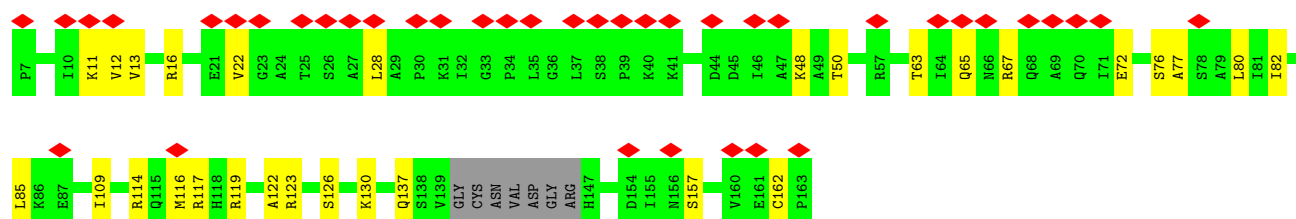
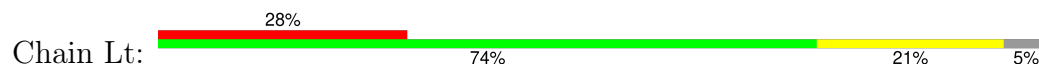
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls:  29% 81% 19%

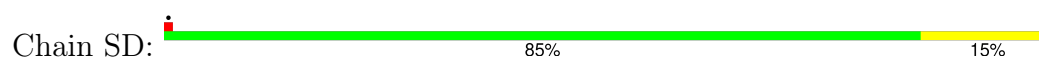




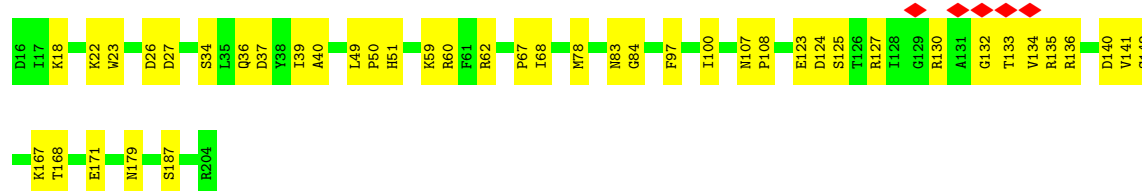
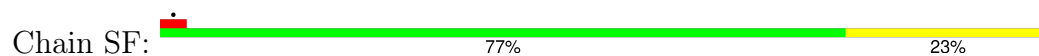
- Molecule 49: Large ribosomal subunit protein uL11



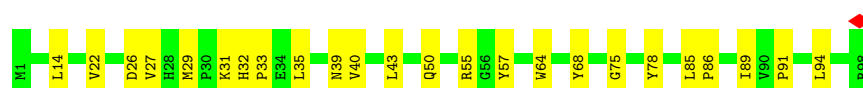
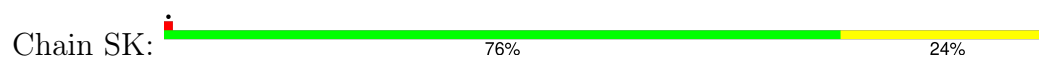
- Molecule 50: Small ribosomal subunit protein uS3



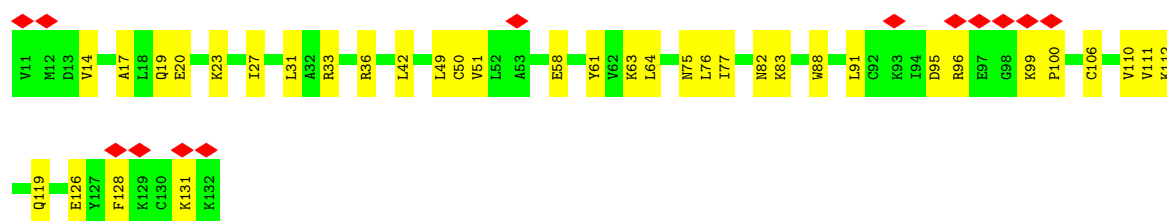
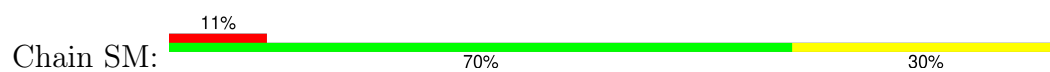
- Molecule 51: 40S ribosomal protein S5



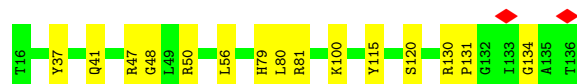
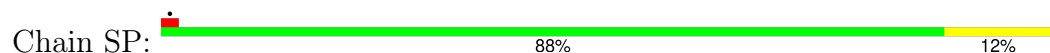
- Molecule 52: 40S ribosomal protein S10



- Molecule 53: Small ribosomal subunit protein eS12



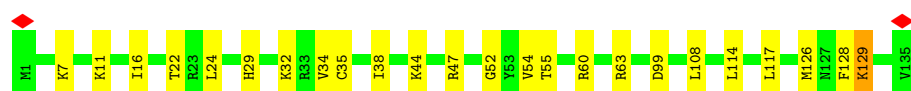
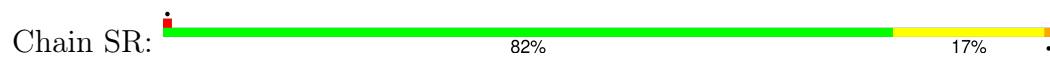
- Molecule 54: Small ribosomal subunit protein uS19



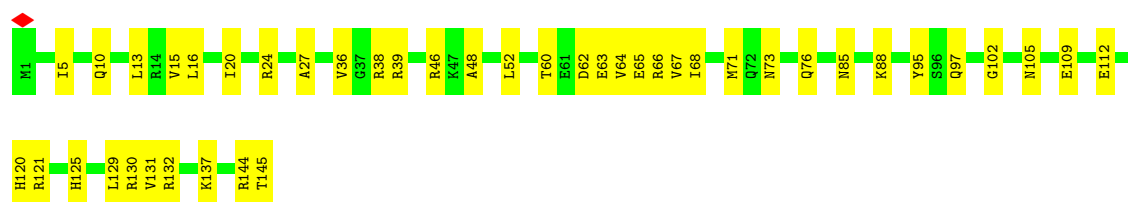
- Molecule 55: Small ribosomal subunit protein uS9



- Molecule 56: Small ribosomal subunit protein eS17

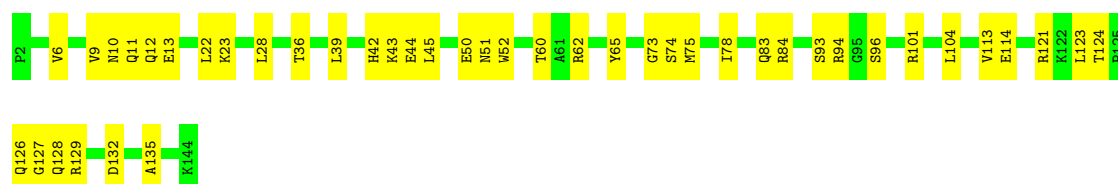


- Molecule 57: 40S ribosomal protein S18

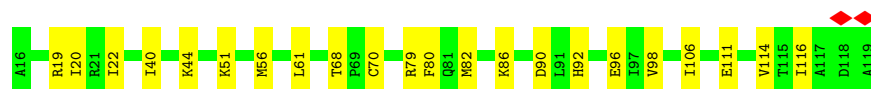
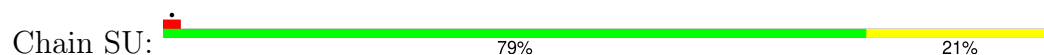


- Molecule 58: 40S ribosomal protein S19

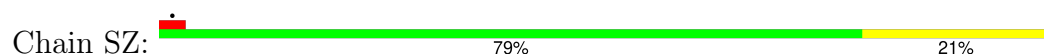




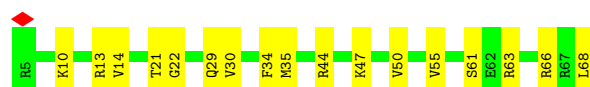
- Molecule 59: 40S ribosomal protein S20



- Molecule 60: Small ribosomal subunit protein eS25



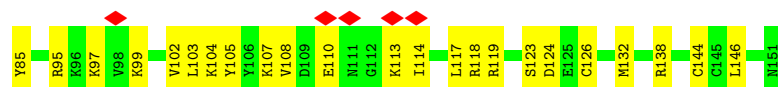
- Molecule 61: 40S ribosomal protein S28



- Molecule 62: 40S ribosomal protein S29

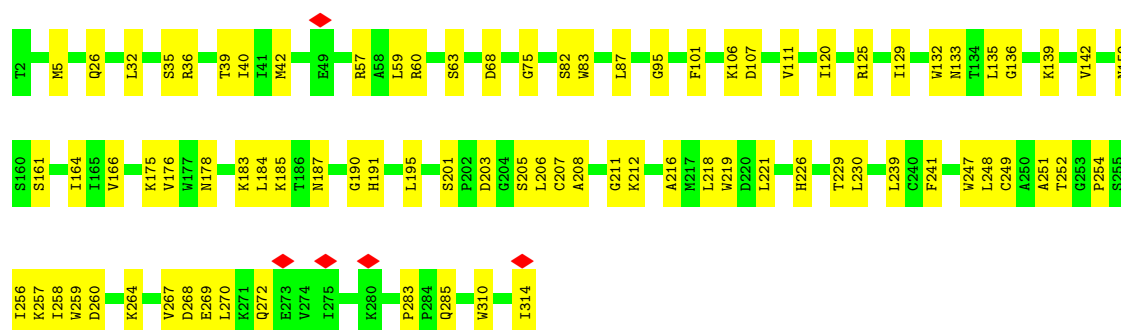


- Molecule 63: Ubiquitin-40S ribosomal protein S27a



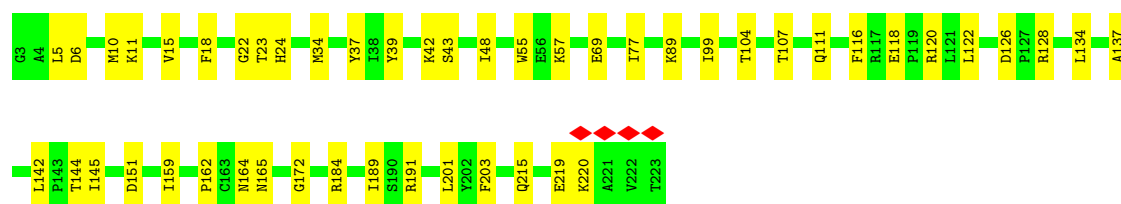
- Molecule 64: Receptor of activated protein C kinase 1





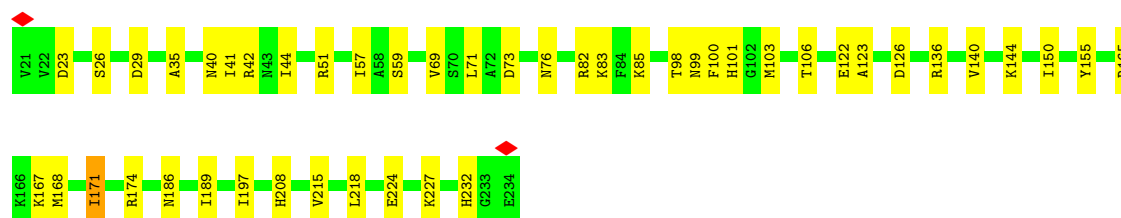
- Molecule 65: 40S ribosomal protein SA

Chain SA: 78% 22%



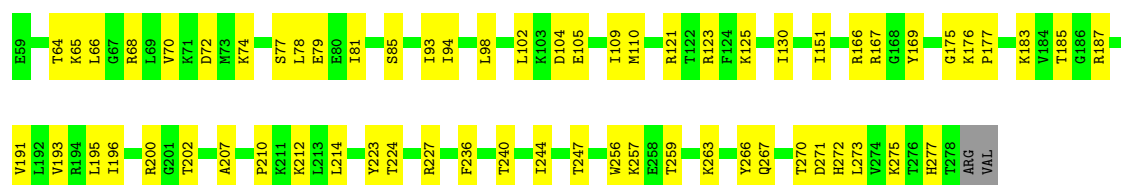
- Molecule 66: 40S ribosomal protein S3a

Chain SB: 79% 21%



- Molecule 67: 40S ribosomal protein S2

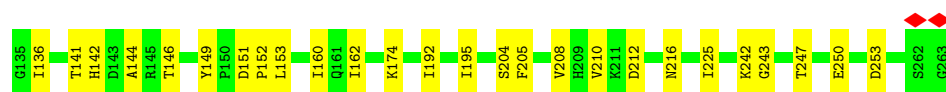
Chain SC: 71% 28%



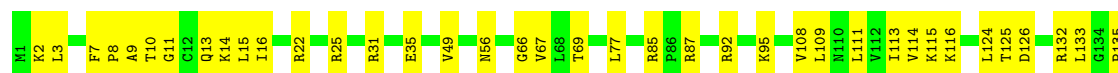
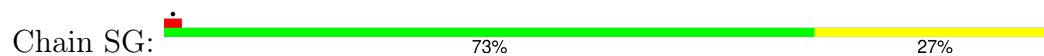
- Molecule 68: Small ribosomal subunit protein eS4, X isoform

Chain SE: 77% 23%

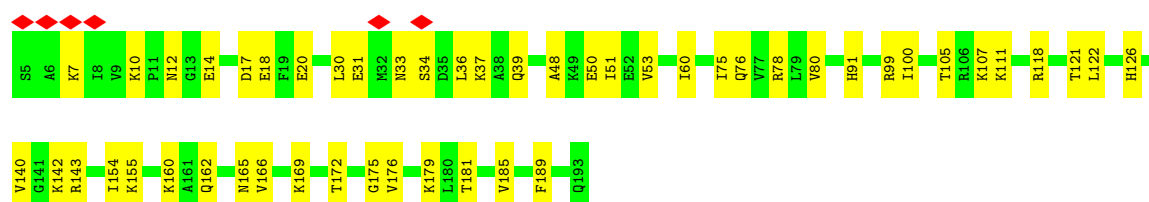
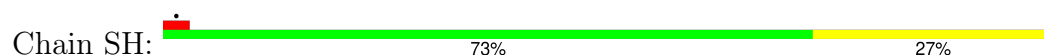




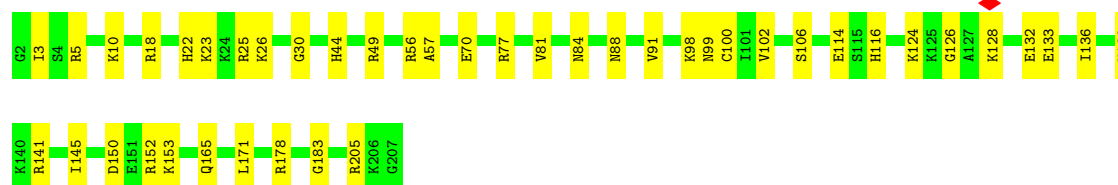
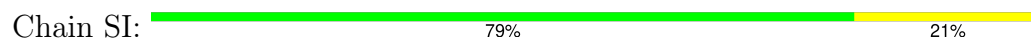
- Molecule 69: 40S ribosomal protein S6



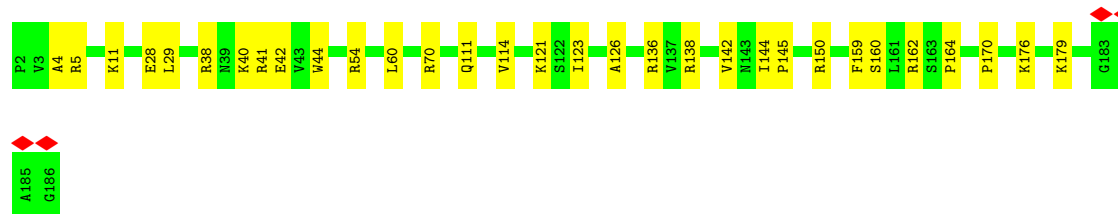
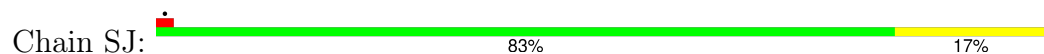
- Molecule 70: Small ribosomal subunit protein eS7



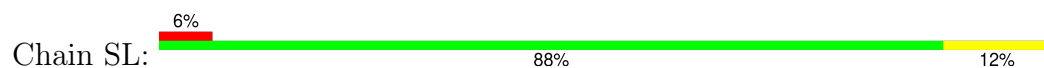
- Molecule 71: 40S ribosomal protein S8

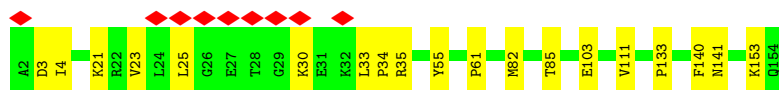


- Molecule 72: 40S ribosomal protein S9



- Molecule 73: 40S ribosomal protein S11





- Molecule 74: 40S ribosomal protein S13

Chain SN: 89% 11%



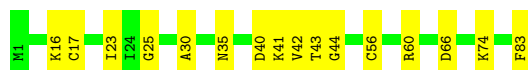
- Molecule 75: Small ribosomal subunit protein uS11

Chain SO: 81% 16%



- Molecule 76: Small ribosomal subunit protein eS21

Chain SV: 81% 19%



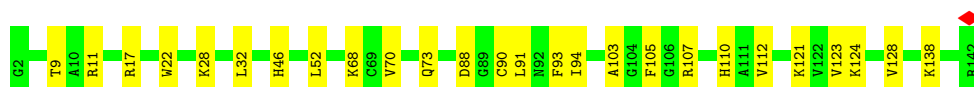
- Molecule 77: 40S ribosomal protein S15a

Chain SW: 79% 21%



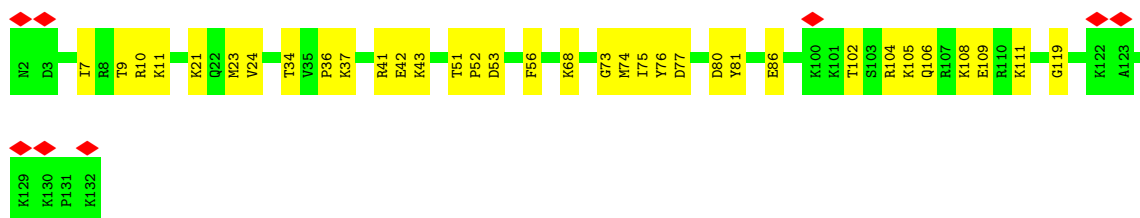
- Molecule 78: 40S ribosomal protein S23

Chain SX: 82% 18%

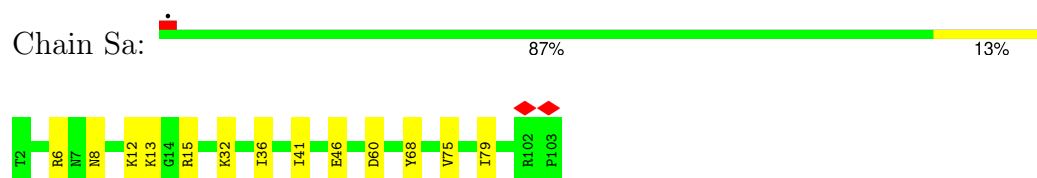


- Molecule 79: 40S ribosomal protein S24

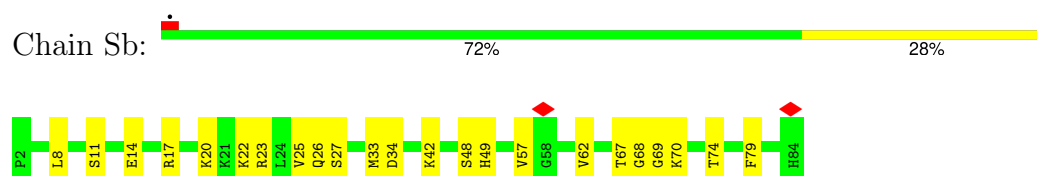
Chain SY: 6% 74% 26%



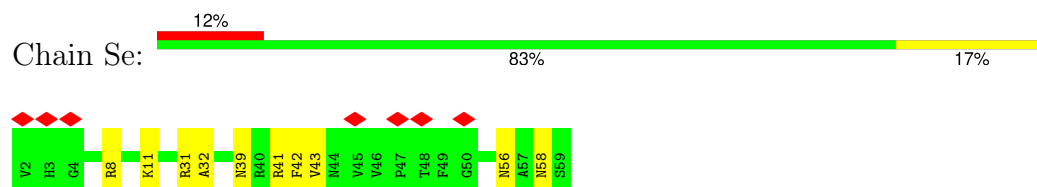
- Molecule 80: 40S ribosomal protein S26



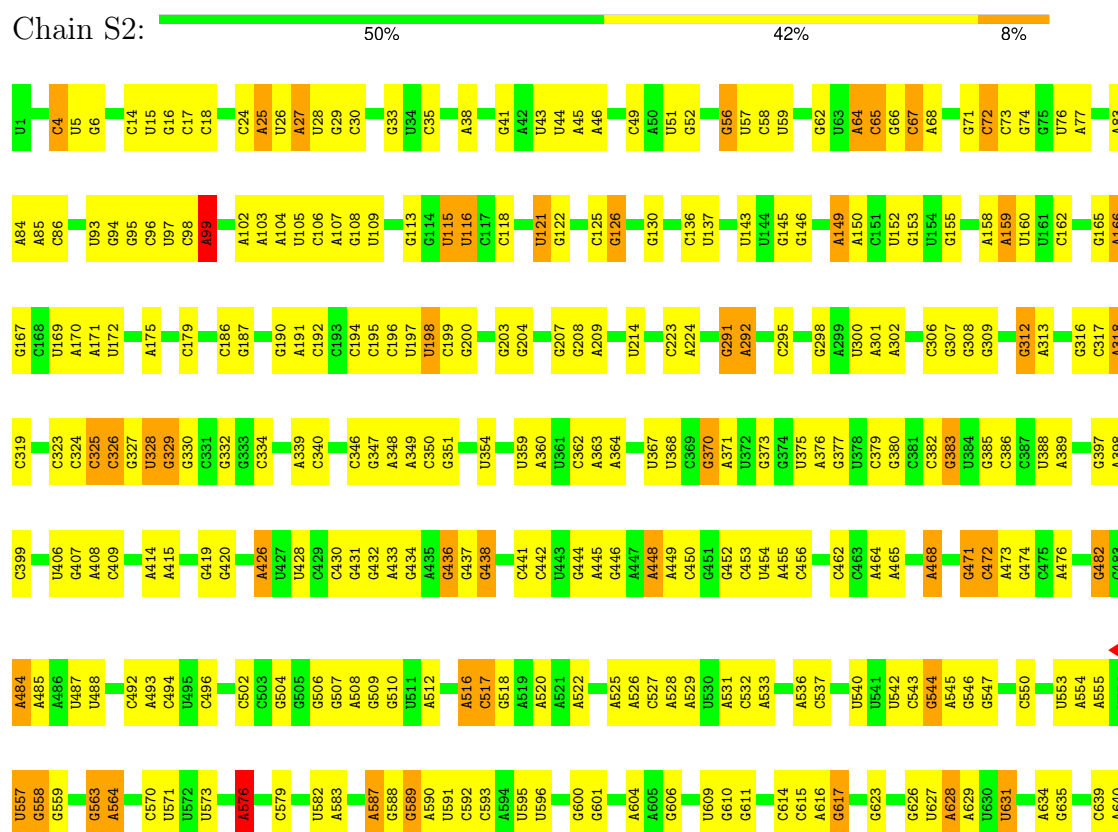
- Molecule 81: Small ribosomal subunit protein eS27

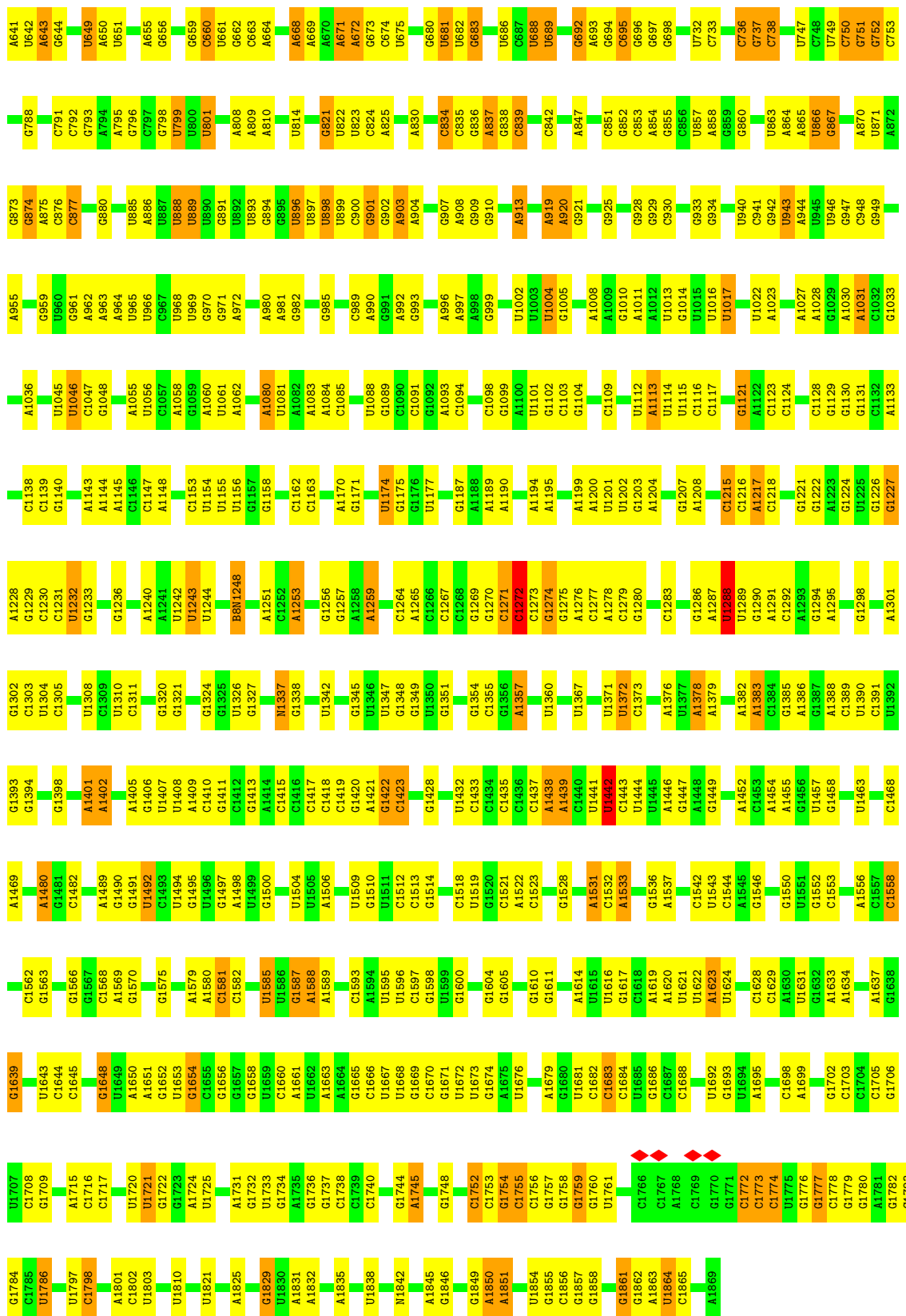


- Molecule 82: Small ribosomal subunit protein eS30

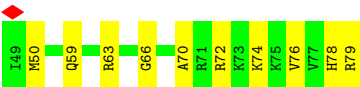


- Molecule 83: 18S rRNA





• Molecule 84: Transcription factor BTF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67622	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	0.164	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0128	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Pt	0.12	0/1761	0.26	0/2741
2	Et	0.14	0/1778	0.31	0/2767
3	L5	0.19	0/85098	0.30	0/132762
4	L7	0.16	0/2861	0.25	0/4459
5	L8	0.17	0/3631	0.28	0/5657
6	LA	0.20	0/1936	0.38	0/2596
7	LB	0.18	0/3306	0.36	0/4424
8	LC	0.18	0/2981	0.35	0/4002
9	LD	0.16	0/2428	0.33	0/3252
10	LE	0.17	0/1973	0.41	0/2645
11	LF	0.18	0/1905	0.32	0/2539
12	LG	0.17	0/1960	0.39	0/2637
13	LH	0.16	0/1537	0.34	0/2066
14	LI	0.17	0/1751	0.33	0/2340
15	LJ	0.16	0/1385	0.36	0/1852
16	LL	0.17	0/1732	0.32	0/2315
17	LM	0.18	0/1161	0.36	0/1554
18	LN	0.19	0/1746	0.33	0/2338
19	LO	0.20	0/1682	0.35	0/2250
20	LP	0.19	0/1268	0.39	0/1701
21	LQ	0.19	0/1537	0.35	0/2052
22	LR	0.17	0/1582	0.35	0/2091
23	LS	0.19	0/1493	0.33	0/2003
24	LT	0.18	0/1326	0.32	0/1770
25	LU	0.18	0/839	0.43	0/1126
26	LV	0.17	0/993	0.36	0/1332
27	LW	0.17	0/959	0.37	0/1270
28	LX	0.16	0/1002	0.33	0/1345
29	LY	0.17	0/1132	0.36	0/1504
30	LZ	0.16	0/1130	0.35	0/1507
31	La	0.17	0/1191	0.31	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.16	0/889	0.40	0/1175
33	Lc	0.17	0/774	0.36	0/1038
34	Ld	0.17	0/903	0.34	0/1216
35	Le	0.18	0/1071	0.31	0/1429
36	Lf	0.19	0/895	0.35	0/1198
37	Lg	0.17	0/916	0.35	0/1220
38	Lh	0.15	0/1023	0.32	0/1351
39	Li	0.15	0/843	0.32	0/1115
40	Lj	0.19	0/720	0.36	0/952
41	Lk	0.16	0/575	0.42	0/761
42	Ll	0.17	0/454	0.29	0/599
43	Lm	0.16	0/435	0.33	0/575
44	Ln	0.18	0/231	0.31	0/294
45	Lo	0.18	0/876	0.33	0/1156
46	Lp	0.17	0/718	0.33	0/953
47	Lr	0.17	0/1017	0.32	0/1364
48	Ls	0.12	0/1519	0.33	0/2052
49	Lt	0.17	0/1009	0.50	0/1363
50	SD	0.13	0/1793	0.30	0/2414
51	SF	0.15	0/1516	0.36	0/2037
52	SK	0.14	0/851	0.43	0/1147
53	SM	0.13	0/950	0.37	0/1275
54	SP	0.15	0/1003	0.42	0/1342
55	SQ	0.15	0/1160	0.39	0/1553
56	SR	0.16	0/1105	0.42	0/1484
57	SS	0.15	0/1216	0.36	0/1628
58	ST	0.14	0/1131	0.39	0/1515
59	SU	0.17	0/831	0.44	0/1115
60	SZ	0.16	0/604	0.48	0/810
61	Sc	0.15	0/508	0.36	0/680
62	Sd	0.14	0/470	0.34	0/623
63	Sf	0.15	0/560	0.45	0/745
64	Sg	0.13	0/2493	0.36	0/3394
65	SA	0.14	0/1778	0.34	0/2416
66	SB	0.14	0/1765	0.35	0/2362
67	SC	0.15	0/1744	0.35	0/2357
68	SE	0.14	0/2118	0.35	0/2849
69	SG	0.15	0/1946	0.37	0/2590
70	SH	0.16	0/1519	0.41	0/2033
71	SI	0.16	0/1715	0.36	0/2287
72	SJ	0.13	0/1550	0.32	0/2069
73	SL	0.15	0/1268	0.31	0/1696
74	SN	0.13	0/1232	0.27	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SO	0.17	0/1037	0.38	0/1391
76	SV	0.16	0/643	0.38	0/860
77	SW	0.17	0/1051	0.35	0/1406
78	SX	0.15	0/1116	0.36	0/1490
79	SY	0.15	0/1083	0.40	0/1438
80	Sa	0.17	0/836	0.33	0/1121
81	Sb	0.14	0/665	0.35	0/891
82	Se	0.14	0/465	0.41	0/612
83	S2	0.18	0/39756	0.28	0/61939
84	CI	0.16	0/247	0.30	0/323
All	All	0.17	0/231657	0.32	0/339847

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
55	SQ	0	1
66	SB	0	1
75	SO	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	SB	171	ILE	Peptide
75	SO	137	SER	Peptide
55	SQ	107	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Pt	1576	0	803	20	0
2	Et	1593	0	810	37	0
3	L5	78444	0	39719	907	0
4	L7	2561	0	1295	21	0
5	L8	3315	0	1685	35	0
6	LA	1898	0	1993	45	0
7	LB	3238	0	3376	78	0
8	LC	2927	0	3104	32	0
9	LD	2382	0	2410	32	0
10	LE	1935	0	2096	25	0
11	LF	1870	0	1996	29	0
12	LG	1927	0	2074	21	0
13	LH	1518	0	1601	18	0
14	LI	1711	0	1749	21	0
15	LJ	1362	0	1399	22	0
16	LL	1701	0	1818	24	0
17	LM	1138	0	1204	20	0
18	LN	1701	0	1749	23	0
19	LO	1650	0	1794	29	0
20	LP	1242	0	1269	20	0
21	LQ	1513	0	1628	25	0
22	LR	1566	0	1729	21	0
23	LS	1453	0	1490	15	0
24	LT	1298	0	1366	17	0
25	LU	825	0	850	14	0
26	LV	979	0	1039	11	0
27	LW	945	0	1003	20	0
28	LX	985	0	1066	4	0
29	LY	1115	0	1205	13	0
30	LZ	1107	0	1182	18	0
31	La	1162	0	1213	12	0
32	Lb	876	0	948	17	0
33	Lc	764	0	804	13	0
34	Ld	888	0	930	17	0
35	Le	1053	0	1147	10	0
36	Lf	876	0	912	8	0
37	Lg	906	0	998	8	0
38	Lh	1015	0	1148	17	0
39	Li	832	0	917	7	0
40	Lj	705	0	737	16	0
41	Lk	569	0	637	14	0
42	Ll	444	0	483	5	0
43	Lm	429	0	465	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Ln	230	0	276	2	0
45	Lo	862	0	929	11	0
46	Lp	708	0	756	7	0
47	Lr	1002	0	1068	9	0
48	Ls	1496	0	1540	25	0
49	Lt	998	0	1032	20	0
50	SD	1765	0	1865	23	0
51	SF	1495	0	1549	38	0
52	SK	827	0	854	17	0
53	SM	940	0	965	23	0
54	SP	985	0	1031	13	0
55	SQ	1142	0	1213	29	0
56	SR	1090	0	1149	16	0
57	SS	1198	0	1261	32	0
58	ST	1112	0	1146	31	0
59	SU	821	0	883	16	0
60	SZ	598	0	656	15	0
61	Sc	506	0	536	11	0
62	Sd	459	0	452	16	0
63	Sf	548	0	551	19	0
64	Sg	2436	0	2393	58	0
65	SA	1741	0	1746	32	0
66	SB	1738	0	1809	29	0
67	SC	1707	0	1791	45	0
68	SE	2076	0	2177	41	0
69	SG	1923	0	2089	56	0
70	SH	1497	0	1590	32	0
71	SI	1686	0	1772	34	0
72	SJ	1525	0	1640	25	0
73	SL	1247	0	1323	14	0
74	SN	1208	0	1294	11	0
75	SO	1024	0	1050	15	0
76	SV	636	0	637	13	0
77	SW	1034	0	1080	25	0
78	SX	1098	0	1167	23	0
79	SY	1065	0	1142	26	0
80	Sa	821	0	870	10	0
81	Sb	651	0	672	16	0
82	Se	459	0	503	11	0
83	S2	36953	0	18679	529	0
84	CI	247	0	283	18	0
85	L5	179	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L7	3	0	0	0	0
85	L8	5	0	0	0	0
85	LA	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0
85	Le	1	0	0	0	0
85	S2	27	0	0	0	0
85	SS	1	0	0	0	0
86	L5	98	0	182	7	0
87	L5	90	0	171	5	0
87	LN	10	0	19	0	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lm	1	0	0	0	0
88	Lo	1	0	0	0	0
88	Lp	1	0	0	0	0
88	Sa	1	0	0	0	0
All	All	219971	0	163632	2637	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 2637 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2708:U:O2'	84:CI:79:ARG:NH1	1.63	1.30
34:Ld:70:LYS:NZ	84:CI:66:GLY:HA3	1.81	0.96
83:S2:1033:G:H1	83:S2:1080:A:HO2'	1.07	0.95
83:S2:928:G:H1	83:S2:1013:U:H3	1.15	0.93
3:L5:1759:G:H1	3:L5:1773:U:H3	1.05	0.93

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	
6	LA	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
7	LB	400/402 (100%)	386 (96%)	14 (4%)	0	100	100
8	LC	366/368 (100%)	354 (97%)	12 (3%)	0	100	100
9	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
10	LE	236/240 (98%)	221 (94%)	15 (6%)	0	100	100
11	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
12	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
13	LH	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
14	LI	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
15	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
16	LL	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
17	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
18	LN	201/203 (99%)	199 (99%)	2 (1%)	0	100	100
19	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
20	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
21	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
22	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
23	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
26	LV	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
27	LW	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
28	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
29	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
30	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
31	La	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
32	Lb	105/109 (96%)	100 (95%)	5 (5%)	0	100	100
33	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
34	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
35	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lf	107/109 (98%)	107 (100%)	0	0	100	100
37	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
38	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
39	Li	100/102 (98%)	100 (100%)	0	0	100	100
40	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
42	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
46	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
47	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
48	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
49	Lt	128/141 (91%)	112 (88%)	16 (12%)	0	100	100
50	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
51	SF	187/189 (99%)	174 (93%)	13 (7%)	0	100	100
52	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
53	SM	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
54	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
55	SQ	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
56	SR	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	44
57	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
58	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
59	SU	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
60	SZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
61	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
62	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
63	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
64	Sg	311/313 (99%)	295 (95%)	16 (5%)	0	100	100
65	SA	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
66	SB	212/214 (99%)	205 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	SC	218/222 (98%)	207 (95%)	11 (5%)	0	100	100
68	SE	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
69	SG	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
70	SH	182/186 (98%)	169 (93%)	13 (7%)	0	100	100
71	SI	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
72	SJ	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	24	55
73	SL	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
74	SN	148/150 (99%)	147 (99%)	1 (1%)	0	100	100
75	SO	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
76	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
77	SW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
78	SX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
79	SY	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
80	Sa	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
81	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
82	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
84	CI	29/31 (94%)	29 (100%)	0	0	100	100
All	All	11672/11860 (98%)	11194 (96%)	476 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
56	SR	129	LYS
72	SJ	138	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	LA	190/190 (100%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/212 (100%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	180/180 (100%)	180 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	176 (100%)	0	100	100
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/97 (98%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/90 (98%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/115 (93%)	107 (100%)	0	100	100
50	SD	190/190 (100%)	190 (100%)	0	100	100
51	SF	159/159 (100%)	159 (100%)	0	100	100
52	SK	89/89 (100%)	89 (100%)	0	100	100
53	SM	102/104 (98%)	102 (100%)	0	100	100
54	SP	107/107 (100%)	107 (100%)	0	100	100
55	SQ	119/119 (100%)	119 (100%)	0	100	100
56	SR	122/122 (100%)	122 (100%)	0	100	100
57	SS	126/126 (100%)	126 (100%)	0	100	100
58	ST	113/113 (100%)	113 (100%)	0	100	100
59	SU	94/94 (100%)	94 (100%)	0	100	100
60	SZ	66/66 (100%)	66 (100%)	0	100	100
61	Sc	57/57 (100%)	57 (100%)	0	100	100
62	Sd	48/48 (100%)	48 (100%)	0	100	100
63	Sf	60/60 (100%)	60 (100%)	0	100	100
64	Sg	272/272 (100%)	272 (100%)	0	100	100
65	SA	183/183 (100%)	183 (100%)	0	100	100
66	SB	195/195 (100%)	195 (100%)	0	100	100
67	SC	186/188 (99%)	186 (100%)	0	100	100
68	SE	224/224 (100%)	224 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	SG	207/207 (100%)	207 (100%)	0	100	100
70	SH	166/166 (100%)	166 (100%)	0	100	100
71	SI	178/178 (100%)	178 (100%)	0	100	100
72	SJ	161/161 (100%)	161 (100%)	0	100	100
73	SL	137/137 (100%)	137 (100%)	0	100	100
74	SN	130/130 (100%)	130 (100%)	0	100	100
75	SO	107/110 (97%)	107 (100%)	0	100	100
76	SV	67/67 (100%)	67 (100%)	0	100	100
77	SW	112/112 (100%)	112 (100%)	0	100	100
78	SX	113/113 (100%)	113 (100%)	0	100	100
79	SY	113/113 (100%)	113 (100%)	0	100	100
80	Sa	89/89 (100%)	89 (100%)	0	100	100
81	Sb	75/75 (100%)	75 (100%)	0	100	100
82	Se	47/47 (100%)	47 (100%)	0	100	100
84	CI	25/25 (100%)	25 (100%)	0	100	100
All	All	10147/10176 (100%)	10147 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
53	SM	19	GLN
66	SB	76	ASN
57	SS	87	GLN
64	Sg	272	GLN
67	SC	277	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Pt	72/74 (97%)	15 (20%)	0
2	Et	73/75 (97%)	25 (34%)	0
3	L5	3643/3655 (99%)	726 (19%)	16 (0%)
4	L7	119/120 (99%)	9 (7%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L8	155/156 (99%)	21 (13%)	0
83	S2	1714/1740 (98%)	369 (21%)	3 (0%)
All	All	5776/5820 (99%)	1165 (20%)	19 (0%)

5 of 1165 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Pt	9	A
1	Pt	13	U
1	Pt	19	G
1	Pt	21	A
1	Pt	46	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4699	U
83	S2	563	G
83	S2	688	U
83	S2	291	G
3	L5	2416	G

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	$\# Z > 2$
3	A2M	L5	2363	85,3	22,25,26	1.24	2 (9%)	30,36,39	1.50	6 (20%)
83	OMG	S2	509	83	23,26,27	0.47	0	32,38,41	0.50	0
3	OMC	L5	1340	3	19,22,23	0.55	0	25,31,34	0.76	0
3	PSU	L5	1744	85,3	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
3	OMU	L5	3925	3	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
3	PSU	L5	4673	85,3	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	PSU	S2	93	83	18,21,22	1.11	1 (5%)	21,30,33	1.74	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	1004	83	18,21,22	1.14	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
3	OMU	L5	2837	3	19,22,23	3.37	7 (36%)	25,31,34	1.85	4 (16%)
83	OMC	S2	1391	83	19,22,23	0.50	0	25,31,34	0.69	0
83	OMG	S2	1490	83	23,26,27	0.52	0	32,38,41	0.49	0
3	PSU	L5	3853	85,3	18,21,22	1.05	1 (5%)	21,30,33	1.79	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
3	A2M	L5	3785	85,3	22,25,26	1.16	1 (4%)	30,36,39	1.62	9 (30%)
3	OMC	L5	3808	3	19,22,23	0.58	0	25,31,34	0.85	1 (4%)
83	OMU	S2	1288	83	19,22,23	3.37	7 (36%)	25,31,34	1.78	5 (20%)
3	PSU	L5	3844	3	18,21,22	1.14	1 (5%)	21,30,33	1.81	4 (19%)
3	PSU	L5	1782	3	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
83	4AC	S2	1842	83	21,24,25	0.37	0	28,34,37	0.46	0
3	OMG	L5	1316	3	23,26,27	0.51	0	32,38,41	0.57	0
3	UR3	L5	4530	3	19,22,23	2.73	7 (36%)	26,32,35	1.57	3 (11%)
83	PSU	S2	801	83	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
83	A2M	S2	484	83	22,25,26	1.21	1 (4%)	30,36,39	1.47	6 (20%)
3	PSU	L5	1683	3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	2839	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
83	OMU	S2	1442	83	19,22,23	3.39	7 (36%)	25,31,34	1.76	4 (16%)
3	PSU	L5	1781	3	18,21,22	1.05	1 (5%)	21,30,33	1.75	4 (19%)
83	A2M	S2	576	83	22,25,26	1.26	2 (9%)	30,36,39	1.54	5 (16%)
3	PSU	L5	4442	3	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)
3	A2M	L5	4571	3	22,25,26	1.31	2 (9%)	30,36,39	1.56	6 (20%)
3	OMU	L5	4306	3	19,22,23	3.33	7 (36%)	25,31,34	1.82	4 (16%)
83	PSU	S2	814	83	18,21,22	1.12	1 (5%)	21,30,33	1.82	4 (19%)
83	PSU	S2	1244	83	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	3920	85,3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
83	OMU	S2	354	83	19,22,23	3.34	7 (36%)	25,31,34	1.84	5 (20%)
3	A2M	L5	400	3	22,25,26	1.31	1 (4%)	30,36,39	1.54	6 (20%)
3	A2M	L5	3830	3	22,25,26	1.24	1 (4%)	30,36,39	1.59	5 (16%)
83	OMU	S2	116	83	19,22,23	3.35	7 (36%)	25,31,34	1.73	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	OMU	S2	1326	83	19,22,23	3.35	7 (36%)	25,31,34	1.85	5 (20%)
3	PSU	L5	3639	3	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
3	PSU	L5	4493	3	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
83	PSU	S2	105	83	18,21,22	1.12	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L5	2422	85,3	19,22,23	0.53	0	25,31,34	0.71	0
3	A2M	L5	3867	3	22,25,26	1.27	1 (4%)	30,36,39	1.43	6 (20%)
83	OMG	S2	644	83	23,26,27	0.46	0	32,38,41	0.50	0
3	OMG	L5	4499	3	23,26,27	0.47	0	32,38,41	0.49	0
3	A2M	L5	2401	3	22,25,26	1.25	1 (4%)	30,36,39	1.56	6 (20%)
83	A2M	S2	668	85,83	22,25,26	1.34	2 (9%)	30,36,39	1.54	6 (20%)
3	1MA	L5	1322	85,3	21,25,26	0.56	0	30,37,40	0.78	1 (3%)
3	OMG	L5	2424	3	23,26,27	0.50	0	32,38,41	0.48	0
83	OMG	S2	683	83	23,26,27	0.50	0	32,38,41	0.47	0
3	OMG	L5	4637	3	23,26,27	0.49	0	32,38,41	0.50	0
5	PSU	L8	69	5	18,21,22	1.10	1 (5%)	21,30,33	1.87	5 (23%)
3	PSU	L5	4457	3	18,21,22	1.08	1 (5%)	21,30,33	1.88	5 (23%)
3	PSU	L5	4576	3	18,21,22	1.10	1 (5%)	21,30,33	1.81	4 (19%)
3	A2M	L5	1534	85,3	22,25,26	1.21	1 (4%)	30,36,39	1.43	7 (23%)
3	PSU	L5	4299	3	18,21,22	1.05	1 (5%)	21,30,33	1.91	5 (23%)
83	OMG	S2	1328	83	23,26,27	0.45	0	32,38,41	0.46	0
83	PSU	S2	863	83	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
3	OMC	L5	2861	3	19,22,23	0.54	0	25,31,34	0.86	1 (4%)
3	OMC	L5	4456	3	19,22,23	0.59	0	25,31,34	0.91	1 (4%)
3	PSU	L5	1860	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	1367	83	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	2815	3	22,25,26	1.26	1 (4%)	30,36,39	1.46	6 (20%)
3	PSU	L5	4521	85,3	18,21,22	1.10	1 (5%)	21,30,33	2.01	5 (23%)
83	PSU	S2	109	83	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
83	PSU	S2	406	83	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
83	A2M	S2	99	85,83	22,25,26	1.25	1 (4%)	30,36,39	1.54	5 (16%)
3	A2M	L5	3718	3	22,25,26	1.18	1 (4%)	30,36,39	1.48	5 (16%)
5	OMG	L8	75	5	23,26,27	0.47	0	32,38,41	0.52	0
3	PSU	L5	4636	3	18,21,22	1.13	1 (5%)	21,30,33	2.04	6 (28%)
3	PSU	L5	4973	3	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
83	PSU	S2	1177	83	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
83	PSU	S2	866	83	18,21,22	1.11	1 (5%)	21,30,33	1.86	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	OMC	S2	517	83	19,22,23	0.50	0	25,31,34	0.65	0
3	PSU	L5	5001	3	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4500	3	18,21,22	1.13	1 (5%)	21,30,33	2.01	5 (23%)
3	OMU	L5	4620	3	19,22,23	3.28	7 (36%)	25,31,34	1.72	4 (16%)
3	OMG	L5	3792	3	23,26,27	0.49	0	32,38,41	0.51	0
3	PSU	L5	4579	3	18,21,22	1.07	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
3	OMG	L5	3744	3	23,26,27	0.49	0	32,38,41	0.51	0
3	OMC	L5	3701	3	19,22,23	0.65	0	25,31,34	1.70	4 (16%)
83	MA6	S2	1851	83	23,26,27	1.27	2 (8%)	33,38,41	3.38	13 (39%)
3	OMG	L5	3627	3	23,26,27	0.47	0	32,38,41	0.56	0
3	OMG	L5	1522	3	23,26,27	0.49	0	32,38,41	0.60	0
3	PSU	L5	1792	3	18,21,22	1.07	1 (5%)	21,30,33	1.80	4 (19%)
3	OMU	L5	4498	3	19,22,23	3.33	7 (36%)	25,31,34	1.83	5 (20%)
83	PSU	S2	651	83	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
3	5MC	L5	3782	85,3	19,22,23	0.59	0	26,32,35	0.71	0
3	OMG	L5	4494	3	23,26,27	0.50	0	32,38,41	0.53	0
3	OMG	L5	1625	3	23,26,27	0.48	0	32,38,41	0.48	0
83	PSU	S2	686	83	18,21,22	1.13	1 (5%)	21,30,33	1.92	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.33	2 (9%)	30,36,39	1.51	6 (20%)
3	OMC	L5	2351	85,3	19,22,23	0.60	0	25,31,34	1.19	2 (8%)
3	OMC	L5	3869	3	19,22,23	0.55	0	25,31,34	0.72	0
83	B8N	S2	1248	83	25,29,30	3.27	6 (24%)	28,42,45	1.99	7 (25%)
3	OMU	L5	4227	3	19,22,23	3.36	7 (36%)	25,31,34	1.83	4 (16%)
83	A2M	S2	27	83	22,25,26	1.25	1 (4%)	30,36,39	1.53	6 (20%)
3	PSU	L5	4293	3	18,21,22	1.11	1 (5%)	21,30,33	1.98	4 (19%)
3	A2M	L5	4590	3	22,25,26	1.23	1 (4%)	30,36,39	1.52	5 (16%)
5	PSU	L8	55	5	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
83	OMC	S2	1703	83	19,22,23	0.52	0	25,31,34	0.60	0
83	OMG	S2	867	83	23,26,27	0.49	0	32,38,41	0.47	0
83	PSU	S2	649	83	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	1046	83	18,21,22	1.11	1 (5%)	21,30,33	1.83	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
83	PSU	S2	681	83	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)
3	OMC	L5	2804	3	19,22,23	0.59	0	25,31,34	0.97	1 (4%)
3	A2M	L5	1871	85,3	22,25,26	1.31	1 (4%)	30,36,39	1.63	6 (20%)
3	6MZ	L5	4220	3	22,25,26	3.94	11 (50%)	29,36,39	2.43	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	4370	3	23,26,27	0.48	0	32,38,41	0.53	0
83	OMU	S2	627	83	19,22,23	3.40	7 (36%)	25,31,34	1.79	5 (20%)
83	OMC	S2	174	83	19,22,23	0.49	0	25,31,34	0.64	0
3	OMC	L5	2365	85,3	19,22,23	0.53	0	25,31,34	0.62	0
3	OMC	L5	3887	3	19,22,23	0.54	0	25,31,34	0.77	0
83	PSU	S2	1174	83	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4532	3	18,21,22	1.10	1 (5%)	21,30,33	1.81	4 (19%)
83	MA6	S2	1850	83	23,26,27	1.27	2 (8%)	33,38,41	3.32	12 (36%)
3	PSU	L5	4972	3	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
83	PSU	S2	1045	83	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.08	1 (5%)	21,30,33	1.79	4 (19%)
3	OMG	L5	3899	3	23,26,27	0.53	0	32,38,41	0.55	0
83	A2M	S2	159	83	22,25,26	1.22	2 (9%)	30,36,39	1.50	6 (20%)
3	PSU	L5	1582	3	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
83	OMG	S2	436	83	23,26,27	0.48	0	32,38,41	0.53	0
83	6MZ	S2	1832	85,83	26,26,26	2.83	4 (15%)	36,39,39	2.10	11 (30%)
3	PSU	L5	3822	3	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
3	PSU	L5	3637	3	18,21,22	1.11	1 (5%)	21,30,33	1.97	4 (19%)
83	OMC	S2	1272	83	19,22,23	0.56	0	25,31,34	1.05	2 (8%)
83	OMU	S2	121	83	19,22,23	3.36	7 (36%)	25,31,34	1.81	5 (20%)
83	A2M	S2	1031	83	22,25,26	1.23	1 (4%)	30,36,39	1.54	5 (16%)
83	A2M	S2	468	83	22,25,26	1.28	1 (4%)	30,36,39	1.53	6 (20%)
3	PSU	L5	4403	3	18,21,22	1.09	1 (5%)	21,30,33	1.97	6 (28%)
3	PSU	L5	3851	3	18,21,22	1.11	1 (5%)	21,30,33	1.86	4 (19%)
83	OMU	S2	172	83	19,22,23	3.36	7 (36%)	25,31,34	1.85	5 (20%)
3	OMC	L5	4536	3	19,22,23	0.55	0	25,31,34	0.71	0
3	PSU	L5	3695	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	5 (23%)
3	A2M	L5	1326	3	22,25,26	1.25	1 (4%)	30,36,39	1.43	6 (20%)
83	PSU	S2	1081	83	18,21,22	1.08	1 (5%)	21,30,33	1.88	5 (23%)
3	UY1	L5	3818	3	19,22,23	4.93	10 (52%)	21,31,34	2.02	6 (28%)
3	OMC	L5	3841	3	19,22,23	0.54	0	25,31,34	0.65	0
3	5MC	L5	4447	3	19,22,23	0.72	0	26,32,35	0.62	0
3	PSU	L5	4312	3	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
3	OMG	L5	4392	3	23,26,27	0.47	0	32,38,41	0.51	0
3	A2M	L5	4523	85,3	22,25,26	1.32	2 (9%)	30,36,39	1.57	6 (20%)
3	PSU	L5	1536	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
3	A2M	L5	398	3	22,25,26	1.26	1 (4%)	30,36,39	1.60	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	OMC	S2	462	83	19,22,23	0.53	0	25,31,34	0.73	0
83	A2M	S2	166	83	22,25,26	1.30	1 (4%)	30,36,39	1.54	6 (20%)
3	PSU	L5	1677	3	18,21,22	1.08	1 (5%)	21,30,33	2.01	5 (23%)
3	A2M	L5	1323	3	22,25,26	1.32	3 (13%)	30,36,39	1.57	7 (23%)
3	OMG	L5	4196	1,3	23,26,27	0.46	0	32,38,41	0.48	0
3	OMG	L5	2364	85,3	23,26,27	0.49	0	32,38,41	0.51	0
3	OMG	L5	4228	3	23,26,27	0.48	0	32,38,41	0.58	0
3	PSU	L5	5010	3	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
83	PSU	S2	1232	83	18,21,22	1.15	1 (5%)	21,30,33	1.92	4 (19%)
3	OMG	L5	2876	3	23,26,27	0.49	0	32,38,41	0.49	0
3	PSU	L5	4628	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	5 (23%)
83	OMU	S2	799	83	19,22,23	3.40	7 (36%)	25,31,34	1.80	4 (16%)
83	OMG	S2	601	83	23,26,27	0.47	0	32,38,41	0.47	0
83	OMU	S2	428	83	19,22,23	3.37	7 (36%)	25,31,34	1.83	5 (20%)
3	PSU	L5	2632	3	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
83	G7M	S2	1639	1,83	23,26,27	2.66	9 (39%)	34,39,42	2.59	11 (32%)
3	OMG	L5	4623	3	23,26,27	0.49	0	32,38,41	0.57	0
83	A2M	S2	1383	83	22,25,26	1.24	1 (4%)	30,36,39	1.59	5 (16%)
83	PSU	S2	966	85,83	18,21,22	1.09	1 (5%)	21,30,33	1.83	4 (19%)
3	A2M	L5	2787	3	22,25,26	1.22	1 (4%)	30,36,39	1.49	6 (20%)
83	4AC	S2	1337	83	21,24,25	0.39	0	28,34,37	0.74	1 (3%)
3	A2M	L5	3825	3	22,25,26	1.26	1 (4%)	30,36,39	1.54	5 (16%)
83	PSU	S2	1056	83	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
3	OMC	L5	2824	3	19,22,23	0.55	0	25,31,34	0.72	0
3	OMG	L5	4618	3	23,26,27	0.50	0	32,38,41	0.54	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
3	A2M	L5	2363	85,3	-	0/9/27/28	0/3/3/3
83	OMG	S2	509	83	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	1744	85,3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4673	85,3	-	0/7/25/26	0/2/2/2
83	PSU	S2	93	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1004	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
83	OMC	S2	1391	83	-	0/9/27/28	0/2/2/2
83	OMG	S2	1490	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	3853	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	85,3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
83	OMU	S2	1288	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
83	4AC	S2	1842	83	-	0/11/29/30	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	801	83	-	2/7/25/26	0/2/2/2
83	A2M	S2	484	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	1442	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
83	A2M	S2	576	83	-	3/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4306	3	-	1/9/27/28	0/2/2/2
83	PSU	S2	814	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1244	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	85,3	-	0/7/25/26	0/2/2/2
83	OMU	S2	354	83	-	0/9/27/28	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
83	OMU	S2	116	83	-	1/9/27/28	0/2/2/2
83	OMU	S2	1326	83	-	0/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	105	83	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	2422	85,3	-	2/9/27/28	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
83	OMG	S2	644	83	-	3/9/27/28	0/3/3/3
3	OMG	L5	4499	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
83	A2M	S2	668	85,83	-	2/9/27/28	0/3/3/3
3	1MA	L5	1322	85,3	-	2/7/25/26	0/3/3/3
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
83	OMG	S2	683	83	-	2/9/27/28	0/3/3/3
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	85,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	1328	83	-	1/9/27/28	0/3/3/3
83	PSU	S2	863	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1367	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4521	85,3	-	0/7/25/26	0/2/2/2
83	PSU	S2	109	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	406	83	-	0/7/25/26	0/2/2/2
83	A2M	S2	99	85,83	-	3/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1177	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	866	83	-	0/7/25/26	0/2/2/2
83	OMC	S2	517	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
83	MA6	S2	1851	83	-	1/11/29/30	0/3/3/3
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	651	83	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	85,3	-	1/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
83	PSU	S2	686	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	2351	85,3	-	3/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
83	B8N	S2	1248	83	-	4/16/34/35	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
83	A2M	S2	27	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	3/9/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
83	OMC	S2	1703	83	-	1/9/27/28	0/2/2/2
83	OMG	S2	867	83	-	2/9/27/28	0/3/3/3
83	PSU	S2	649	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1046	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	681	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	1871	85,3	-	0/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
83	OMU	S2	627	83	-	4/9/27/28	0/2/2/2
83	OMC	S2	174	83	-	0/9/27/28	0/2/2/2
3	OMC	L5	2365	85,3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
83	PSU	S2	1174	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
83	MA6	S2	1850	83	-	0/11/29/30	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1045	83	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	3/9/27/28	0/3/3/3
83	A2M	S2	159	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	436	83	-	2/9/27/28	0/3/3/3
83	6MZ	S2	1832	85,83	-	3/12/28/28	0/3/3/3
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
83	OMC	S2	1272	83	-	5/9/27/28	0/2/2/2
83	OMU	S2	121	83	-	0/9/27/28	0/2/2/2
83	A2M	S2	1031	83	-	0/9/27/28	0/3/3/3
83	A2M	S2	468	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
83	OMU	S2	172	83	-	0/9/27/28	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	4/9/27/28	0/3/3/3
83	PSU	S2	1081	83	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4523	85,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
83	OMC	S2	462	83	-	1/9/27/28	0/2/2/2
83	A2M	S2	166	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	4/7/25/26	0/2/2/2
3	A2M	L5	1323	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4196	1,3	-	1/9/27/28	0/3/3/3
3	OMG	L5	2364	85,3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1232	83	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	799	83	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	OMG	S2	601	83	-	1/9/27/28	0/3/3/3
83	OMU	S2	428	83	-	4/9/27/28	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
83	G7M	S2	1639	1,83	-	0/7/25/26	0/3/3/3
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
83	A2M	S2	1383	83	-	1/9/27/28	0/3/3/3
83	PSU	S2	966	85,83	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
83	4AC	S2	1337	83	-	1/11/29/30	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
83	PSU	S2	1056	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3

The worst 5 of 273 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C6-C5	12.91	1.49	1.35
83	S2	1832	6MZ	C6-N6	12.80	1.48	1.34
3	L5	4220	6MZ	C6-N6	12.11	1.48	1.34
3	L5	3818	UY1	C2-N1	11.87	1.52	1.36
83	S2	799	OMU	C2-N1	8.50	1.51	1.38

The worst 5 of 637 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1851	MA6	N1-C6-N6	-11.87	102.39	116.86
83	S2	1850	MA6	N1-C6-N6	-11.57	102.75	116.86
83	S2	1851	MA6	C5-C6-N6	7.95	137.92	125.33
83	S2	1850	MA6	C5-C6-N6	7.74	137.58	125.33
83	S2	1639	G7M	C1'-N9-C4	7.62	148.99	126.49

There are no chirality outliers.

5 of 145 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1340	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

80 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2363	A2M	1	0
83	S2	509	OMG	3	0
3	L5	1340	OMC	2	0
3	L5	3925	OMU	1	0
83	S2	1004	PSU	2	0
3	L5	4689	PSU	1	0
83	S2	1391	OMC	1	0
3	L5	4431	PSU	1	0
3	L5	3785	A2M	1	0
83	S2	1288	OMU	1	0
83	S2	1842	4AC	1	0
83	S2	484	A2M	1	0
3	L5	1683	PSU	2	0
83	S2	1442	OMU	1	0
83	S2	576	A2M	2	0
3	L5	4571	A2M	1	0
3	L5	4306	OMU	1	0
3	L5	400	A2M	1	0
83	S2	116	OMU	2	0
3	L5	2422	OMC	1	0
3	L5	3867	A2M	5	0
3	L5	2424	OMG	1	0
83	S2	683	OMG	1	0
3	L5	4637	OMG	1	0
3	L5	4457	PSU	1	0
3	L5	1534	A2M	1	0
3	L5	4456	OMC	1	0
83	S2	99	A2M	1	0
3	L5	3718	A2M	3	0
5	L8	75	OMG	2	0
3	L5	4636	PSU	1	0
83	S2	866	PSU	2	0
83	S2	517	OMC	1	0
3	L5	4620	OMU	2	0
3	L5	4579	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3701	OMC	1	0
3	L5	2351	OMC	1	0
83	S2	27	A2M	3	0
3	L5	4293	PSU	1	0
3	L5	4590	A2M	1	0
83	S2	1703	OMC	1	0
83	S2	867	OMG	3	0
83	S2	649	PSU	2	0
83	S2	1046	PSU	1	0
83	S2	681	PSU	1	0
3	L5	2804	OMC	1	0
3	L5	1871	A2M	1	0
3	L5	4220	6MZ	1	0
83	S2	1174	PSU	2	0
83	S2	1850	MA6	1	0
83	S2	159	A2M	2	0
83	S2	436	OMG	1	0
3	L5	3822	PSU	1	0
83	S2	1272	OMC	1	0
83	S2	121	OMU	1	0
83	S2	1031	A2M	1	0
83	S2	468	A2M	1	0
3	L5	4536	OMC	1	0
3	L5	1326	A2M	5	0
3	L5	3818	UY1	1	0
3	L5	3841	OMC	1	0
3	L5	4392	OMG	1	0
3	L5	4523	A2M	2	0
3	L5	398	A2M	1	0
83	S2	462	OMC	1	0
83	S2	166	A2M	2	0
3	L5	1677	PSU	1	0
3	L5	4196	OMG	1	0
3	L5	2364	OMG	1	0
3	L5	4228	OMG	1	0
83	S2	1232	PSU	1	0
3	L5	2876	OMG	1	0
83	S2	601	OMG	2	0
3	L5	3884	PSU	1	0
83	S2	1639	G7M	1	0
83	S2	1383	A2M	1	0
83	S2	1337	4AC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3825	A2M	1	0
3	L5	2824	OMC	1	0
3	L5	4618	OMG	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	$\# Z > 2$
87	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.84	0
86	SPM	L5	5293	-	13,13,13	0.36	0	12,12,12	0.87	0
87	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.94	0
87	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.88	0
86	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.99	0
86	SPM	L5	5263	-	13,13,13	0.34	0	12,12,12	0.98	0
87	SPD	L5	5288	-	9,9,9	0.31	0	8,8,8	0.83	0
87	SPD	LN	301	-	9,9,9	0.31	0	8,8,8	0.91	0
87	SPD	L5	5283	-	9,9,9	0.34	0	8,8,8	0.86	0
87	SPD	L5	5291	-	9,9,9	0.31	0	8,8,8	0.81	0
86	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	1.09	0
87	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.79	0
87	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.85	0
87	SPD	L5	5290	-	9,9,9	0.33	0	8,8,8	0.85	0
86	SPM	L5	5264	-	13,13,13	0.34	0	12,12,12	1.01	0
86	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.90	0
86	SPM	L5	5289	-	13,13,13	0.37	0	12,12,12	1.01	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
87	SPD	L5	5286	-	-	0/7/7/7	-
86	SPM	L5	5293	-	-	5/11/11/11	-
87	SPD	L5	5261	-	-	1/7/7/7	-
87	SPD	L5	5285	-	-	4/7/7/7	-
86	SPM	L5	5259	-	-	2/11/11/11	-
86	SPM	L5	5263	-	-	2/11/11/11	-
87	SPD	L5	5288	-	-	3/7/7/7	-
87	SPD	LN	301	-	-	1/7/7/7	-
87	SPD	L5	5283	-	-	1/7/7/7	-
87	SPD	L5	5291	-	-	4/7/7/7	-
86	SPM	L5	5267	-	-	4/11/11/11	-
87	SPD	L5	5284	-	-	1/7/7/7	-
87	SPD	L5	5287	-	-	3/7/7/7	-
87	SPD	L5	5290	-	-	2/7/7/7	-
86	SPM	L5	5264	-	-	4/11/11/11	-
86	SPM	L5	5292	-	-	4/11/11/11	-
86	SPM	L5	5289	-	-	5/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	L5	5264	SPM	N5-C6-C7-C8
87	L5	5285	SPD	C3-C4-C5-N6
86	L5	5292	SPM	C7-C8-C9-N10
87	L5	5285	SPD	N6-C7-C8-C9
86	L5	5264	SPM	C7-C6-N5-C4

There are no ring outliers.

8 monomers are involved in 12 short contacts:

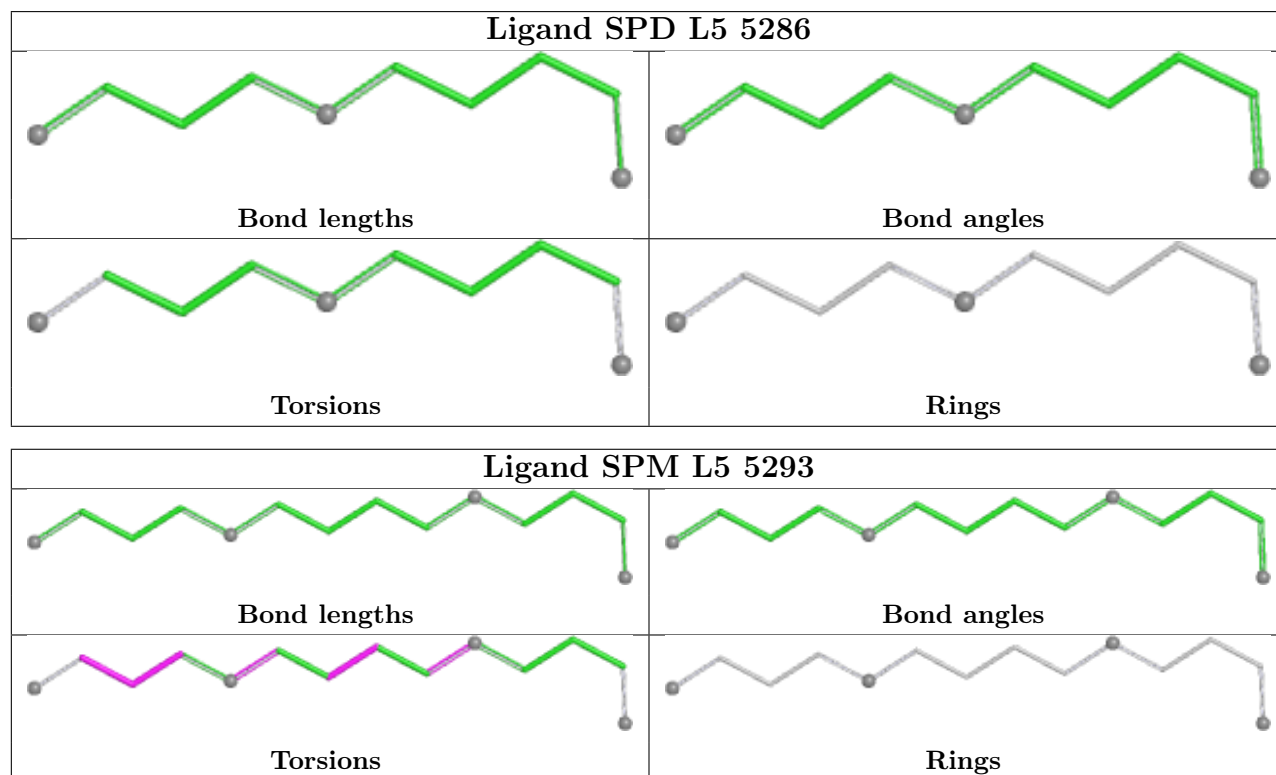
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5293	SPM	2	0
87	L5	5261	SPD	2	0

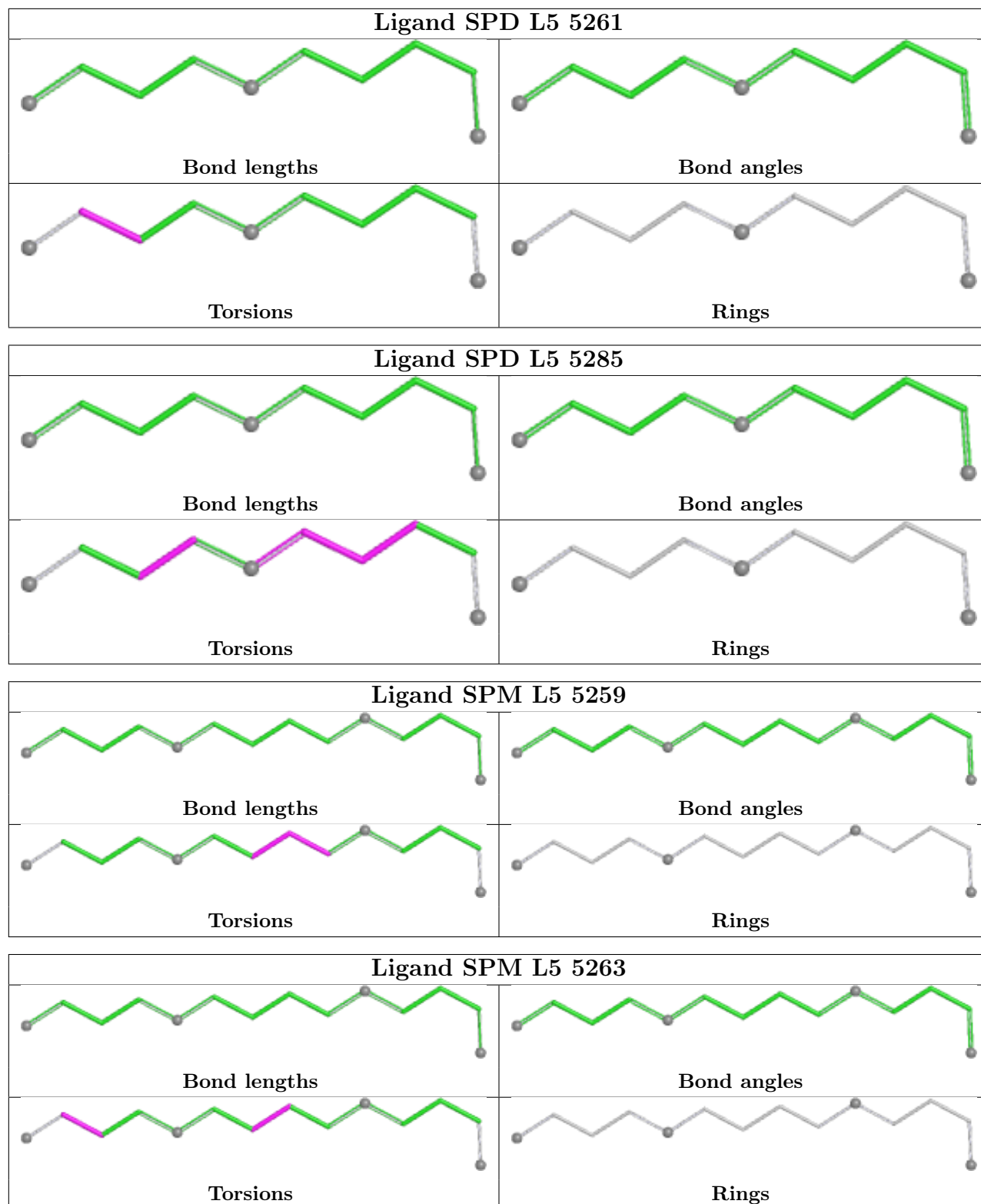
Continued on next page...

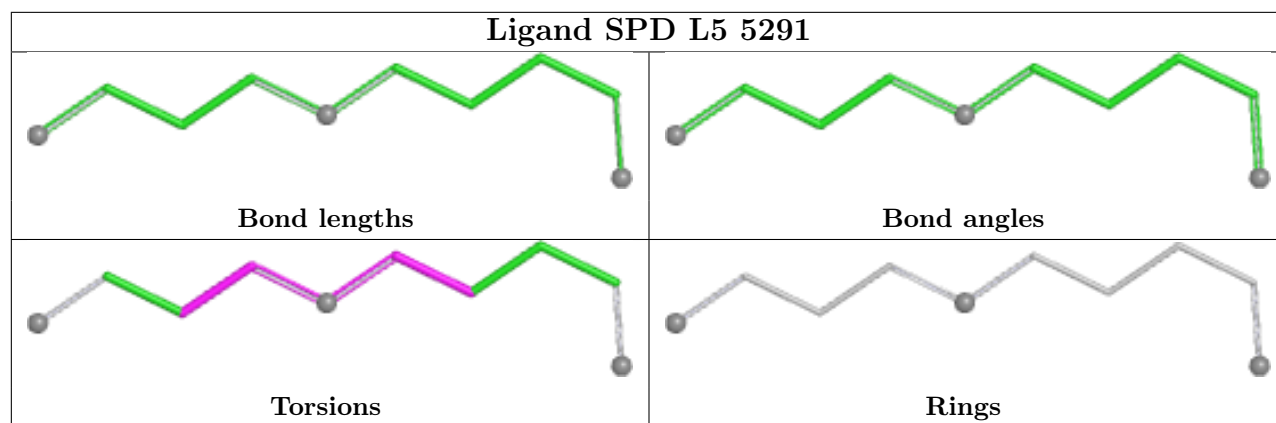
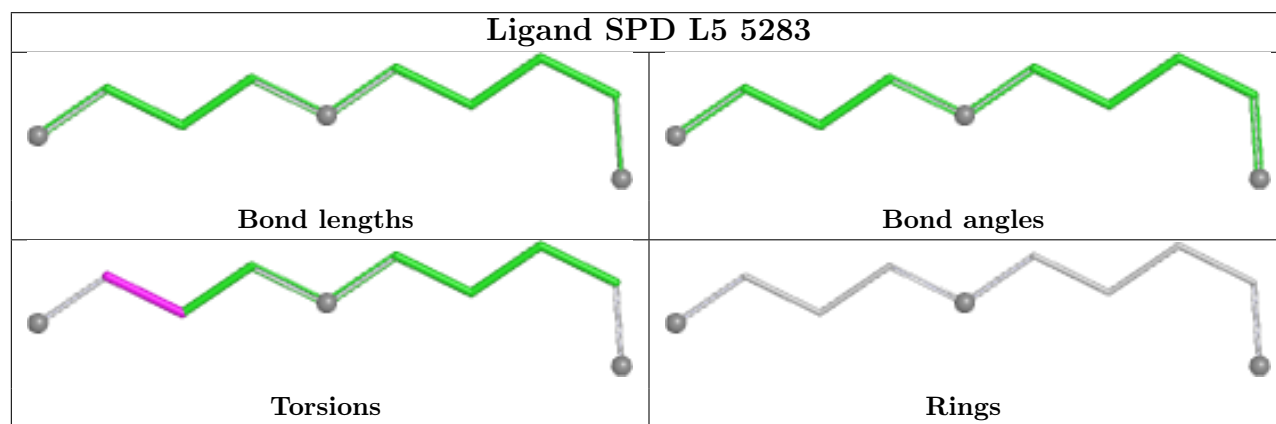
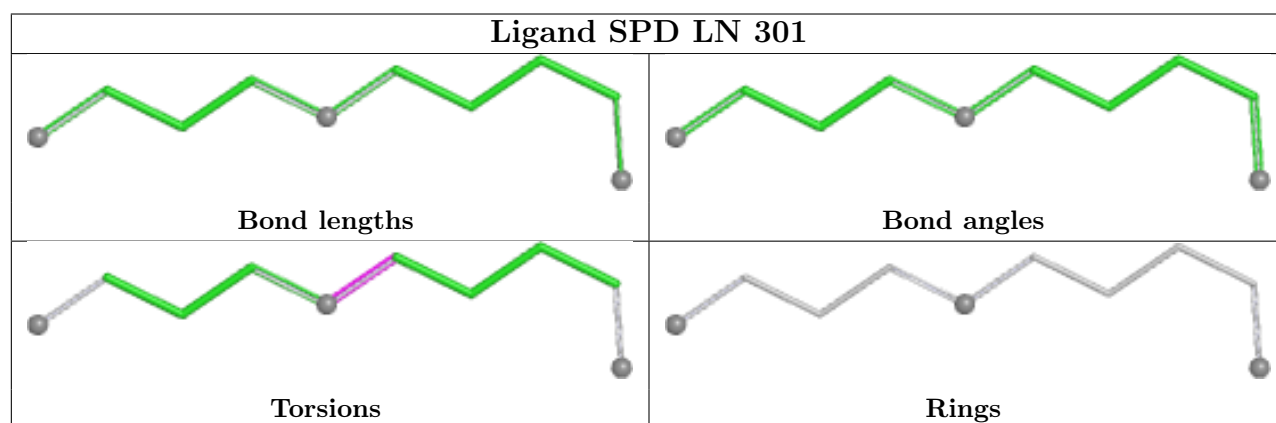
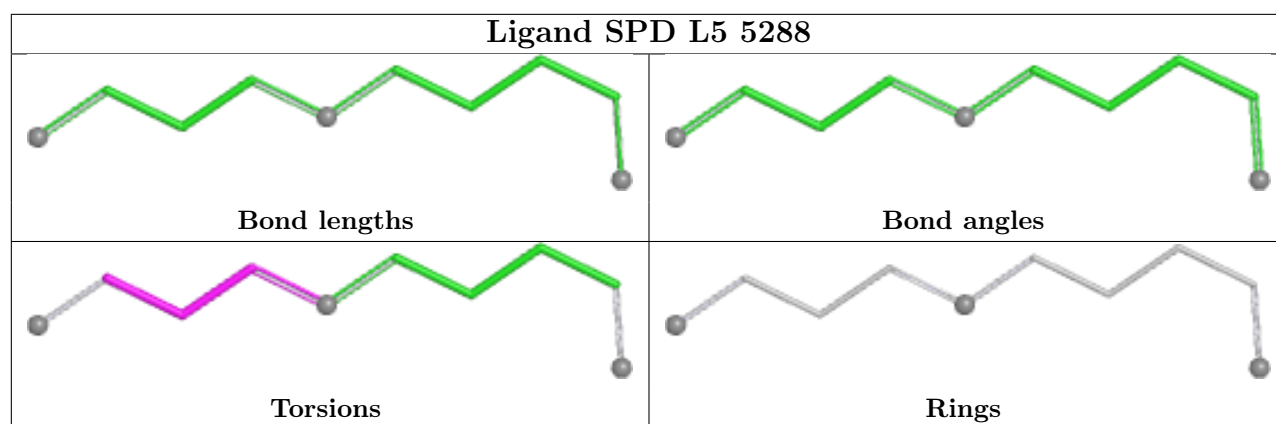
Continued from previous page...

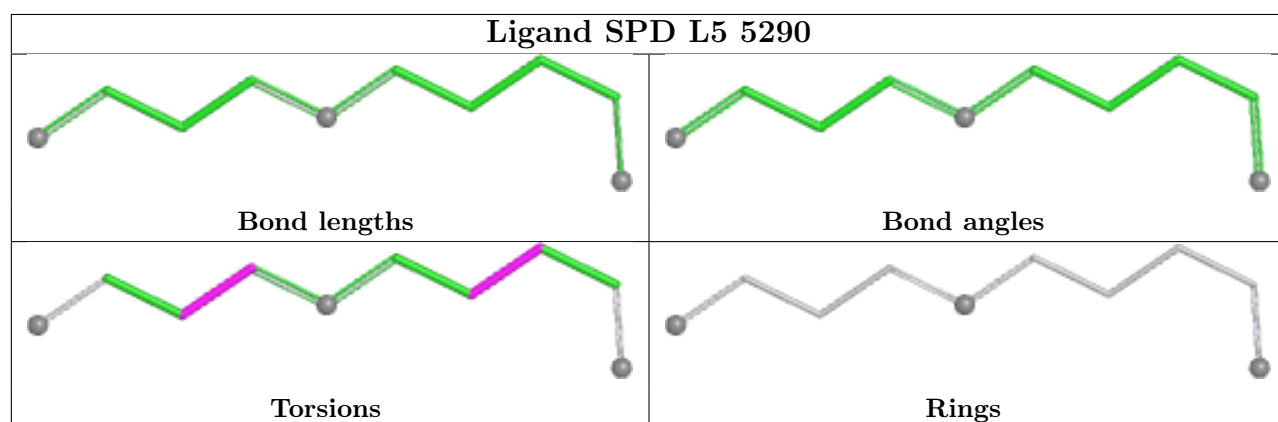
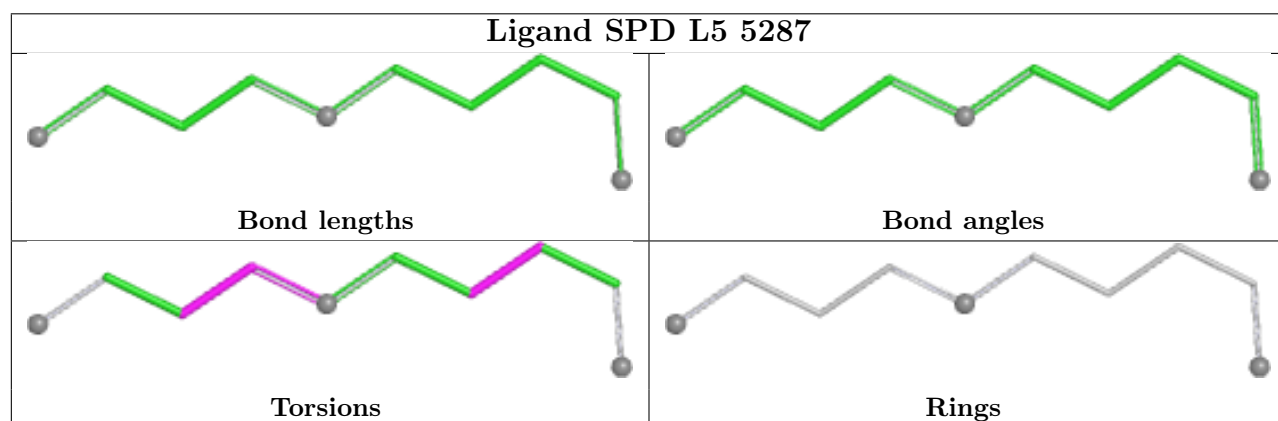
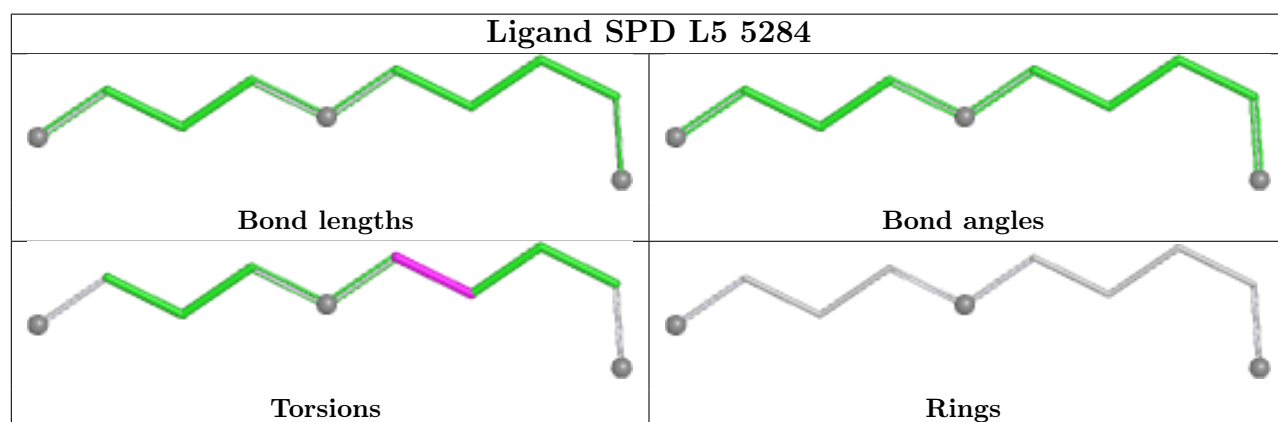
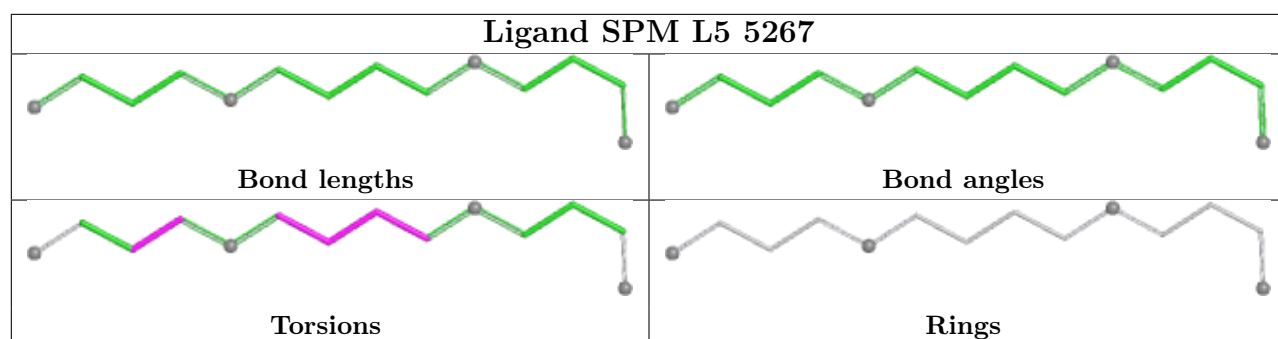
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5259	SPM	1	0
86	L5	5263	SPM	1	0
87	L5	5284	SPD	2	0
87	L5	5290	SPD	1	0
86	L5	5264	SPM	2	0
86	L5	5292	SPM	1	0

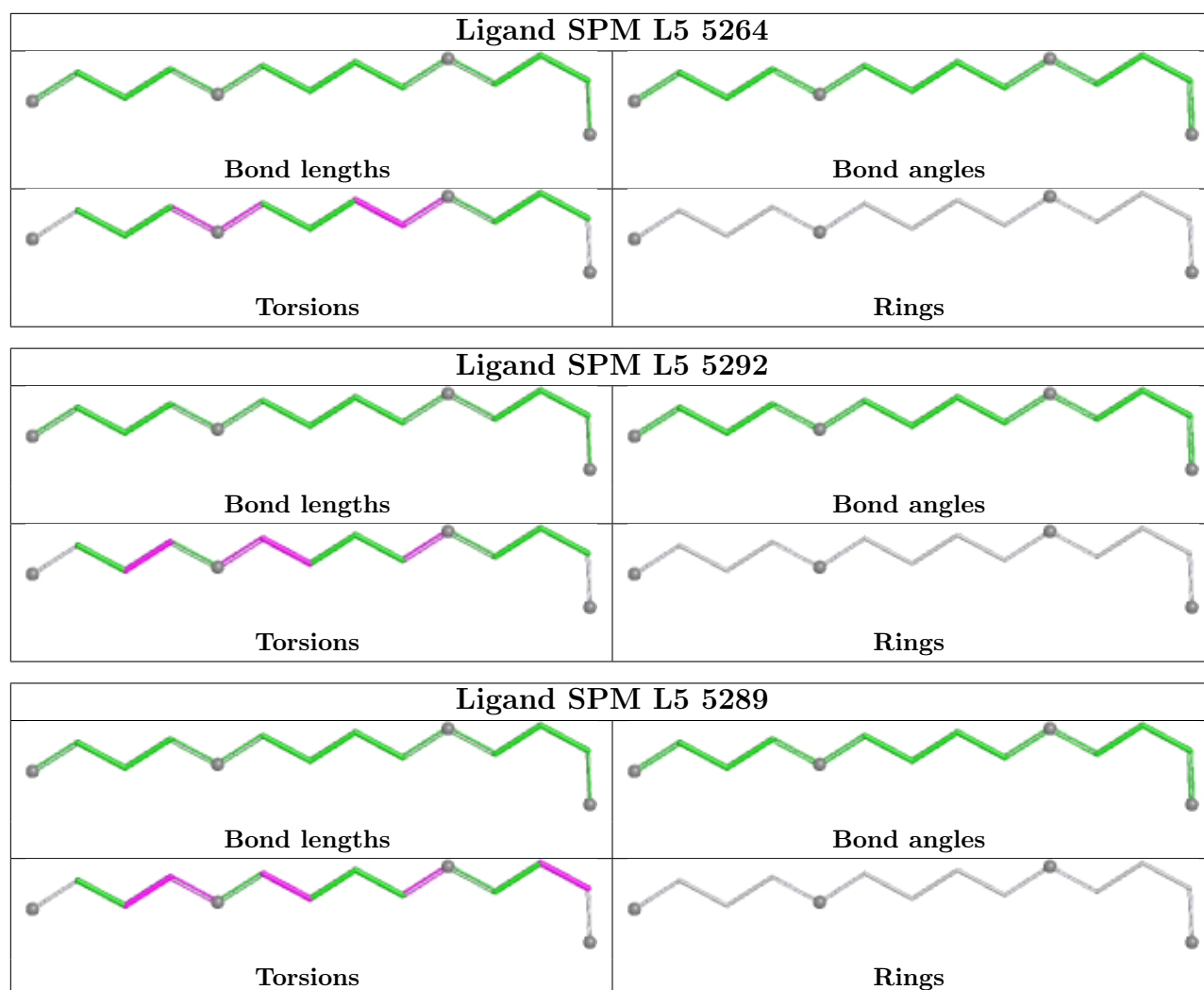
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	L5	10
83	S2	5
32	Lb	1
10	LE	1
49	Lt	1
70	SH	1
1	Pt	1

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Mol	Chain	Number of breaks
2	Et	1

The worst 5 of 21 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	35.06
1	S2	753:C	O3'	785:C	P	29.06
1	LE	76:ALA	C	87:LYS	N	21.90
1	L5	2910:G	O3'	3584:C	P	21.12
1	L5	1706:A	O3'	1716:G	P	20.98

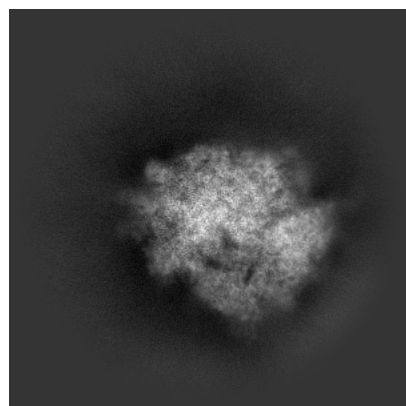
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71331. These allow visual inspection of the internal detail of the map and identification of artifacts.

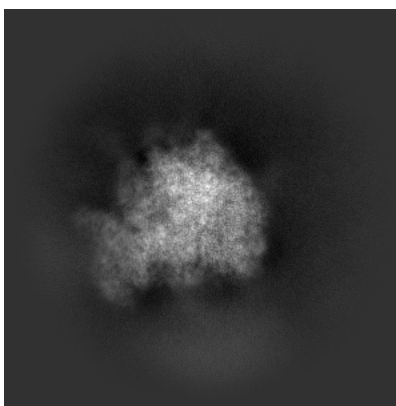
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

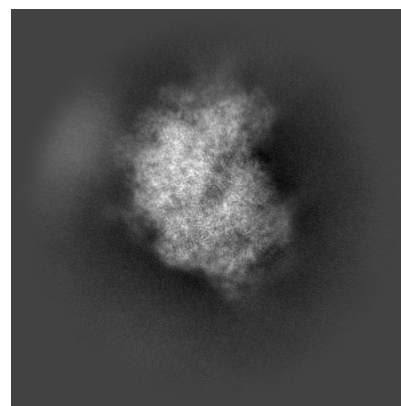
6.1.1 Primary map



X

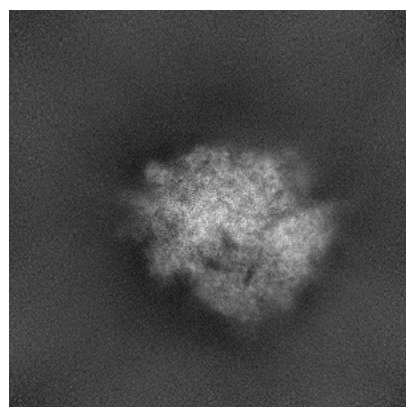


Y

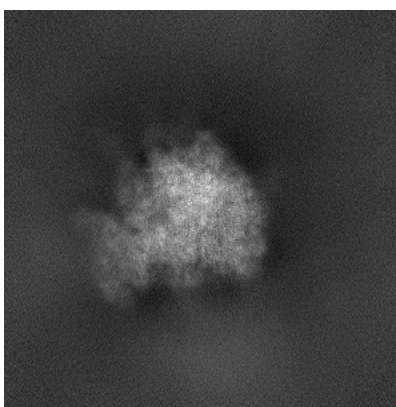


Z

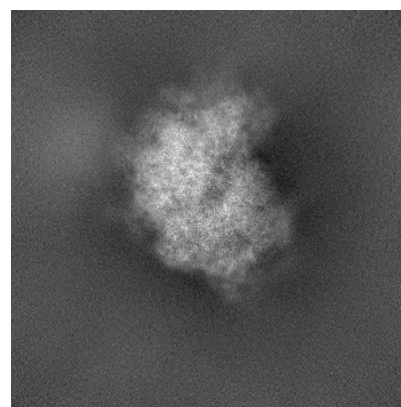
6.1.2 Raw map



X



Y

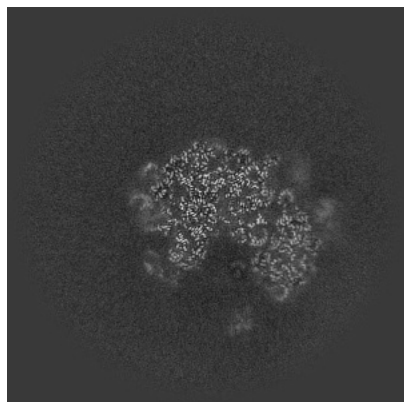


Z

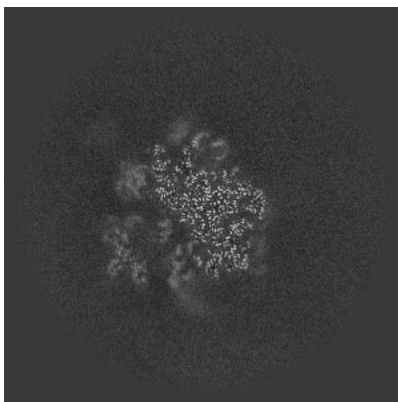
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

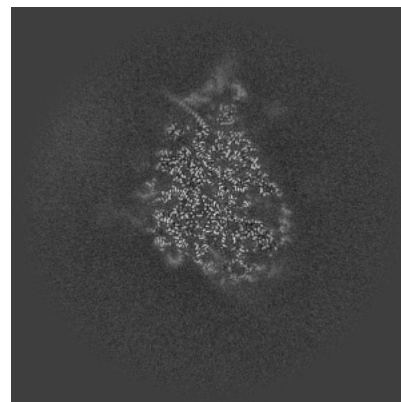
6.2.1 Primary map



X Index: 256

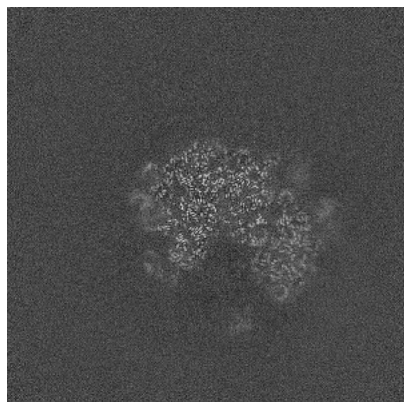


Y Index: 256

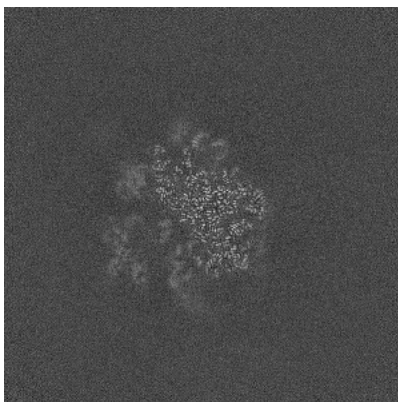


Z Index: 256

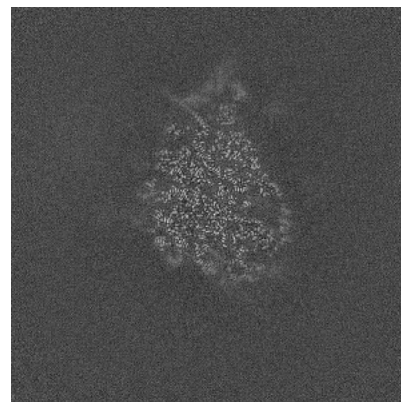
6.2.2 Raw map



X Index: 256



Y Index: 256

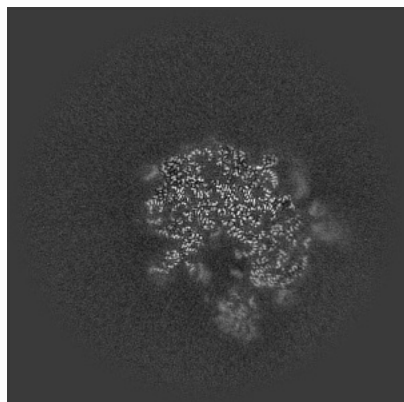


Z Index: 256

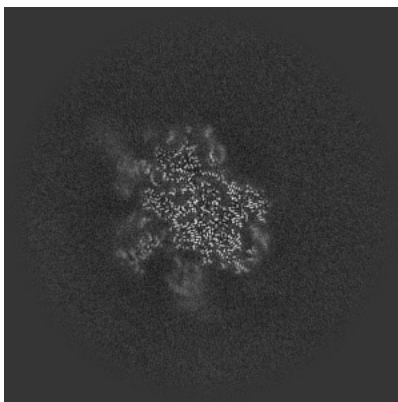
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

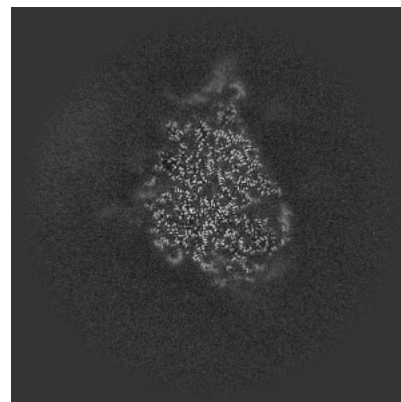
6.3.1 Primary map



X Index: 243

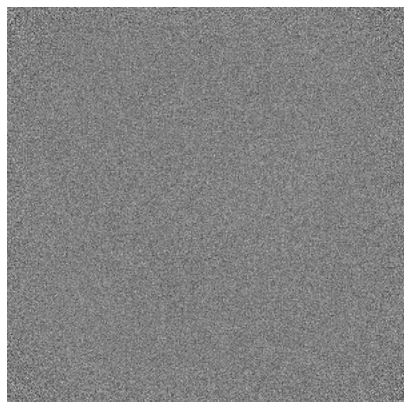


Y Index: 243

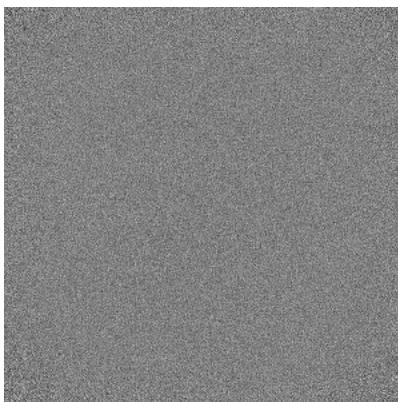


Z Index: 258

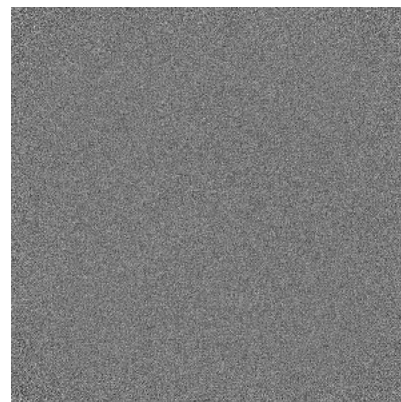
6.3.2 Raw map



X Index: 0



Y Index: 0

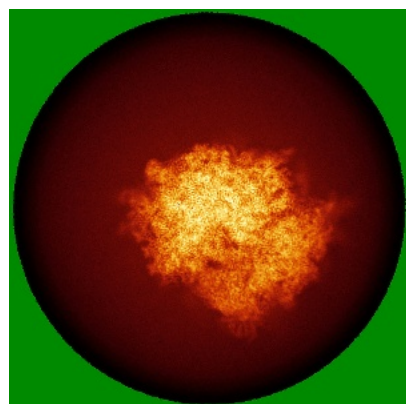


Z Index: 0

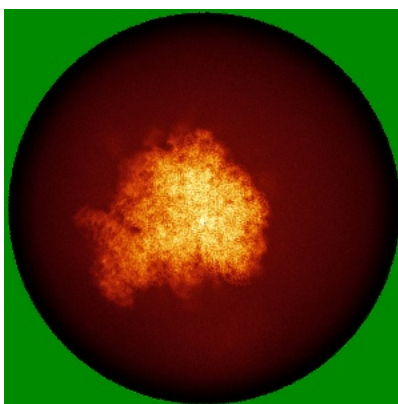
The images above show the largest variance slices of the map in three orthogonal directions.

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

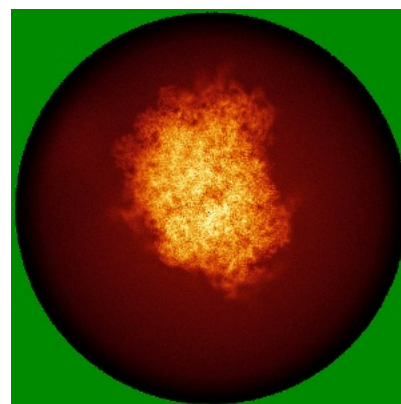
6.4.1 Primary map



X

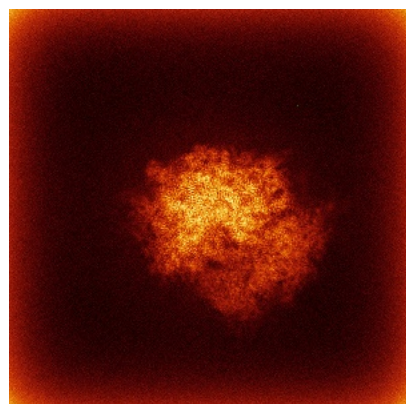


Y

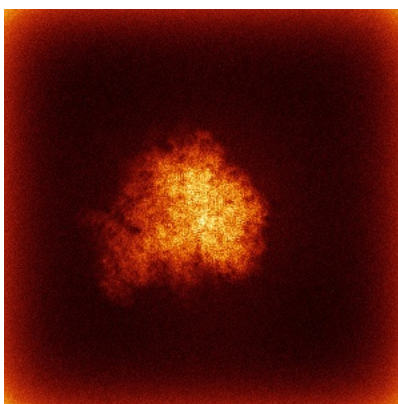


Z

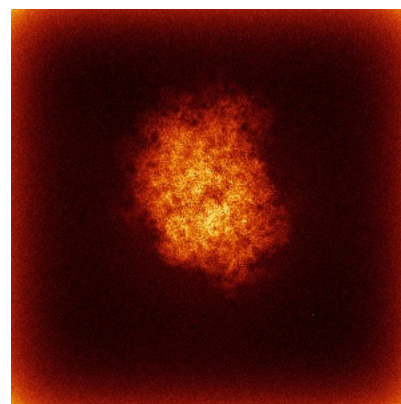
6.4.2 Raw map



X



Y

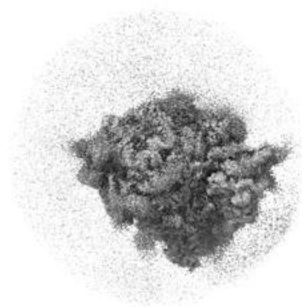


Z

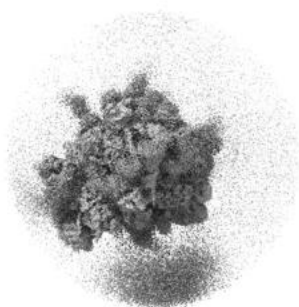
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

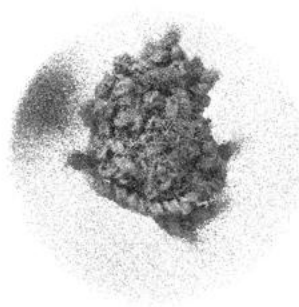
6.5.1 Primary map



X



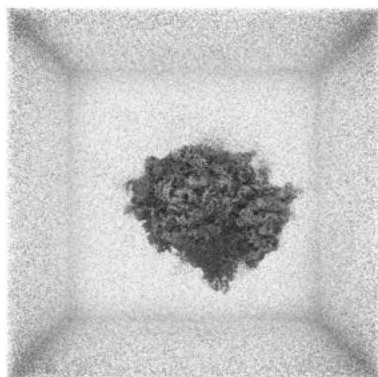
Y



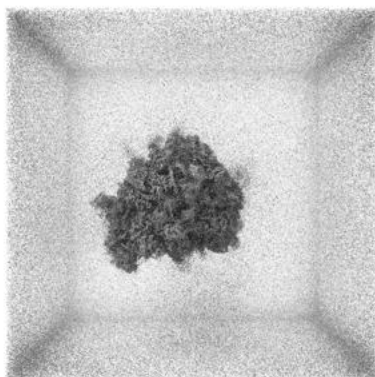
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

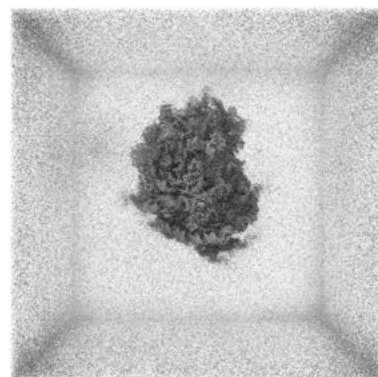
6.5.2 Raw map



X



Y



Z

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

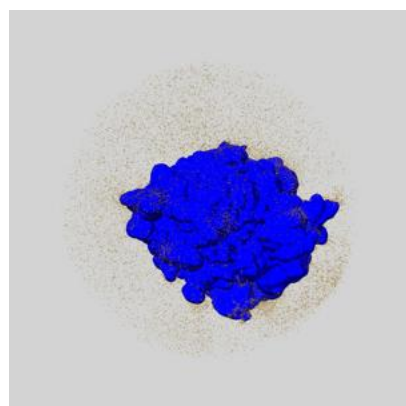
6.6 Mask visualisation [i](#)

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

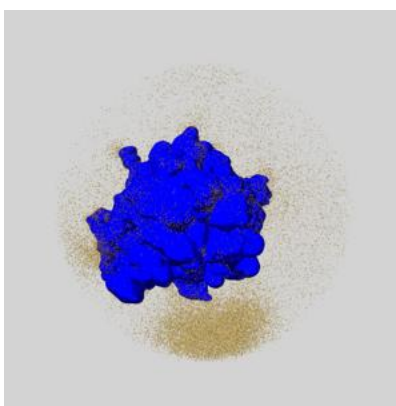
A mask typically either:

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

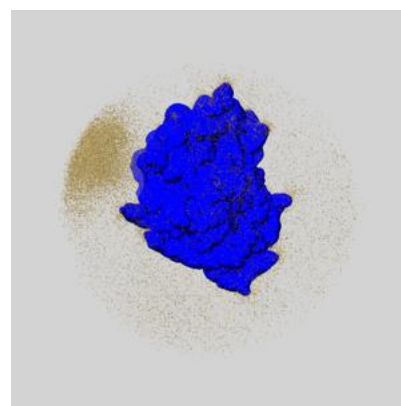
6.6.1 emd_71331_msk_1.map [i](#)



X



Y

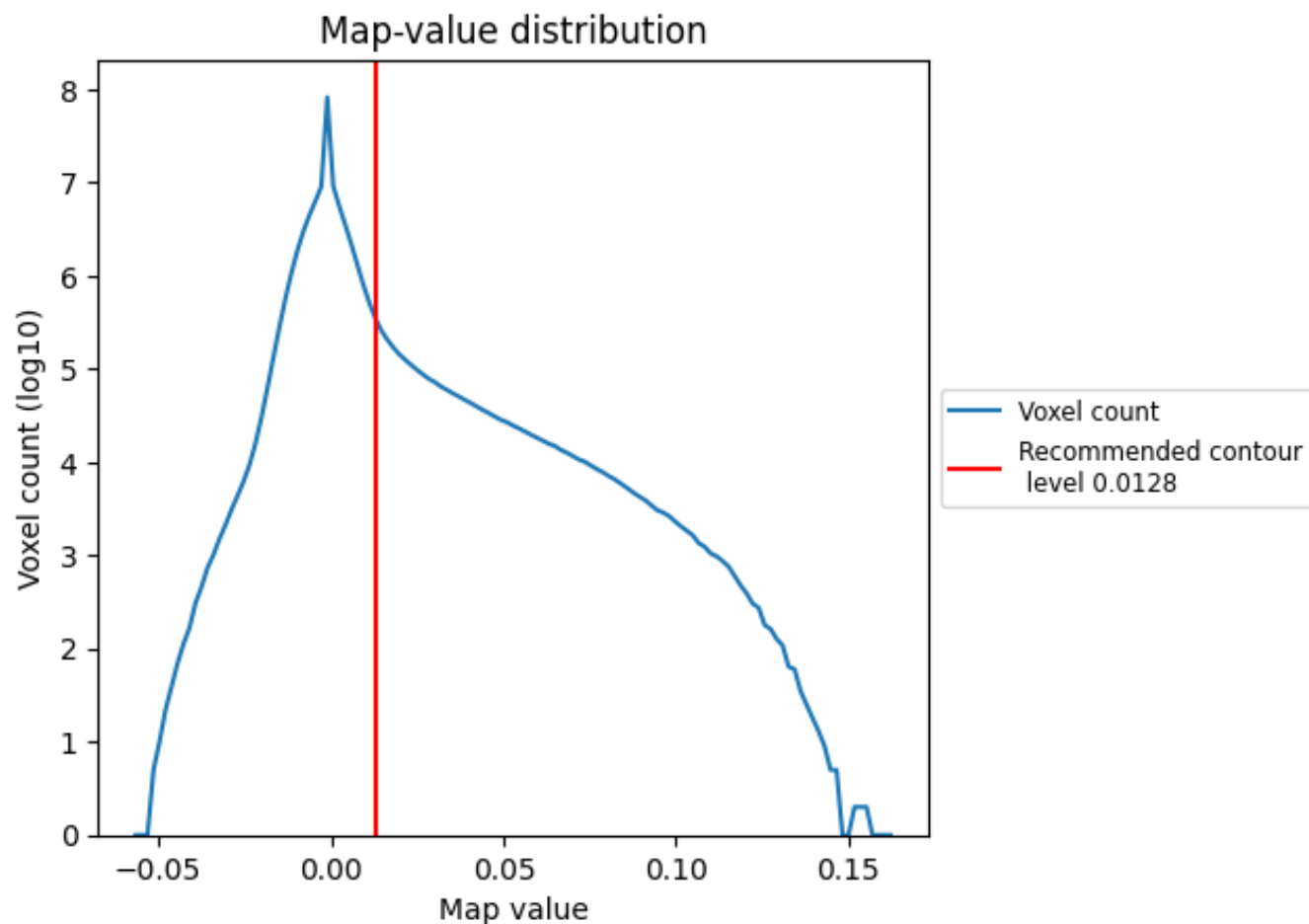


Z

7 Map analysis [i](#)

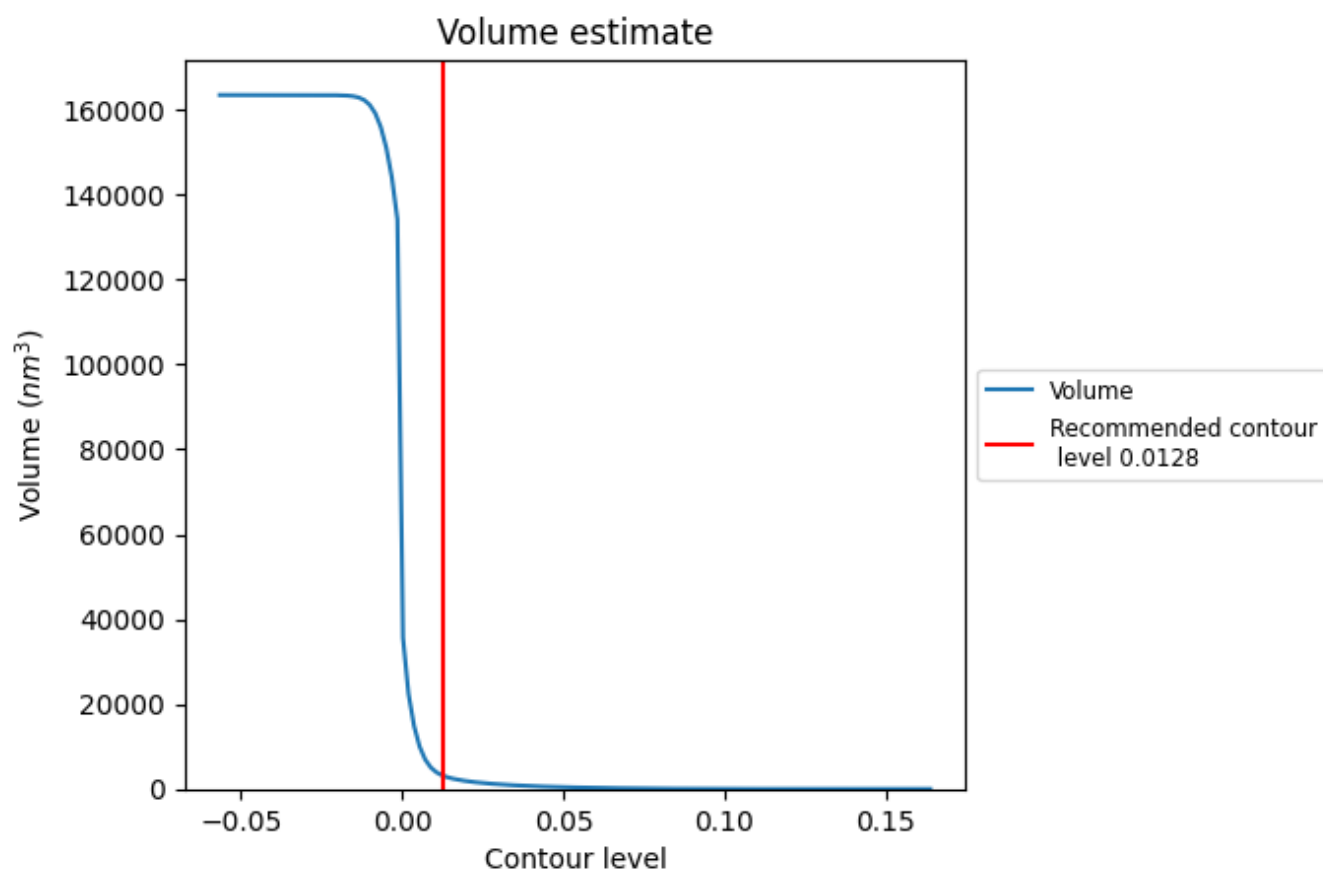
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

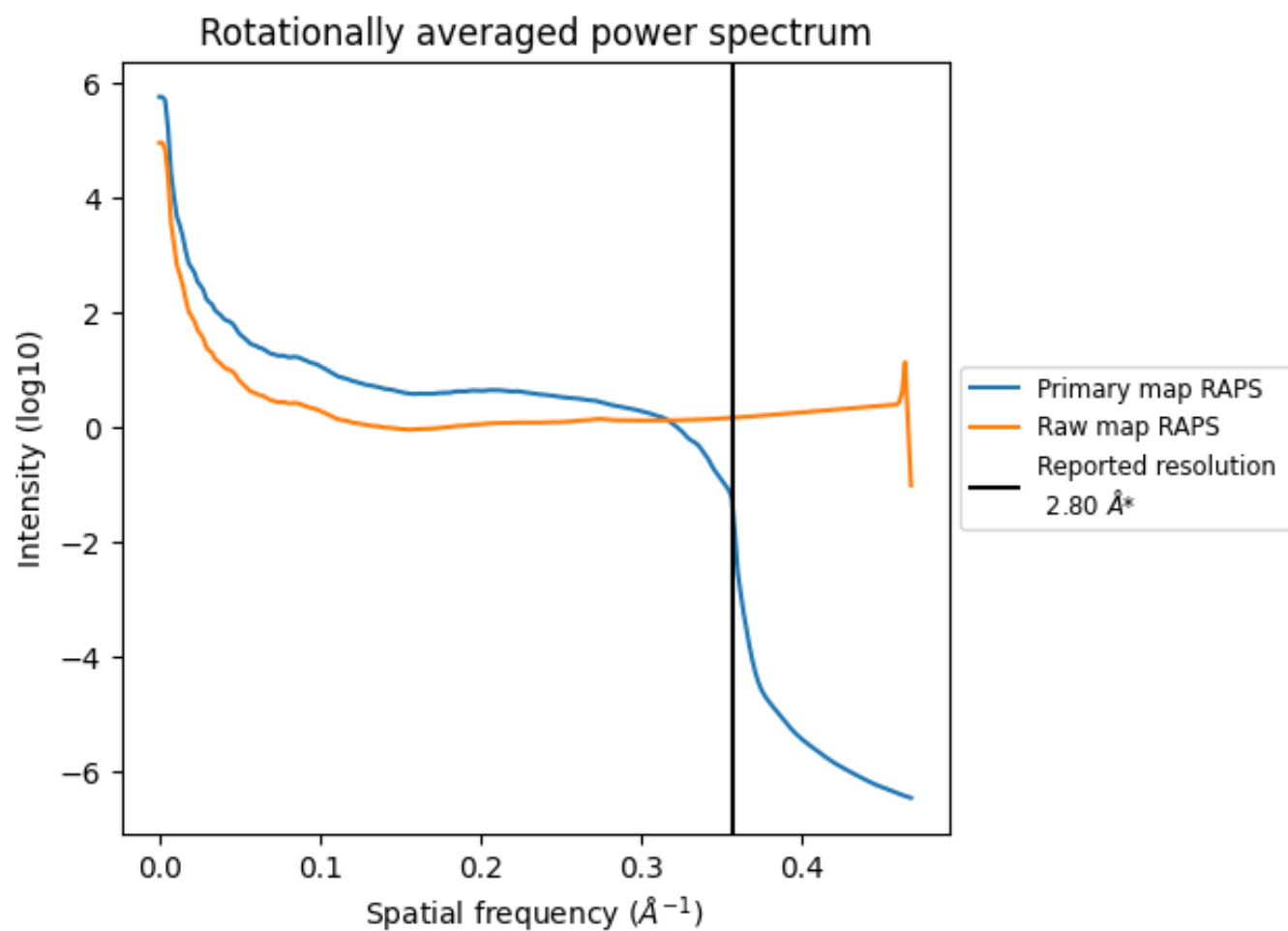
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3105 nm^3 ; this corresponds to an approximate mass of 2804 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 [i](#)

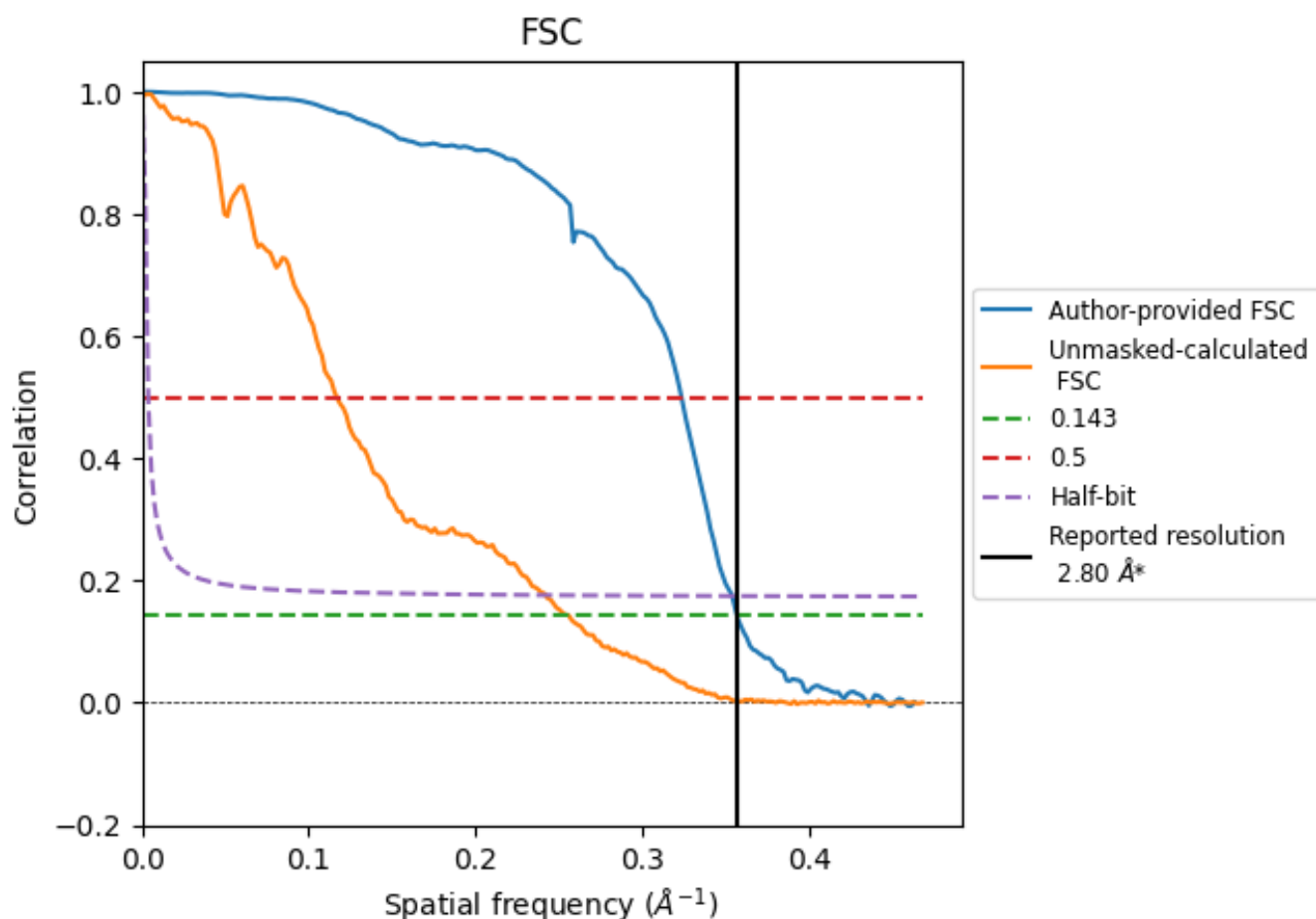


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

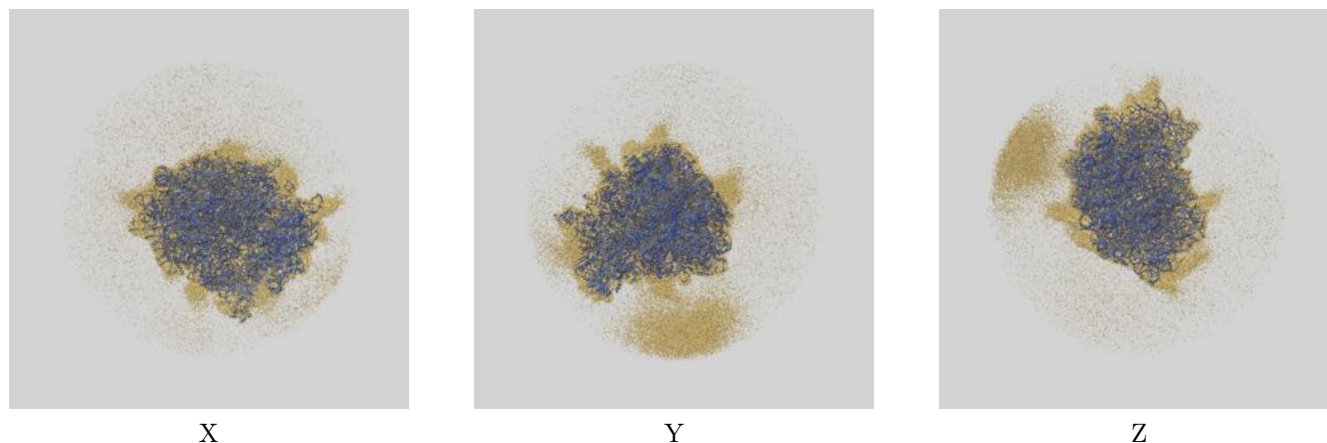
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.09	2.82
Unmasked-calculated*	3.91	8.56	4.13

*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 3.91 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

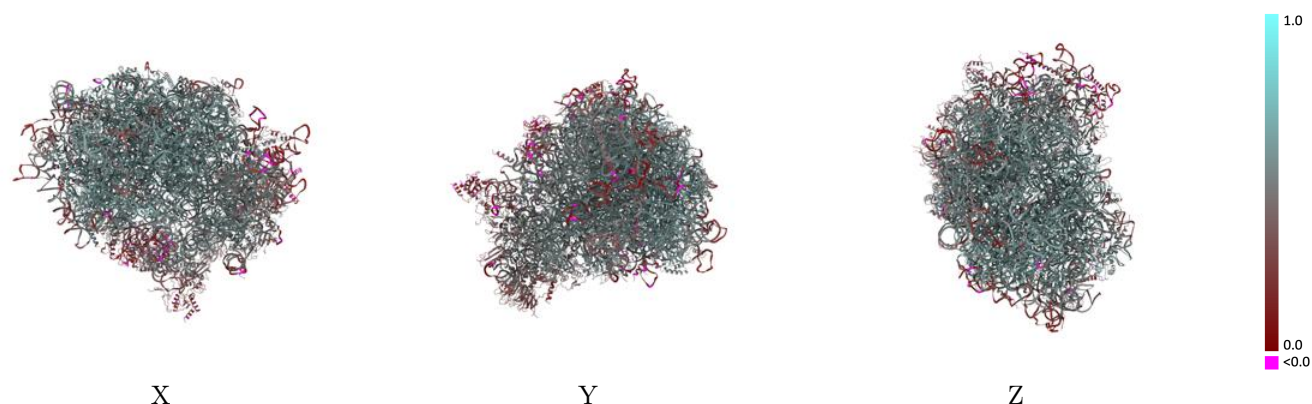
This section contains information regarding the fit between EMDB map EMD-71331 and PDB model 9P72. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



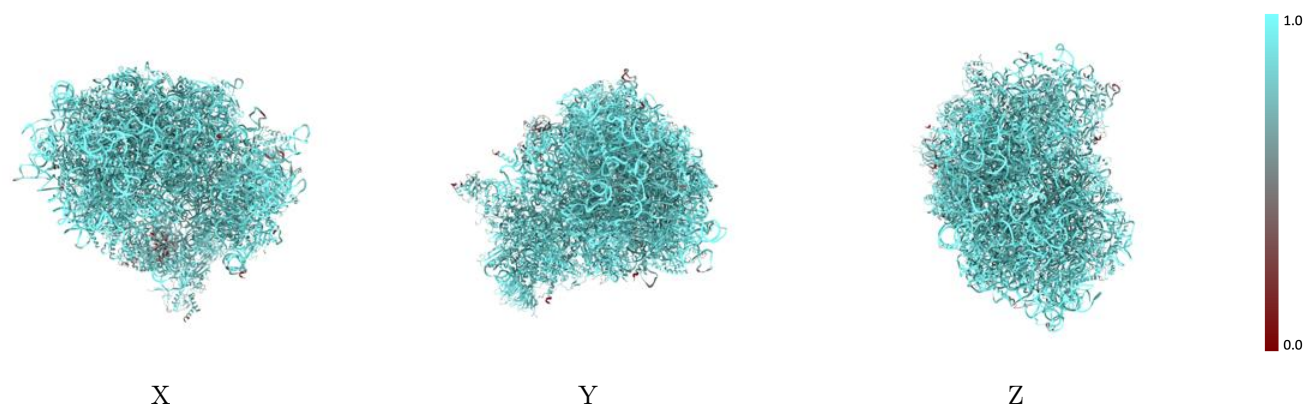
The images above show the 3D surface view of the map at the recommended contour level 0.0128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



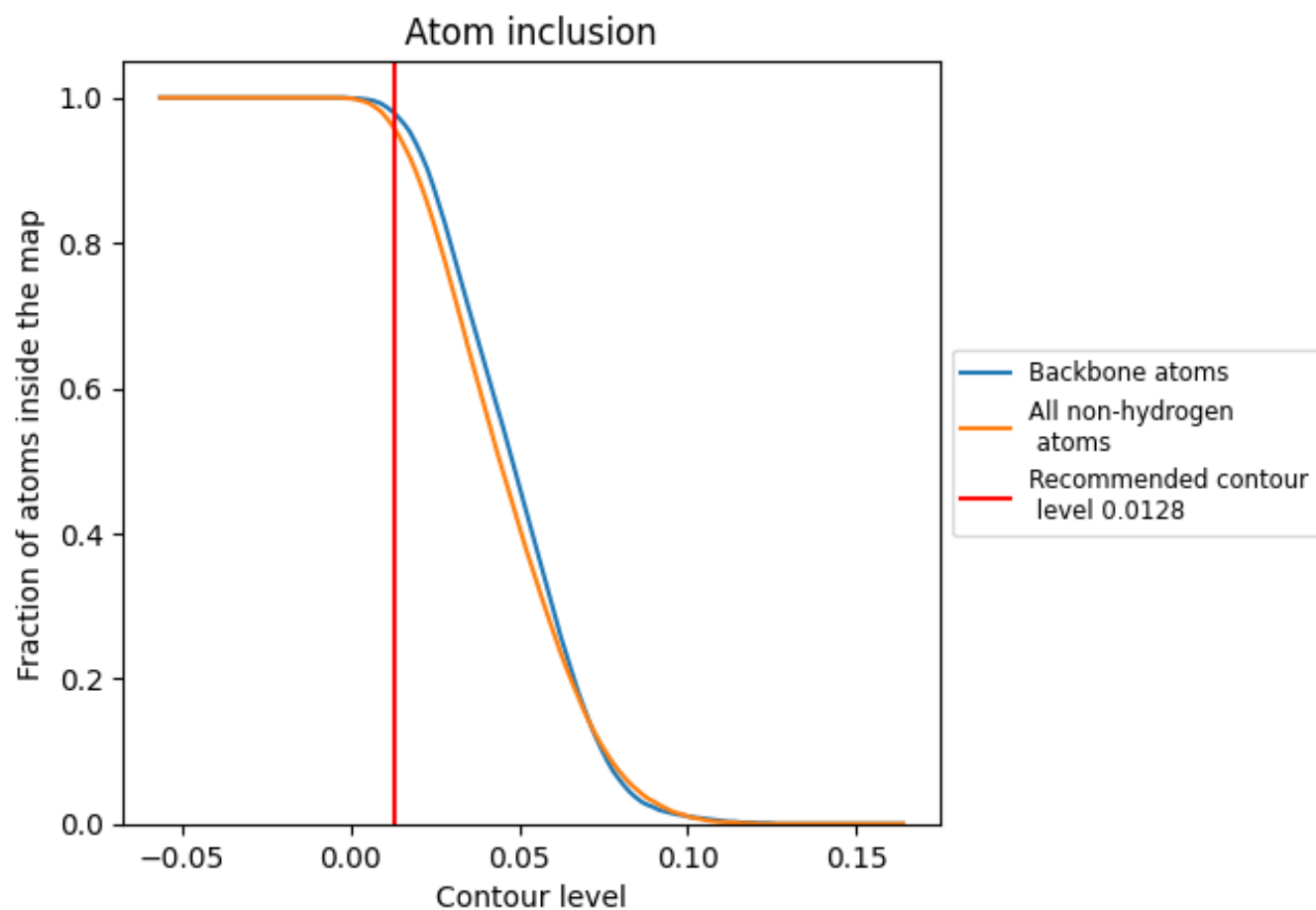
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0128).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.0128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.5080
CI	 0.8160	 0.4450
Et	 0.9350	 0.2290
L5	 0.9820	 0.5310
L7	 0.9980	 0.5770
L8	 0.9880	 0.5580
LA	 0.9790	 0.5940
LB	 0.9580	 0.5730
LC	 0.9580	 0.5710
LD	 0.9480	 0.5330
LE	 0.9200	 0.5110
LF	 0.9770	 0.5740
LG	 0.9110	 0.5130
LH	 0.9570	 0.5630
LI	 0.9550	 0.5640
LJ	 0.9390	 0.5100
LL	 0.9360	 0.5470
LM	 0.9670	 0.5530
LN	 0.9910	 0.6080
LO	 0.9700	 0.5700
LP	 0.9710	 0.5830
LQ	 0.9790	 0.5950
LR	 0.9130	 0.5200
LS	 0.9840	 0.5940
LT	 0.9530	 0.5570
LU	 0.9460	 0.4940
LV	 0.9650	 0.5810
LW	 0.8710	 0.4130
LX	 0.9500	 0.5530
LY	 0.9530	 0.5540
LZ	 0.9640	 0.5460
La	 0.9760	 0.6000
Lb	 0.9130	 0.4960
Lc	 0.9650	 0.5450
Ld	 0.9480	 0.5610



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Chain	Atom inclusion	Q-score
Le	 0.9780	 0.5940
Lf	 0.9850	 0.5990
Lg	 0.9630	 0.5700
Lh	 0.9450	 0.5470
Li	 0.9590	 0.5480
Lj	 0.9900	 0.5940
Lk	 0.9080	 0.5030
Ll	 0.9810	 0.5800
Lm	 0.9590	 0.5700
Ln	 0.9860	 0.5700
Lo	 0.9570	 0.5690
Lp	 0.9670	 0.5720
Lr	 0.9710	 0.5780
Ls	 0.6350	 0.2060
Lt	 0.5870	 0.1380
Pt	 0.9680	 0.4760
S2	 0.9840	 0.4850
SA	 0.9120	 0.4780
SB	 0.9200	 0.5060
SC	 0.9530	 0.5110
SD	 0.8970	 0.4140
SE	 0.9520	 0.4840
SF	 0.9110	 0.4370
SG	 0.8790	 0.3930
SH	 0.8590	 0.4030
SI	 0.9170	 0.4900
SJ	 0.9230	 0.4660
SK	 0.8920	 0.3600
SL	 0.9070	 0.5120
SM	 0.7000	 0.1900
SN	 0.9520	 0.5360
SO	 0.9370	 0.5230
SP	 0.8710	 0.3920
SQ	 0.9070	 0.4350
SR	 0.8660	 0.4110
SS	 0.9050	 0.4280
ST	 0.9310	 0.4340
SU	 0.8950	 0.3700
SV	 0.9490	 0.4870
SW	 0.9720	 0.5350
SX	 0.9470	 0.5250
SY	 0.8710	 0.3920

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Chain	Atom inclusion	Q-score
SZ	 0.8490	 0.4040
Sa	 0.9400	 0.5230
Sb	 0.9190	 0.4810
Sc	 0.8870	 0.4320
Sd	 0.9500	 0.4760
Se	 0.8110	 0.4000
Sf	 0.7790	 0.2470
Sg	 0.8920	 0.3480