



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 06:15 PM EDT

PDB ID : 9P8H / pdb_00009p8h
EMDB ID : EMD-71377
Title : In situ human A/P-P/E state 80S ribosome
Authors : Zheng, W.; Xiong, Y.
Deposited on : 2025-06-23
Resolution : 2.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

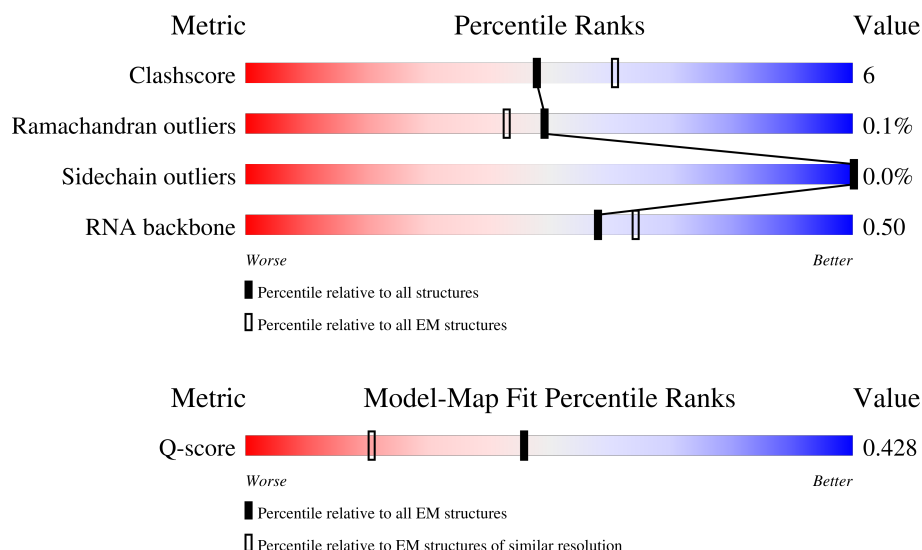
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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.



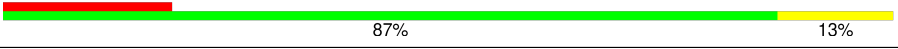
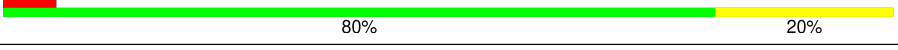
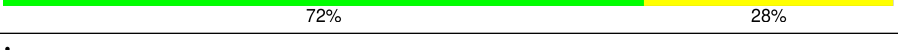
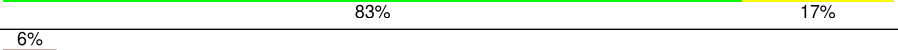
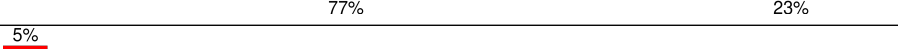
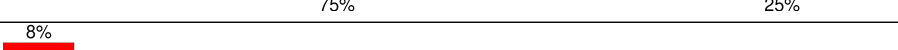
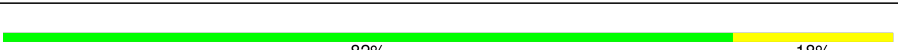
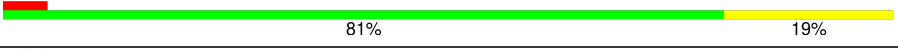
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 (2.48 - 3.48)

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	AP	142	
2	PE	150	
3	SD	454	

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Mol	Chain	Length	Quality of chain
4	SF	189	
5	SK	98	
6	SM	122	
7	SP	127	
8	SQ	144	
9	SR	135	
10	SS	145	
11	ST	143	
12	SU	104	
13	SZ	75	
14	Sc	64	
15	Sd	55	
16	Sf	67	
17	Sg	313	
18	SA	221	
19	SB	214	
20	SC	222	
21	SE	262	
22	SG	237	
23	SH	186	
24	SI	206	
25	SJ	185	
26	SL	153	
27	SN	150	
28	SO	140	

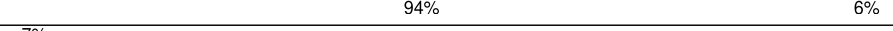
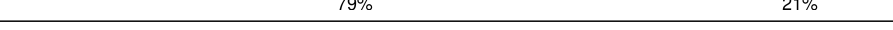
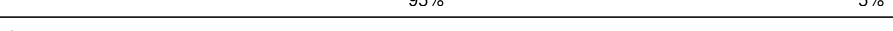
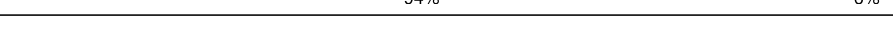
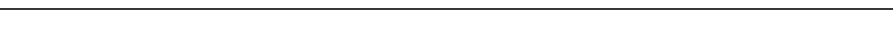
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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SW	129	
31	SX	141	
32	SY	131	
33	Sa	102	
34	Sb	83	
35	S2	1740	
36	LR	187	
37	LW	118	
38	CI	31	
39	L5	3655	
40	L7	120	
41	L8	156	
42	LA	248	
43	LB	402	
44	LC	368	
45	LD	293	
46	LE	250	
47	LF	225	
48	LG	241	
49	LH	190	
50	LI	213	
51	LJ	176	
52	LL	210	
53	LM	139	

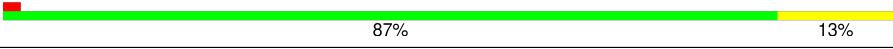
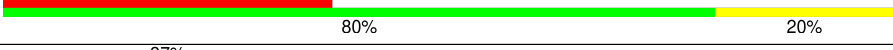
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Mol	Chain	Length	Quality of chain
54	LN	203	
55	LO	201	
56	LP	153	
57	LQ	187	
58	LS	175	
59	LT	159	
60	LU	101	
61	LV	131	
62	LX	120	
63	LY	134	
64	LZ	135	
65	La	147	
66	Lb	109	
67	Lc	98	
68	Ld	107	
69	Le	128	
70	Lf	109	
71	Lg	114	
72	Lh	122	
73	Li	102	
74	Lj	86	
75	Lk	69	
76	Ll	50	
77	Lm	52	
78	Ln	24	

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Mol	Chain	Length	Quality of chain
79	Lo	105	
80	Lp	91	
81	Lr	125	
82	Ls	196	
83	Lt	141	
84	CH	132	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 220526 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 A/P site tRNA.

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

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

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

- Molecule 3 is a protein called 40S ribosomal protein S3.

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

- Molecule 4 is a protein called 40S ribosomal protein S5.

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

- Molecule 5 is a protein called 40S ribosomal protein S10.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 7 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 9 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 10 is a protein called 40S ribosomal protein S18.

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

- Molecule 11 is a protein called 40S ribosomal protein S19.

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

- Molecule 12 is a protein called 40S ribosomal protein S20.

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

- Molecule 13 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 14 is a protein called 40S ribosomal protein S28.

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

- Molecule 15 is a protein called 40S ribosomal protein S29.

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

- Molecule 16 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 17 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 18 is a protein called 40S ribosomal protein SA.

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

- Molecule 19 is a protein called 40S ribosomal protein S3a.

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

- Molecule 20 is a protein called 40S ribosomal protein S2.

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

- Molecule 21 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 22 is a protein called 40S ribosomal protein S6.

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

- Molecule 23 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	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 24 is a protein called 40S ribosomal protein S8.

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

- Molecule 25 is a protein called 40S ribosomal protein S9.

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

- Molecule 26 is a protein called 40S ribosomal protein S11.

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

- Molecule 27 is a protein called 40S ribosomal protein S13.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 29 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 30 is a protein called 40S ribosomal protein S15a.

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

- Molecule 31 is a protein called 40S ribosomal protein S23.

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

- Molecule 32 is a protein called 40S ribosomal protein S24.

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

- Molecule 33 is a protein called 40S ribosomal protein S26.

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

- Molecule 34 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 35 is a RNA chain called 18S rRNA.

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

- Molecule 36 is a protein called 60S ribosomal protein L19.

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

- Molecule 37 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	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 38 is a protein called Transcription factor BTF3.

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

- Molecule 39 is a RNA chain called 28S rRNA.

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

- Molecule 40 is a RNA chain called 5S rRNA.

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

- Molecule 41 is a RNA chain called 5.8S rRNA.

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

- Molecule 42 is a protein called 60S ribosomal protein L8.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 44 is a protein called 60S ribosomal protein L4.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 46 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 47 is a protein called 60S ribosomal protein L7.

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

- Molecule 48 is a protein called 60S ribosomal protein L7a.

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

- Molecule 49 is a protein called 60S ribosomal protein L9.

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

- Molecule 50 is a protein called Ribosomal protein uL16-like.

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

- Molecule 51 is a protein called 60S ribosomal protein L11.

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

- Molecule 52 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 53 is a protein called 60S ribosomal protein L14.

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

- Molecule 54 is a protein called 60S ribosomal protein L15.

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

- Molecule 55 is a protein called 60S ribosomal protein L13a.

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

- Molecule 56 is a protein called 60S ribosomal protein L17.

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

- Molecule 57 is a protein called 60S ribosomal protein L18.

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

- Molecule 58 is a protein called 60S ribosomal protein L18a.

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

- Molecule 59 is a protein called 60S ribosomal protein L21.

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

- Molecule 60 is a protein called Heparin-binding protein HBp15.

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

- Molecule 61 is a protein called 60S ribosomal protein L23.

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

- Molecule 62 is a protein called 60S ribosomal protein L23a.

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

- Molecule 63 is a protein called 60S ribosomal protein L26.

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

- Molecule 64 is a protein called 60S ribosomal protein L27.

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

- Molecule 65 is a protein called 60S ribosomal protein L27a.

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

- Molecule 66 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 67 is a protein called 60S ribosomal protein L30.

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

- Molecule 68 is a protein called 60S ribosomal protein L31.

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

- Molecule 69 is a protein called 60S ribosomal protein L32.

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

- Molecule 70 is a protein called 60S ribosomal protein L35a.

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

- Molecule 71 is a protein called 60S ribosomal protein L34.

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

- Molecule 72 is a protein called 60S ribosomal protein L35.

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

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

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

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

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

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

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

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

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

- Molecule 77 is a protein called Large ribosomal subunit protein eL40.

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

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

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

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

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

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

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

- Molecule 81 is a protein called 60S ribosomal protein L28.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 83 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	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

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

- Molecule 84 is a protein called Endothelial differentiation-related factor 1.

Mol	Chain	Residues	Atoms			AltConf	Trace
84	CH	132	Total	C	N	O	
			1018	625	199	194	
						0	0

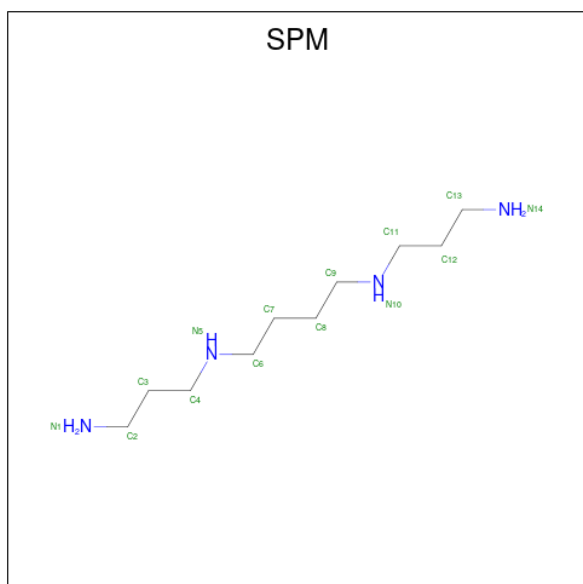
- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
85	SS	1	Total	Mg	0
			1	1	
85	SG	1	Total	Mg	0
			1	1	
85	S2	25	Total	Mg	0
			25	25	
85	L5	178	Total	Mg	0
			178	178	
85	L7	3	Total	Mg	0
			3	3	
85	L8	4	Total	Mg	0
			4	4	
85	LA	1	Total	Mg	0
			1	1	
85	LB	1	Total	Mg	0
			1	1	
85	LI	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	

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



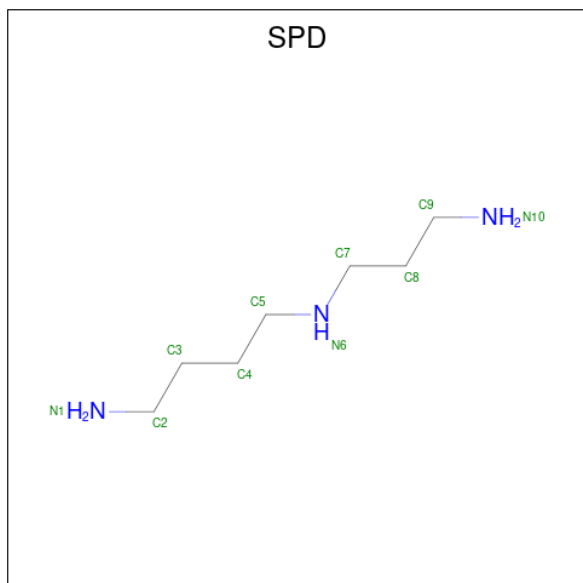
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	

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

- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

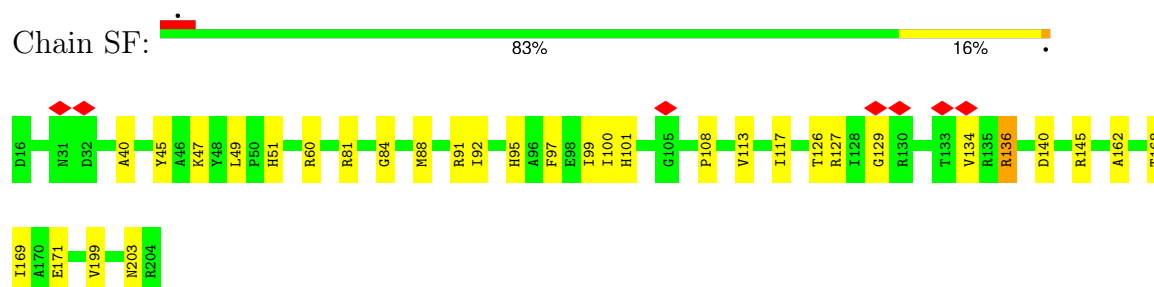
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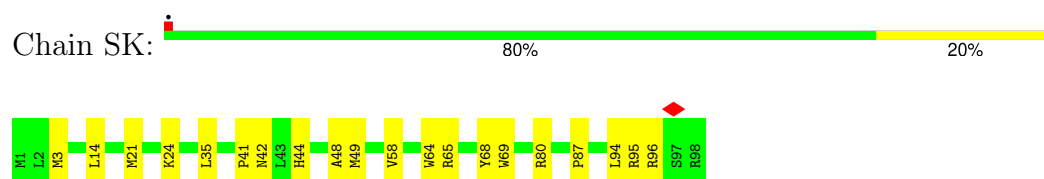
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
88	LN	1	10	7	3	0

ARG	GLY	LEU	CYS	ALA	ILE	ALA	GLN	GLY	ALA	GLU	SER	LEU	ARG	TYR	LYS	LEU	LEU	GLY	GLY	ALA	VAL	ARG	ARG	GLN	CYS	TYR	VAL	GLY	LEU	VAL	ARG	PHE	ILE	ILE	MET	GLU	SER	LEU	GLY	ALA	LYS	GLY	CYS	PRO	THR	GLY	VAL	VAL	VAL	SER	GLY	PRO	LYS	LEU	ARG	GLY	GLN	ASP	HIS	ALA	LYS	SER	ILE	VAL	VAL	GLU	PHE	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
ASP	GLY	LEU	MET	ILE	HIS	SER	GLY	PRO	ASP	VAL	ASN	TYR	TYR	VAL	VAL	THR	ASP	ALA	VAL	ARG	HIS	VAL	LEU	LEU	ARG	GLN	GLY	VAL	LEU	GLY	ILE	LYS	PRO	TRP	ASP	PRO	THR	THR	GLY	LYS	ILE	VAL	VAL	LYS	PRO	LEU	PRO	PRO	ASP	HIS	VAL	SER	ILE	VAL	VAL	GLU	PHE	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
LYS	ASP	GLU	ILE	LEU	PRO	THR	THR	PRO	ILE	SER	GLU	GLN	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	</

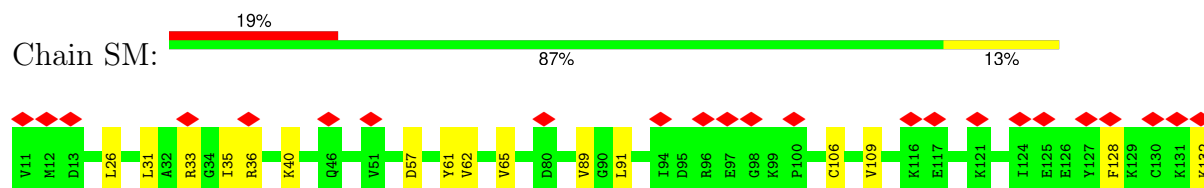
- Molecule 4: 40S ribosomal protein S5



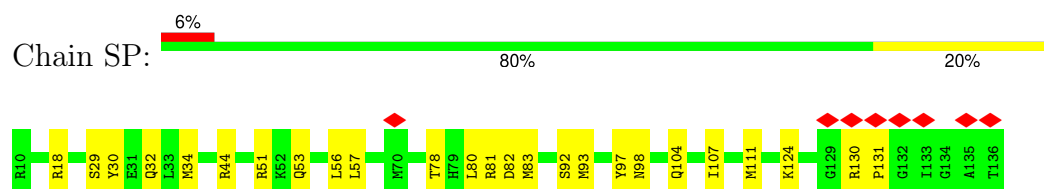
- Molecule 5: 40S ribosomal protein S10



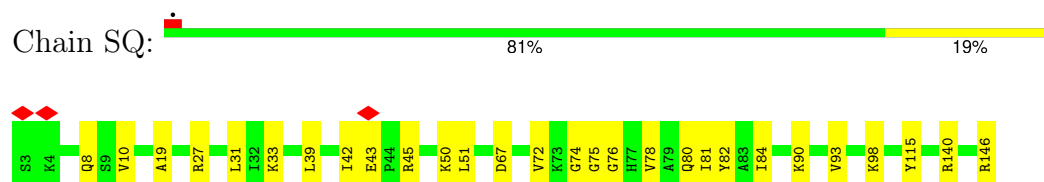
- Molecule 6: Small ribosomal subunit protein eS12



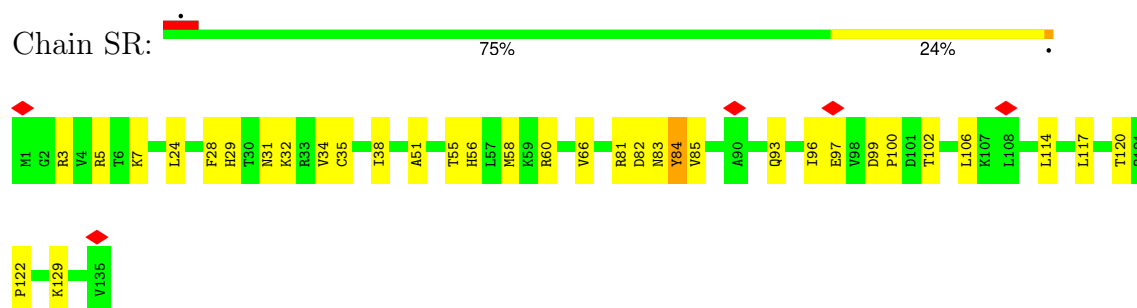
- Molecule 7: 40S ribosomal protein S15



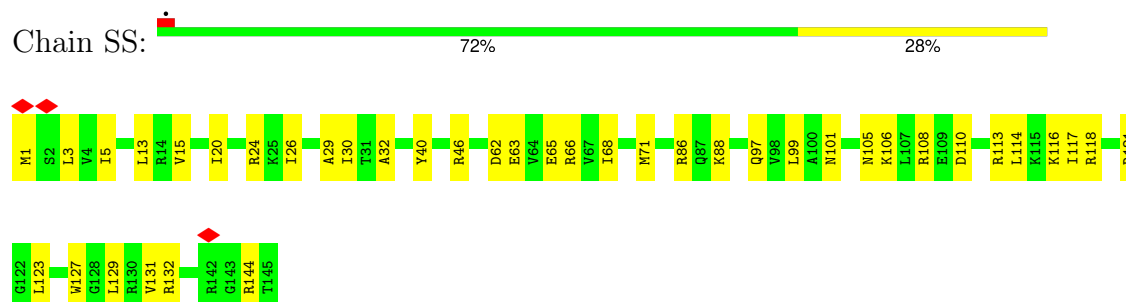
- Molecule 8: Small ribosomal subunit protein uS9



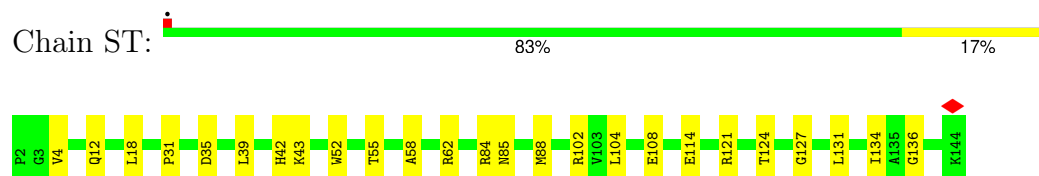
- Molecule 9: Small ribosomal subunit protein eS17



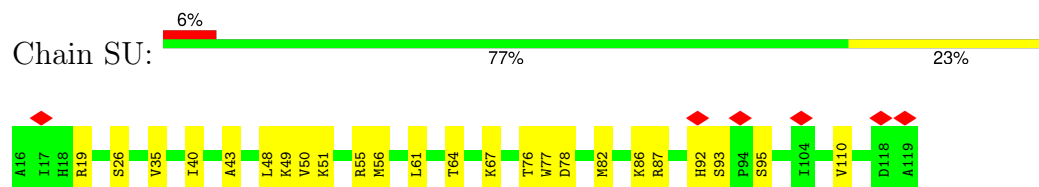
- Molecule 10: 40S ribosomal protein S18



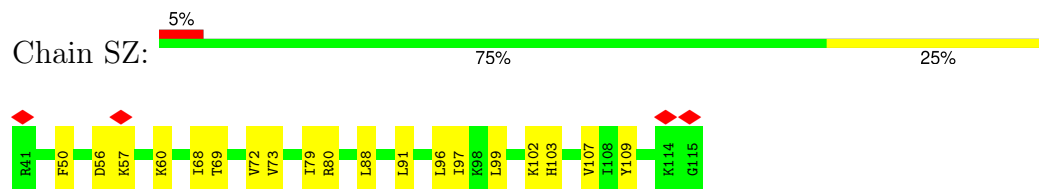
- Molecule 11: 40S ribosomal protein S19



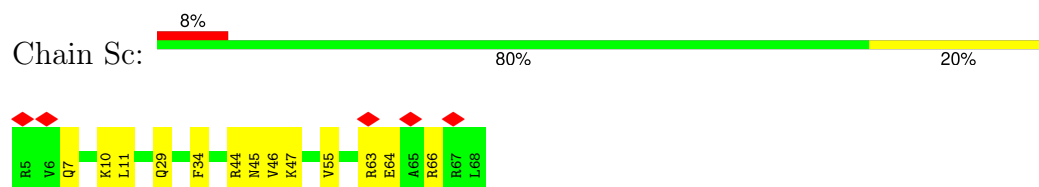
- Molecule 12: 40S ribosomal protein S20



- Molecule 13: Small ribosomal subunit protein eS25



- Molecule 14: 40S ribosomal protein S28



- Molecule 15: 40S ribosomal protein S29

Chain Sd:  89% 11%



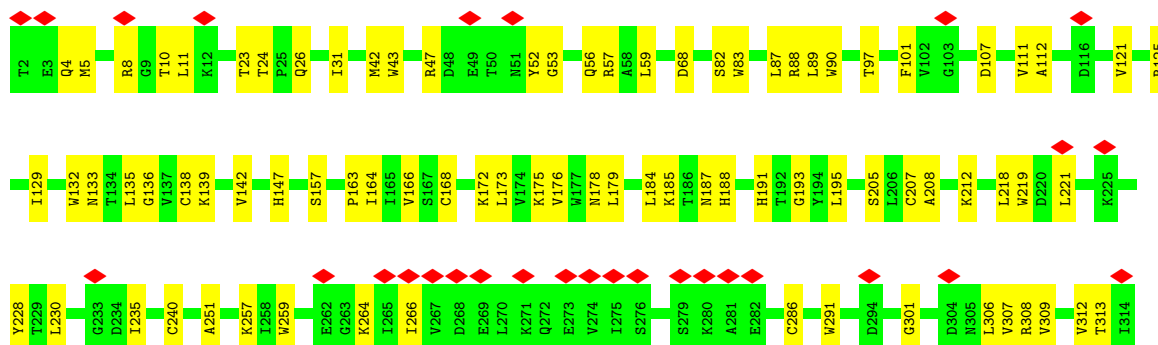
- Molecule 16: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  15% 78% 22%



- Molecule 17: Receptor of activated protein C kinase 1

Chain Sg:  9% 73% 27%



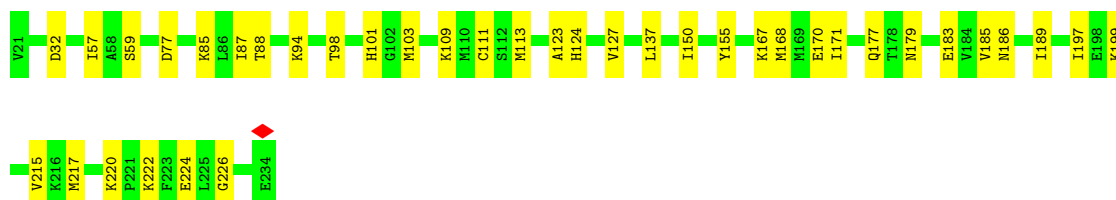
- Molecule 18: 40S ribosomal protein SA

Chain SA:  82% 18%



- Molecule 19: 40S ribosomal protein S3a

Chain SB:  82% 18%



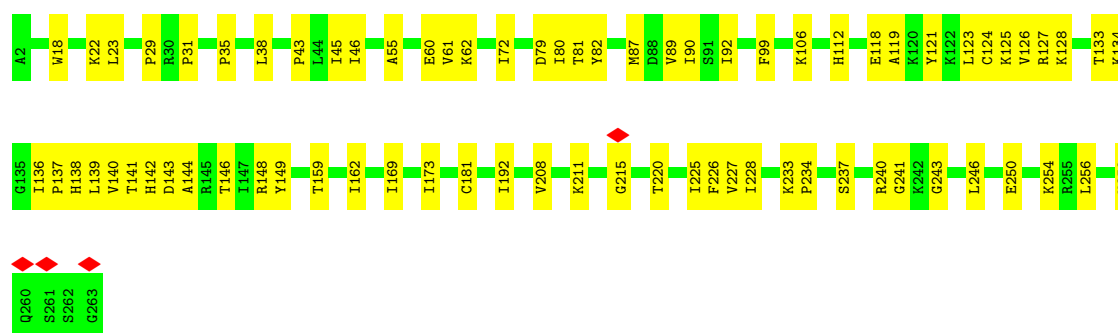
- Molecule 20: 40S ribosomal protein S2

Chain SC:  83% 16%



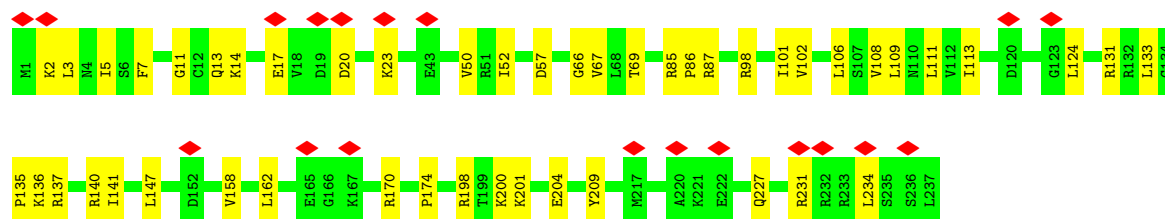
- Molecule 21: Small ribosomal subunit protein eS4, X isoform

Chain SE:  72% 28%



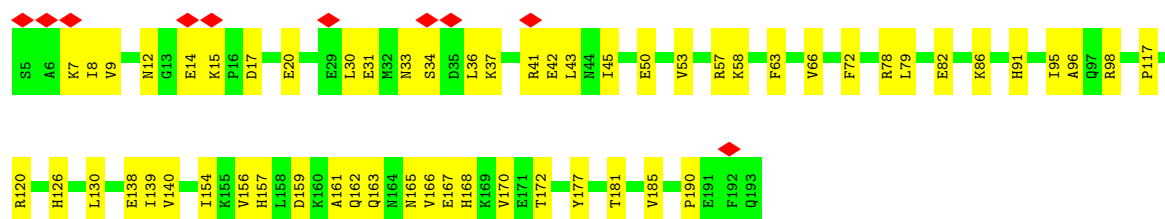
- Molecule 22: 40S ribosomal protein S6

Chain SG:  8% 80% 20%



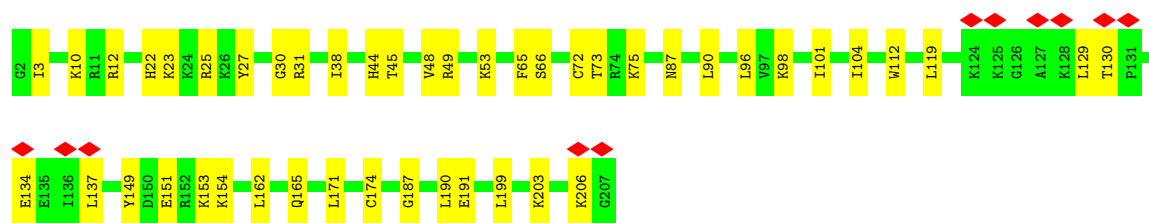
- Molecule 23: Small ribosomal subunit protein eS7

Chain SH:  5% 69% 31%

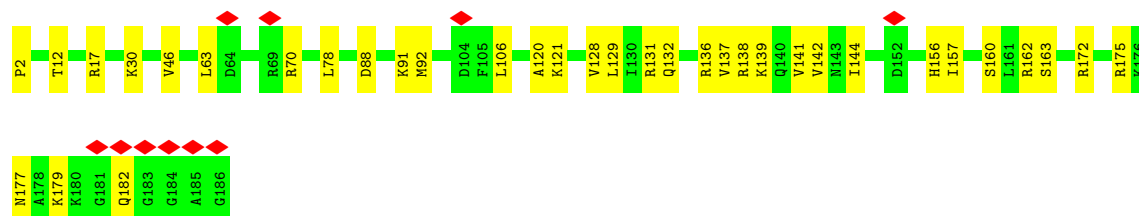
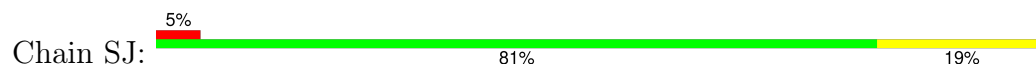


- Molecule 24: 40S ribosomal protein S8

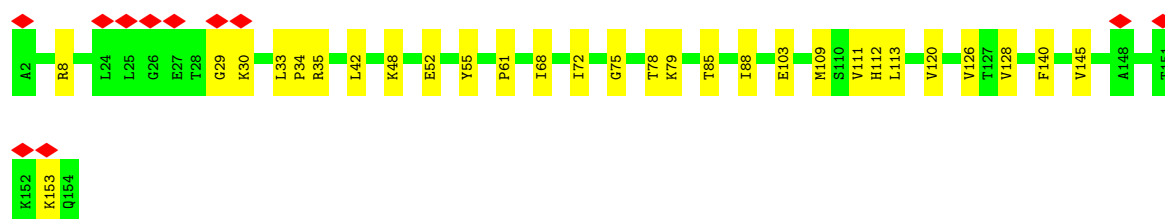
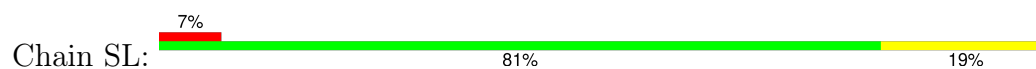
Chain SI:  5% 78% 22%



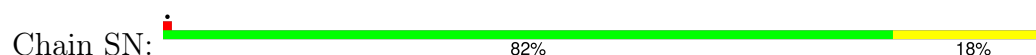
- Molecule 25: 40S ribosomal protein S9



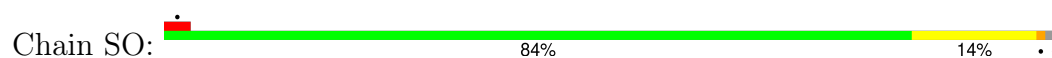
- Molecule 26: 40S ribosomal protein S11



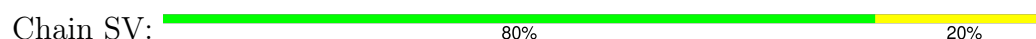
- Molecule 27: 40S ribosomal protein S13



- Molecule 28: Small ribosomal subunit protein uS11



- Molecule 29: Small ribosomal subunit protein eS21





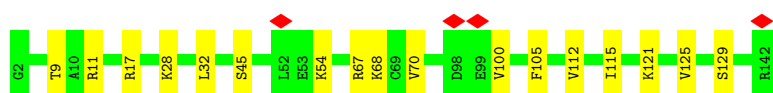
- Molecule 30: 40S ribosomal protein S15a

Chain SW: 81% 19%



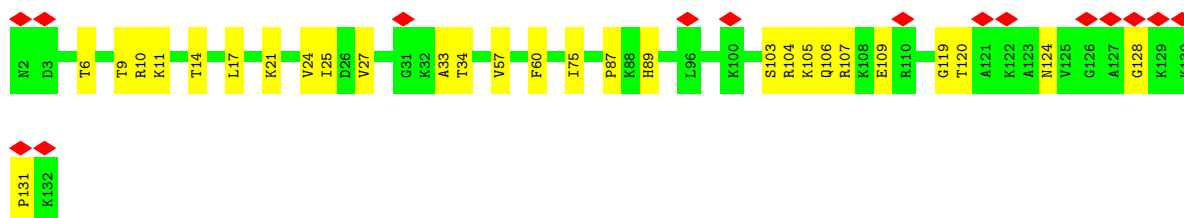
- Molecule 31: 40S ribosomal protein S23

Chain SX: 88% 12%



- Molecule 32: 40S ribosomal protein S24

Chain SY: 11% 79% 21%



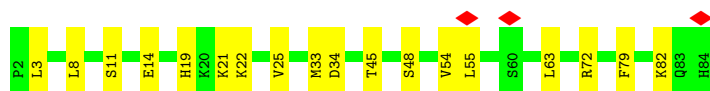
- Molecule 33: 40S ribosomal protein S26

Chain Sa: 82% 18%



- Molecule 34: Small ribosomal subunit protein eS27

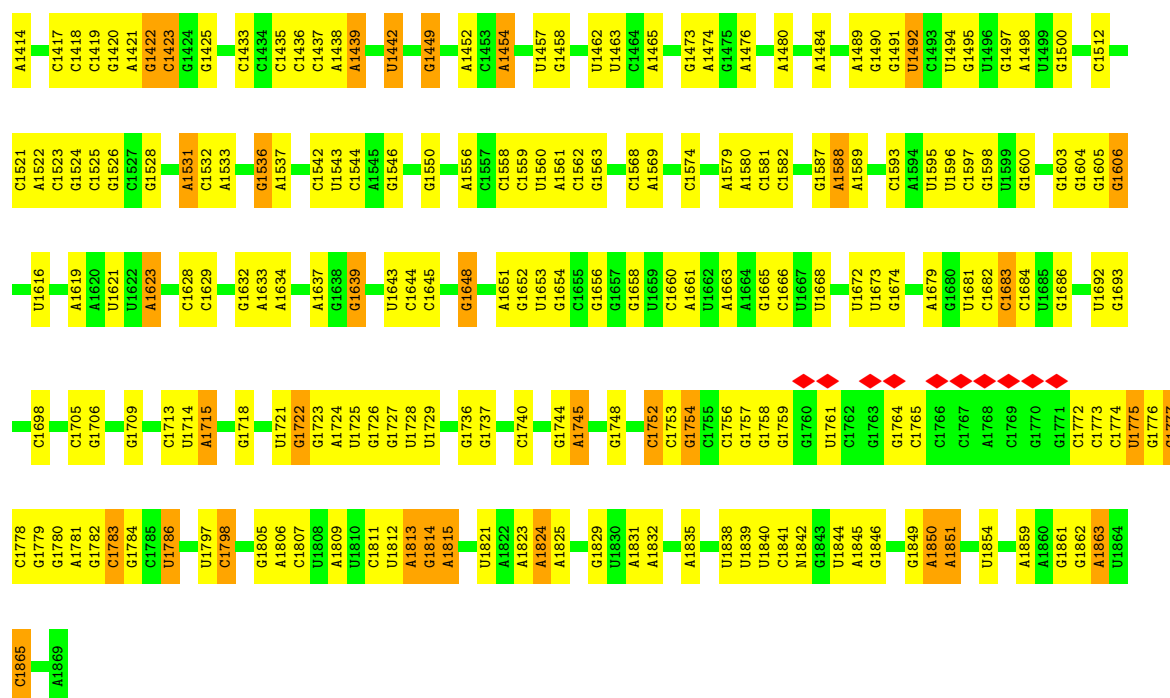
Chain Sb: 78% 22%



- Molecule 35: 18S rRNA

Chain S2: 55% 37% 7%

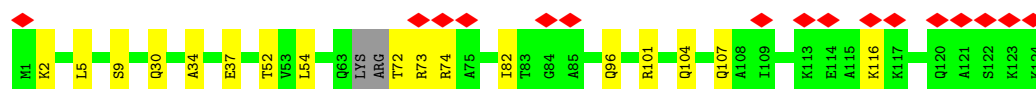
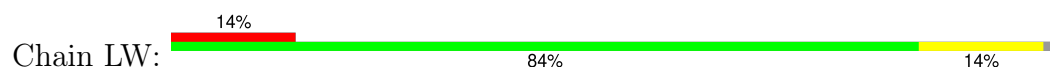
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U1307	A1228	C1116	A1012	A908	A826	C674	U591	A512	G329	A175	C98	C4
U1308	G1229	U1013	U1013	A913	A827	U676	C592	A516	G330	C182	A99	U15
U1310	U1232	A1119	U1017	A916	A830	C677	G601	A520	G332	G186	A102	C14
C1311	G1233	U1120	U1018	A919	C834	U681	A604	A525	A339	G187	A103	U16
G1312	U1237	C1124	C1019	A920	G836	U682	U607	A526	C341	C188	A104	C17
G1320	U1238	G1129	A1020	G925	A837	U686	C908	A528	C342	G190	U189	C18
G1321	U1239	G1130	A1023	G929	G838	U687	U609	A529	A343	G196	G108	U21
U1326	U1242	G1133	A1027	G932	C839	U688	G610	U530	C346	U197	U109	C24
G1328	U1244	G1134	A1028	G939	C840	U689	G611	A531	G347	U198	A25	C25
U1333	BN1248	C1138	G1029	C930	G841	G690	U612	C532	A348	G199	G113	A26
U1337	A1251	C1139	A1030	G933	C842	G691	G613	A533	C350	G200	U115	U27
G1338	C1252	G1140	A1031	G934	G845	G692	C615	G534	C354	G203	U116	A27
U1342	A1253	A1144	G1033	G942	G846	G694	A616	G535	U354	G204	C117	U28
G1348	C1254	A1145	U1045	U943	A847	G695	G617	A536	A364	G205	C118	G29
U1358	G1255	U1149	U1046	U946	C851	G696	G623	C537	A366	G206	U121	C30
G1354	G1256	C1153	U1046	C953	G852	G697	U627	U541	U367	G207	G33	G42
C1355	A1258	U1154	A1085	A962	U857	G731	A628	U542	U368	G208	U124	A42
G1356	A1259	U1171	U1056	A963	G859	C732	U631	C543	U369	A209	C125	U43
A1357	C1260	G1174	C1057	A964	G860	C733	U634	G544	G370	G210	G126	U44
U1358	U1261	U1174	A1058	U965	U863	C736	G635	G545	A371	G211	G130	A45
G1365	C1268	U1177	A1059	U966	A864	C737	G636	C548	G471	G212	U135	U51
G1366	U1269	U1177	A1060	U966	A865	C738	U637	G549	G472	C223	G52	G52
U1367	U1270	G1187	U1061	U969	A866	C739	C638	C550	G473	A224	C142	C53
U1371	C1273	U1187	A1062	G971	G867	C746	C639	A555	G474	G289	U143	G66
C1373	G1275	A1195	C1067	G971	A870	U749	A640	U556	C382	U290	U144	U57
A1376	A1276	A1199	A1080	A980	G874	C750	U642	U557	G383	G291	A147	C58
U1377	C1277	U1201	U1081	A981	A875	G751	A643	G558	G385	G292	U148	G62
A1378	C1279	U1202	A1083	G982	C875	G752	G644	G559	C386	A150	U149	U83
U1378	G1280	G1203	A1084	C984	U883	C785	U649	U560	C387	G153	A151	G86
A1382	C1283	A1204	C1085	C989	C884	G786	A650	U562	U388	U154	C87	C87
A1383	A1284	G1207	U1088	A990	A886	G787	U651	A564	A390	G155	A68	A68
A1388	G1285	A1209	G1089	G991	U887	G788	A655	G565	C391	A158	G71	G71
C1395	A1287	A1209	C1090	A992	U888	G791	G856	U566	A392	C72	C73	C73
A1396	U1289	C1215	A1093	A996	U889	C792	U657	C570	A398	U160	G74	G74
U1401	G1290	C1216	U1093	G997	U890	G796	U658	C570	U406	C310	G75	G75
A1402	U1294	A1217	G1097	U996	C797	U796	C660	U573	G407	G311	U76	U76
C1403	G1298	C1218	C1098	U997	U798	U799	G661	A574	A408	C312	A83	A83
U1404	U1299	A1220	G1099	U998	U799	U800	G662	A575	C409	C317	A164	A84
A1405	C1299	C1221	U1103	U999	U800	U801	C663	A576	C497	A318	A166	A85
G1406	U1300	G1222	U1104	C900	U801	U814	A664	U582	A426	C319	G167	A85
U1407	A1301	A1223	G1104	G901	U802	G821	A668	A583	U427	C323	C168	C168
U1408	C1302	U1224	G1108	A903	A903	U822	A669	A587	U428	C324	U169	A92
G1413	C1303	G1226	C1109	C905	A904	U823	A671	G588	G431	C325	A171	U93
				U906	G905	U824	A672	G589	A433	G327	U172	G94
												G95
												C96



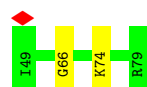
- Molecule 36: 60S ribosomal protein L19



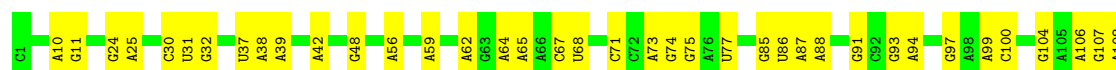
- Molecule 37: Ribosomal protein L24



- Molecule 38: Transcription factor BTF3

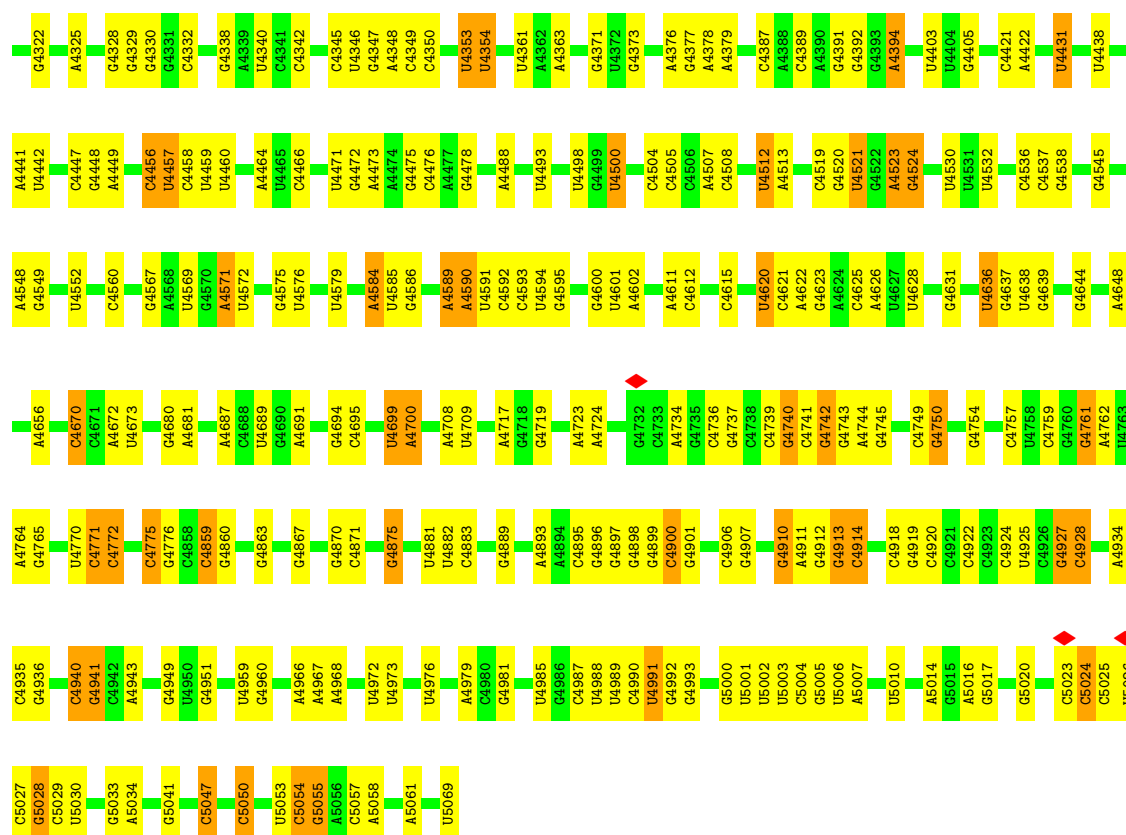


- Molecule 39: 28S rRNA

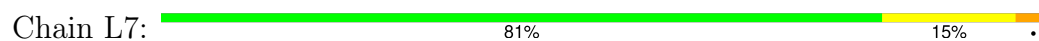


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G1764	A1765	A1766	A1767	U1768	G1769	A1770	U1771	C1772	U1773	C1774	U1777	U1781	U1782	C1785	A1786	A1787	A1788	U1792	A1793	A1794	G1797	U1802	G1803	A1804	A1805	G1806	C1807	G1810	G1811	C1812	G1815	C1820	G1821	U1822	G1823	G1824	A1825	U1834	G1835	G1836	A1837	U1842	G1846	C1847	G1855	C1856							
C1666	A1669	C1676	U1677	U1683	A1684	G1685	G1688	G1691	C1692	U1693	C1694	G1697	C1698	A1699	G1700	A1701	C1702	C1703	C1704	G1705	A1706	G1716	C1717	C1718	A1719	G1720	G1721	U1725	U1726	C1731	C1732	G1733	G1734	G1739	C1740	G1741	A1742	A1743	U1744	A1749	G1750	U1757	G1758	G1759	G1760	G1761	C1762	C1763					
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C1413	C1414	G1415	G1416	C1417	C1418	G1419	A1420	C1437	U1438	C1439	U1440	C1441	C1442	A1443	G1444	U1445	C1446	C1447	C1464	G1465	G1466	G1475	C1476	C1480	G1481	G1482	C1483	G1489	U1494	G1495	G1496	G1497	C1499	G1502	A1503	G1504	C1509	U1514	A1515	G1516	G1517	G1522	A1523	A1524	C1661	C1662	C1663	A1534	U1536				
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U1247	C1248	C1249	C1250	C1251	C1252	G1253	A1254	A1255	G1256	A1257	G1258	G1259	G1260	G1261	G1266	G1267	G1268	G1269	A1270	C1271	C1272	G1273	A1274	G1275	G1276	C1277	C1278	A1279	C1280	G1281	G1282	G1283	G1284	U1285	G1286	G1287	G1293	A1294	C1295	G1296	U1297	C1298	G1299	G1300	C1301	C1304	C1305	C1308	C1309	C1314	U1317	C1318	
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A915	C916	A917	G918	C919	C923	C924	C925	G926	A932	G933	C934	A935	C936	A944	U945	C946	C947	A956	G957	G958	G959	A960	C961	C962	G963	A964	G965	A966	C967	C968	C969	G970	C978	C979	U982	C985	U989	G1070	C1071	C1072	G1075	C1080	C1081	C1082	U1083	C1084	C1085						
G666	A667	C668	C669	C673	C679	G680	A686	U687	C691	A692	C696	G701	U702	G703	C704	G705	G708	C716	U717	C718	C724	G729	G730	G731	C737	C738	G739	G742	A746	U747	G748	U754	C755	G756	C904	C905	C906	C907	A909	G910	U913	U914											
U467	U468	C469	C473	C474	G478	G481	G482	C485	C486	C489	G490	G491	U492	G493	C494	G495	G496	G497	C498	G499	C500	U501	C502	G503	G504	A509	U510	U513	U514	C515	C516	C517	G518	C643	G644	G645	G646	G652	U653	C654	C655	C656	C657	C658	G659	C662	G663	G664	C665				
C210	C216	C217	A218	U233	G234	G253	G254	C255	G256	C257	G258	C259	C260	G261	G262	G263	C264	C265	C266	G267	G268	G269	U270	G271	C275	C276	G280	U297	A300	U301	C302	C303	C304	A305	A306	A307	G308	G312	U315	G315	U316	A317	A318	A319	U325	C326	G330						
G109	C110	C216	C217	A218	A121	U122	C123	C124	G132	C133	G134	G135	C136	G137	G138	G139	G144	C148	A149	U150	G151	U152	G153	G154	A158	C159	A162	A163	G164	A165	C170	U171	C172	C173	C174	C178	G179	G182	C183	U184	C185	G186	U187	G188	G189	G190	G191	U200	U209				

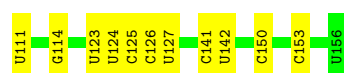
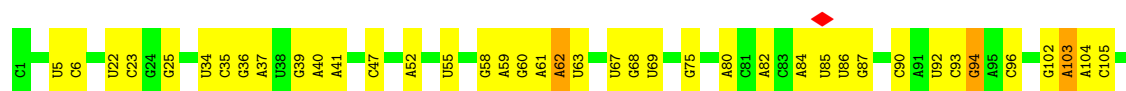




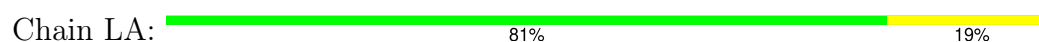
• Molecule 40: 5S rRNA



• Molecule 41: 5.8S rRNA

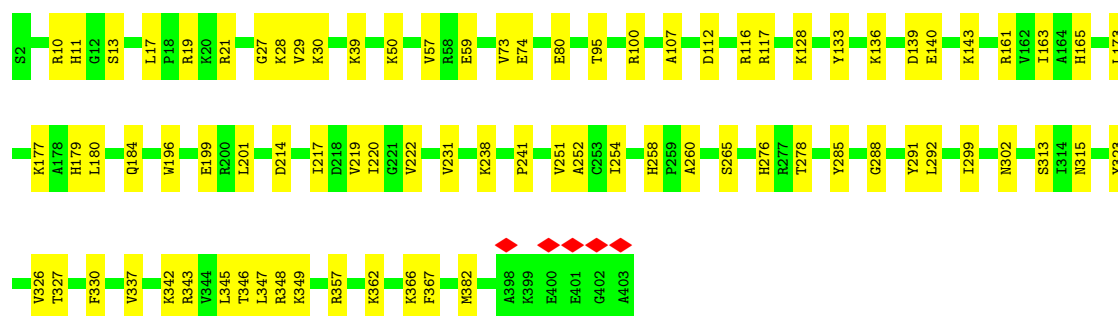
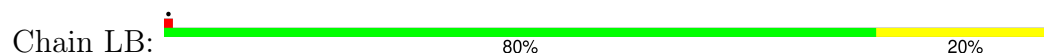


• Molecule 42: 60S ribosomal protein L8

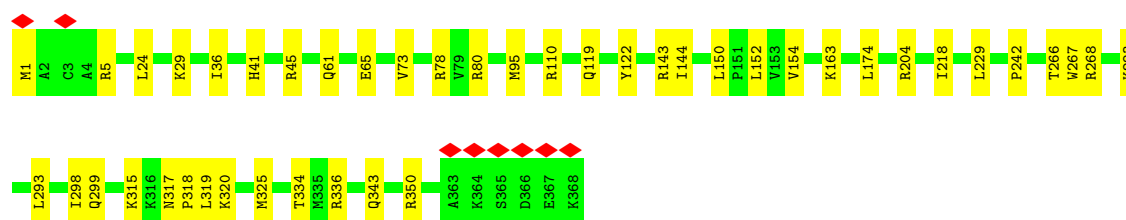




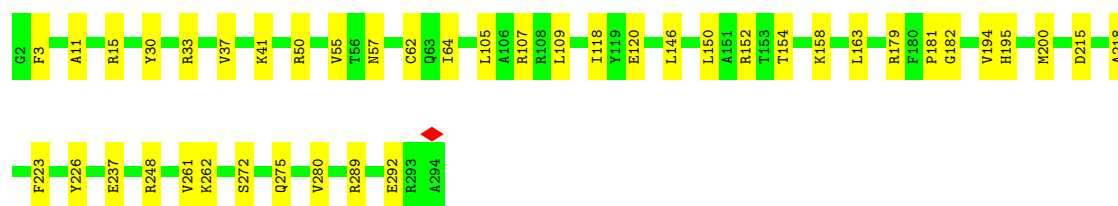
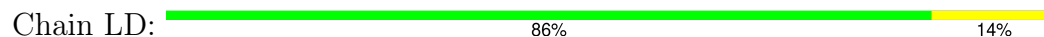
- Molecule 43: Large ribosomal subunit protein uL3



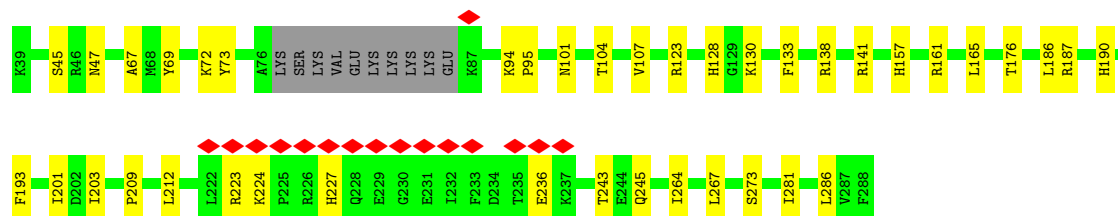
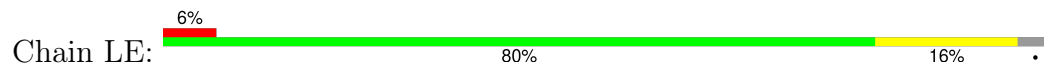
- Molecule 44: 60S ribosomal protein L4



- Molecule 45: Large ribosomal subunit protein uL18



- Molecule 46: Large ribosomal subunit protein eL6



- Molecule 47: 60S ribosomal protein L7

Chain LF:  88% 12%



- Molecule 48: 60S ribosomal protein L7a

Chain LG:  6% 88% 12%



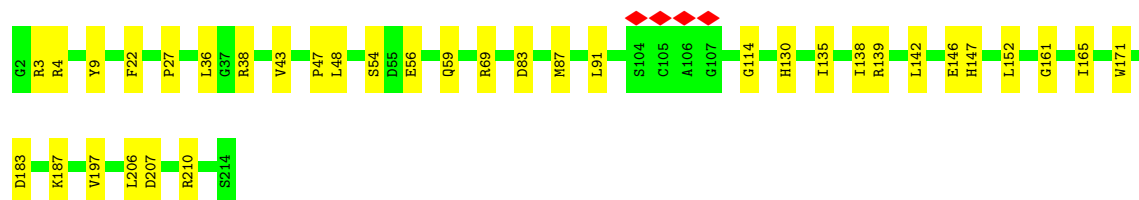
- Molecule 49: 60S ribosomal protein L9

Chain LH:  84% 16%



- Molecule 50: Ribosomal protein uL16-like

Chain LI:  84% 16%



- Molecule 51: 60S ribosomal protein L11

Chain LJ:  82% 15%



- Molecule 52: Large ribosomal subunit protein eL13

Chain LL:  89% 11%



- Molecule 53: 60S ribosomal protein L14

Chain LM:  88% 12%



- Molecule 54: 60S ribosomal protein L15

Chain LN:  89% 11%



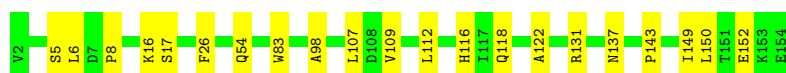
- Molecule 55: 60S ribosomal protein L13a

Chain LO:  82% 18%



- Molecule 56: 60S ribosomal protein L17

Chain LP:  86% 14%



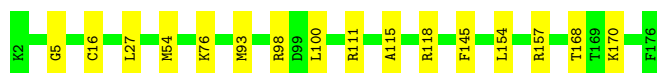
- Molecule 57: 60S ribosomal protein L18

Chain LQ:  91% 9%



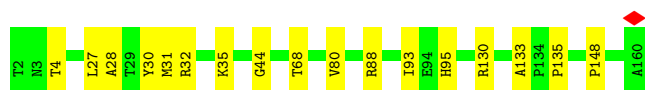
- Molecule 58: 60S ribosomal protein L18a

Chain LS:  91% 9%

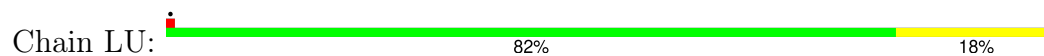


- Molecule 59: 60S ribosomal protein L21

Chain LT:  89% 11%



- Molecule 60: Heparin-binding protein HBp15



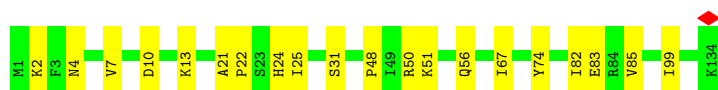
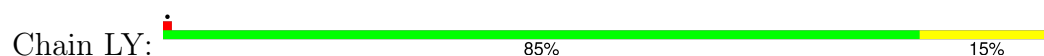
- Molecule 61: 60S ribosomal protein L23



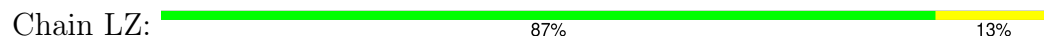
- Molecule 62: 60S ribosomal protein L23a



- Molecule 63: 60S ribosomal protein L26



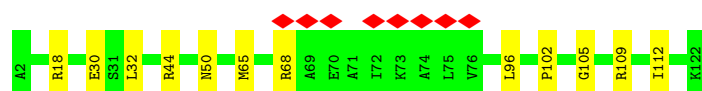
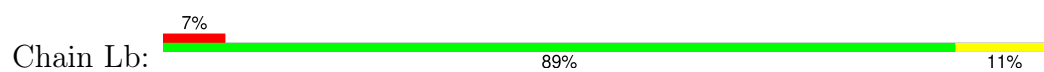
- Molecule 64: 60S ribosomal protein L27



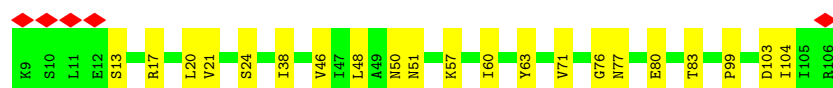
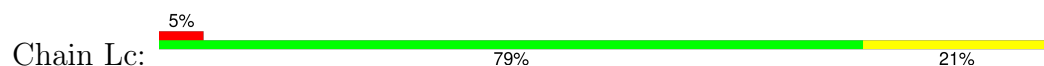
- Molecule 65: 60S ribosomal protein L27a



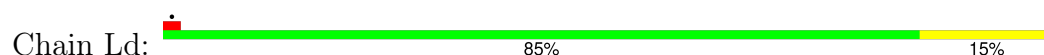
- Molecule 66: Large ribosomal subunit protein eL29



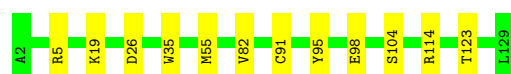
- Molecule 67: 60S ribosomal protein L30



- Molecule 68: 60S ribosomal protein L31



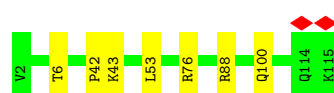
- Molecule 69: 60S ribosomal protein L32



- Molecule 70: 60S ribosomal protein L35a



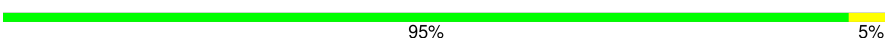
- Molecule 71: 60S ribosomal protein L34



- Molecule 72: 60S ribosomal protein L35



- Molecule 73: 60S ribosomal protein L36

Chain Li:  95% 5%



- Molecule 74: 60S ribosomal protein L37

Chain Lj:  86% 14%



- Molecule 75: 60S ribosomal protein L38

Chain Lk:  86% 14%

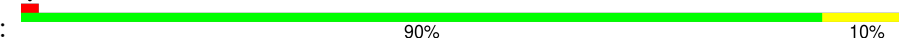


- Molecule 76: 60S ribosomal protein L39

Chain Ll:  80% 20%



- Molecule 77: Large ribosomal subunit protein eL40

Chain Lm:  90% 10%



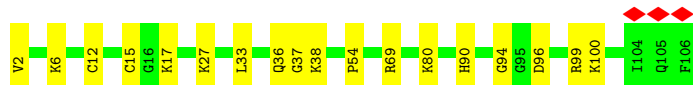
- Molecule 78: 60S ribosomal protein L41

Chain Ln:  79% 21%

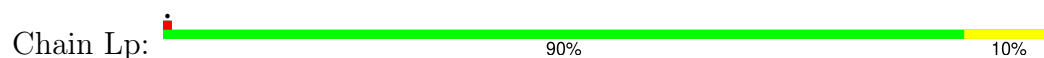


- Molecule 79: 60S ribosomal protein L36a

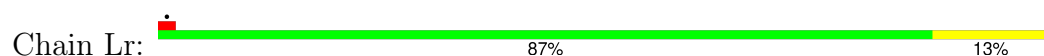
Chain Lo:  83% 17%



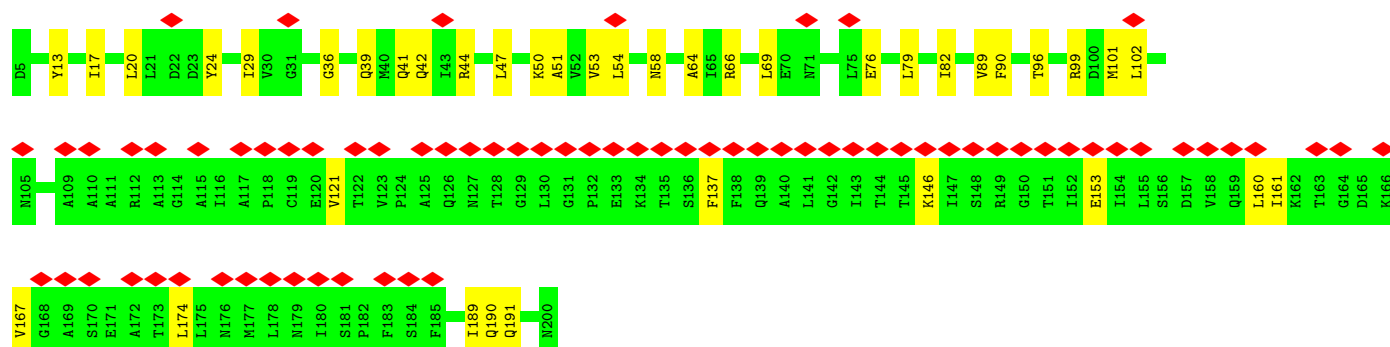
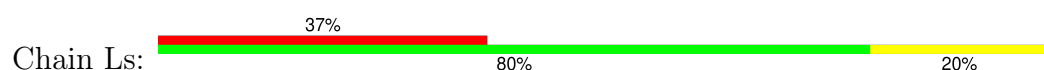
- Molecule 80: 60S ribosomal protein L37a



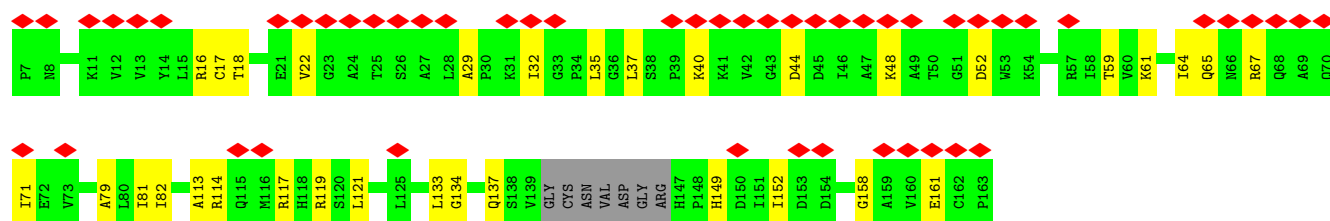
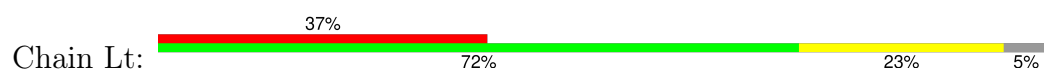
- Molecule 81: 60S ribosomal protein L28



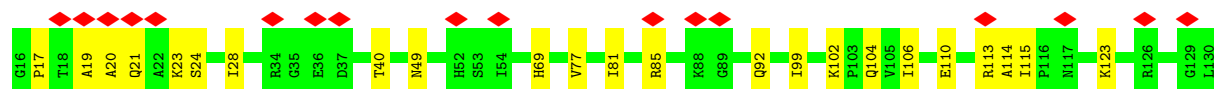
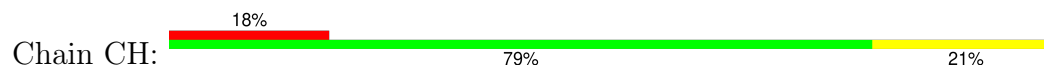
- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: Large ribosomal subunit protein uL11



- Molecule 84: Endothelial differentiation-related factor 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36954	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)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0126	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: OMC, B8N, A2M, MG, SPD, 5MC, UR3, G7M, 6MZ, PSU, OMU, UY1, MA6, SPM, 1MA, 4AC, ZN, OMG

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	AP	0.15	0/1692	0.24	0/2634
2	PE	0.21	0/1778	0.31	0/2767
3	SD	0.19	0/1793	0.31	0/2414
4	SF	0.19	0/1516	0.38	0/2037
5	SK	0.20	0/851	0.42	0/1147
6	SM	0.15	0/950	0.39	0/1275
7	SP	0.18	0/1065	0.31	0/1423
8	SQ	0.18	0/1160	0.37	0/1553
9	SR	0.25	0/1105	0.50	0/1484
10	SS	0.19	0/1216	0.36	0/1628
11	ST	0.18	0/1131	0.32	0/1515
12	SU	0.19	0/831	0.40	0/1115
13	SZ	0.19	0/604	0.38	0/810
14	Sc	0.19	0/508	0.34	0/680
15	Sd	0.21	0/470	0.32	0/623
16	Sf	0.19	0/560	0.44	0/745
17	Sg	0.16	0/2493	0.40	0/3394
18	SA	0.22	0/1778	0.36	0/2416
19	SB	0.21	0/1765	0.38	0/2362
20	SC	0.23	0/1744	0.39	0/2357
21	SE	0.18	0/2118	0.36	0/2849
22	SG	0.16	0/1946	0.32	0/2590
23	SH	0.17	0/1519	0.37	0/2033
24	SI	0.19	0/1715	0.36	0/2287
25	SJ	0.16	0/1550	0.32	0/2069
26	SL	0.20	0/1268	0.30	0/1696
27	SN	0.21	0/1232	0.32	0/1656
28	SO	0.24	0/1037	0.41	0/1391
29	SV	0.18	0/643	0.30	0/860
30	SW	0.23	0/1051	0.37	0/1406
31	SX	0.22	0/1116	0.39	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SY	0.17	0/1083	0.36	0/1438
33	Sa	0.25	0/836	0.39	0/1121
34	Sb	0.19	0/665	0.32	0/891
35	S2	0.25	0/39756	0.28	0/61939
36	LR	0.29	0/1582	0.40	0/2091
37	LW	0.23	0/959	0.31	0/1270
38	CI	0.16	0/247	0.27	0/323
39	L5	0.34	0/85098	0.32	0/132762
40	L7	0.33	0/2861	0.27	0/4459
41	L8	0.34	0/3631	0.29	0/5657
42	LA	0.34	0/1936	0.44	0/2596
43	LB	0.31	0/3306	0.40	0/4424
44	LC	0.32	0/2981	0.38	0/4002
45	LD	0.26	0/2428	0.35	0/3252
46	LE	0.25	0/1973	0.40	0/2645
47	LF	0.32	0/1905	0.34	0/2539
48	LG	0.26	0/1960	0.37	0/2637
49	LH	0.27	0/1537	0.38	0/2066
50	LI	0.28	0/1751	0.32	0/2340
51	LJ	0.24	0/1385	0.39	0/1852
52	LL	0.27	0/1732	0.34	0/2315
53	LM	0.29	0/1161	0.39	0/1554
54	LN	0.33	0/1746	0.36	0/2338
55	LO	0.32	0/1682	0.37	0/2250
56	LP	0.33	0/1268	0.43	0/1701
57	LQ	0.32	0/1537	0.37	0/2052
58	LS	0.31	0/1493	0.36	0/2003
59	LT	0.29	0/1326	0.33	0/1770
60	LU	0.25	0/839	0.48	0/1126
61	LV	0.30	0/993	0.39	0/1332
62	LX	0.28	0/1002	0.34	0/1345
63	LY	0.28	0/1132	0.36	0/1504
64	LZ	0.27	0/1130	0.34	0/1507
65	La	0.31	0/1191	0.34	0/1591
66	Lb	0.24	0/889	0.41	0/1175
67	Lc	0.27	0/774	0.39	0/1038
68	Ld	0.30	0/903	0.38	0/1216
69	Le	0.34	0/1071	0.36	0/1429
70	Lf	0.33	0/895	0.37	0/1198
71	Lg	0.30	0/916	0.35	0/1220
72	Lh	0.27	0/1023	0.38	0/1351
73	Li	0.24	0/843	0.32	0/1115
74	Lj	0.34	0/720	0.42	0/952

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lk	0.24	0/575	0.34	0/761
76	Ll	0.30	0/454	0.28	0/599
77	Lm	0.27	0/435	0.35	0/575
78	Ln	0.23	0/231	0.32	0/294
79	Lo	0.30	0/876	0.34	0/1156
80	Lp	0.30	0/718	0.38	0/953
81	Lr	0.31	0/1017	0.36	0/1364
82	Ls	0.14	0/1519	0.38	0/2052
83	Lt	0.16	0/1009	0.45	0/1363
84	CH	0.16	0/1028	0.40	0/1376
All	All	0.29	0/232213	0.33	0/340585

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
9	SR	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	SR	81	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	AP	1514	0	770	22	0
2	PE	1593	0	810	23	0
3	SD	1765	0	1865	28	0
4	SF	1495	0	1549	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	SK	827	0	854	14	0
6	SM	940	0	965	11	0
7	SP	1045	0	1095	20	0
8	SQ	1142	0	1213	21	0
9	SR	1090	0	1149	21	0
10	SS	1198	0	1261	29	0
11	ST	1112	0	1146	18	0
12	SU	821	0	883	18	0
13	SZ	598	0	656	17	0
14	Sc	506	0	536	8	0
15	Sd	459	0	452	5	0
16	Sf	548	0	551	9	0
17	Sg	2436	0	2393	55	0
18	SA	1741	0	1746	26	0
19	SB	1738	0	1809	25	0
20	SC	1707	0	1791	23	0
21	SE	2076	0	2177	52	0
22	SG	1923	0	2089	41	0
23	SH	1497	0	1590	36	0
24	SI	1686	0	1772	31	0
25	SJ	1525	0	1640	25	0
26	SL	1247	0	1323	18	0
27	SN	1208	0	1294	19	0
28	SO	1024	0	1050	16	0
29	SV	636	0	637	11	0
30	SW	1034	0	1080	19	0
31	SX	1098	0	1167	16	0
32	SY	1065	0	1142	20	0
33	Sa	821	0	870	14	0
34	Sb	651	0	672	14	0
35	S2	36952	0	18678	412	0
36	LR	1566	0	1729	13	0
37	LW	945	0	1003	15	0
38	CI	247	0	283	2	0
39	L5	78444	0	39719	673	0
40	L7	2561	0	1295	13	0
41	L8	3315	0	1685	23	0
42	LA	1898	0	1993	41	0
43	LB	3238	0	3376	61	0
44	LC	2927	0	3104	37	0
45	LD	2382	0	2410	33	0
46	LE	1935	0	2096	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	LF	1870	0	1996	19	0
48	LG	1927	0	2074	19	0
49	LH	1518	0	1601	20	0
50	LI	1711	0	1749	22	0
51	LJ	1362	0	1399	15	0
52	LL	1701	0	1818	20	0
53	LM	1138	0	1204	16	0
54	LN	1701	0	1749	19	0
55	LO	1650	0	1794	29	0
56	LP	1242	0	1269	15	0
57	LQ	1513	0	1628	14	0
58	LS	1453	0	1490	12	0
59	LT	1298	0	1366	16	0
60	LU	825	0	850	13	0
61	LV	979	0	1039	9	0
62	LX	985	0	1066	8	0
63	LY	1115	0	1205	14	0
64	LZ	1107	0	1182	11	0
65	La	1162	0	1213	9	0
66	Lb	876	0	948	10	0
67	Lc	764	0	804	13	0
68	Ld	888	0	930	11	0
69	Le	1053	0	1147	9	0
70	Lf	876	0	912	3	0
71	Lg	906	0	998	6	0
72	Lh	1015	0	1148	14	0
73	Li	832	0	917	5	0
74	Lj	705	0	737	9	0
75	Lk	569	0	637	8	0
76	Ll	444	0	483	7	0
77	Lm	429	0	465	4	0
78	Ln	230	0	276	3	0
79	Lo	862	0	929	12	0
80	Lp	708	0	756	7	0
81	Lr	1002	0	1068	10	0
82	Ls	1496	0	1540	26	0
83	Lt	998	0	1032	25	0
84	CH	1018	0	1064	20	0
85	L5	178	0	0	0	0
85	L7	3	0	0	0	0
85	L8	4	0	0	0	0
85	LA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	LB	1	0	0	0	0
85	LI	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	25	0	0	0	0
85	SG	1	0	0	0	0
85	SS	1	0	0	0	0
86	Lg	1	0	0	0	0
86	Lj	1	0	0	0	0
86	Lm	1	0	0	0	0
86	Lo	1	0	0	0	0
86	Lp	1	0	0	0	0
86	Sa	1	0	0	0	0
87	L5	98	0	182	5	0
88	L5	80	0	152	3	0
88	L8	10	0	19	0	0
88	LN	10	0	19	0	0
All	All	220526	0	164223	2225	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 6.

The worst 5 of 2225 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)
39:L5:1095:A:H2	39:L5:1200:G:N1	1.45	1.15
39:L5:1095:A:C2	39:L5:1200:G:N1	2.19	1.05
2:PE:26:A:H61	2:PE:44:G:H1	1.06	0.91
39:L5:1100:U:H3	39:L5:1194:G:H1	1.23	0.87
35:S2:1815:A:H8	39:L5:3806:G:H21	1.21	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	SD	225/454 (50%)	219 (97%)	6 (3%)	0	100	100
4	SF	187/189 (99%)	168 (90%)	18 (10%)	1 (0%)	24	58
5	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
6	SM	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
7	SP	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
8	SQ	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
9	SR	133/135 (98%)	126 (95%)	5 (4%)	2 (2%)	8	33
10	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
11	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
12	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
13	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
14	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
15	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
16	Sf	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
17	Sg	311/313 (99%)	287 (92%)	24 (8%)	0	100	100
18	SA	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
19	SB	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
20	SC	218/222 (98%)	204 (94%)	14 (6%)	0	100	100
21	SE	260/262 (99%)	246 (95%)	14 (5%)	0	100	100
22	SG	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
23	SH	182/186 (98%)	168 (92%)	14 (8%)	0	100	100
24	SI	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
25	SJ	183/185 (99%)	178 (97%)	5 (3%)	0	100	100
26	SL	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
27	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
28	SO	135/140 (96%)	128 (95%)	6 (4%)	1 (1%)	18	50
29	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
30	SW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
31	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
32	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Sa	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
34	Sb	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
36	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
37	LW	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
38	CI	29/31 (94%)	29 (100%)	0	0	100	100
42	LA	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
43	LB	400/402 (100%)	382 (96%)	18 (4%)	0	100	100
44	LC	366/368 (100%)	350 (96%)	16 (4%)	0	100	100
45	LD	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
46	LE	236/250 (94%)	221 (94%)	15 (6%)	0	100	100
47	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
48	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
49	LH	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
50	LI	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
51	LJ	168/176 (96%)	159 (95%)	8 (5%)	1 (1%)	21	53
52	LL	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
53	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
54	LN	201/203 (99%)	199 (99%)	2 (1%)	0	100	100
55	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
56	LP	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
57	LQ	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
58	LS	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
59	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
60	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
61	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
62	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
63	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
64	LZ	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
65	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
66	Lb	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
67	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	Ld	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
69	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
70	Lf	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
71	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
72	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
73	Li	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
74	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
75	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
76	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
77	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
78	Ln	22/24 (92%)	22 (100%)	0	0	100	100
79	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
80	Lp	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
81	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
82	Ls	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
83	Lt	128/141 (91%)	110 (86%)	18 (14%)	0	100	100
84	CH	130/132 (98%)	108 (83%)	21 (16%)	1 (1%)	16	47
All	All	11752/12177 (96%)	11226 (96%)	520 (4%)	6 (0%)	49	78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	SF	136	ARG
84	CH	114	ALA
9	SR	84	TYR
51	LJ	31	ASP
9	SR	129	LYS

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	
3	SD	190/380 (50%)	190 (100%)	0	100	100
4	SF	159/159 (100%)	159 (100%)	0	100	100
5	SK	89/89 (100%)	89 (100%)	0	100	100
6	SM	102/104 (98%)	102 (100%)	0	100	100
7	SP	113/113 (100%)	113 (100%)	0	100	100
8	SQ	119/119 (100%)	119 (100%)	0	100	100
9	SR	122/122 (100%)	121 (99%)	1 (1%)	73	86
10	SS	126/126 (100%)	126 (100%)	0	100	100
11	ST	113/113 (100%)	113 (100%)	0	100	100
12	SU	94/94 (100%)	94 (100%)	0	100	100
13	SZ	66/66 (100%)	66 (100%)	0	100	100
14	Sc	57/57 (100%)	57 (100%)	0	100	100
15	Sd	48/48 (100%)	48 (100%)	0	100	100
16	Sf	60/60 (100%)	60 (100%)	0	100	100
17	Sg	272/272 (100%)	272 (100%)	0	100	100
18	SA	183/183 (100%)	183 (100%)	0	100	100
19	SB	195/195 (100%)	195 (100%)	0	100	100
20	SC	186/188 (99%)	186 (100%)	0	100	100
21	SE	224/224 (100%)	224 (100%)	0	100	100
22	SG	207/207 (100%)	207 (100%)	0	100	100
23	SH	166/166 (100%)	166 (100%)	0	100	100
24	SI	178/178 (100%)	178 (100%)	0	100	100
25	SJ	161/161 (100%)	161 (100%)	0	100	100
26	SL	137/137 (100%)	137 (100%)	0	100	100
27	SN	130/130 (100%)	130 (100%)	0	100	100
28	SO	107/110 (97%)	107 (100%)	0	100	100
29	SV	67/67 (100%)	67 (100%)	0	100	100
30	SW	112/112 (100%)	112 (100%)	0	100	100
31	SX	113/113 (100%)	113 (100%)	0	100	100
32	SY	113/113 (100%)	113 (100%)	0	100	100
33	Sa	89/89 (100%)	89 (100%)	0	100	100
34	Sb	75/75 (100%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	LR	166/166 (100%)	166 (100%)	0	100	100
37	LW	95/97 (98%)	95 (100%)	0	100	100
38	CI	25/25 (100%)	25 (100%)	0	100	100
42	LA	190/190 (100%)	190 (100%)	0	100	100
43	LB	348/348 (100%)	348 (100%)	0	100	100
44	LC	306/306 (100%)	306 (100%)	0	100	100
45	LD	246/247 (100%)	246 (100%)	0	100	100
46	LE	212/222 (96%)	212 (100%)	0	100	100
47	LF	194/194 (100%)	194 (100%)	0	100	100
48	LG	203/205 (99%)	203 (100%)	0	100	100
49	LH	169/169 (100%)	169 (100%)	0	100	100
50	LI	180/180 (100%)	180 (100%)	0	100	100
51	LJ	143/148 (97%)	143 (100%)	0	100	100
52	LL	176/176 (100%)	176 (100%)	0	100	100
53	LM	118/118 (100%)	118 (100%)	0	100	100
54	LN	171/171 (100%)	171 (100%)	0	100	100
55	LO	173/173 (100%)	173 (100%)	0	100	100
56	LP	134/134 (100%)	134 (100%)	0	100	100
57	LQ	164/164 (100%)	164 (100%)	0	100	100
58	LS	156/156 (100%)	156 (100%)	0	100	100
59	LT	139/139 (100%)	139 (100%)	0	100	100
60	LU	91/91 (100%)	91 (100%)	0	100	100
61	LV	101/101 (100%)	101 (100%)	0	100	100
62	LX	108/108 (100%)	108 (100%)	0	100	100
63	LY	124/124 (100%)	124 (100%)	0	100	100
64	LZ	117/117 (100%)	117 (100%)	0	100	100
65	La	120/120 (100%)	120 (100%)	0	100	100
66	Lb	88/90 (98%)	88 (100%)	0	100	100
67	Lc	83/83 (100%)	83 (100%)	0	100	100
68	Ld	98/98 (100%)	98 (100%)	0	100	100
69	Le	114/114 (100%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	Lf	88/88 (100%)	88 (100%)	0	100	100
71	Lg	98/98 (100%)	98 (100%)	0	100	100
72	Lh	109/109 (100%)	109 (100%)	0	100	100
73	Li	86/86 (100%)	86 (100%)	0	100	100
74	Lj	73/73 (100%)	73 (100%)	0	100	100
75	Lk	64/64 (100%)	64 (100%)	0	100	100
76	Ll	47/47 (100%)	47 (100%)	0	100	100
77	Lm	48/48 (100%)	48 (100%)	0	100	100
78	Ln	23/23 (100%)	23 (100%)	0	100	100
79	Lo	93/93 (100%)	93 (100%)	0	100	100
80	Lp	74/74 (100%)	74 (100%)	0	100	100
81	Lr	109/109 (100%)	109 (100%)	0	100	100
82	Ls	162/164 (99%)	162 (100%)	0	100	100
83	Lt	107/115 (93%)	107 (100%)	0	100	100
84	CH	106/106 (100%)	106 (100%)	0	100	100
All	All	10212/10441 (98%)	10211 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	SR	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
50	LI	92	HIS
65	La	60	HIS
53	LM	34	ASN
56	LP	97	ASN
67	Lc	72	HIS

5.3.3 RNA [i](#)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AP	69/142 (48%)	11 (15%)	0
2	PE	74/150 (49%)	21 (28%)	1 (1%)
35	S2	1715/1740 (98%)	374 (21%)	3 (0%)
39	L5	3643/3655 (99%)	729 (20%)	15 (0%)
40	L7	119/120 (99%)	10 (8%)	0
41	L8	155/156 (99%)	24 (15%)	0
All	All	5775/5963 (96%)	1169 (20%)	19 (0%)

5 of 1169 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AP	8	U
1	AP	9	A
1	AP	11	U
1	AP	13	U
1	AP	14	A

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	L5	2760	G
39	L5	4699	U
39	L5	4913	G
39	L5	4600	G
39	L5	1633	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	$\# Z > 2$
35	PSU	S2	681	35	18,21,22	1.04	1 (5%)	21,30,33	1.94	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	PSU	L8	55	41	18,21,22	1.04	1 (5%)	21,30,33	1.86	4 (19%)
35	OMC	S2	517	35	19,22,23	0.56	0	25,31,34	0.67	0
35	OMU	S2	116	35	19,22,23	3.30	7 (36%)	25,31,34	1.68	4 (16%)
39	PSU	L5	3920	39,85	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
35	OMG	S2	867	35	23,26,27	0.51	0	32,38,41	0.47	0
39	PSU	L5	3639	39	18,21,22	1.13	2 (11%)	21,30,33	2.05	4 (19%)
39	OMG	L5	4370	39	23,26,27	0.61	0	32,38,41	0.54	0
35	PSU	S2	1367	35	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
39	OMG	L5	1316	39	23,26,27	0.69	0	32,38,41	0.56	0
39	A2M	L5	398	39	22,25,26	1.18	1 (4%)	30,36,39	1.67	7 (23%)
39	A2M	L5	1534	39,85	22,25,26	1.20	2 (9%)	30,36,39	1.42	7 (23%)
39	PSU	L5	1744	39,85	18,21,22	1.06	2 (11%)	21,30,33	1.95	4 (19%)
39	PSU	L5	4296	39	18,21,22	1.09	1 (5%)	21,30,33	1.98	4 (19%)
35	OMC	S2	1391	35	19,22,23	0.58	0	25,31,34	0.63	0
39	PSU	L5	3637	39	18,21,22	1.06	2 (11%)	21,30,33	2.00	5 (23%)
39	OMG	L5	3744	39	23,26,27	0.60	0	32,38,41	0.47	0
39	OMC	L5	4536	39	19,22,23	0.69	0	25,31,34	0.72	0
39	OMC	L5	3869	39	19,22,23	0.67	0	25,31,34	0.70	0
39	OMC	L5	4456	39	19,22,23	0.76	1 (5%)	25,31,34	0.77	0
35	A2M	S2	27	35	22,25,26	1.21	1 (4%)	30,36,39	1.52	8 (26%)
39	PSU	L5	1677	39	18,21,22	1.13	3 (16%)	21,30,33	2.13	5 (23%)
35	OMU	S2	428	35	19,22,23	3.31	7 (36%)	25,31,34	1.84	5 (20%)
39	PSU	L5	1781	39	18,21,22	1.05	1 (5%)	21,30,33	1.85	4 (19%)
39	A2M	L5	2815	39	22,25,26	1.19	2 (9%)	30,36,39	1.53	9 (30%)
35	OMG	S2	601	35	23,26,27	0.52	0	32,38,41	0.41	0
35	PSU	S2	814	35	18,21,22	1.07	1 (5%)	21,30,33	1.81	4 (19%)
39	PSU	L5	3822	39	18,21,22	1.01	1 (5%)	21,30,33	1.98	5 (23%)
39	PSU	L5	3844	39	18,21,22	1.08	2 (11%)	21,30,33	1.91	4 (19%)
39	A2M	L5	3867	39	22,25,26	1.37	3 (13%)	30,36,39	1.52	8 (26%)
39	PSU	L5	4493	39	18,21,22	1.04	1 (5%)	21,30,33	1.91	4 (19%)
39	PSU	L5	1683	39	18,21,22	1.06	2 (11%)	21,30,33	2.00	4 (19%)
39	PSU	L5	4579	39	18,21,22	1.06	2 (11%)	21,30,33	1.91	4 (19%)
39	PSU	L5	4471	39	18,21,22	1.05	2 (11%)	21,30,33	1.95	4 (19%)
35	PSU	S2	93	35	18,21,22	1.05	1 (5%)	21,30,33	1.76	4 (19%)
39	OMC	L5	2351	39,85	19,22,23	0.74	1 (5%)	25,31,34	0.88	1 (4%)
39	PSU	L5	4299	39	18,21,22	1.04	1 (5%)	21,30,33	1.94	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	A2M	L5	4523	39,85	22,25,26	1.27	3 (13%)	30,36,39	1.57	8 (26%)
39	A2M	L5	1524	39	22,25,26	1.31	3 (13%)	30,36,39	1.52	6 (20%)
39	OMG	L5	4196	39	23,26,27	0.60	0	32,38,41	0.42	0
35	PSU	S2	1232	35	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
35	MA6	S2	1850	35	23,26,27	2.68	9 (39%)	33,38,41	3.34	13 (39%)
39	6MZ	L5	4220	39	22,25,26	2.89	6 (27%)	29,36,39	2.46	10 (34%)
39	PSU	L5	4500	39	18,21,22	1.09	2 (11%)	21,30,33	2.04	6 (28%)
35	A2M	S2	576	35	22,25,26	1.20	1 (4%)	30,36,39	1.54	5 (16%)
35	PSU	S2	863	35	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
35	PSU	S2	1056	35	18,21,22	1.06	2 (11%)	21,30,33	2.01	5 (23%)
39	OMG	L5	4623	39	23,26,27	0.61	0	32,38,41	0.60	0
39	PSU	L5	4552	39	18,21,22	1.08	2 (11%)	21,30,33	2.01	4 (19%)
39	PSU	L5	4442	39	18,21,22	1.04	2 (11%)	21,30,33	2.07	6 (28%)
39	OMG	L5	4637	39	23,26,27	0.60	0	32,38,41	0.48	0
39	PSU	L5	4689	39	18,21,22	1.03	2 (11%)	21,30,33	1.97	4 (19%)
35	OMC	S2	174	35	19,22,23	0.57	0	25,31,34	0.79	1 (4%)
35	PSU	S2	1045	35	18,21,22	1.07	1 (5%)	21,30,33	1.95	4 (19%)
39	A2M	L5	3830	39	22,25,26	1.21	2 (9%)	30,36,39	1.58	6 (20%)
39	OMC	L5	3841	39	19,22,23	0.67	0	25,31,34	0.67	0
39	PSU	L5	4532	39	18,21,22	1.09	2 (11%)	21,30,33	1.95	4 (19%)
35	PSU	S2	109	35	18,21,22	1.11	2 (11%)	21,30,33	2.04	6 (28%)
39	PSU	L5	4636	39	18,21,22	1.08	2 (11%)	21,30,33	2.10	6 (28%)
39	UR3	L5	4530	39	19,22,23	2.61	7 (36%)	26,32,35	1.66	3 (11%)
35	OMU	S2	172	35	19,22,23	3.31	7 (36%)	25,31,34	1.83	5 (20%)
39	OMG	L5	3899	39	23,26,27	0.66	0	32,38,41	0.54	0
39	5MC	L5	3782	39,85	19,22,23	0.77	0	26,32,35	0.77	1 (3%)
35	PSU	S2	105	35	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
39	PSU	L5	4293	39	18,21,22	1.08	2 (11%)	21,30,33	2.07	4 (19%)
39	PSU	L5	4353	39	18,21,22	1.09	2 (11%)	21,30,33	2.04	6 (28%)
35	PSU	S2	801	35	18,21,22	1.12	1 (5%)	21,30,33	1.79	4 (19%)
39	OMC	L5	2365	39,85	19,22,23	0.66	0	25,31,34	0.59	0
39	1MA	L5	1322	39,85	21,25,26	0.67	0	30,37,40	0.83	2 (6%)
35	OMU	S2	1288	35	19,22,23	3.35	7 (36%)	25,31,34	1.76	5 (20%)
39	A2M	L5	1323	39	22,25,26	1.27	2 (9%)	30,36,39	1.60	9 (30%)
39	A2M	L5	2401	39	22,25,26	1.24	2 (9%)	30,36,39	1.61	8 (26%)
35	PSU	S2	1046	35	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	L5	5001	39	18,21,22	1.05	1 (5%)	21,30,33	1.92	4 (19%)
35	OMC	S2	462	35	19,22,23	0.60	0	25,31,34	0.78	0
39	PSU	L5	1782	39	18,21,22	1.07	1 (5%)	21,30,33	1.97	4 (19%)
39	OMG	L5	4228	39	23,26,27	0.59	0	32,38,41	0.60	0
39	OMG	L5	3792	39	23,26,27	0.60	0	32,38,41	0.49	0
39	PSU	L5	3884	39	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
35	PSU	S2	1081	35	18,21,22	1.03	1 (5%)	21,30,33	1.81	4 (19%)
39	A2M	L5	2787	39	22,25,26	1.19	1 (4%)	30,36,39	1.53	8 (26%)
39	OMG	L5	3627	39	23,26,27	0.59	0	32,38,41	0.59	0
35	OMG	S2	1328	35	23,26,27	0.51	0	32,38,41	0.45	0
35	OMG	S2	509	35	23,26,27	0.51	0	32,38,41	0.51	0
39	PSU	L5	1862	39	18,21,22	1.08	1 (5%)	21,30,33	2.01	4 (19%)
39	PSU	L5	1792	39	18,21,22	1.07	2 (11%)	21,30,33	1.92	4 (19%)
35	MA6	S2	1851	35	23,26,27	1.30	2 (8%)	33,38,41	3.41	12 (36%)
39	OMC	L5	3701	39	19,22,23	0.75	1 (5%)	25,31,34	1.83	4 (16%)
39	OMU	L5	4306	39	19,22,23	3.22	7 (36%)	25,31,34	1.89	4 (16%)
39	PSU	L5	4361	39	18,21,22	1.01	1 (5%)	21,30,33	1.81	4 (19%)
39	PSU	L5	3853	39,85	18,21,22	1.02	1 (5%)	21,30,33	1.90	4 (19%)
39	OMU	L5	4498	39	19,22,23	3.21	7 (36%)	25,31,34	1.93	5 (20%)
39	A2M	L5	4571	39	22,25,26	1.32	3 (13%)	30,36,39	1.60	8 (26%)
39	PSU	L5	4576	39	18,21,22	1.02	1 (5%)	21,30,33	1.93	4 (19%)
39	PSU	L5	4673	39,85	18,21,22	1.08	2 (11%)	21,30,33	1.97	4 (19%)
39	PSU	L5	4972	39	18,21,22	1.07	2 (11%)	21,30,33	1.92	4 (19%)
35	OMG	S2	1490	35	23,26,27	0.56	0	32,38,41	0.47	0
39	OMG	L5	1625	39	23,26,27	0.59	0	32,38,41	0.46	0
35	PSU	S2	1177	35	18,21,22	1.03	2 (11%)	21,30,33	1.97	4 (19%)
35	OMU	S2	1442	35	19,22,23	3.31	7 (36%)	25,31,34	1.80	5 (20%)
39	A2M	L5	1871	39,85	22,25,26	1.35	3 (13%)	30,36,39	1.64	7 (23%)
39	A2M	L5	400	39	22,25,26	1.30	3 (13%)	30,36,39	1.55	8 (26%)
35	A2M	S2	166	35	22,25,26	1.24	1 (4%)	30,36,39	1.62	7 (23%)
39	OMC	L5	2824	39	19,22,23	0.63	0	25,31,34	0.66	0
39	PSU	L5	4628	39	18,21,22	1.05	2 (11%)	21,30,33	2.03	4 (19%)
35	OMU	S2	354	35	19,22,23	3.27	7 (36%)	25,31,34	1.92	5 (20%)
41	PSU	L8	69	41	18,21,22	1.09	2 (11%)	21,30,33	2.04	6 (28%)
35	A2M	S2	99	35,85	22,25,26	1.17	1 (4%)	30,36,39	1.57	7 (23%)
39	A2M	L5	3825	39	22,25,26	1.20	2 (9%)	30,36,39	1.59	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	A2M	L5	3785	39,85	22,25,26	1.23	1 (4%)	30,36,39	1.65	10 (33%)
39	OMG	L5	2876	39	23,26,27	0.58	0	32,38,41	0.52	0
39	A2M	L5	3718	39	22,25,26	1.18	2 (9%)	30,36,39	1.57	8 (26%)
39	OMC	L5	2422	39,85	19,22,23	0.66	0	25,31,34	0.73	1 (4%)
39	A2M	L5	4590	39	22,25,26	1.24	2 (9%)	30,36,39	1.58	5 (16%)
39	OMG	L5	4618	39	23,26,27	0.61	0	32,38,41	0.52	0
39	PSU	L5	4973	39	18,21,22	1.04	2 (11%)	21,30,33	1.99	5 (23%)
35	6MZ	S2	1832	35,85	22,25,26	4.04	11 (50%)	29,36,39	2.33	9 (31%)
35	A2M	S2	484	35	22,25,26	1.18	1 (4%)	30,36,39	1.47	8 (26%)
39	PSU	L5	3851	39	18,21,22	1.08	1 (5%)	21,30,33	1.97	4 (19%)
39	PSU	L5	4457	39	18,21,22	1.03	2 (11%)	21,30,33	2.03	5 (23%)
35	OMG	S2	683	35	23,26,27	0.55	0	32,38,41	0.46	0
39	OMC	L5	3808	39	19,22,23	0.72	0	25,31,34	0.88	2 (8%)
35	PSU	S2	686	35	18,21,22	1.07	1 (5%)	21,30,33	1.97	5 (23%)
41	OMG	L8	75	41	23,26,27	0.56	0	32,38,41	0.53	0
39	UY1	L5	3818	39	19,22,23	4.79	9 (47%)	21,31,34	2.00	5 (23%)
39	OMU	L5	2837	39	19,22,23	3.26	7 (36%)	25,31,34	1.91	5 (20%)
39	PSU	L5	4431	39	18,21,22	1.04	2 (11%)	21,30,33	1.95	4 (19%)
35	OMG	S2	644	35	23,26,27	0.50	0	32,38,41	0.46	0
39	PSU	L5	4312	39	18,21,22	1.08	2 (11%)	21,30,33	1.91	4 (19%)
35	A2M	S2	1383	35	22,25,26	1.16	1 (4%)	30,36,39	1.64	8 (26%)
39	OMG	L5	4499	39	23,26,27	0.58	0	32,38,41	0.47	0
35	B8N	S2	1248	35	25,29,30	3.24	7 (28%)	28,42,45	2.01	8 (28%)
39	PSU	L5	1536	39	18,21,22	1.06	2 (11%)	21,30,33	1.93	4 (19%)
35	PSU	S2	1244	35	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
39	OMC	L5	2861	39	19,22,23	0.68	0	25,31,34	0.81	1 (4%)
39	PSU	L5	3695	39	18,21,22	1.04	2 (11%)	21,30,33	1.97	4 (19%)
39	PSU	L5	4521	39,85	18,21,22	1.08	2 (11%)	21,30,33	1.99	5 (23%)
39	5MC	L5	4447	39	19,22,23	0.97	1 (5%)	26,32,35	0.69	0
35	OMU	S2	627	35	19,22,23	3.36	7 (36%)	25,31,34	1.79	4 (16%)
35	PSU	S2	406	35	18,21,22	1.07	2 (11%)	21,30,33	2.02	5 (23%)
39	OMU	L5	4620	39	19,22,23	3.13	7 (36%)	25,31,34	1.72	5 (20%)
35	4AC	S2	1337	35	21,24,25	0.42	0	28,34,37	0.79	2 (7%)
35	PSU	S2	1004	35	18,21,22	1.09	2 (11%)	21,30,33	1.95	4 (19%)
39	OMC	L5	3887	39	19,22,23	0.67	0	25,31,34	0.66	0
35	PSU	S2	649	35	18,21,22	1.10	1 (5%)	21,30,33	1.96	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	L5	1860	39	18,21,22	1.07	2 (11%)	21,30,33	1.96	4 (19%)
39	PSU	L5	2839	39	18,21,22	1.07	2 (11%)	21,30,33	2.01	4 (19%)
35	G7M	S2	1639	35,2	23,26,27	2.63	9 (39%)	34,39,42	2.58	11 (32%)
35	PSU	S2	1174	35	18,21,22	1.07	2 (11%)	21,30,33	1.90	4 (19%)
39	OMG	L5	4392	39	23,26,27	0.64	0	32,38,41	0.48	0
35	OMU	S2	799	35	19,22,23	3.39	7 (36%)	25,31,34	1.83	5 (20%)
39	OMG	L5	2364	39,85	23,26,27	0.62	0	32,38,41	0.45	0
35	OMG	S2	436	35	23,26,27	0.53	0	32,38,41	0.55	0
39	OMC	L5	2804	39	19,22,23	0.68	0	25,31,34	0.64	0
39	OMG	L5	4494	39	23,26,27	0.60	0	32,38,41	0.48	0
35	OMC	S2	1703	35	19,22,23	0.64	0	25,31,34	0.69	0
35	PSU	S2	966	35,85	18,21,22	1.07	1 (5%)	21,30,33	1.98	4 (19%)
39	OMG	L5	2424	39	23,26,27	0.61	0	32,38,41	0.41	0
39	OMC	L5	1340	39	19,22,23	0.71	0	25,31,34	0.78	0
35	OMU	S2	121	35	19,22,23	3.32	7 (36%)	25,31,34	1.85	5 (20%)
35	A2M	S2	668	35,85	22,25,26	1.31	2 (9%)	30,36,39	1.67	8 (26%)
35	OMC	S2	1272	35	19,22,23	0.62	0	25,31,34	0.84	1 (4%)
35	OMU	S2	1326	35	19,22,23	3.28	7 (36%)	25,31,34	1.88	5 (20%)
35	PSU	S2	651	35	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
39	OMU	L5	3925	39	19,22,23	3.19	7 (36%)	25,31,34	1.92	5 (20%)
35	A2M	S2	1031	35	22,25,26	1.15	1 (4%)	30,36,39	1.56	7 (23%)
39	OMU	L5	4227	39	19,22,23	3.20	7 (36%)	25,31,34	1.85	4 (16%)
35	A2M	S2	159	35	22,25,26	1.18	1 (4%)	30,36,39	1.51	8 (26%)
39	PSU	L5	4403	39	18,21,22	1.05	2 (11%)	21,30,33	2.09	6 (28%)
39	A2M	L5	2363	39,85	22,25,26	1.25	2 (9%)	30,36,39	1.56	9 (30%)
39	PSU	L5	5010	39	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
35	A2M	S2	468	35	22,25,26	1.24	1 (4%)	30,36,39	1.58	7 (23%)
35	4AC	S2	1842	35	21,24,25	0.40	0	28,34,37	0.46	0
39	PSU	L5	1582	39	18,21,22	1.04	1 (5%)	21,30,33	1.82	4 (19%)
39	OMG	L5	1522	39	23,26,27	0.63	0	32,38,41	0.65	1 (3%)
39	PSU	L5	2632	39	18,21,22	1.06	2 (11%)	21,30,33	2.03	5 (23%)
39	A2M	L5	1326	39	22,25,26	1.26	2 (9%)	30,36,39	1.52	9 (30%)
35	PSU	S2	866	35	18,21,22	1.09	2 (11%)	21,30,33	2.01	6 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	S2	681	35	-	0/7/25/26	0/2/2/2
41	PSU	L8	55	41	-	0/7/25/26	0/2/2/2
35	OMC	S2	517	35	-	0/9/27/28	0/2/2/2
35	OMU	S2	116	35	-	0/9/27/28	0/2/2/2
39	PSU	L5	3920	39,85	-	0/7/25/26	0/2/2/2
35	OMG	S2	867	35	-	2/9/27/28	0/3/3/3
39	PSU	L5	3639	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	4370	39	-	0/9/27/28	0/3/3/3
35	PSU	S2	1367	35	-	0/7/25/26	0/2/2/2
39	OMG	L5	1316	39	-	0/9/27/28	0/3/3/3
39	A2M	L5	398	39	-	0/9/27/28	0/3/3/3
39	A2M	L5	1534	39,85	-	1/9/27/28	0/3/3/3
39	PSU	L5	1744	39,85	-	0/7/25/26	0/2/2/2
39	PSU	L5	4296	39	-	2/7/25/26	0/2/2/2
35	OMC	S2	1391	35	-	0/9/27/28	0/2/2/2
39	PSU	L5	3637	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	3744	39	-	0/9/27/28	0/3/3/3
39	OMC	L5	4536	39	-	0/9/27/28	0/2/2/2
39	OMC	L5	3869	39	-	0/9/27/28	0/2/2/2
39	OMC	L5	4456	39	-	0/9/27/28	0/2/2/2
35	A2M	S2	27	35	-	1/9/27/28	0/3/3/3
39	PSU	L5	1677	39	-	1/7/25/26	0/2/2/2
35	OMU	S2	428	35	-	4/9/27/28	0/2/2/2
39	PSU	L5	1781	39	-	1/7/25/26	0/2/2/2
39	A2M	L5	2815	39	-	2/9/27/28	0/3/3/3
35	OMG	S2	601	35	-	1/9/27/28	0/3/3/3
35	PSU	S2	814	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	3822	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	3844	39	-	1/7/25/26	0/2/2/2
39	A2M	L5	3867	39	-	2/9/27/28	0/3/3/3
39	PSU	L5	4493	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	1683	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4579	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4471	39	-	0/7/25/26	0/2/2/2
35	PSU	S2	93	35	-	0/7/25/26	0/2/2/2
39	OMC	L5	2351	39,85	-	1/9/27/28	0/2/2/2
39	PSU	L5	4299	39	-	0/7/25/26	0/2/2/2
39	A2M	L5	4523	39,85	-	0/9/27/28	0/3/3/3
39	A2M	L5	1524	39	-	3/9/27/28	0/3/3/3
39	OMG	L5	4196	39	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	S2	1232	35	-	0/7/25/26	0/2/2/2
35	MA6	S2	1850	35	-	0/11/29/30	0/3/3/3
39	6MZ	L5	4220	39	-	2/9/27/28	0/3/3/3
39	PSU	L5	4500	39	-	3/7/25/26	0/2/2/2
35	A2M	S2	576	35	-	3/9/27/28	0/3/3/3
35	PSU	S2	863	35	-	0/7/25/26	0/2/2/2
35	PSU	S2	1056	35	-	0/7/25/26	0/2/2/2
39	OMG	L5	4623	39	-	0/9/27/28	0/3/3/3
39	PSU	L5	4552	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4442	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	4637	39	-	2/9/27/28	0/3/3/3
39	PSU	L5	4689	39	-	0/7/25/26	0/2/2/2
35	OMC	S2	174	35	-	0/9/27/28	0/2/2/2
35	PSU	S2	1045	35	-	2/7/25/26	0/2/2/2
39	A2M	L5	3830	39	-	0/9/27/28	0/3/3/3
39	OMC	L5	3841	39	-	0/9/27/28	0/2/2/2
39	PSU	L5	4532	39	-	0/7/25/26	0/2/2/2
35	PSU	S2	109	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	4636	39	-	2/7/25/26	0/2/2/2
39	UR3	L5	4530	39	-	0/7/25/26	0/2/2/2
35	OMU	S2	172	35	-	0/9/27/28	0/2/2/2
39	OMG	L5	3899	39	-	3/9/27/28	0/3/3/3
39	5MC	L5	3782	39,85	-	1/7/25/26	0/2/2/2
35	PSU	S2	105	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	4293	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4353	39	-	0/7/25/26	0/2/2/2
35	PSU	S2	801	35	-	2/7/25/26	0/2/2/2
39	OMC	L5	2365	39,85	-	0/9/27/28	0/2/2/2
39	1MA	L5	1322	39,85	-	2/7/25/26	0/3/3/3
35	OMU	S2	1288	35	-	2/9/27/28	0/2/2/2
39	A2M	L5	1323	39	-	2/9/27/28	0/3/3/3
39	A2M	L5	2401	39	-	1/9/27/28	0/3/3/3
35	PSU	S2	1046	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	5001	39	-	0/7/25/26	0/2/2/2
35	OMC	S2	462	35	-	1/9/27/28	0/2/2/2
39	PSU	L5	1782	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	4228	39	-	2/9/27/28	0/3/3/3
39	OMG	L5	3792	39	-	2/9/27/28	0/3/3/3
39	PSU	L5	3884	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	S2	1081	35	-	1/7/25/26	0/2/2/2
39	A2M	L5	2787	39	-	5/9/27/28	0/3/3/3
39	OMG	L5	3627	39	-	0/9/27/28	0/3/3/3
35	OMG	S2	1328	35	-	0/9/27/28	0/3/3/3
35	OMG	S2	509	35	-	0/9/27/28	0/3/3/3
39	PSU	L5	1862	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	1792	39	-	0/7/25/26	0/2/2/2
35	MA6	S2	1851	35	-	1/11/29/30	0/3/3/3
39	OMC	L5	3701	39	-	5/9/27/28	0/2/2/2
39	OMU	L5	4306	39	-	0/9/27/28	0/2/2/2
39	PSU	L5	4361	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	3853	39,85	-	0/7/25/26	0/2/2/2
39	OMU	L5	4498	39	-	0/9/27/28	0/2/2/2
39	A2M	L5	4571	39	-	0/9/27/28	0/3/3/3
39	PSU	L5	4576	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4673	39,85	-	0/7/25/26	0/2/2/2
39	PSU	L5	4972	39	-	0/7/25/26	0/2/2/2
35	OMG	S2	1490	35	-	1/9/27/28	0/3/3/3
39	OMG	L5	1625	39	-	2/9/27/28	0/3/3/3
35	PSU	S2	1177	35	-	0/7/25/26	0/2/2/2
35	OMU	S2	1442	35	-	2/9/27/28	0/2/2/2
39	A2M	L5	1871	39,85	-	0/9/27/28	0/3/3/3
39	A2M	L5	400	39	-	1/9/27/28	0/3/3/3
35	A2M	S2	166	35	-	0/9/27/28	0/3/3/3
39	OMC	L5	2824	39	-	1/9/27/28	0/2/2/2
39	PSU	L5	4628	39	-	0/7/25/26	0/2/2/2
35	OMU	S2	354	35	-	0/9/27/28	0/2/2/2
41	PSU	L8	69	41	-	0/7/25/26	0/2/2/2
35	A2M	S2	99	35,85	-	2/9/27/28	0/3/3/3
39	A2M	L5	3825	39	-	0/9/27/28	0/3/3/3
39	A2M	L5	3785	39,85	-	2/9/27/28	0/3/3/3
39	OMG	L5	2876	39	-	0/9/27/28	0/3/3/3
39	A2M	L5	3718	39	-	0/9/27/28	0/3/3/3
39	OMC	L5	2422	39,85	-	2/9/27/28	0/2/2/2
39	A2M	L5	4590	39	-	3/9/27/28	0/3/3/3
39	OMG	L5	4618	39	-	1/9/27/28	0/3/3/3
39	PSU	L5	4973	39	-	0/7/25/26	0/2/2/2
35	6MZ	S2	1832	35,85	-	2/9/27/28	0/3/3/3
35	A2M	S2	484	35	-	0/9/27/28	0/3/3/3
39	PSU	L5	3851	39	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	L5	4457	39	-	0/7/25/26	0/2/2/2
35	OMG	S2	683	35	-	2/9/27/28	0/3/3/3
39	OMC	L5	3808	39	-	1/9/27/28	0/2/2/2
35	PSU	S2	686	35	-	0/7/25/26	0/2/2/2
41	OMG	L8	75	41	-	1/9/27/28	0/3/3/3
39	UY1	L5	3818	39	-	3/9/27/28	0/2/2/2
39	OMU	L5	2837	39	-	0/9/27/28	0/2/2/2
39	PSU	L5	4431	39	-	0/7/25/26	0/2/2/2
35	OMG	S2	644	35	-	3/9/27/28	0/3/3/3
39	PSU	L5	4312	39	-	0/7/25/26	0/2/2/2
35	A2M	S2	1383	35	-	3/9/27/28	0/3/3/3
39	OMG	L5	4499	39	-	0/9/27/28	0/3/3/3
35	B8N	S2	1248	35	-	1/16/34/35	0/2/2/2
39	PSU	L5	1536	39	-	2/7/25/26	0/2/2/2
35	PSU	S2	1244	35	-	0/7/25/26	0/2/2/2
39	OMC	L5	2861	39	-	0/9/27/28	0/2/2/2
39	PSU	L5	3695	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	4521	39,85	-	0/7/25/26	0/2/2/2
39	5MC	L5	4447	39	-	4/7/25/26	0/2/2/2
35	OMU	S2	627	35	-	6/9/27/28	0/2/2/2
35	PSU	S2	406	35	-	0/7/25/26	0/2/2/2
39	OMU	L5	4620	39	-	0/9/27/28	0/2/2/2
35	4AC	S2	1337	35	-	1/11/29/30	0/2/2/2
35	PSU	S2	1004	35	-	0/7/25/26	0/2/2/2
39	OMC	L5	3887	39	-	1/9/27/28	0/2/2/2
35	PSU	S2	649	35	-	0/7/25/26	0/2/2/2
39	PSU	L5	1860	39	-	0/7/25/26	0/2/2/2
39	PSU	L5	2839	39	-	0/7/25/26	0/2/2/2
35	G7M	S2	1639	35,2	-	1/7/25/26	0/3/3/3
35	PSU	S2	1174	35	-	0/7/25/26	0/2/2/2
39	OMG	L5	4392	39	-	0/9/27/28	0/3/3/3
35	OMU	S2	799	35	-	2/9/27/28	0/2/2/2
39	OMG	L5	2364	39,85	-	3/9/27/28	0/3/3/3
35	OMG	S2	436	35	-	0/9/27/28	0/3/3/3
39	OMC	L5	2804	39	-	0/9/27/28	0/2/2/2
39	OMG	L5	4494	39	-	1/9/27/28	0/3/3/3
35	OMC	S2	1703	35	-	1/9/27/28	0/2/2/2
35	PSU	S2	966	35,85	-	0/7/25/26	0/2/2/2
39	OMG	L5	2424	39	-	0/9/27/28	0/3/3/3
39	OMC	L5	1340	39	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	OMU	S2	121	35	-	0/9/27/28	0/2/2/2
35	A2M	S2	668	35,85	-	3/9/27/28	0/3/3/3
35	OMC	S2	1272	35	-	2/9/27/28	0/2/2/2
35	OMU	S2	1326	35	-	0/9/27/28	0/2/2/2
35	PSU	S2	651	35	-	0/7/25/26	0/2/2/2
39	OMU	L5	3925	39	-	1/9/27/28	0/2/2/2
35	A2M	S2	1031	35	-	1/9/27/28	0/3/3/3
39	OMU	L5	4227	39	-	0/9/27/28	0/2/2/2
35	A2M	S2	159	35	-	1/9/27/28	0/3/3/3
39	PSU	L5	4403	39	-	0/7/25/26	0/2/2/2
39	A2M	L5	2363	39,85	-	0/9/27/28	0/3/3/3
39	PSU	L5	5010	39	-	0/7/25/26	0/2/2/2
35	A2M	S2	468	35	-	0/9/27/28	0/3/3/3
35	4AC	S2	1842	35	-	0/11/29/30	0/2/2/2
39	PSU	L5	1582	39	-	0/7/25/26	0/2/2/2
39	OMG	L5	1522	39	-	0/9/27/28	0/3/3/3
39	PSU	L5	2632	39	-	0/7/25/26	0/2/2/2
39	A2M	L5	1326	39	-	4/9/27/28	0/3/3/3
35	PSU	S2	866	35	-	0/7/25/26	0/2/2/2

The worst 5 of 342 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S2	1832	6MZ	C6-N6	12.85	1.48	1.34
39	L5	3818	UY1	C6-C5	12.42	1.49	1.35
39	L5	4220	6MZ	C6-N6	11.50	1.47	1.34
39	L5	3818	UY1	C2-N1	11.43	1.51	1.36
35	S2	799	OMU	C2-N1	8.53	1.51	1.38

The worst 5 of 700 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S2	1851	MA6	N1-C6-N6	-12.19	102.00	116.86
35	S2	1850	MA6	N1-C6-N6	-11.44	102.91	116.86
35	S2	1851	MA6	C5-C6-N6	8.08	138.12	125.33
35	S2	1850	MA6	C5-C6-N6	7.74	137.59	125.33
35	S2	1639	G7M	C1'-N9-C4	7.42	148.40	126.49

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	L8	75	OMG	C1'-C2'-O2'-CM2
35	S2	27	A2M	C1'-C2'-O2'-CM'
35	S2	159	A2M	C1'-C2'-O2'-CM'
35	S2	462	OMC	C1'-C2'-O2'-CM2
35	S2	601	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

61 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	S2	681	PSU	1	0
35	S2	116	OMU	3	0
39	L5	3920	PSU	1	0
35	S2	867	OMG	1	0
39	L5	1534	A2M	1	0
39	L5	4536	OMC	1	0
39	L5	4456	OMC	1	0
35	S2	27	A2M	2	0
35	S2	428	OMU	2	0
39	L5	1781	PSU	1	0
35	S2	601	OMG	1	0
39	L5	3822	PSU	2	0
39	L5	3867	A2M	3	0
39	L5	1683	PSU	1	0
35	S2	93	PSU	1	0
39	L5	2351	OMC	2	0
39	L5	4523	A2M	1	0
39	L5	4196	OMG	1	0
35	S2	1232	PSU	2	0
35	S2	1850	MA6	2	0
35	S2	576	A2M	2	0
39	L5	4623	OMG	1	0
39	L5	3830	A2M	1	0
39	L5	3782	5MC	1	0
39	L5	4353	PSU	1	0
35	S2	1288	OMU	1	0
35	S2	462	OMC	2	0
35	S2	1328	OMG	1	0
35	S2	509	OMG	1	0
39	L5	3701	OMC	1	0
39	L5	4571	A2M	1	0
39	L5	1871	A2M	1	0
39	L5	400	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	S2	166	A2M	1	0
39	L5	2824	OMC	1	0
35	S2	99	A2M	2	0
39	L5	3718	A2M	2	0
39	L5	2422	OMC	1	0
35	S2	484	A2M	1	0
39	L5	4457	PSU	1	0
39	L5	3808	OMC	1	0
41	L8	75	OMG	2	0
39	L5	3818	UY1	1	0
39	L5	4431	PSU	1	0
35	S2	644	OMG	1	0
35	S2	1383	A2M	1	0
39	L5	4521	PSU	1	0
39	L5	4620	OMU	2	0
35	S2	1337	4AC	3	0
35	S2	649	PSU	1	0
35	S2	1639	G7M	1	0
39	L5	4392	OMG	1	0
39	L5	2364	OMG	1	0
39	L5	1340	OMC	2	0
35	S2	121	OMU	1	0
35	S2	1031	A2M	2	0
35	S2	159	A2M	2	0
39	L5	2363	A2M	1	0
35	S2	1842	4AC	1	0
39	L5	2632	PSU	1	0
39	L5	1326	A2M	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 241 ligands modelled in this entry, 224 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.90	0
88	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.86	0
88	SPD	L5	5287	-	9,9,9	0.33	0	8,8,8	0.81	0
87	SPM	L5	5291	-	13,13,13	0.34	0	12,12,12	0.83	0
87	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	0.94	0
88	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.97	0
87	SPM	L5	5263	-	13,13,13	0.34	0	12,12,12	0.96	0
88	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.83	0
87	SPM	L5	5264	-	13,13,13	0.37	0	12,12,12	1.07	0
88	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.85	0
87	SPM	L5	5288	-	13,13,13	0.35	0	12,12,12	0.98	0
88	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.77	0
87	SPM	L5	5258	-	13,13,13	0.36	0	12,12,12	0.93	0
88	SPD	L8	201	-	9,9,9	0.32	0	8,8,8	0.90	0
88	SPD	L5	5285	-	9,9,9	0.34	0	8,8,8	0.94	0
88	SPD	LN	301	-	9,9,9	0.35	0	8,8,8	0.92	0
87	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L5	5283	-	-	1/7/7/7	-
88	SPD	L5	5286	-	-	2/7/7/7	-
88	SPD	L5	5287	-	-	2/7/7/7	-
87	SPM	L5	5291	-	-	4/11/11/11	-
87	SPM	L5	5267	-	-	4/11/11/11	-
88	SPD	L5	5261	-	-	0/7/7/7	-
87	SPM	L5	5263	-	-	4/11/11/11	-
88	SPD	L5	5290	-	-	4/7/7/7	-
87	SPM	L5	5264	-	-	7/11/11/11	-
88	SPD	L5	5289	-	-	3/7/7/7	-
87	SPM	L5	5288	-	-	4/11/11/11	-
88	SPD	L5	5284	-	-	3/7/7/7	-
87	SPM	L5	5258	-	-	4/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L8	201	-	-	4/7/7/7	-
88	SPD	L5	5285	-	-	4/7/7/7	-
88	SPD	LN	301	-	-	2/7/7/7	-
87	SPM	L5	5292	-	-	4/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5264	SPM	N5-C6-C7-C8
88	L5	5284	SPD	C3-C4-C5-N6
87	L5	5263	SPM	N10-C11-C12-C13
87	L5	5292	SPM	N10-C11-C12-C13
88	L5	5285	SPD	N6-C7-C8-C9

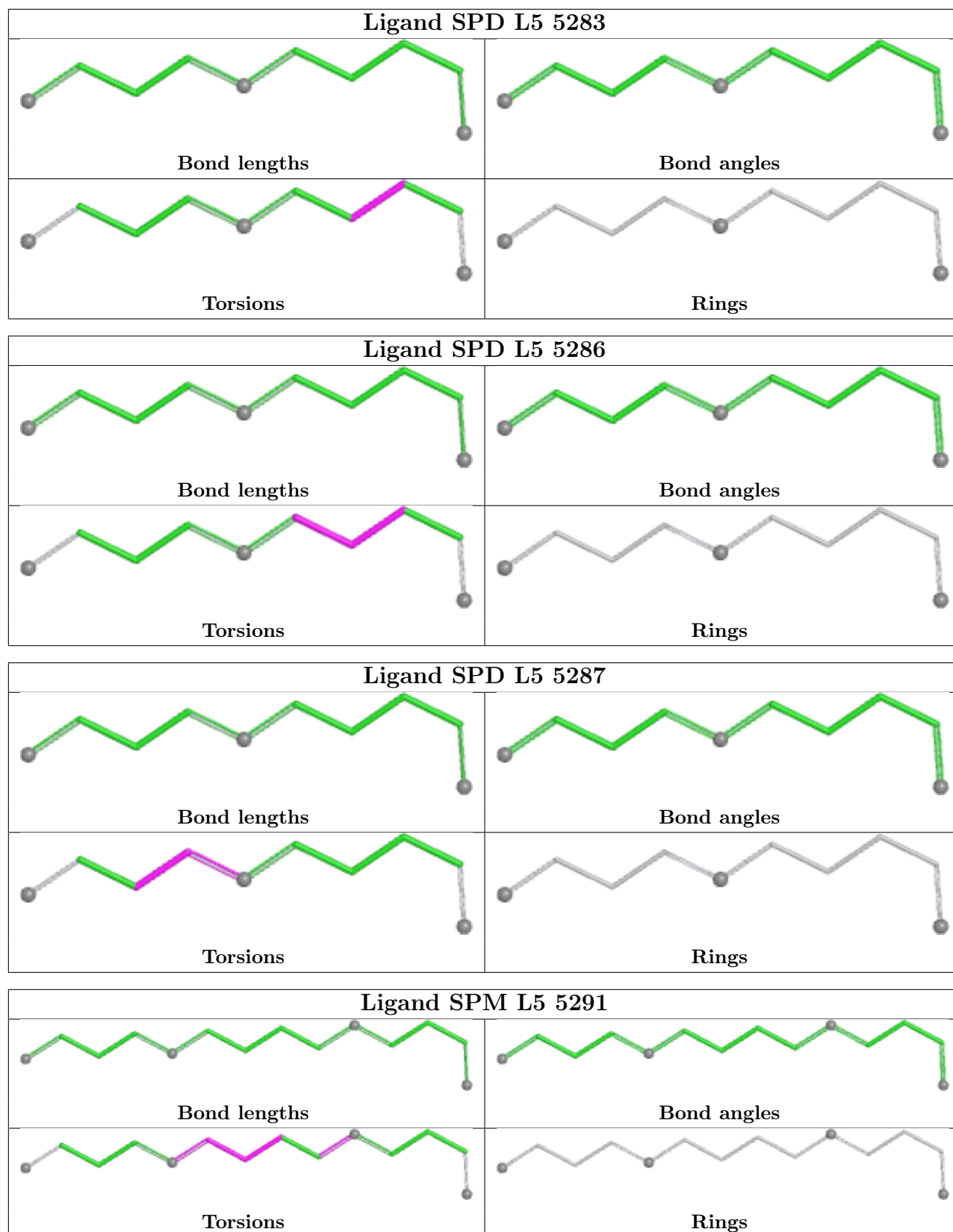
There are no ring outliers.

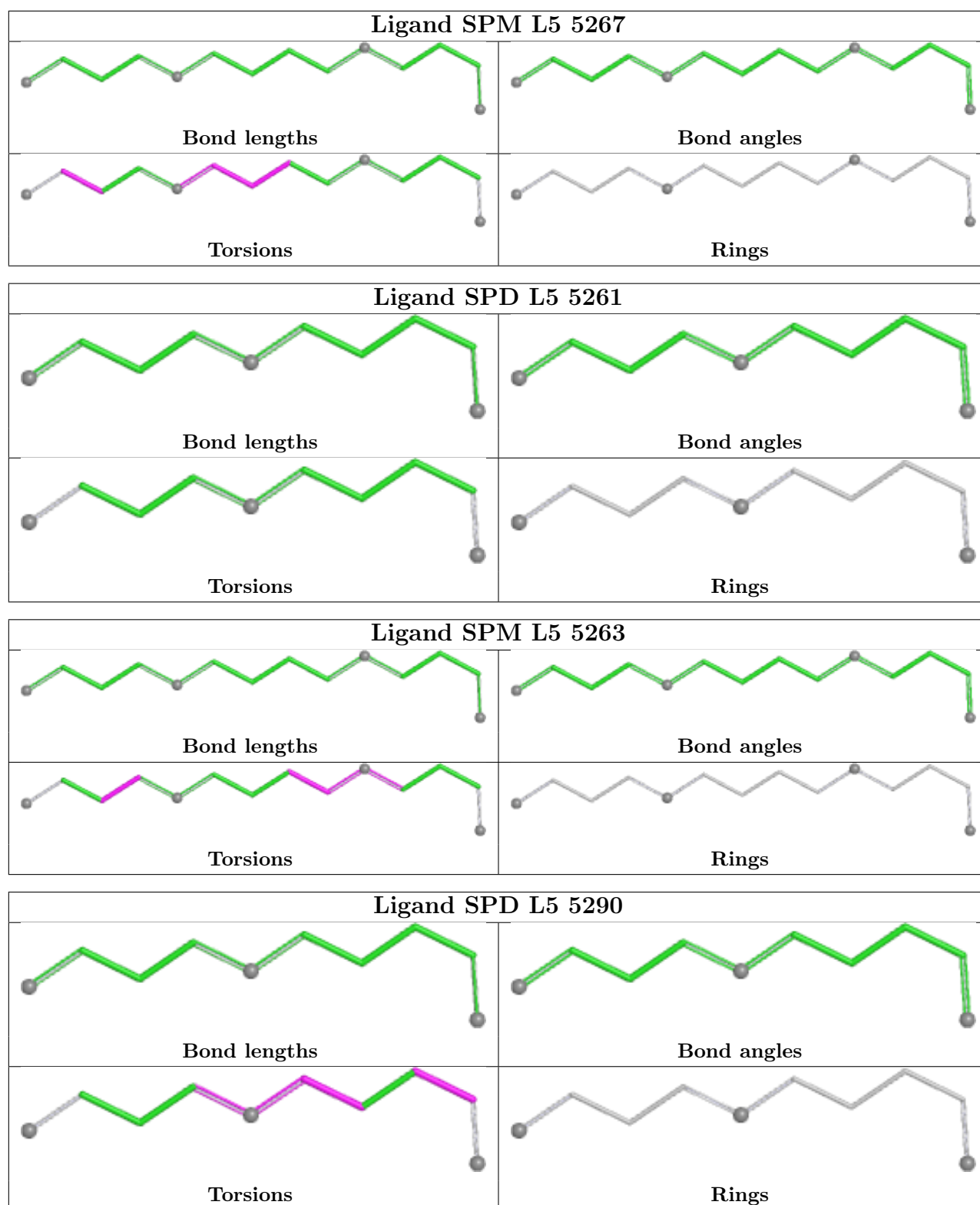
7 monomers are involved in 8 short contacts:

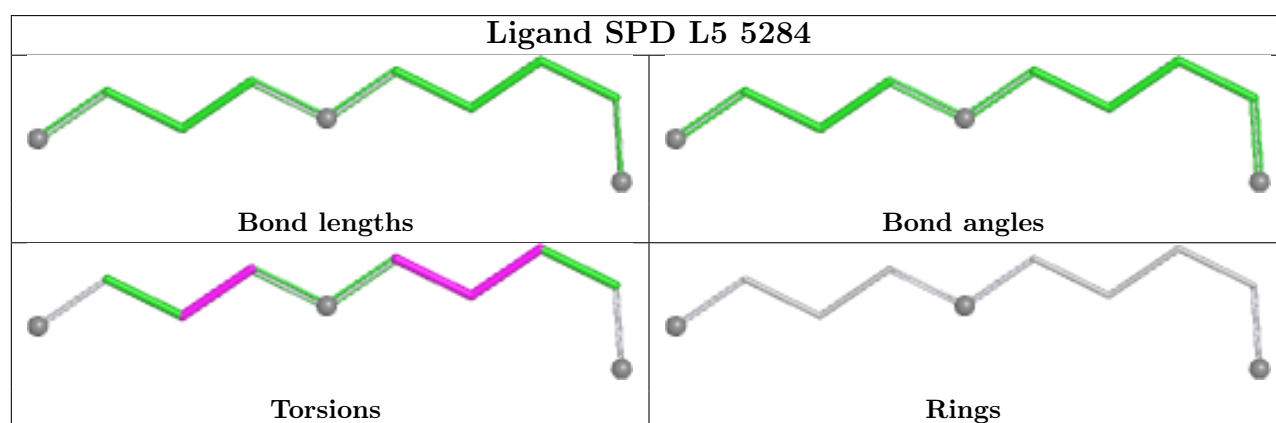
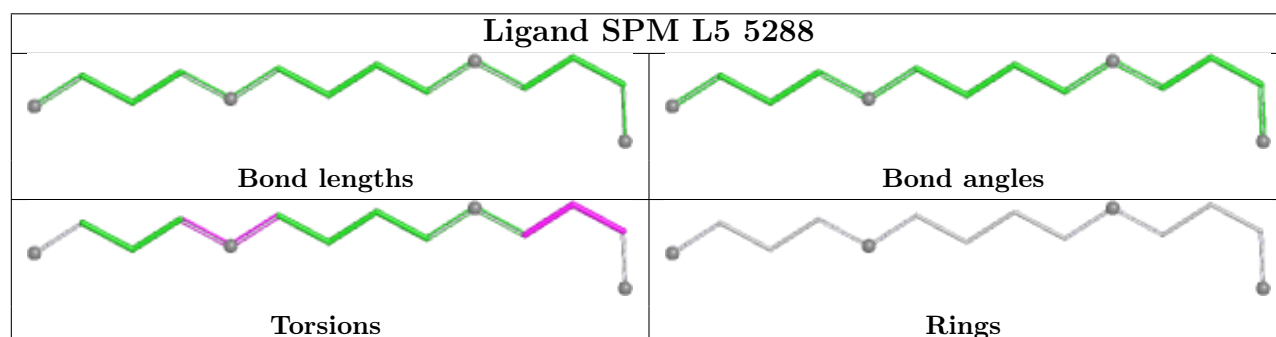
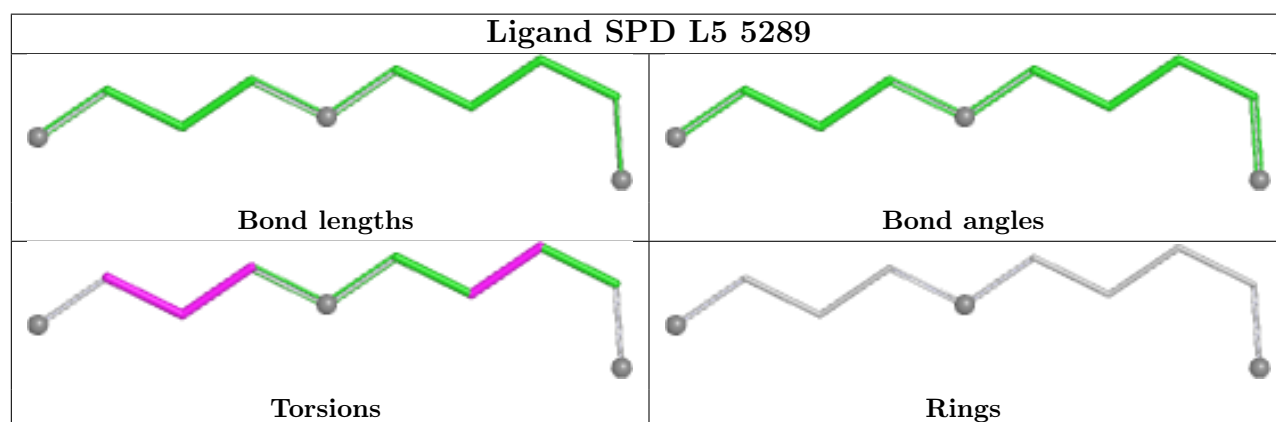
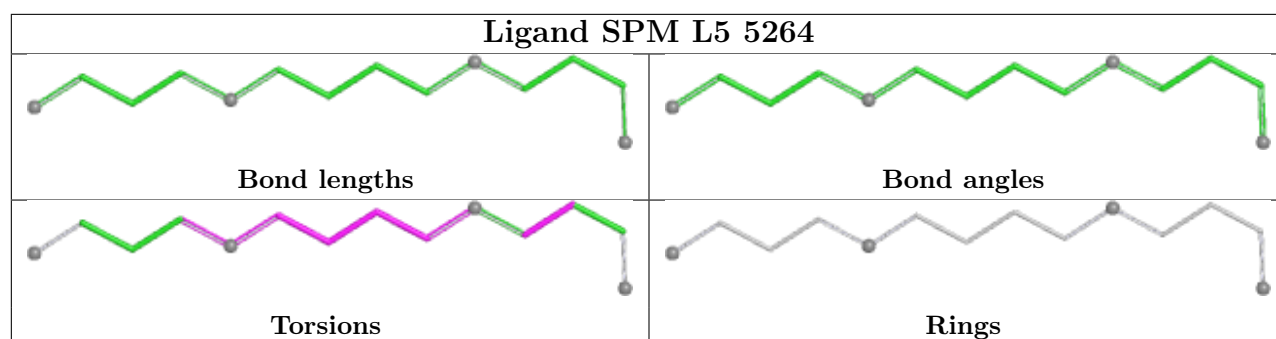
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5286	SPD	1	0
87	L5	5291	SPM	2	0
88	L5	5261	SPD	1	0
87	L5	5263	SPM	1	0
87	L5	5264	SPM	1	0
88	L5	5284	SPD	1	0
87	L5	5292	SPM	1	0

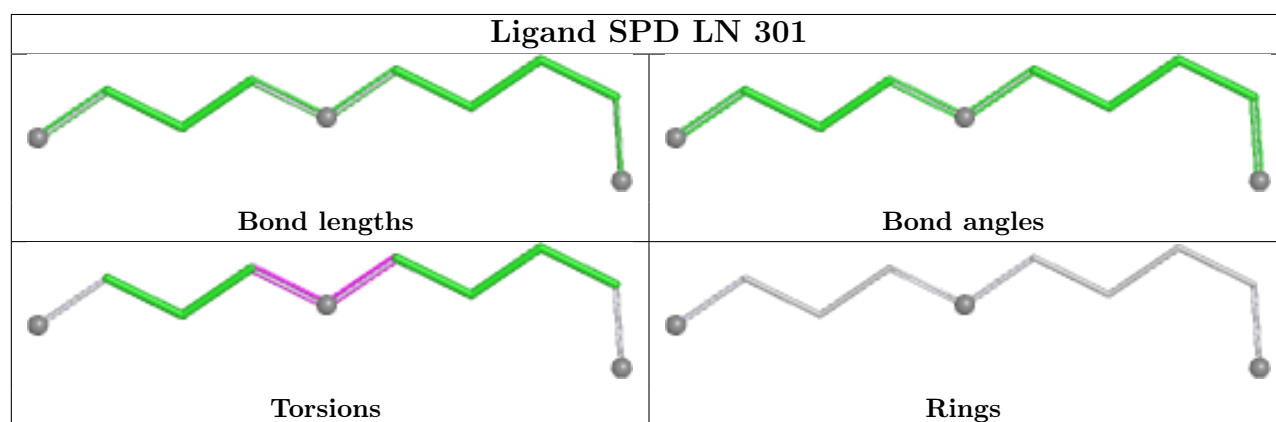
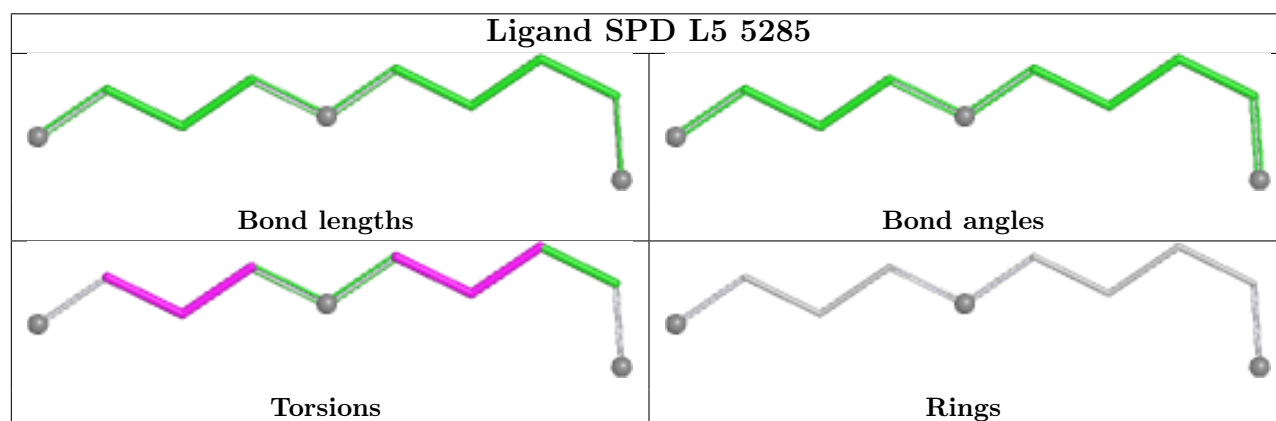
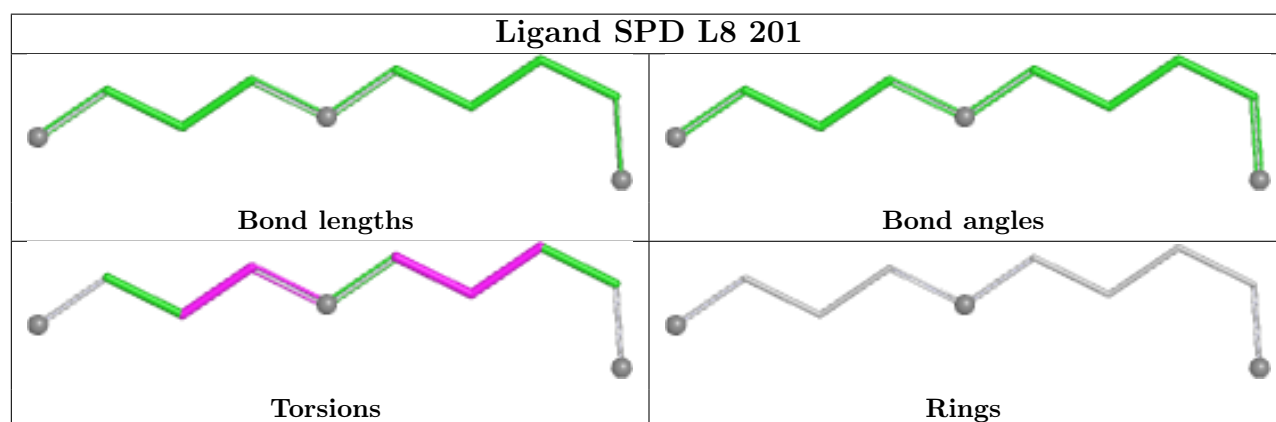
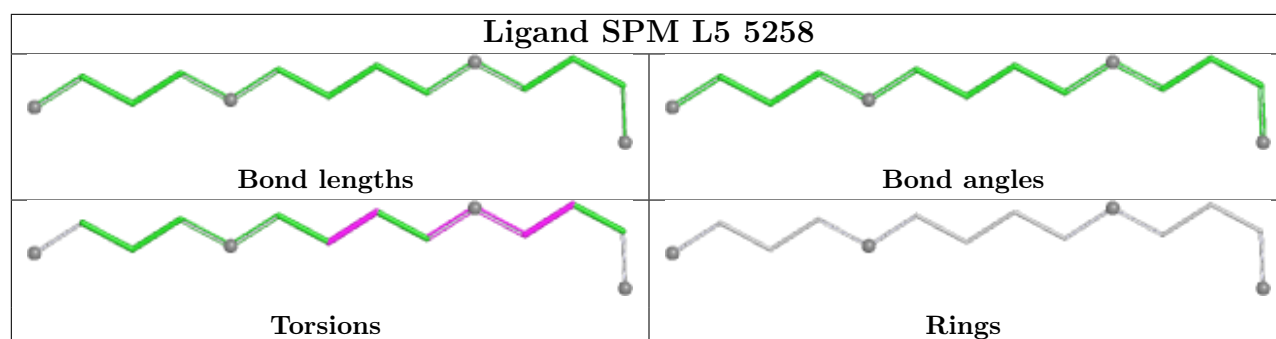
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

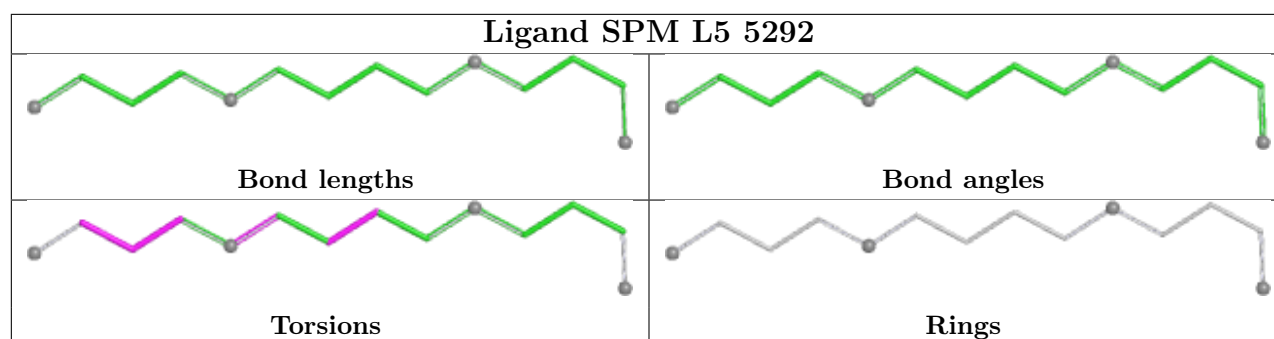
equivalents in the CSD to analyse the geometry.











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
39	L5	10
35	S2	4
66	Lb	1
83	Lt	1
23	SH	1
1	AP	1
2	PE	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	34.81
1	S2	753:C	O3'	785:C	P	28.44
1	L5	2910:G	O3'	3584:C	P	20.91
1	L5	1706:A	O3'	1716:G	P	20.70
1	L5	760:G	O3'	903:C	P	17.16

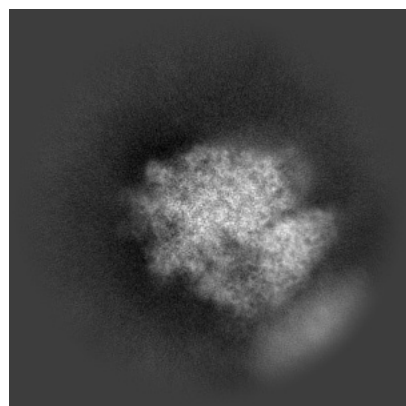
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71377. These allow visual inspection of the internal detail of the map and identification of artifacts.

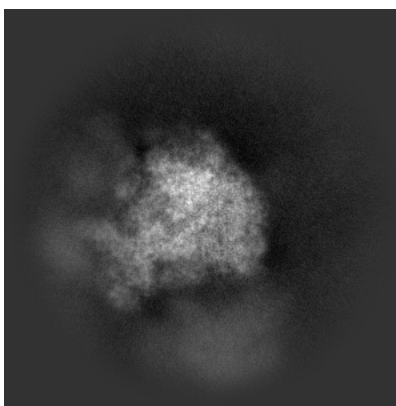
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

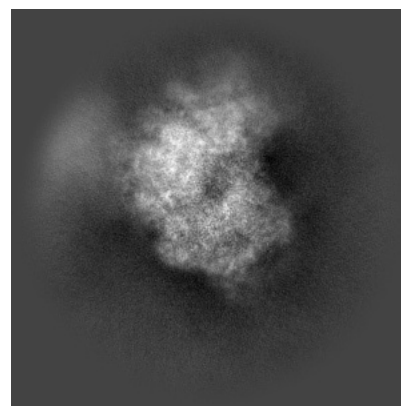
6.1.1 Primary map



X

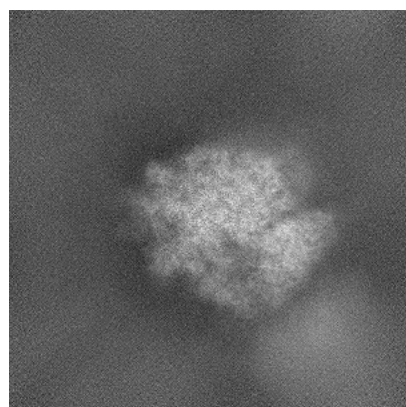


Y

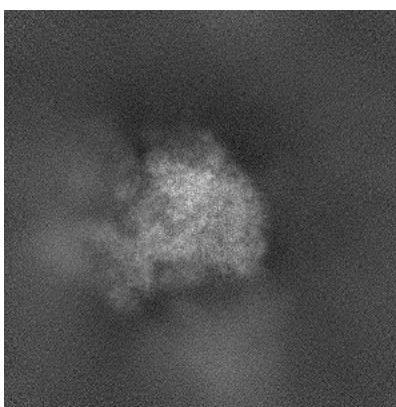


Z

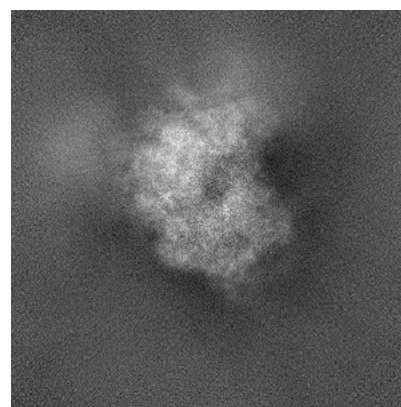
6.1.2 Raw map



X



Y

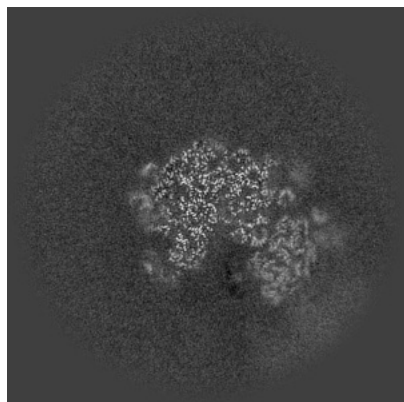


Z

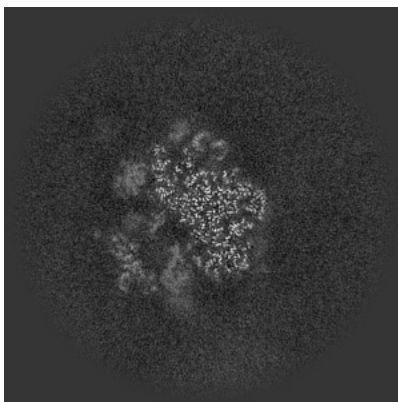
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

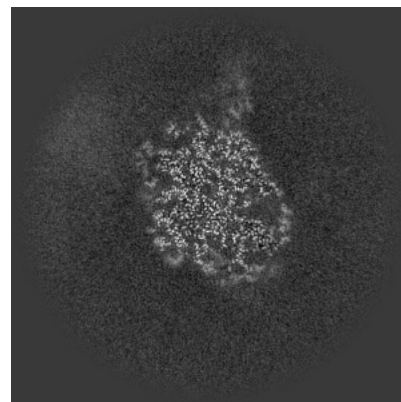
6.2.1 Primary map



X Index: 256

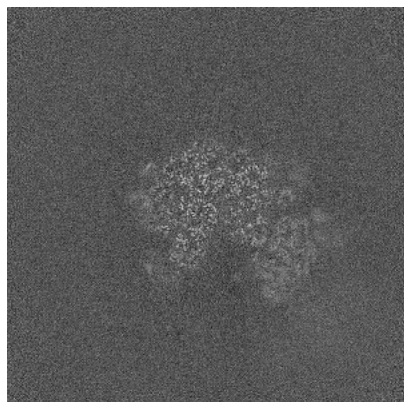


Y Index: 256

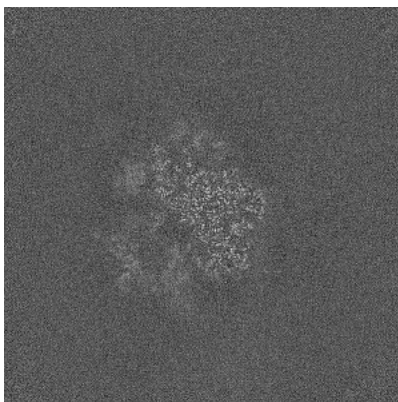


Z Index: 256

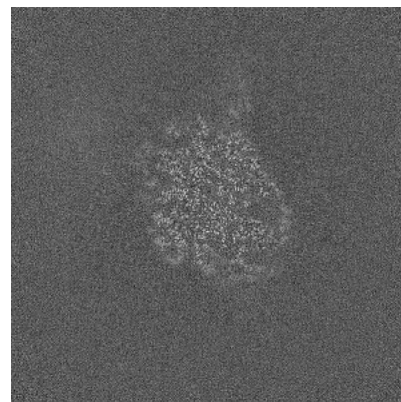
6.2.2 Raw map



X Index: 256



Y Index: 256

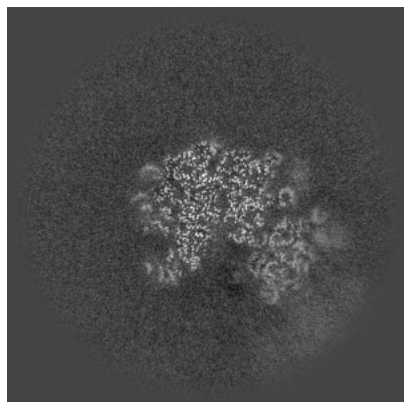


Z Index: 256

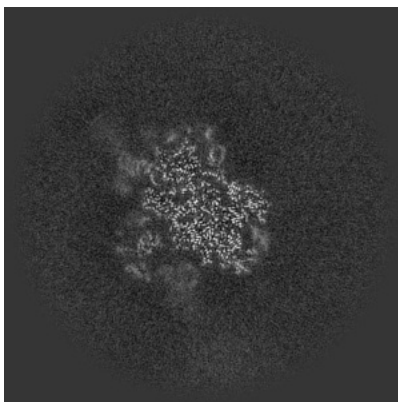
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

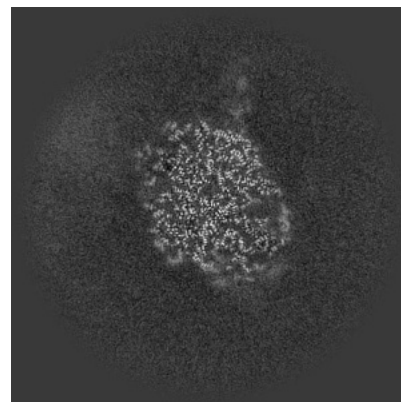
6.3.1 Primary map



X Index: 253

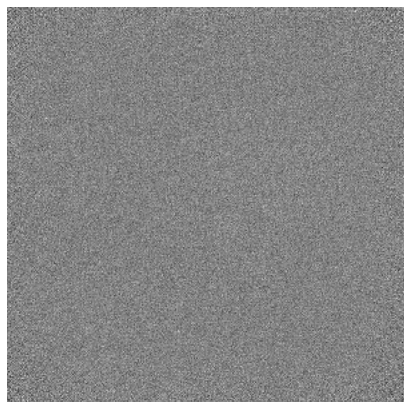


Y Index: 243

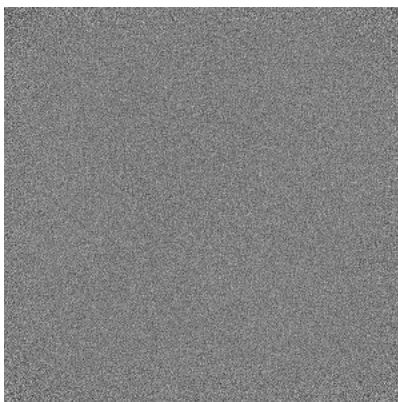


Z Index: 258

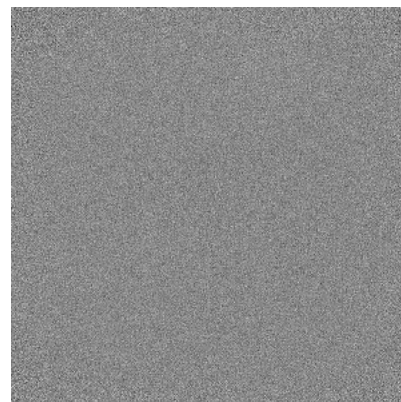
6.3.2 Raw map



X Index: 0



Y Index: 0

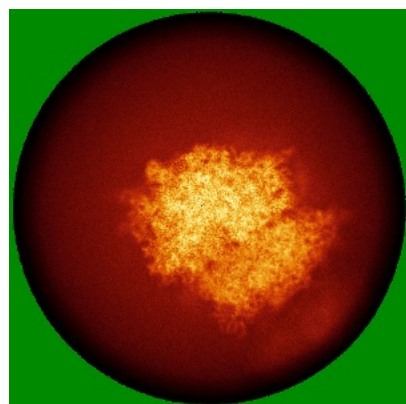


Z Index: 0

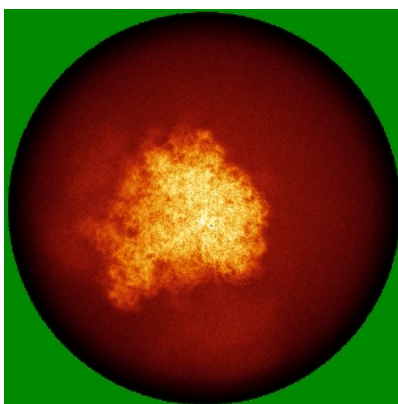
The images above show the largest variance slices of the map in three orthogonal directions.

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

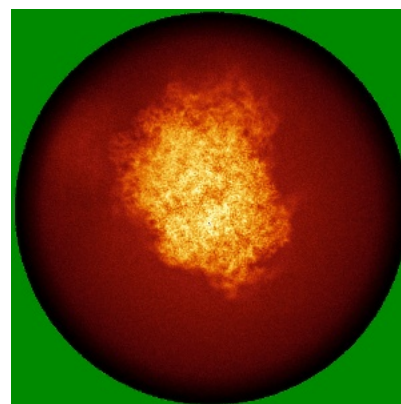
6.4.1 Primary map



X

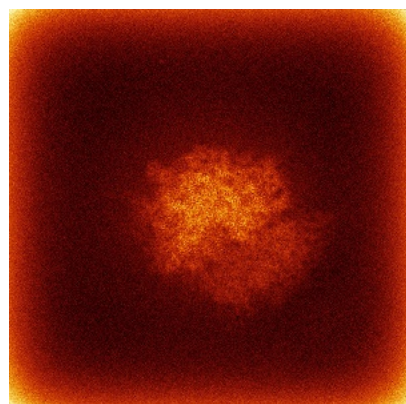


Y

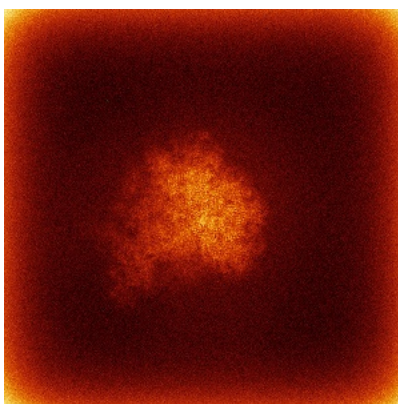


Z

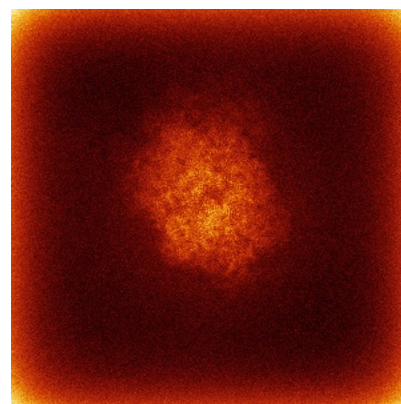
6.4.2 Raw map



X



Y

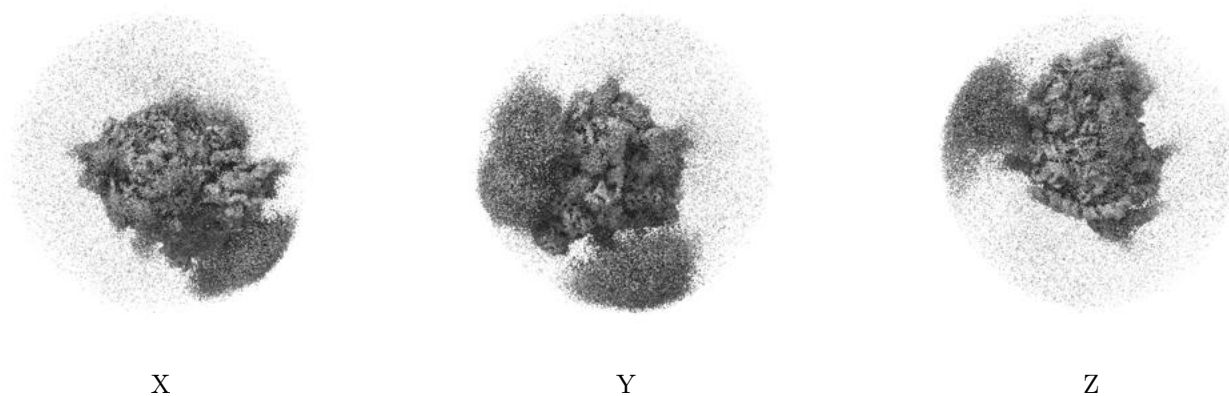


Z

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.

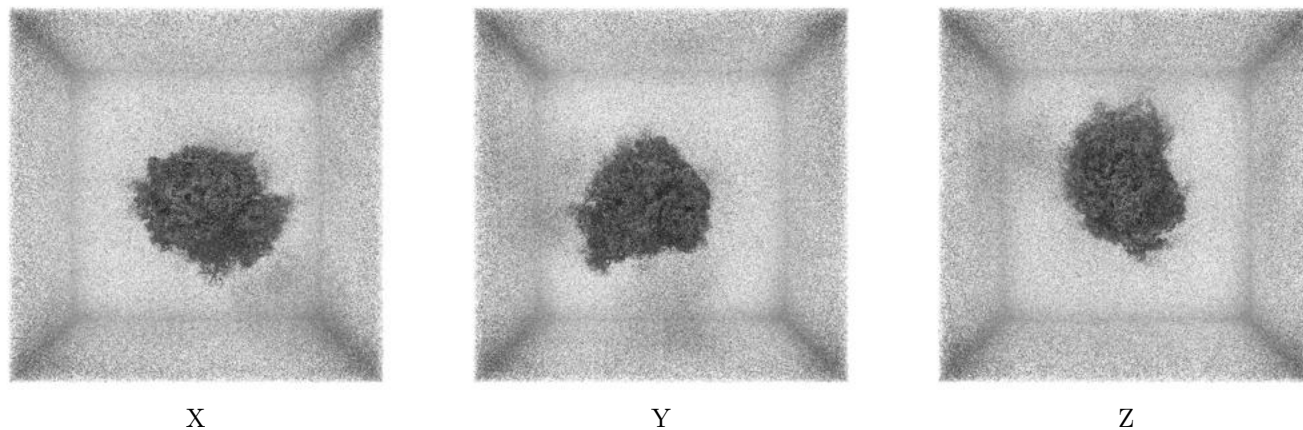
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

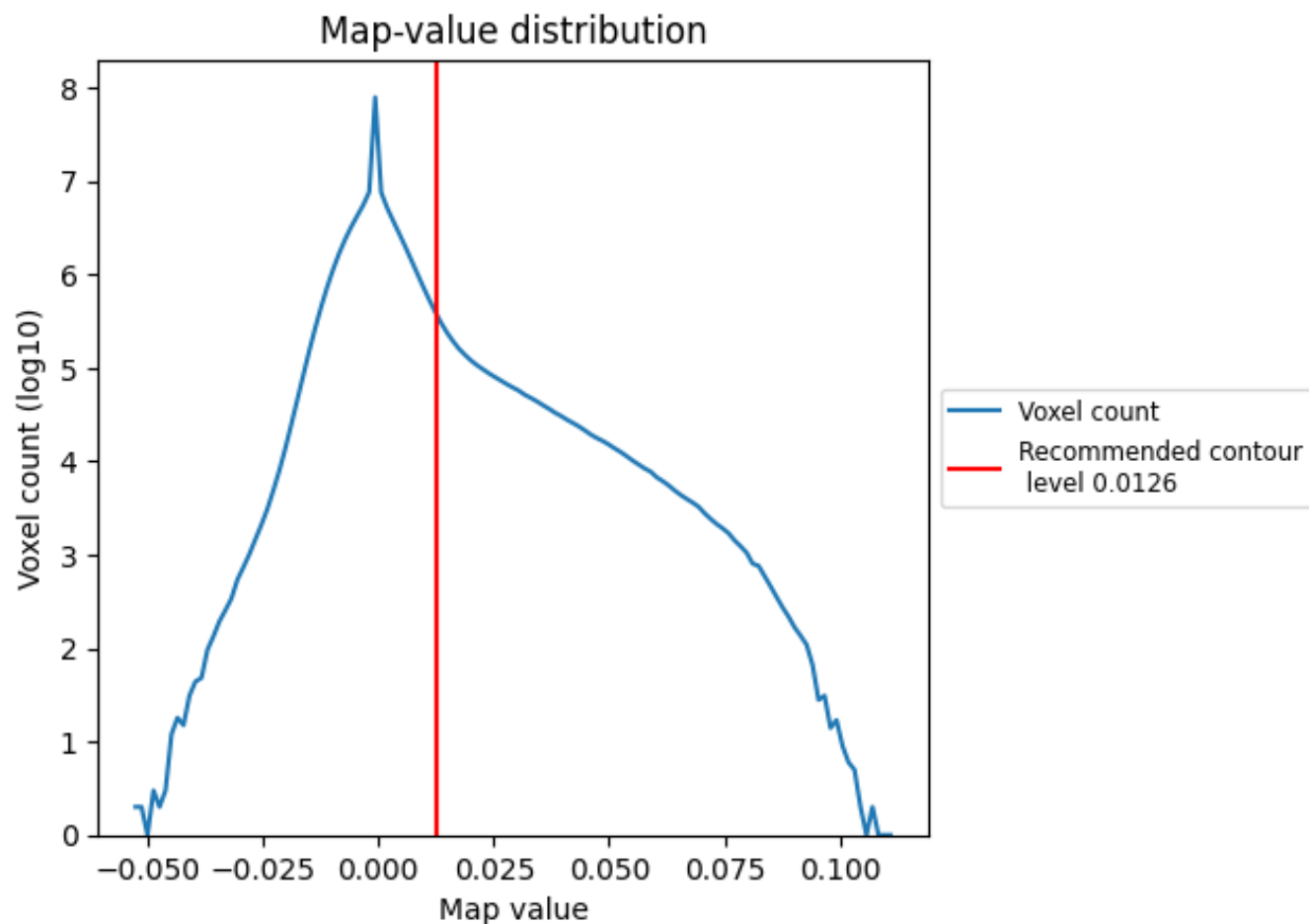
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

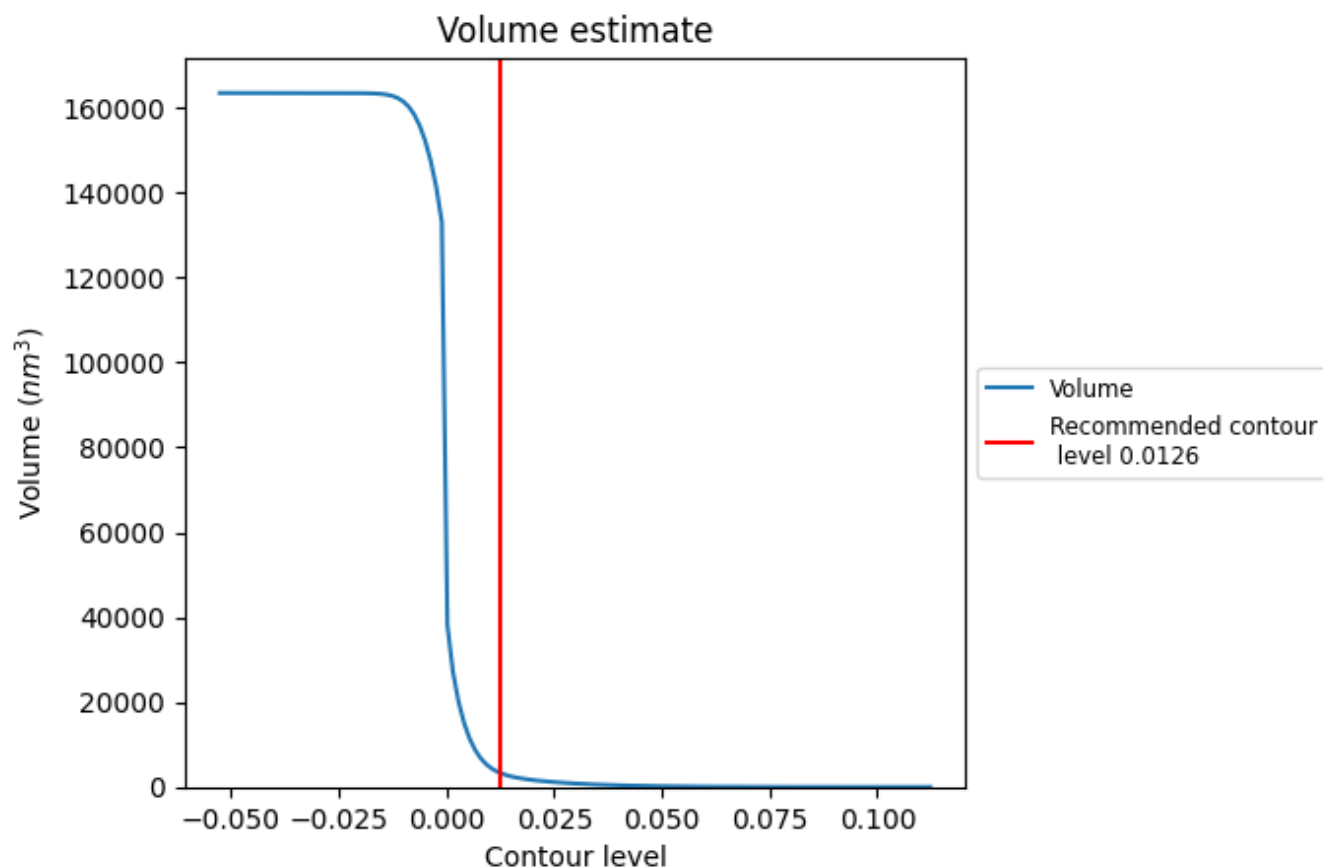
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

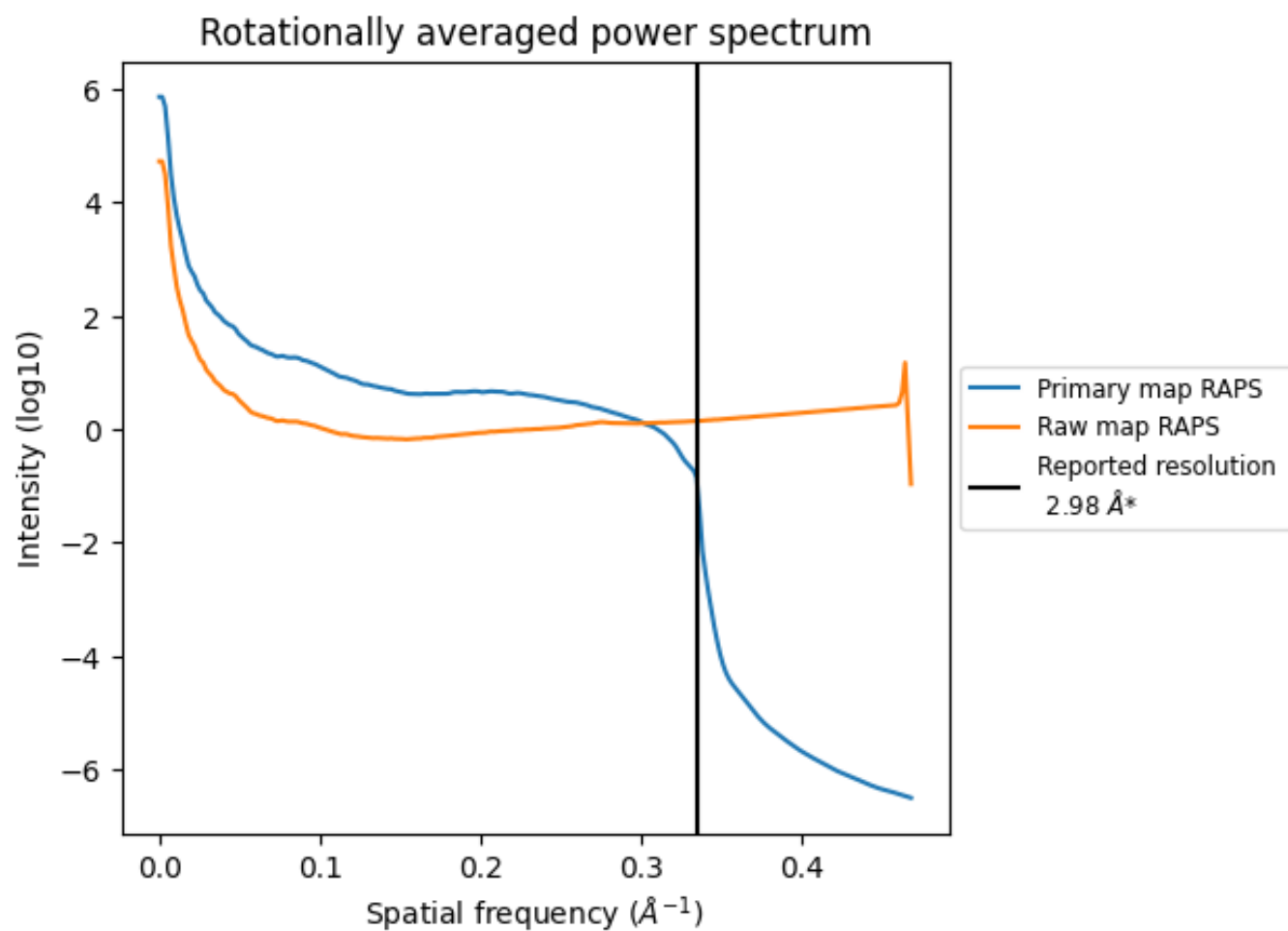
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3255 nm^3 ; this corresponds to an approximate mass of 2941 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

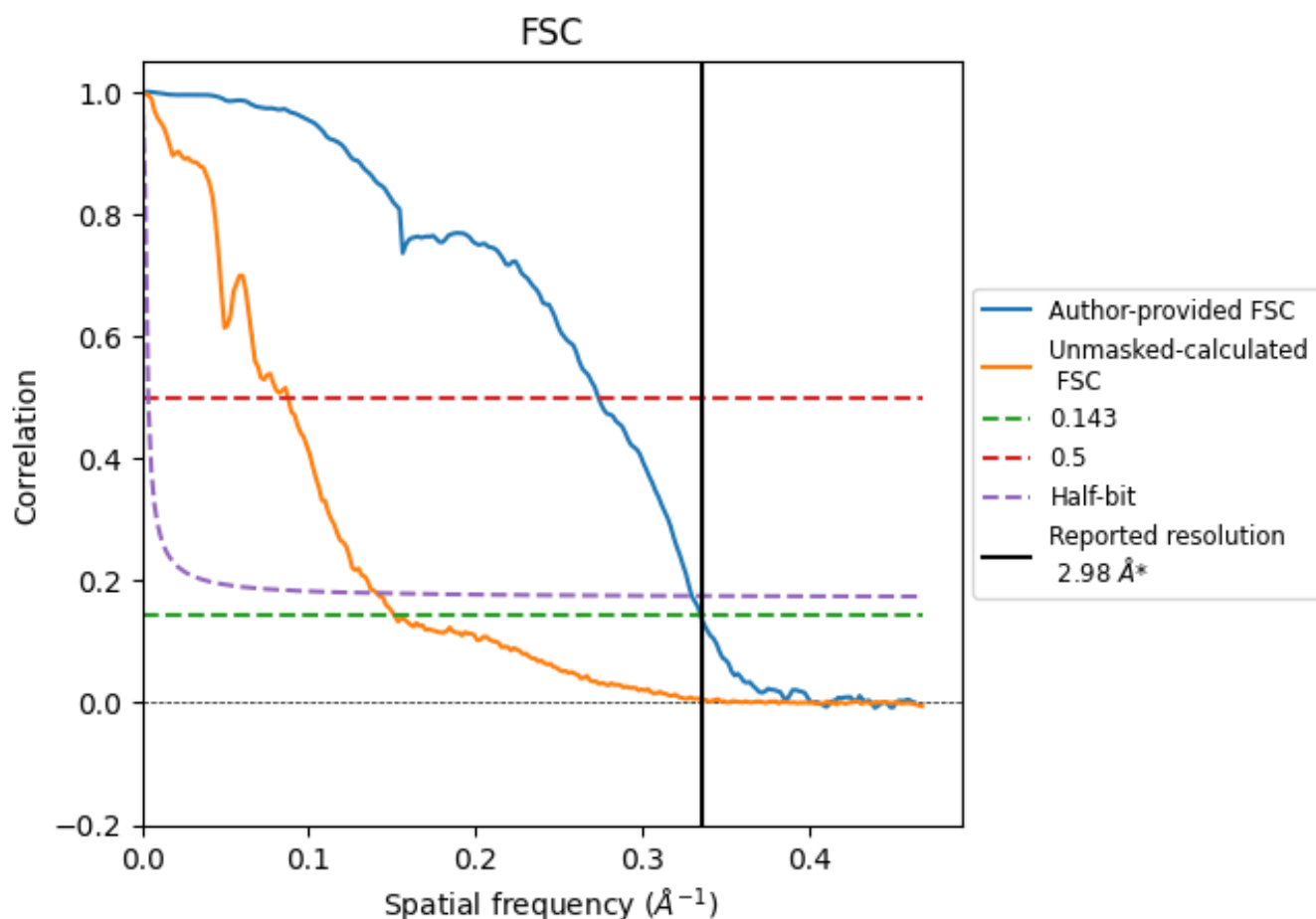


*Reported resolution corresponds to spatial frequency of 0.336 $\text{\AA}^{-1}$

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 0.336 Å⁻¹

8.2 Resolution estimates [i](#)

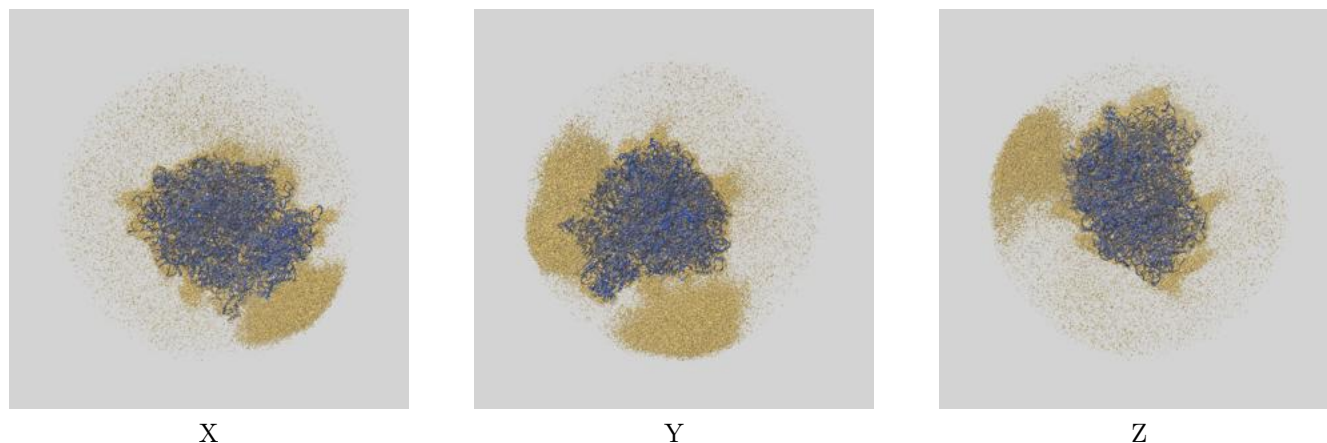
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.65	3.03
Unmasked-calculated*	6.61	11.45	7.10

*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 6.61 differs from the reported value 2.98 by more than 10 %

9 Map-model fit [i](#)

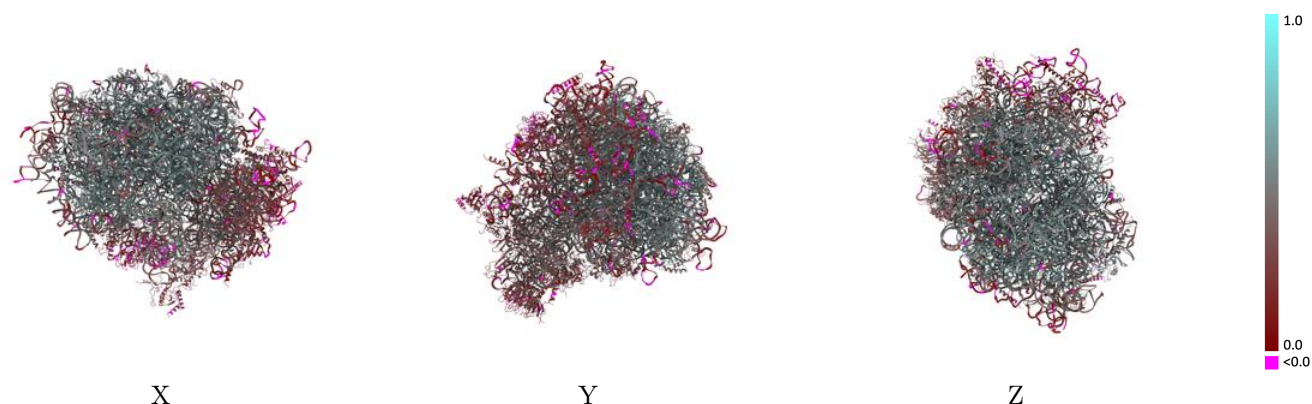
This section contains information regarding the fit between EMDB map EMD-71377 and PDB model 9P8H. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



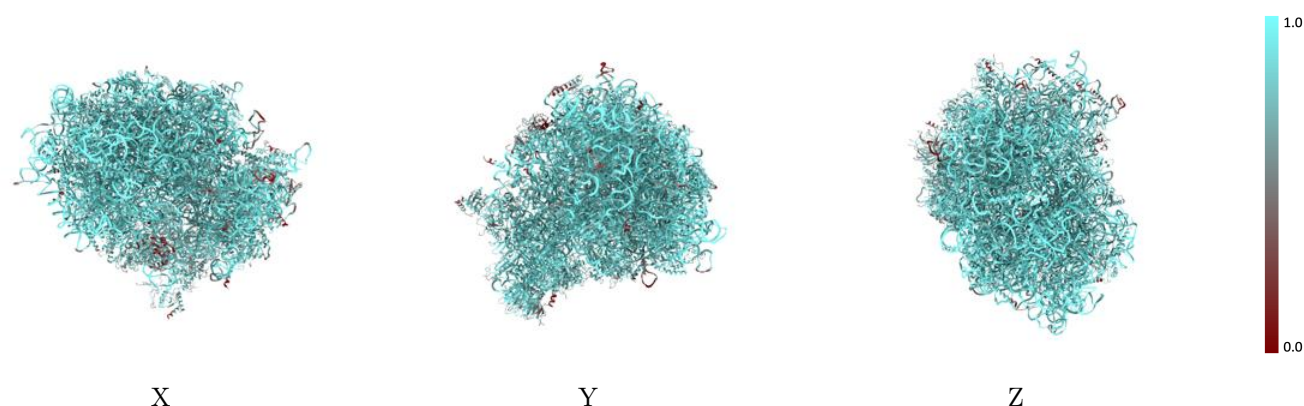
The images above show the 3D surface view of the map at the recommended contour level 0.0126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



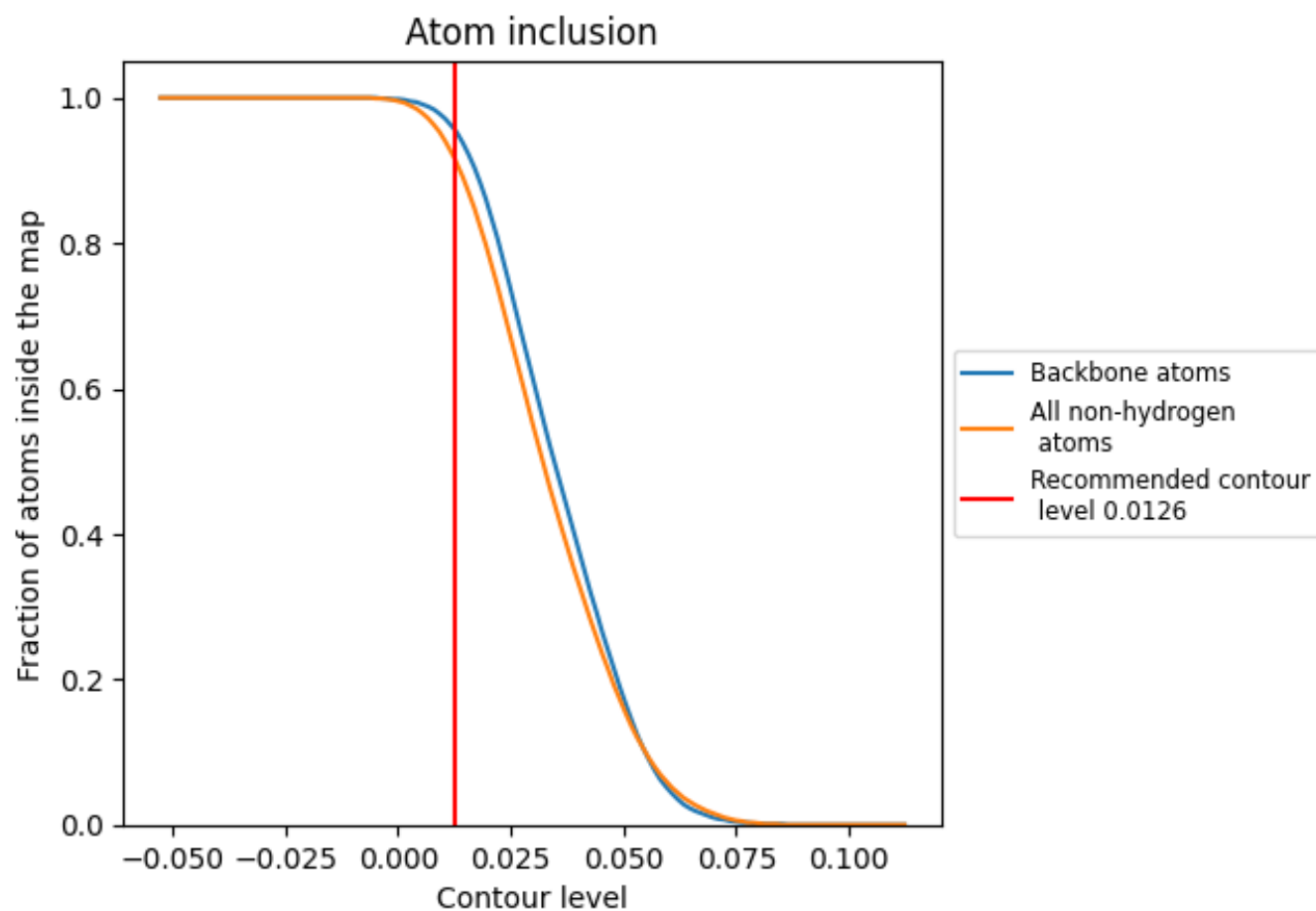
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.4280
AP	 0.7640	 0.2740
CH	 0.6280	 0.2100
CI	 0.7450	 0.3890
L5	 0.9650	 0.4780
L7	 0.9940	 0.5270
L8	 0.9750	 0.5010
LA	 0.9570	 0.5420
LB	 0.9240	 0.5150
LC	 0.9240	 0.5220
LD	 0.9030	 0.4580
LE	 0.8590	 0.4350
LF	 0.9310	 0.5220
LG	 0.8660	 0.4480
LH	 0.8940	 0.4800
LI	 0.8980	 0.4960
LJ	 0.8650	 0.4220
LL	 0.8840	 0.4770
LM	 0.9180	 0.4890
LN	 0.9710	 0.5560
LO	 0.9250	 0.5130
LP	 0.9290	 0.5330
LQ	 0.9490	 0.5460
LR	 0.8820	 0.4480
LS	 0.9420	 0.5410
LT	 0.9010	 0.5060
LU	 0.8750	 0.4200
LV	 0.9210	 0.5210
LW	 0.7530	 0.3210
LX	 0.9030	 0.4950
LY	 0.9190	 0.5040
LZ	 0.9250	 0.4770
La	 0.9470	 0.5420
Lb	 0.8510	 0.4230
Lc	 0.8680	 0.4490



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Chain	Atom inclusion	Q-score
Ld	 0.9040	 0.4960
Le	 0.9460	 0.5440
Lf	 0.9580	 0.5540
Lg	 0.9220	 0.5070
Lh	 0.8920	 0.4840
Li	 0.9080	 0.4720
Lj	 0.9640	 0.5440
Lk	 0.8550	 0.4380
Ll	 0.9270	 0.5200
Lm	 0.9280	 0.5070
Ln	 0.9040	 0.4480
Lo	 0.8850	 0.5060
Lp	 0.9230	 0.5100
Lr	 0.9250	 0.5220
Ls	 0.4990	 0.1240
Lt	 0.4800	 0.0890
PE	 0.9170	 0.3130
S2	 0.9600	 0.3760
SA	 0.8210	 0.3370
SB	 0.8300	 0.3960
SC	 0.8750	 0.3760
SD	 0.8260	 0.3130
SE	 0.8530	 0.2740
SF	 0.8010	 0.3130
SG	 0.7470	 0.2080
SH	 0.7870	 0.2680
SI	 0.8300	 0.3210
SJ	 0.7990	 0.2620
SK	 0.7970	 0.2870
SL	 0.8410	 0.3770
SM	 0.6140	 0.1470
SN	 0.8780	 0.4030
SO	 0.8580	 0.4000
SP	 0.8080	 0.3500
SQ	 0.8360	 0.3080
SR	 0.8000	 0.2860
SS	 0.8110	 0.3490
ST	 0.8300	 0.3240
SU	 0.8060	 0.2770
SV	 0.8330	 0.3340
SW	 0.8910	 0.4240
SX	 0.8210	 0.3750

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Chain	Atom inclusion	Q-score
SY	 0.7140	 0.1870
SZ	 0.7480	 0.2800
Sa	 0.8540	 0.4130
Sb	 0.8260	 0.3540
Sc	 0.7690	 0.2950
Sd	 0.9070	 0.3800
Sf	 0.6620	 0.2080
Sg	 0.7560	 0.2320