



# wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 02:19 AM EDT

PDB ID : 9PBE / pdb\_00009pbe  
EMDB ID : EMD-71477  
Title : In situ human 80S ribosome (composite map)  
Authors : Wei, Z.; Yong, X.  
Deposited on : 2025-06-26  
Resolution : 2.19 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](mailto: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>.

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

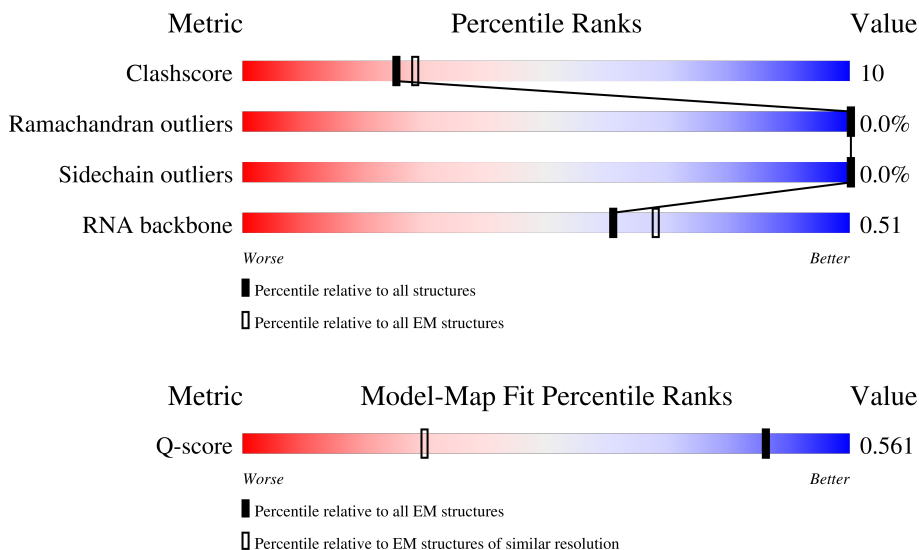
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 2.19 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	2745 ( 1.70 - 2.69 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	CD	50	
2	CI	31	
3	L5	5070	

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Mol	Chain	Length	Quality of chain
4	L7	120	74% 20% 6%
5	L8	156	53% 44%
6	LA	248	70% 29%
7	LB	402	72% 28%
8	LC	368	82% 17%
9	LD	293	82% 18%
10	LE	250	72% 24%
11	LF	225	81% 19%
12	LG	241	78% 22%
13	LH	190	78% 22%
14	LI	213	76% 24%
15	LJ	176	66% 30%
16	LL	210	80% 20%
17	LM	139	79% 21%
18	LN	203	84% 15%
19	LO	201	80% 20%
20	LP	153	75% 24%
21	LQ	187	88% 12%
22	LR	187	74% 26%
23	LS	175	83% 17%
24	LT	159	78% 22%
25	LU	101	74% 26%
26	LV	131	81% 19%
27	LW	118	64% 32%
28	LX	120	91% 9%


























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Mol	Chain	Length	Quality of chain
29	LY	134	76% 23%
30	LZ	135	74% 26%
31	La	147	82% 17%
32	Lb	109	83% 17%
33	Lc	98	76% 24%
34	Ld	107	75% 25%
35	Le	128	88% 12%
36	Lf	109	84% 16%
37	Lg	114	86% 14%
38	Lh	122	84% 16%
39	Li	102	92% 8%
40	Lj	86	77% 23%
41	Lk	69	78% 22%
42	Ll	50	70% 28%
43	Lm	52	79% 21%
44	Ln	24	75% 21%
45	Lo	105	78% 22%
46	Lp	91	82% 18%
47	Lr	125	88% 12%
48	Ls	196	70% 30%
49	Lt	141	15% 64% 31% 5%
50	Pt	74	50% 42% 8%
51	S2	1740	45% 44% 11%
52	SA	221	68% 31%
53	SB	214	71% 29%







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Mol	Chain	Length	Quality of chain
54	SC	222	 73% 26%
55	SD	227	 76% 23%
56	SE	262	 63% 37%
57	SF	189	 63% 37%
58	SG	237	 57% 42%
59	SH	186	 65% 35%
60	SI	206	 72% 28%
61	SJ	185	 76% 23%
62	SK	98	 67% 32%
63	SL	153	 5% 66% 34%
64	SM	122	 18% 54% 46%
65	SN	150	 80% 19%
66	SO	140	 73% 25%
67	SP	121	 73% 27%
68	SQ	144	 61% 38%
69	SR	135	 61% 39%
70	SS	145	 63% 37%
71	ST	143	 64% 34%
72	SU	104	 63% 36%
73	SV	83	 67% 33%
74	SW	129	 73% 26%
75	SX	141	 76% 24%
76	SY	131	 5% 65% 35%
77	SZ	75	 67% 33%
78	Sa	102	 81% 19%

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Mol	Chain	Length	Quality of chain
79	Sb	83	 76% 24%
80	Sc	64	 73% 27%
81	Sd	55	 58% 42%
82	Se	58	 7% 88% 12%
83	Sf	67	 61% 39%
84	Sg	313	 67% 33%

## 2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 223497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Isoform 2 of SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	CD	50	385	243	61	80	1	0	0

- Molecule 2 is a protein called Transcription factor BTF3.

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

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

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

- Molecule 4 is a RNA chain called 5S rRNA [Homo sapiens].

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 28 is a protein called 60S ribosomal protein L23a.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called 60S ribosomal protein L30.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 50 is a RNA chain called P site tRNA.

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

- Molecule 51 is a RNA chain called 18S rRNA.

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

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

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

- Molecule 53 is a protein called 40S ribosomal protein S3a.

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

- Molecule 54 is a protein called 40S ribosomal protein S2.

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

- Molecule 55 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 57 is a protein called 40S ribosomal protein S5.

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

- Molecule 58 is a protein called 40S ribosomal protein S6.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS7.

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

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 60 is a protein called 40S ribosomal protein S8.

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

- Molecule 61 is a protein called 40S ribosomal protein S9.

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

- Molecule 62 is a protein called 40S ribosomal protein S10.

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

- Molecule 63 is a protein called 40S ribosomal protein S11.

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

- Molecule 64 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 65 is a protein called 40S ribosomal protein S13.

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

- Molecule 66 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 69 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 70 is a protein called 40S ribosomal protein S18.

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

- Molecule 71 is a protein called 40S ribosomal protein S19.

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

- Molecule 72 is a protein called 40S ribosomal protein S20.

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

- Molecule 73 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 74 is a protein called 40S ribosomal protein S15a.

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

- Molecule 75 is a protein called 40S ribosomal protein S23.

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

- Molecule 76 is a protein called 40S ribosomal protein S24.

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

- Molecule 77 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 78 is a protein called 40S ribosomal protein S26.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 80 is a protein called 40S ribosomal protein S28.

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

- Molecule 81 is a protein called 40S ribosomal protein S29.

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

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

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

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

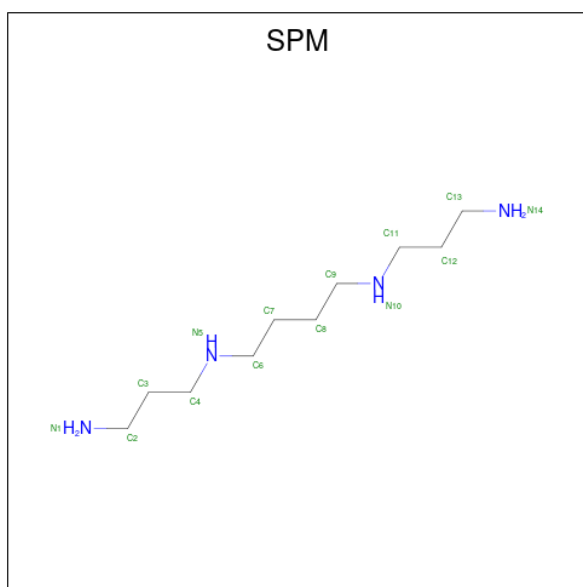
- Molecule 84 is a protein called Receptor of activated protein C kinase 1.

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

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

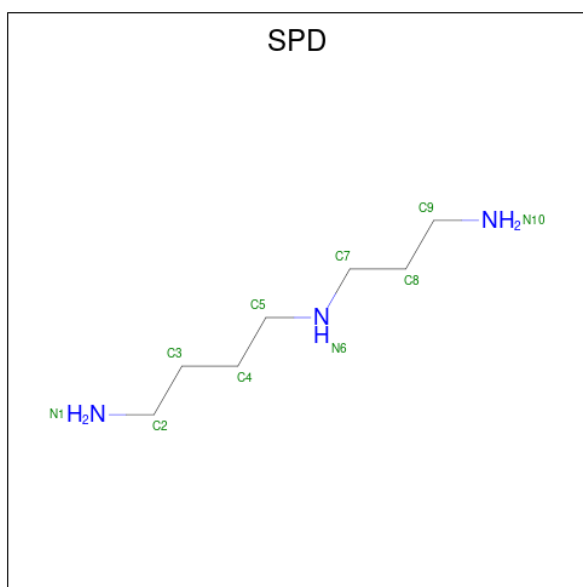
Mol	Chain	Residues	Atoms		AltConf
85	L5	185	Total 185	Mg 185	0
85	L7	3	Total 3	Mg 3	0
85	L8	5	Total 5	Mg 5	0
85	LA	1	Total 1	Mg 1	0
85	LP	1	Total 1	Mg 1	0
85	LV	1	Total 1	Mg 1	0
85	Le	1	Total 1	Mg 1	0
85	S2	28	Total 28	Mg 28	0

- Molecule 86 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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

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



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

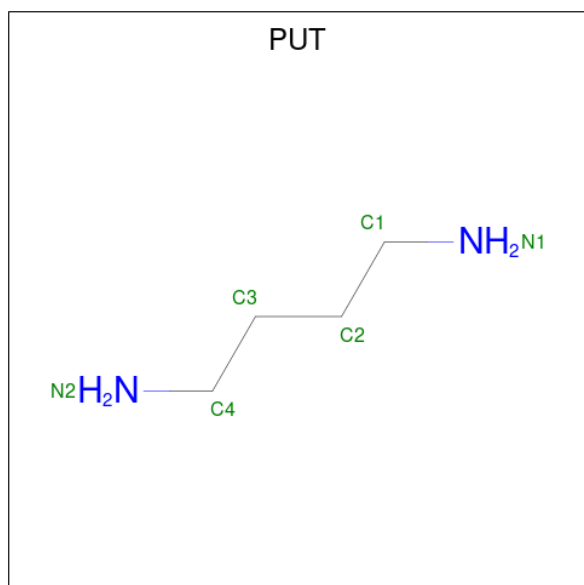
- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 90 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
91	L5	3311	Total	O	0
			3311	3311	
91	L7	16	Total	O	0
			16	16	
91	L8	118	Total	O	0
			118	118	
91	LA	43	Total	O	0
			43	43	
91	LB	66	Total	O	0
			66	66	
91	LC	45	Total	O	0
			45	45	
91	LD	1	Total	O	0
			1	1	
91	LG	13	Total	O	0
			13	13	
91	LH	1	Total	O	0
			1	1	
91	LI	7	Total	O	0
			7	7	
91	LL	33	Total	O	0
			33	33	
91	LN	99	Total	O	0
			99	99	
91	LO	58	Total	O	0
			58	58	
91	LP	38	Total	O	0
			38	38	
91	LQ	21	Total	O	0
			21	21	
91	LR	12	Total	O	0
			12	12	
91	LS	2	Total	O	0
			2	2	
91	LT	8	Total	O	0
			8	8	
91	LU	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
91	LV	41	Total 41	O 41	0
91	LW	15	Total 15	O 15	0
91	LX	10	Total 10	O 10	0
91	La	38	Total 38	O 38	0
91	Lb	14	Total 14	O 14	0
91	Ld	1	Total 1	O 1	0
91	Le	50	Total 50	O 50	0
91	Lf	13	Total 13	O 13	0
91	Lg	2	Total 2	O 2	0
91	Lh	8	Total 8	O 8	0
91	Li	10	Total 10	O 10	0
91	Lj	29	Total 29	O 29	0
91	Ll	5	Total 5	O 5	0
91	Ln	2	Total 2	O 2	0
91	Lo	37	Total 37	O 37	0
91	Lp	4	Total 4	O 4	0
91	Lr	3	Total 3	O 3	0
91	Pt	6	Total 6	O 6	0
91	S2	341	Total 341	O 341	0
91	SE	12	Total 12	O 12	0
91	SF	5	Total 5	O 5	0

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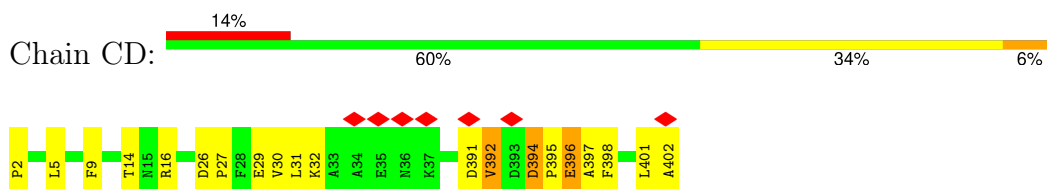
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Mol	Chain	Residues	Atoms		AltConf
91	SH	1	Total 1	O 1	0
91	SI	14	Total 14	O 14	0
91	SJ	1	Total 1	O 1	0
91	SL	22	Total 22	O 22	0
91	SP	1	Total 1	O 1	0
91	SQ	7	Total 7	O 7	0
91	SS	8	Total 8	O 8	0
91	ST	2	Total 2	O 2	0
91	SU	3	Total 3	O 3	0
91	SX	8	Total 8	O 8	0
91	SZ	1	Total 1	O 1	0
91	Sc	1	Total 1	O 1	0
91	Sd	3	Total 3	O 3	0

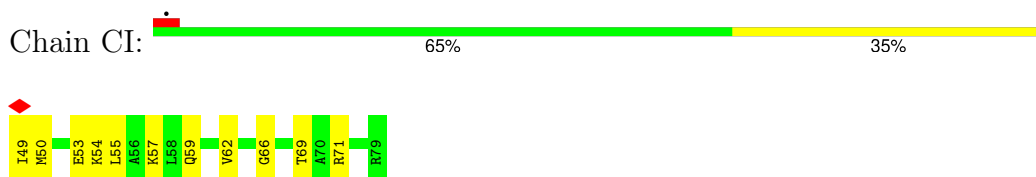
### 3 Residue-property plots [i](#)

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

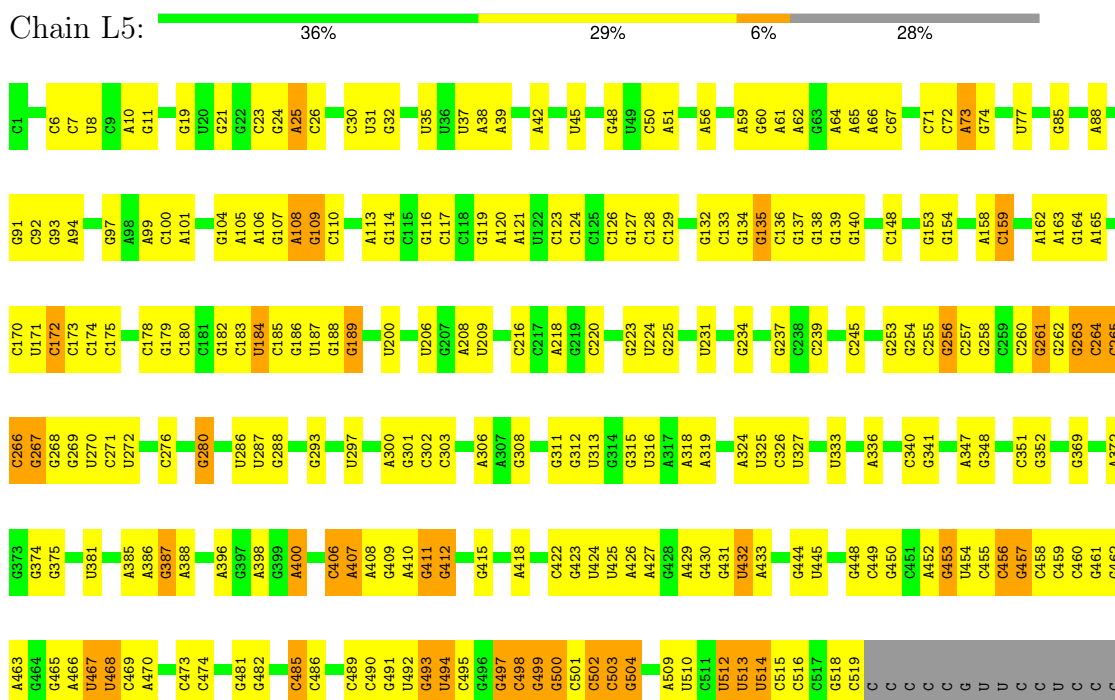
- Molecule 1: Isoform 2 of SERPINE1 mRNA-binding protein 1



- Molecule 2: Transcription factor BTF3



- Molecule 3: 28S rRNA





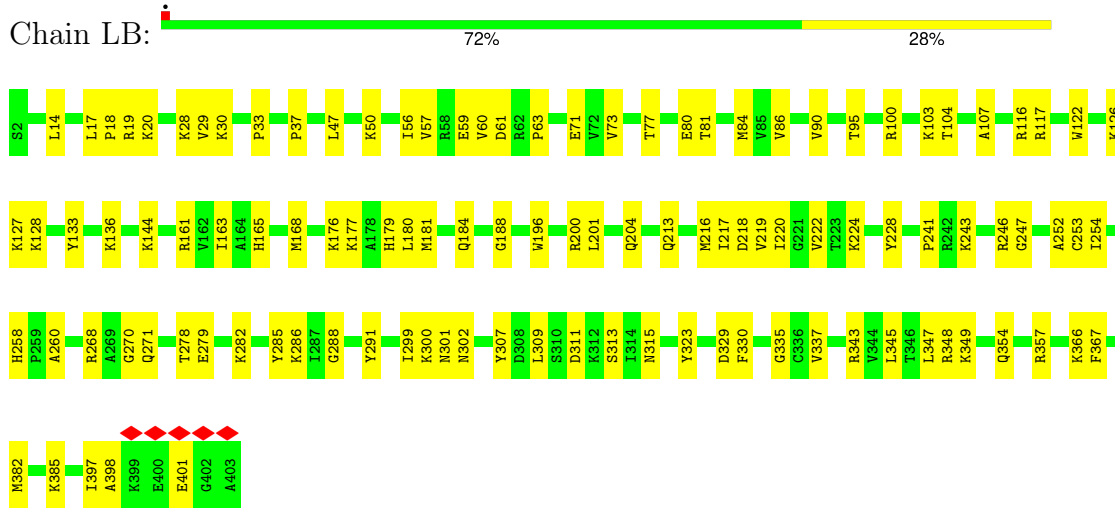




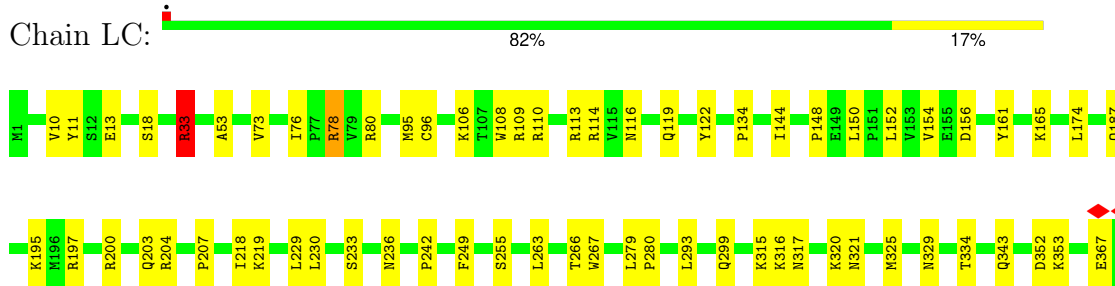




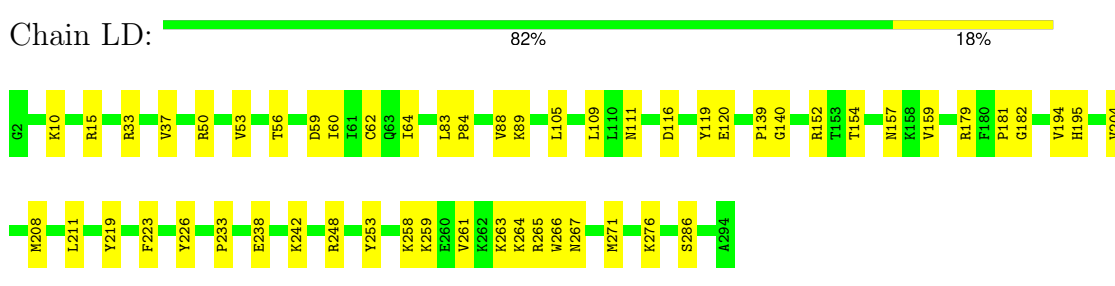
• Molecule 7: Large ribosomal subunit protein uL3



• Molecule 8: 60S ribosomal protein L4

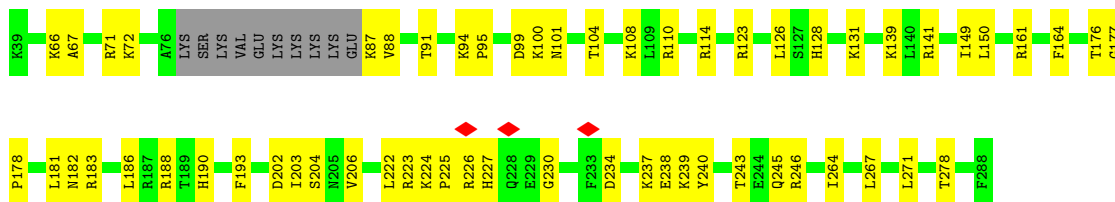


• Molecule 9: Large ribosomal subunit protein uL18



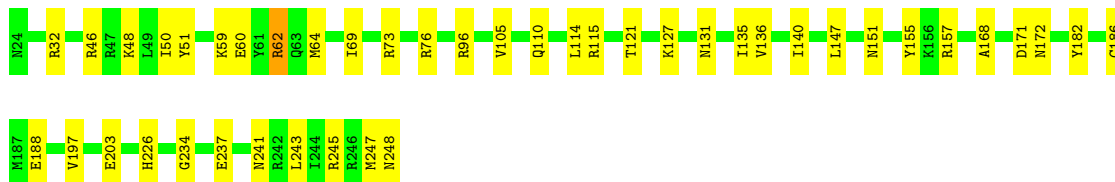
• Molecule 10: Large ribosomal subunit protein eL6





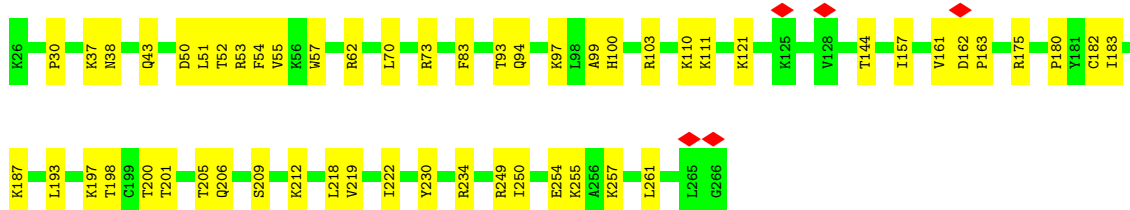
- Molecule 11: 60S ribosomal protein L7

Chain LF: 81% 19%



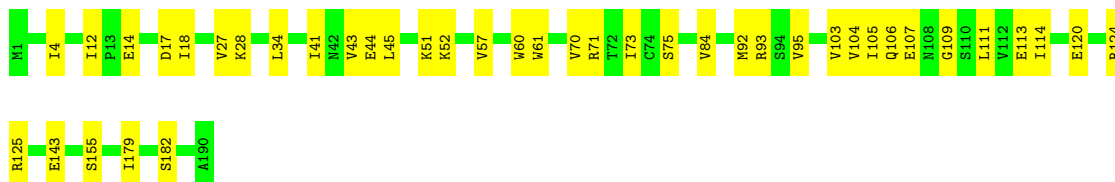
- Molecule 12: 60S ribosomal protein L7a

Chain LG: 78% 22%



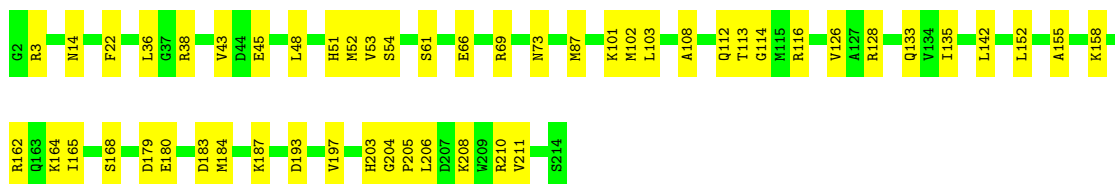
- Molecule 13: 60S ribosomal protein L9

Chain LH: 78% 22%



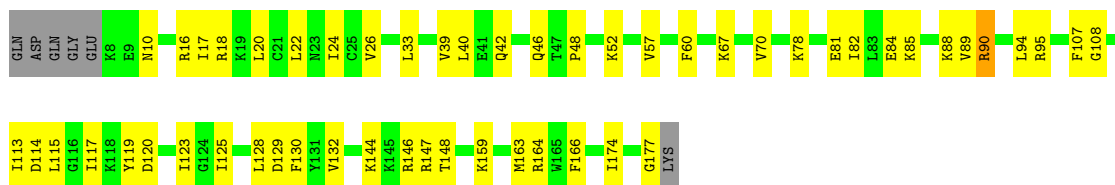
- Molecule 14: Ribosomal protein uL16-like

Chain LI: 76% 24%




- Molecule 15: 60S ribosomal protein L11

Chain LJ:  66% 30%




- Molecule 16: Large ribosomal subunit protein eL13

Chain LL:  80% 20%




- Molecule 17: 60S ribosomal protein L14

Chain LM:  79% 21%




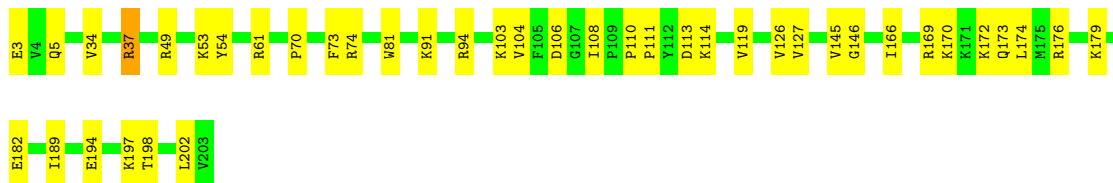
- Molecule 18: 60S ribosomal protein L15

Chain LN:  84% 15%




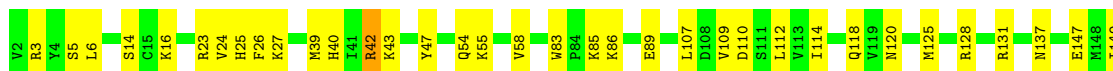
- Molecule 19: 60S ribosomal protein L13a

Chain LO:  80% 20%




- Molecule 20: 60S ribosomal protein L17

Chain LP:  75% 24%




L150  
T151  
E152  
K153  
E154

- Molecule 21: 60S ribosomal protein L18

Chain LQ:  88% 12%

G2 V3 D4 I5 K12 W13 R14 D22 L35 T39 F43 M70 V82 I86 T87 A102 R115 G133 V137 R172 K173 F174 E175 R176 A177 R178 R184 M188


- Molecule 22: 60S ribosomal protein L19

Chain LR:  74% 26%

S2 M3 L4 R5 K20 K21 T29 M30 E31 K43 L44 L49 V55 R60 M76 G77 I78 G79 K80 R81 V93 M96 R103 R104 L105 R108 S112 K113 K114 R117 Y124 V127 F132 K133 M134 R136 I137 D148 K149 K152 K153


L154 L155 Q158 K167 E168 A169 R170 K171 R172 R173 E174 E175 R176 L177 K181 E182 E183 I184 I185 K186 T187 L188

- Molecule 23: 60S ribosomal protein L18a

Chain LS:  83% 17%

K2 G5 K11 C16 T19 P20 K21 L27 Y28 M30 K52 K53 R54 F68 E69 K70 K76 R83 S86 G89 T90 M93 R98 D99 L100 R111 R118 Q125 I150 P153 L154 R157 R161 T168 F176

- Molecule 24: 60S ribosomal protein L21

Chain LT:  78% 22%

T2 R3 T4 K7 R8 R9 Y13 M14 L27 M81 K35 K43 G44 V48 K65 H68 H70 V75 K83 I84 L85 A86 K87 R88 E94 H95 R102 L106 K107 K115 A119 K122 G123 T124 L128 K129 R130 A133 P148


Y156 E157 F158 M159 A160

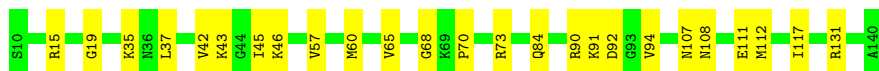
- Molecule 25: Heparin-binding protein HBp15

Chain LU:  74% 26%

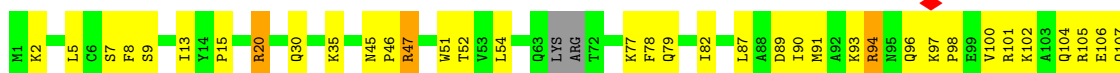
Q17 V18 L19 K20 F21 T22 L23 K48 A53 T62 I63 E64 R65 S66 K67 I70 T71 V72 T73 K80 K88 K89 Y90 N94 R97 D98 W99 L100 R101 Y110 E111 L112 I117

- Molecule 26: 60S ribosomal protein L23

Chain LV:  81% 19%



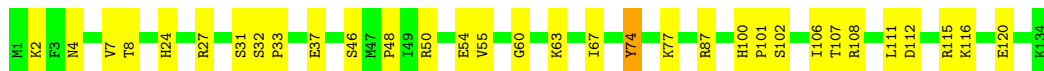
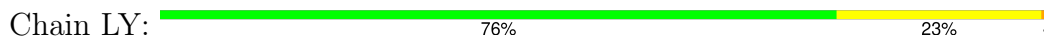
- Molecule 27: Ribosomal protein L24



- Molecule 28: 60S ribosomal protein L23a



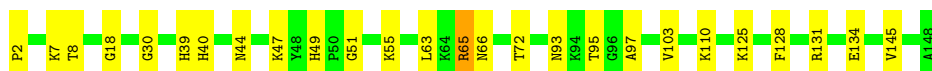
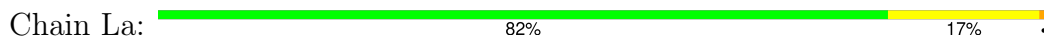
- Molecule 29: 60S ribosomal protein L26



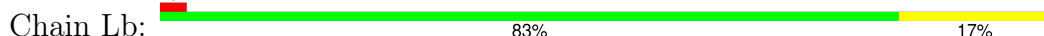
- Molecule 30: 60S ribosomal protein L27



- Molecule 31: 60S ribosomal protein L27a

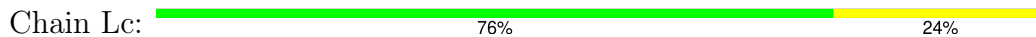


- Molecule 32: Large ribosomal subunit protein eL29





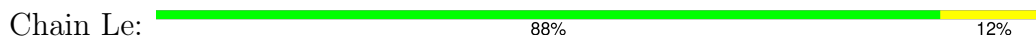
- Molecule 33: 60S ribosomal protein L30



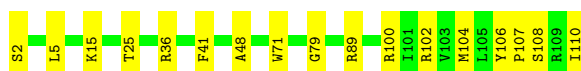
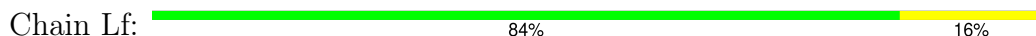
- Molecule 34: 60S ribosomal protein L31



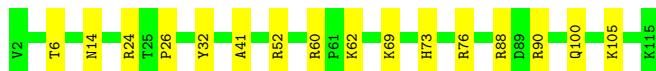
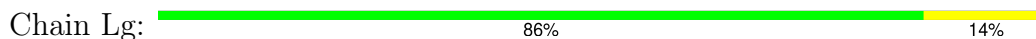
- Molecule 35: 60S ribosomal protein L32



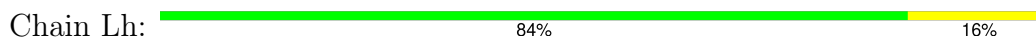
- Molecule 36: 60S ribosomal protein L35a



- Molecule 37: 60S ribosomal protein L34

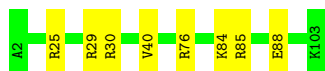


- Molecule 38: 60S ribosomal protein L35

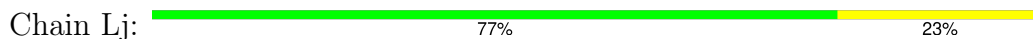


- Molecule 39: 60S ribosomal protein L36

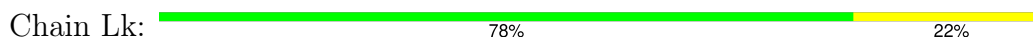




- Molecule 40: 60S ribosomal protein L37



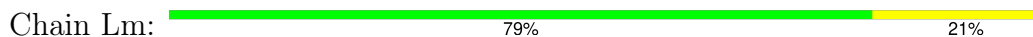
- Molecule 41: 60S ribosomal protein L38



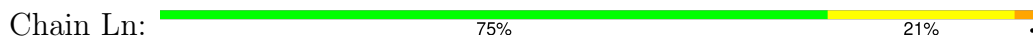
- Molecule 42: 60S ribosomal protein L39



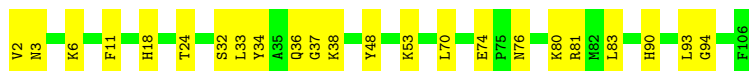
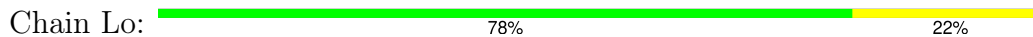
- Molecule 43: Large ribosomal subunit protein eL40



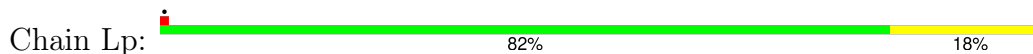
- Molecule 44: 60S ribosomal protein L41



- Molecule 45: 60S ribosomal protein L36a

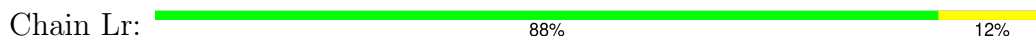


- Molecule 46: 60S ribosomal protein L37a

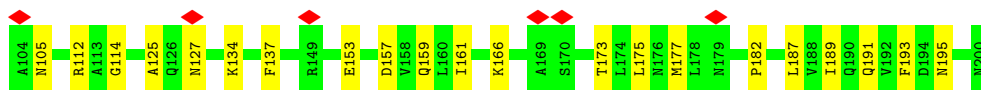
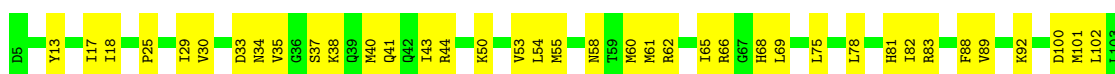




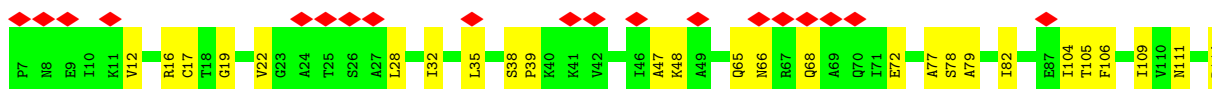
- Molecule 47: 60S ribosomal protein L28



- Molecule 48: 60S acidic ribosomal protein P0



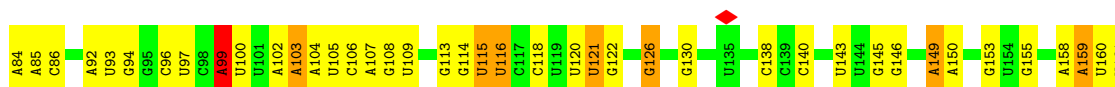
- Molecule 49: Large ribosomal subunit protein uL11

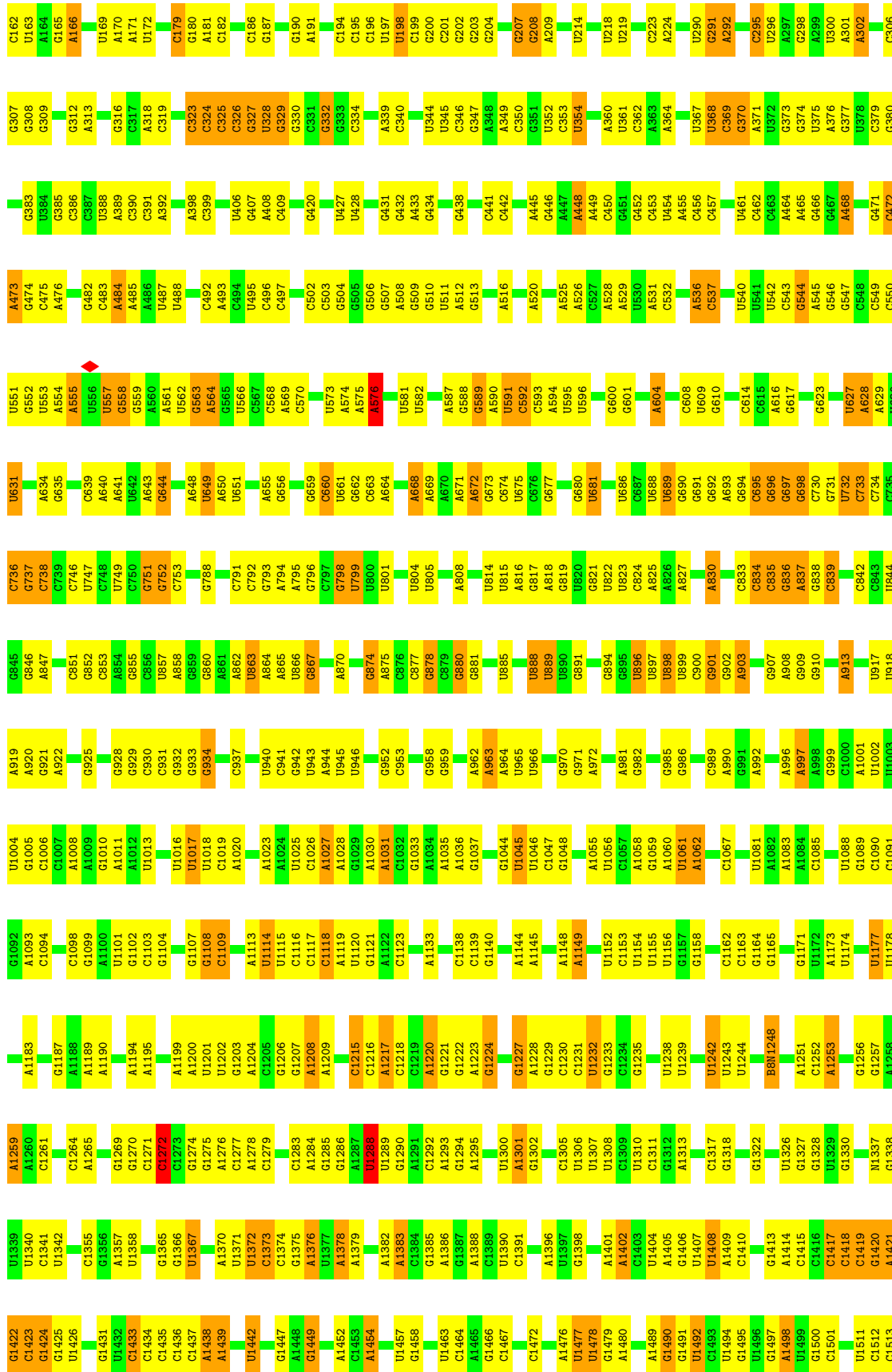


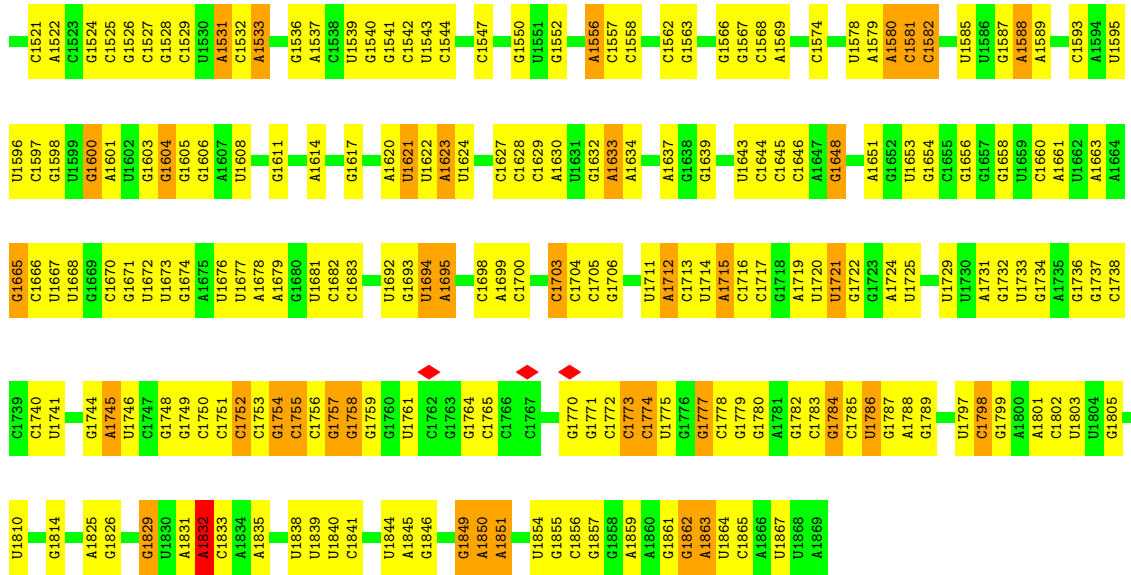
- Molecule 50: P site tRNA



- Molecule 51: 18S rRNA

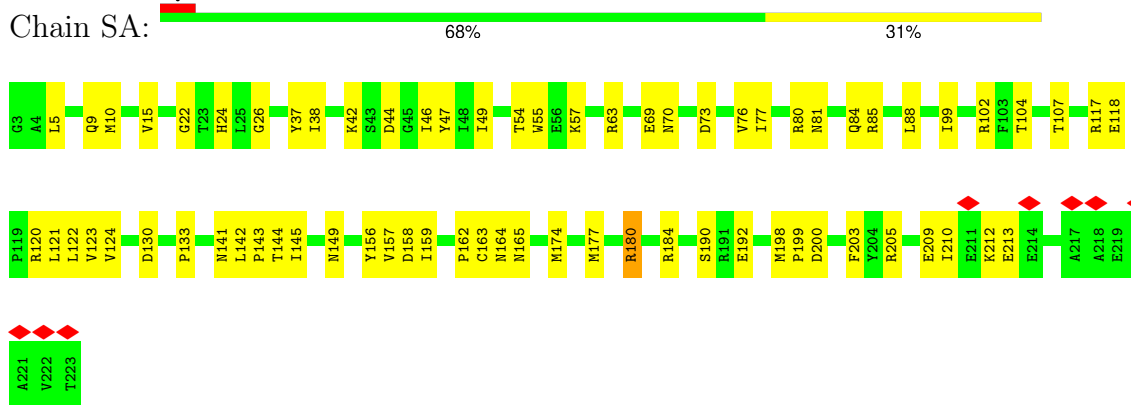






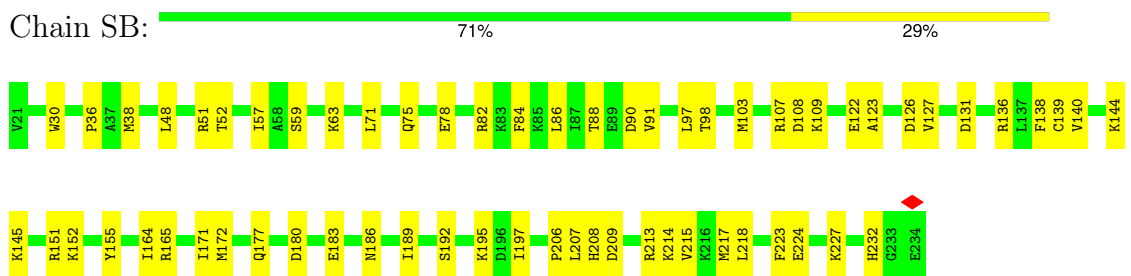
- Molecule 52: 40S ribosomal protein SA

Chain SA:



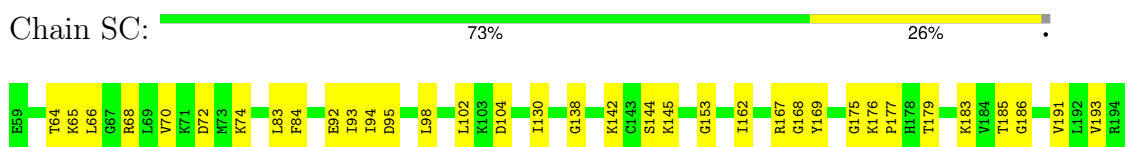
- Molecule 53: 40S ribosomal protein S3a

Chain SB:



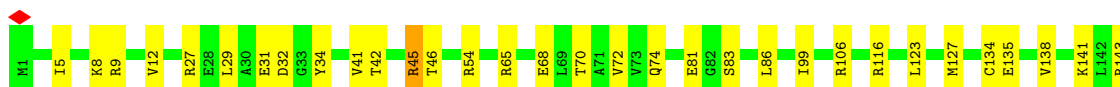
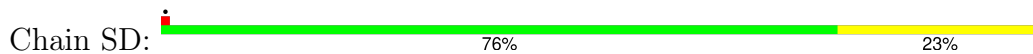
- Molecule 54: 40S ribosomal protein S2

Chain SC:





- Molecule 55: Small ribosomal subunit protein uS3



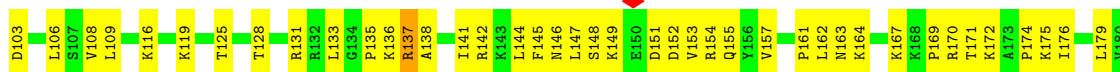
- Molecule 56: Small ribosomal subunit protein eS4, X isoform

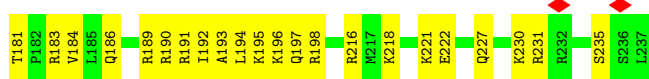


- Molecule 57: 40S ribosomal protein S5



- Molecule 58: 40S ribosomal protein S6

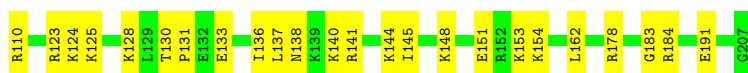




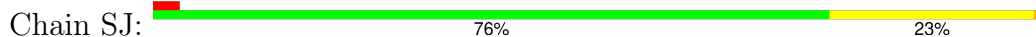
- Molecule 59: Small ribosomal subunit protein eS7



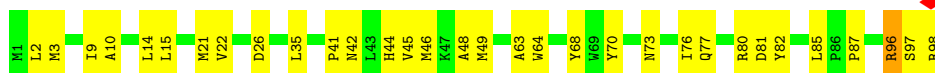
- Molecule 60: 40S ribosomal protein S8



- Molecule 61: 40S ribosomal protein S9



- Molecule 62: 40S ribosomal protein S10

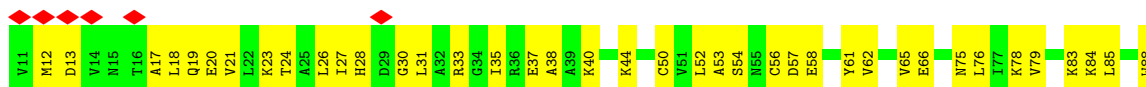


- Molecule 63: 40S ribosomal protein S11

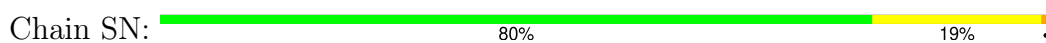




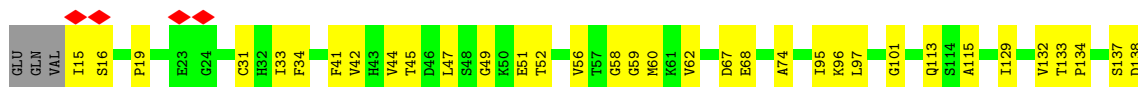
- Molecule 64: Small ribosomal subunit protein eS12



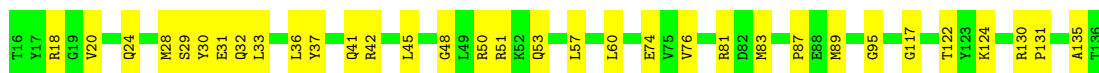
- Molecule 65: 40S ribosomal protein S13



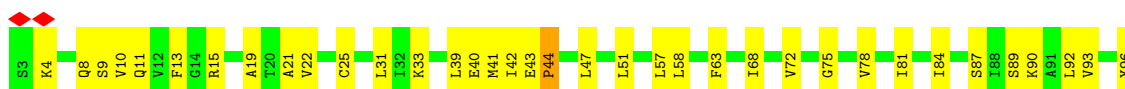
- Molecule 66: Small ribosomal subunit protein uS11



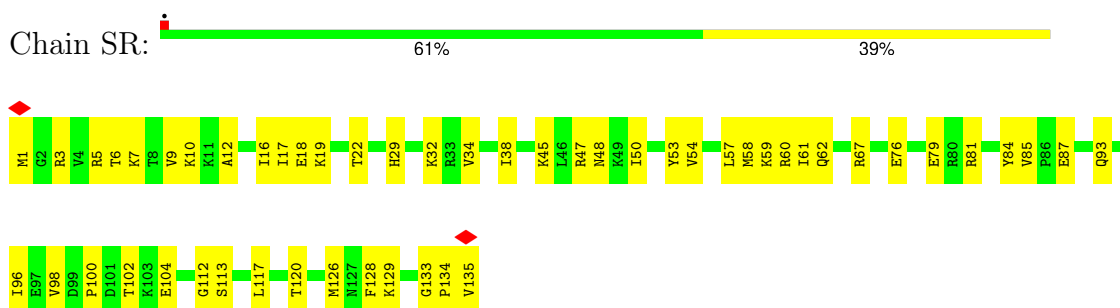
- Molecule 67: Small ribosomal subunit protein uS19



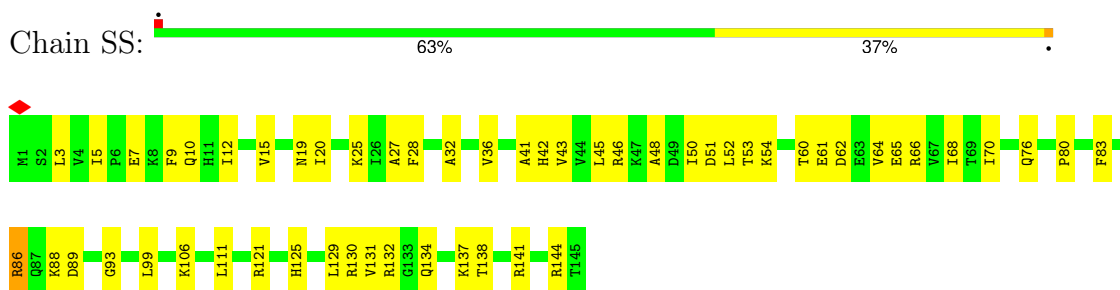
- Molecule 68: Small ribosomal subunit protein uS9



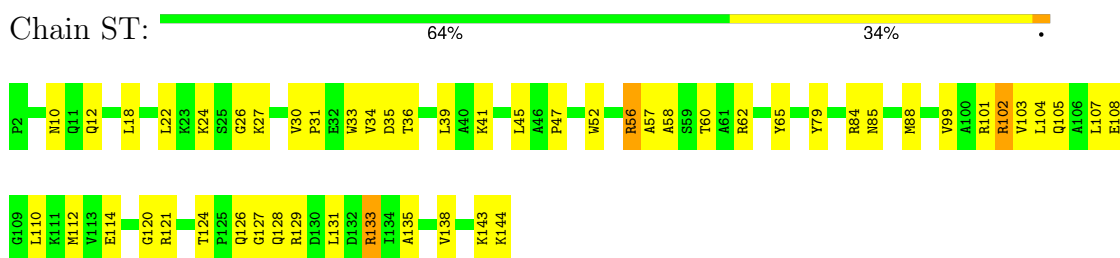
- Molecule 69: Small ribosomal subunit protein eS17



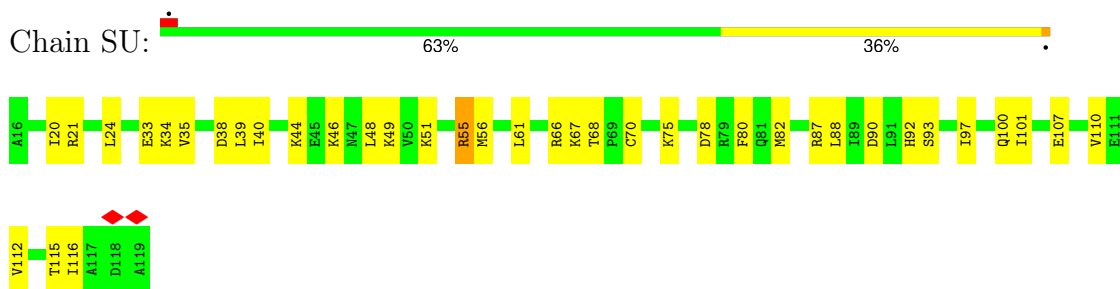
- Molecule 70: 40S ribosomal protein S18



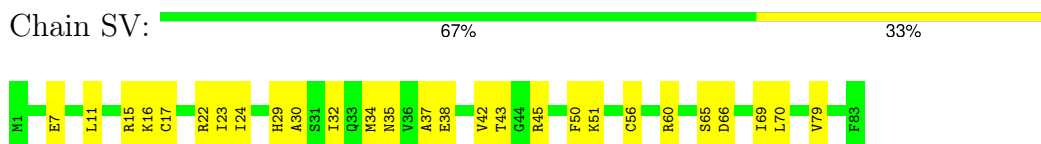
- Molecule 71: 40S ribosomal protein S19



- Molecule 72: 40S ribosomal protein S20

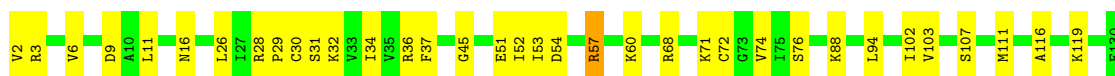


- Molecule 73: Small ribosomal subunit protein eS21




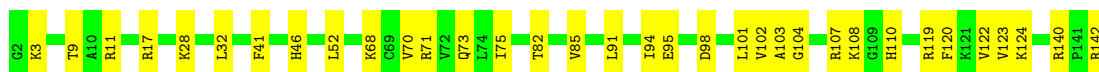
- Molecule 74: 40S ribosomal protein S15a

Chain SW:  73% 26%



- Molecule 75: 40S ribosomal protein S23

Chain SX:  76% 24%



- Molecule 76: 40S ribosomal protein S24

Chain SY:  5% 65% 35%




- Molecule 77: Small ribosomal subunit protein eS25

Chain SZ:  67% 33%




- Molecule 78: 40S ribosomal protein S26

Chain Sa:  81% 19%

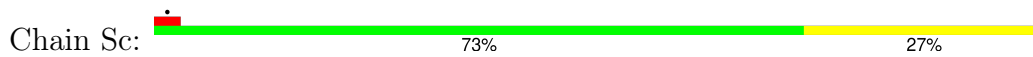


- Molecule 79: Small ribosomal subunit protein eS27

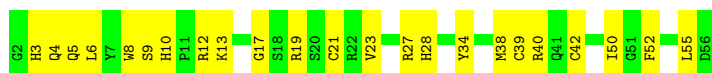
Chain Sb:  76% 24%



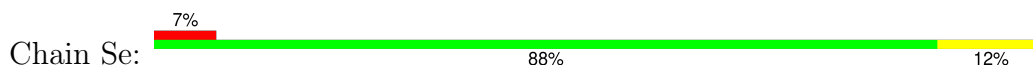
- Molecule 80: 40S ribosomal protein S28



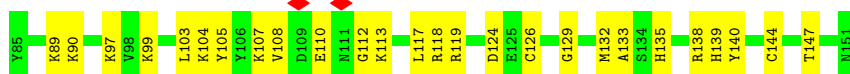
- Molecule 81: 40S ribosomal protein S29



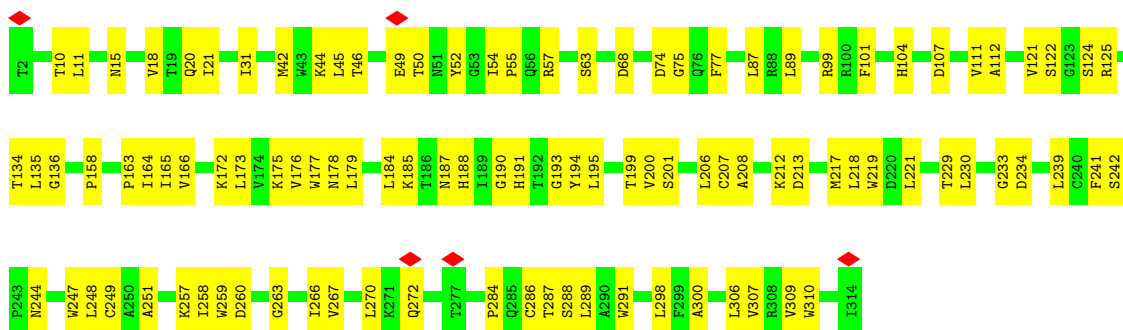
- Molecule 82: Small ribosomal subunit protein eS30



- Molecule 83: Ubiquitin-40S ribosomal protein S27a



- Molecule 84: Receptor of activated protein C kinase 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1272627	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.451	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0169	Depositor
Map size (Å)	512.64, 512.64, 512.64	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89000005, 0.89000005, 0.89000005	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: 5MC, A2M, G7M, SPD, 6MZ, OMG, 1MA, MA6, OMU, UY1, B8N, UR3, SPM, 4AC, OMC, ZN, PUT, MG, PSU, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	CD	0.42	0/394	0.61	0/534
2	CI	0.16	0/247	0.44	0/323
3	L5	0.16	0/85098	0.30	0/132762
4	L7	0.12	0/2861	0.23	0/4459
5	L8	0.13	0/3631	0.26	0/5657
6	LA	0.19	0/1936	0.39	0/2596
7	LB	0.18	0/3306	0.42	0/4424
8	LC	0.21	0/2981	0.45	1/4002 (0.0%)
9	LD	0.18	0/2428	0.36	0/3252
10	LE	0.18	0/1973	0.43	0/2645
11	LF	0.16	0/1905	0.31	0/2539
12	LG	0.21	0/1960	0.42	0/2637
13	LH	0.18	0/1537	0.39	0/2066
14	LI	0.15	0/1751	0.37	0/2340
15	LJ	0.19	0/1385	0.44	0/1852
16	LL	0.16	0/1732	0.36	0/2315
17	LM	0.18	0/1161	0.35	0/1554
18	LN	0.16	0/1746	0.37	1/2338 (0.0%)
19	LO	0.18	0/1682	0.36	0/2250
20	LP	0.19	0/1268	0.38	0/1701
21	LQ	0.16	0/1537	0.33	0/2052
22	LR	0.16	0/1582	0.38	0/2091
23	LS	0.14	0/1493	0.31	0/2003
24	LT	0.19	0/1326	0.43	0/1770
25	LU	0.21	0/839	0.53	0/1126
26	LV	0.21	0/993	0.40	0/1332
27	LW	0.18	0/959	0.48	1/1270 (0.1%)
28	LX	0.16	0/1002	0.33	0/1345
29	LY	0.19	0/1132	0.46	0/1504
30	LZ	0.18	0/1130	0.38	0/1507
31	La	0.16	0/1191	0.38	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Lb	0.17	0/889	0.38	0/1175
33	Lc	0.16	0/774	0.39	0/1038
34	Ld	0.18	0/903	0.35	0/1216
35	Le	0.15	0/1071	0.35	0/1429
36	Lf	0.17	0/895	0.37	0/1198
37	Lg	0.14	0/916	0.36	0/1220
38	Lh	0.18	0/1023	0.34	0/1351
39	Li	0.17	0/843	0.40	0/1115
40	Lj	0.17	0/720	0.41	0/952
41	Lk	0.17	0/575	0.46	0/761
42	Ll	0.18	0/454	0.39	0/599
43	Lm	0.14	0/435	0.36	0/575
44	Ln	0.18	0/231	0.32	0/294
45	Lo	0.21	0/876	0.43	0/1156
46	Lp	0.16	0/718	0.39	0/953
47	Lr	0.19	0/1017	0.35	0/1364
48	Ls	0.20	0/1519	0.44	0/2052
49	Lt	0.20	0/1009	0.54	0/1363
50	Pt	0.10	0/1761	0.24	0/2741
51	S2	0.17	0/39755	0.28	0/61935
52	SA	0.18	0/1778	0.41	0/2416
53	SB	0.20	0/1765	0.44	0/2362
54	SC	0.18	0/1744	0.42	0/2357
55	SD	0.17	0/1793	0.39	0/2414
56	SE	0.19	0/2118	0.42	0/2849
57	SF	0.21	0/1516	0.43	0/2037
58	SG	0.19	0/1946	0.42	0/2590
59	SH	0.21	0/1519	0.46	0/2033
60	SI	0.18	0/1715	0.44	0/2287
61	SJ	0.16	0/1550	0.38	0/2069
62	SK	0.19	0/851	0.41	0/1147
63	SL	0.17	0/1268	0.40	0/1696
64	SM	0.20	0/950	0.52	0/1275
65	SN	0.16	0/1232	0.33	0/1656
66	SO	0.19	0/1037	0.41	0/1391
67	SP	0.22	0/1003	0.48	0/1342
68	SQ	0.21	0/1160	0.46	0/1553
69	SR	0.18	0/1105	0.48	0/1484
70	SS	0.19	0/1216	0.44	0/1628
71	ST	0.19	0/1131	0.53	0/1515
72	SU	0.21	0/831	0.48	0/1115
73	SV	0.21	0/643	0.46	0/860
74	SW	0.22	0/1051	0.40	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	SX	0.15	0/1116	0.39	0/1490
76	SY	0.18	0/1083	0.43	0/1438
77	SZ	0.22	0/604	0.47	0/810
78	Sa	0.21	0/836	0.47	0/1121
79	Sb	0.18	0/665	0.40	0/891
80	Sc	0.21	0/508	0.46	0/680
81	Sd	0.18	0/470	0.43	0/623
82	Se	0.18	0/465	0.41	0/612
83	Sf	0.34	0/560	0.60	0/745
84	Sg	0.17	0/2493	0.40	0/3394
All	All	0.17	0/230272	0.34	3/337610 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	LA	0	2
8	LC	0	2
11	LF	0	1
15	LJ	0	1
18	LN	0	1
19	LO	0	1
20	LP	0	1
27	LW	0	2
29	LY	0	1
30	LZ	0	1
31	La	0	1
32	Lb	0	1
35	Le	0	1
42	Ll	0	1
44	Ln	0	1
52	SA	0	1
53	SB	0	1
55	SD	0	1
58	SG	0	3
60	SI	0	2
61	SJ	0	1
62	SK	0	1
65	SN	0	1
68	SQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
70	SS	0	1
71	ST	0	3
72	SU	0	1
73	SV	0	1
74	SW	0	1
82	Se	0	1
All	All	0	38

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
18	LN	143	ARG	CG-CD-NE	5.87	124.91	112.00
8	LC	33	ARG	CB-CA-C	5.46	118.46	110.87
27	LW	47	ARG	CB-CG-CD	5.17	123.20	111.30

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LA	147	ARG	Sidechain
6	LA	245	ARG	Sidechain
8	LC	33	ARG	Sidechain
8	LC	78	ARG	Sidechain
11	LF	62	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	CD	385	0	347	18	0
2	CI	247	0	283	8	0
3	L5	78445	0	39700	1235	0
4	L7	2561	0	1295	24	0
5	L8	3315	0	1685	49	0
6	LA	1898	0	1993	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	LB	3238	0	3375	102	0
8	LC	2927	0	3104	55	0
9	LD	2382	0	2410	37	0
10	LE	1935	0	2096	50	0
11	LF	1870	0	1996	33	0
12	LG	1927	0	2074	43	0
13	LH	1518	0	1601	30	0
14	LI	1711	0	1749	37	0
15	LJ	1362	0	1399	41	0
16	LL	1701	0	1818	35	0
17	LM	1138	0	1204	25	0
18	LN	1701	0	1749	28	0
19	LO	1650	0	1794	33	0
20	LP	1242	0	1269	30	0
21	LQ	1513	0	1628	20	0
22	LR	1566	0	1729	36	0
23	LS	1453	0	1490	21	0
24	LT	1298	0	1366	32	0
25	LU	825	0	850	24	0
26	LV	979	0	1039	23	0
27	LW	945	0	1003	34	0
28	LX	985	0	1066	9	0
29	LY	1115	0	1205	26	0
30	LZ	1107	0	1182	24	0
31	La	1162	0	1213	24	0
32	Lb	876	0	948	22	0
33	Lc	764	0	804	16	0
34	Ld	888	0	930	19	0
35	Le	1053	0	1147	12	0
36	Lf	876	0	912	13	0
37	Lg	906	0	998	16	0
38	Lh	1015	0	1148	20	0
39	Li	832	0	917	9	0
40	Lj	705	0	737	17	0
41	Lk	569	0	637	17	0
42	Ll	444	0	483	13	0
43	Lm	429	0	465	9	0
44	Ln	230	0	276	7	0
45	Lo	862	0	929	16	0
46	Lp	708	0	756	14	0
47	Lr	1002	0	1068	11	0
48	Ls	1496	0	1540	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Lt	998	0	1032	46	0
50	Pt	1576	0	802	20	0
51	S2	36953	0	18679	720	0
52	SA	1741	0	1746	66	0
53	SB	1738	0	1809	49	0
54	SC	1707	0	1791	44	0
55	SD	1765	0	1865	35	0
56	SE	2076	0	2177	76	0
57	SF	1495	0	1549	57	0
58	SG	1923	0	2089	93	0
59	SH	1497	0	1590	51	0
60	SI	1686	0	1772	54	0
61	SJ	1525	0	1640	37	0
62	SK	827	0	854	29	0
63	SL	1247	0	1323	44	0
64	SM	940	0	965	49	0
65	SN	1208	0	1294	24	0
66	SO	1024	0	1050	27	0
67	SP	985	0	1031	28	0
68	SQ	1142	0	1213	49	0
69	SR	1090	0	1149	48	0
70	SS	1198	0	1261	46	0
71	ST	1112	0	1146	42	0
72	SU	821	0	883	43	0
73	SV	636	0	637	28	0
74	SW	1034	0	1080	38	0
75	SX	1098	0	1167	25	0
76	SY	1065	0	1142	45	0
77	SZ	598	0	656	22	0
78	Sa	821	0	870	16	0
79	Sb	651	0	672	16	0
80	Sc	506	0	536	22	0
81	Sd	459	0	448	23	0
82	Se	459	0	503	7	0
83	Sf	548	0	551	28	0
84	Sg	2436	0	2393	78	0
85	L5	185	0	0	0	0
85	L7	3	0	0	0	0
85	L8	5	0	0	0	0
85	LA	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	Le	1	0	0	0	0
85	S2	28	0	0	0	0
86	L5	98	0	182	10	0
86	S2	14	0	26	2	0
87	L5	80	0	151	3	0
87	L8	10	0	19	0	0
87	LN	10	0	19	0	0
87	S2	20	0	38	0	0
88	L5	74	0	0	0	0
88	Lg	1	0	0	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	1	0	0	0	0
90	S2	6	0	12	0	0
91	L5	3311	0	0	17	0
91	L7	16	0	0	0	0
91	L8	118	0	0	0	0
91	LA	43	0	0	0	0
91	LB	66	0	0	1	0
91	LC	45	0	0	0	0
91	LD	1	0	0	0	0
91	LG	13	0	0	0	0
91	LH	1	0	0	0	0
91	LI	7	0	0	0	0
91	LL	33	0	0	0	0
91	LN	99	0	0	2	0
91	LO	58	0	0	1	0
91	LP	38	0	0	2	0
91	LQ	21	0	0	0	0
91	LR	12	0	0	0	0
91	LS	2	0	0	0	0
91	LT	8	0	0	0	0
91	LU	1	0	0	0	0
91	LV	41	0	0	3	0
91	LW	15	0	0	0	0
91	LX	10	0	0	0	0
91	La	38	0	0	0	0
91	Lb	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	Ld	1	0	0	0	0
91	Le	50	0	0	0	0
91	Lf	13	0	0	0	0
91	Lg	2	0	0	0	0
91	Lh	8	0	0	1	0
91	Li	10	0	0	1	0
91	Lj	29	0	0	0	0
91	Ll	5	0	0	0	0
91	Ln	2	0	0	0	0
91	Lo	37	0	0	1	0
91	Lp	4	0	0	0	0
91	Lr	3	0	0	0	0
91	Pt	6	0	0	1	0
91	S2	341	0	0	5	0
91	SE	12	0	0	2	0
91	SF	5	0	0	1	0
91	SH	1	0	0	0	0
91	SI	14	0	0	4	0
91	SJ	1	0	0	0	0
91	SL	22	0	0	0	0
91	SP	1	0	0	0	0
91	SQ	7	0	0	0	0
91	SS	8	0	0	0	0
91	ST	2	0	0	0	0
91	SU	3	0	0	0	0
91	SX	8	0	0	0	0
91	SZ	1	0	0	1	0
91	Sc	1	0	0	0	0
91	Sd	3	0	0	0	0
All	All	223497	0	163219	3936	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 10.

The worst 5 of 3936 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)
49:Lt:16:ARG:HE	49:Lt:17:CYS:H	1.12	0.94
49:Lt:16:ARG:HH12	49:Lt:28:LEU:HB3	1.31	0.94
3:L5:1974:U:OP1	49:Lt:77:ALA:HB1	1.68	0.94
68:SQ:43:GLU:HG3	68:SQ:44:PRO:HD3	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2017:A:HO2'	3:L5:2018:C:H6	0.96	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	46/50 (92%)	43 (94%)	3 (6%)	0	100	100
2	CI	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	LA	246/248 (99%)	223 (91%)	23 (9%)	0	100	100
7	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
8	LC	366/368 (100%)	347 (95%)	19 (5%)	0	100	100
9	LD	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
10	LE	236/250 (94%)	216 (92%)	20 (8%)	0	100	100
11	LF	223/225 (99%)	216 (97%)	6 (3%)	1 (0%)	30	34
12	LG	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
13	LH	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
14	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
15	LJ	168/176 (96%)	164 (98%)	4 (2%)	0	100	100
16	LL	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
17	LM	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
18	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
19	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
20	LP	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
21	LQ	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	LS	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
24	LT	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
25	LU	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
26	LV	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
27	LW	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
28	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
29	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
30	LZ	133/135 (98%)	124 (93%)	9 (7%)	0	100	100
31	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
32	Lb	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
33	Lc	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	12	11
34	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
35	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
36	Lf	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
37	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
38	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
39	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
42	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
46	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
47	Lr	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
48	Ls	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
49	Lt	128/141 (91%)	107 (84%)	21 (16%)	0	100	100
52	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
53	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
54	SC	218/222 (98%)	204 (94%)	14 (6%)	0	100	100
55	SD	225/227 (99%)	213 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	SE	260/262 (99%)	244 (94%)	16 (6%)	0	100	100
57	SF	187/189 (99%)	173 (92%)	14 (8%)	0	100	100
58	SG	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
59	SH	182/186 (98%)	166 (91%)	15 (8%)	1 (0%)	24	27
60	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
61	SJ	183/185 (99%)	169 (92%)	14 (8%)	0	100	100
62	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
63	SL	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
64	SM	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
65	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
66	SO	135/140 (96%)	129 (96%)	6 (4%)	0	100	100
67	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
68	SQ	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	18	19
69	SR	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
70	SS	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
71	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
72	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
73	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
74	SW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
75	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
76	SY	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
77	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
78	Sa	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
79	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
80	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
81	Sd	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
82	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
83	Sf	65/67 (97%)	54 (83%)	11 (17%)	0	100	100
84	Sg	311/313 (99%)	286 (92%)	25 (8%)	0	100	100
All	All	11718/11920 (98%)	11085 (95%)	629 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	LF	197	VAL
33	Lc	99	PRO
68	SQ	44	PRO
59	SH	15	LYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	41/41 (100%)	37 (90%)	4 (10%)	7	8
2	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	180/180 (100%)	180 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	176 (100%)	0	100	100
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/97 (98%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/90 (98%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/115 (93%)	107 (100%)	0	100	100
52	SA	183/183 (100%)	183 (100%)	0	100	100
53	SB	195/195 (100%)	195 (100%)	0	100	100
54	SC	186/188 (99%)	186 (100%)	0	100	100
55	SD	190/190 (100%)	190 (100%)	0	100	100
56	SE	224/224 (100%)	224 (100%)	0	100	100
57	SF	159/159 (100%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	SG	207/207 (100%)	207 (100%)	0	100	100
59	SH	166/166 (100%)	166 (100%)	0	100	100
60	SI	178/178 (100%)	178 (100%)	0	100	100
61	SJ	161/161 (100%)	161 (100%)	0	100	100
62	SK	89/89 (100%)	89 (100%)	0	100	100
63	SL	137/137 (100%)	137 (100%)	0	100	100
64	SM	102/104 (98%)	102 (100%)	0	100	100
65	SN	130/130 (100%)	130 (100%)	0	100	100
66	SO	107/110 (97%)	107 (100%)	0	100	100
67	SP	107/107 (100%)	107 (100%)	0	100	100
68	SQ	119/119 (100%)	119 (100%)	0	100	100
69	SR	122/122 (100%)	122 (100%)	0	100	100
70	SS	126/126 (100%)	126 (100%)	0	100	100
71	ST	113/113 (100%)	113 (100%)	0	100	100
72	SU	94/94 (100%)	94 (100%)	0	100	100
73	SV	67/67 (100%)	67 (100%)	0	100	100
74	SW	112/112 (100%)	112 (100%)	0	100	100
75	SX	113/113 (100%)	113 (100%)	0	100	100
76	SY	113/113 (100%)	113 (100%)	0	100	100
77	SZ	66/66 (100%)	66 (100%)	0	100	100
78	Sa	89/89 (100%)	89 (100%)	0	100	100
79	Sb	75/75 (100%)	75 (100%)	0	100	100
80	Sc	57/57 (100%)	57 (100%)	0	100	100
81	Sd	48/48 (100%)	48 (100%)	0	100	100
82	Se	47/47 (100%)	47 (100%)	0	100	100
83	Sf	60/60 (100%)	60 (100%)	0	100	100
84	Sg	272/272 (100%)	272 (100%)	0	100	100
All	All	10188/10227 (100%)	10184 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CD	391	ASP

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Mol	Chain	Res	Type
1	CD	392	VAL
1	CD	394	ASP
1	CD	396	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
61	SJ	156	HIS
79	Sb	65	GLN
64	SM	119	GLN
72	SU	92	HIS
84	Sg	226	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/5070 (71%)	706 (19%)	24 (0%)
4	L7	119/120 (99%)	10 (8%)	0
5	L8	155/156 (99%)	24 (15%)	0
50	Pt	72/74 (97%)	16 (22%)	0
51	S2	1715/1740 (98%)	379 (22%)	9 (0%)
All	All	5704/7160 (79%)	1135 (19%)	33 (0%)

5 of 1135 RNA backbone outliers are listed below:

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

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	S2	688	U
51	S2	1418	C
51	S2	1556	A
3	L5	2587	A
3	L5	2485	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMU	L5	2837	3	19,22,23	3.39	7 (36%)	25,31,34	1.83	5 (20%)
3	PSU	L5	3695	3,88	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
51	6MZ	S2	1832	85,51	26,26,26	2.80	5 (19%)	36,39,39	2.47	13 (36%)
3	A2M	L5	3830	3	22,25,26	1.24	1 (4%)	30,36,39	1.60	6 (20%)
3	A2M	L5	1534	85,3	22,25,26	1.24	2 (9%)	30,36,39	1.46	6 (20%)
51	OMU	S2	1326	51	19,22,23	3.36	7 (36%)	25,31,34	1.82	5 (20%)
51	PSU	S2	1174	51	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
3	5MC	L5	3782	85,3	19,22,23	0.51	0	26,32,35	0.67	0
3	PSU	L5	4312	3	18,21,22	1.14	1 (5%)	21,30,33	1.90	5 (23%)
51	OMU	S2	1288	51	19,22,23	3.34	7 (36%)	25,31,34	1.75	5 (20%)
3	OMG	L5	4623	3	23,26,27	0.48	0	32,38,41	0.61	0
3	PSU	L5	4973	3	18,21,22	1.12	1 (5%)	21,30,33	1.92	5 (23%)
3	PSU	L5	5001	3	18,21,22	1.17	1 (5%)	21,30,33	1.79	4 (19%)
51	PSU	S2	93	51	18,21,22	1.13	1 (5%)	21,30,33	1.84	4 (19%)
51	OMG	S2	436	51	23,26,27	0.47	0	32,38,41	0.54	0
3	A2M	L5	3867	3	22,25,26	1.24	1 (4%)	30,36,39	1.50	8 (26%)
3	OMC	L5	4456	3	19,22,23	0.55	0	25,31,34	0.63	0
3	OMG	L5	2364	85,3	23,26,27	0.47	0	32,38,41	0.45	0
51	MA6	S2	1851	51	23,26,27	1.27	2 (8%)	33,38,41	3.23	12 (36%)
3	6MZ	L5	4220	3	26,26,26	2.78	5 (19%)	36,39,39	2.83	17 (47%)
51	A2M	S2	668	85,51	22,25,26	1.34	2 (9%)	30,36,39	1.59	6 (20%)
51	4AC	S2	1842	51	21,24,25	0.36	0	28,34,37	0.40	0
3	PSU	L5	4689	3	18,21,22	1.12	1 (5%)	21,30,33	1.99	4 (19%)
3	OMC	L5	3869	3	19,22,23	0.50	0	25,31,34	0.69	0
3	PSU	L5	4293	3	18,21,22	1.15	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L5	4471	3	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
51	PSU	S2	651	51	18,21,22	1.12	1 (5%)	21,30,33	1.89	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	PSU	S2	1045	51	18,21,22	1.11	1 (5%)	21,30,33	1.81	4 (19%)
3	PSU	L5	3853	85,3,88	18,21,22	1.09	1 (5%)	21,30,33	1.78	4 (19%)
3	PSU	L5	4403	3,88	18,21,22	1.13	1 (5%)	21,30,33	1.96	6 (28%)
51	PSU	S2	686	51	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
51	OMG	S2	867	51	23,26,27	0.50	0	32,38,41	0.48	0
51	PSU	S2	109	51	18,21,22	1.15	1 (5%)	21,30,33	1.90	5 (23%)
51	OMU	S2	172	51	19,22,23	3.40	7 (36%)	25,31,34	1.84	5 (20%)
3	A2M	L5	1871	85,3	22,25,26	1.22	1 (4%)	30,36,39	1.48	6 (20%)
3	OMG	L5	1316	3	23,26,27	0.48	0	32,38,41	0.56	0
3	OMC	L5	3841	3	19,22,23	0.49	0	25,31,34	0.60	0
3	PSU	L5	4361	3	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
51	PSU	S2	105	51	18,21,22	1.14	1 (5%)	21,30,33	1.80	4 (19%)
3	1MA	L5	1322	85,3	21,25,26	0.50	0	30,37,40	0.77	1 (3%)
3	PSU	L5	1683	3,88	18,21,22	1.15	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L5	5010	3	18,21,22	1.14	1 (5%)	21,30,33	1.88	5 (23%)
3	PSU	L5	4442	3	18,21,22	1.14	1 (5%)	21,30,33	1.94	6 (28%)
3	PSU	L5	4521	85,3,88	18,21,22	1.15	1 (5%)	21,30,33	1.92	5 (23%)
3	A2M	L5	4571	3	22,25,26	1.28	2 (9%)	30,36,39	1.59	7 (23%)
3	A2M	L5	1326	3	22,25,26	1.23	2 (9%)	30,36,39	1.36	5 (16%)
3	PSU	L5	1582	3	18,21,22	1.11	1 (5%)	21,30,33	1.79	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
51	PSU	S2	1177	51	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
3	OMC	L5	2861	3	19,22,23	0.51	0	25,31,34	0.82	1 (4%)
3	PSU	L5	3851	3	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
3	UY1	L5	3818	3,88	19,22,23	4.92	10 (52%)	21,31,34	2.01	5 (23%)
51	OMC	S2	1391	51	19,22,23	0.50	0	25,31,34	0.71	0
3	A2M	L5	2815	3	22,25,26	1.23	2 (9%)	30,36,39	1.41	6 (20%)
51	OMC	S2	174	51	19,22,23	0.48	0	25,31,34	0.65	0
3	OMG	L5	3792	3	23,26,27	0.46	0	32,38,41	0.51	0
3	PSU	L5	4299	3	18,21,22	1.11	1 (5%)	21,30,33	1.87	5 (23%)
3	PSU	L5	4628	3	18,21,22	1.08	1 (5%)	21,30,33	1.86	4 (19%)
3	A2M	L5	3785	85,3	22,25,26	1.18	1 (4%)	30,36,39	1.63	10 (33%)
3	OMU	L5	3925	3	19,22,23	3.39	7 (36%)	25,31,34	1.81	4 (16%)
51	OMG	S2	509	51	23,26,27	0.46	0	32,38,41	0.51	0
3	PSU	L5	3822	3	18,21,22	1.14	1 (5%)	21,30,33	1.89	6 (28%)
3	A2M	L5	398	3	22,25,26	1.26	2 (9%)	30,36,39	1.59	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	L5	1677	3	18,21,22	1.21	2 (11%)	21,30,33	1.99	6 (28%)
3	OMG	L5	4499	3	23,26,27	0.44	0	32,38,41	0.47	0
3	OMG	L5	4618	3	23,26,27	0.48	0	32,38,41	0.53	0
3	OMG	L5	2876	3	23,26,27	0.47	0	32,38,41	0.51	0
51	OMG	S2	1328	51	23,26,27	0.46	0	32,38,41	0.46	0
3	PSU	L5	4532	3	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
3	OMG	L5	3744	3	23,26,27	0.46	0	32,38,41	0.49	0
51	B8N	S2	1248	51	25,29,30	3.27	6 (24%)	28,42,45	1.99	8 (28%)
51	PSU	S2	1244	51	18,21,22	1.11	1 (5%)	21,30,33	1.88	5 (23%)
3	PSU	L5	3844	3	18,21,22	1.18	1 (5%)	21,30,33	1.87	4 (19%)
51	G7M	S2	1639	50,51	23,26,27	2.68	8 (34%)	34,39,42	2.61	11 (32%)
5	PSU	L8	55	5	18,21,22	1.14	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L5	2632	3	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.13	1 (5%)	21,30,33	1.92	5 (23%)
51	PSU	S2	814	51	18,21,22	1.09	1 (5%)	21,30,33	1.76	4 (19%)
3	OMG	L5	2424	3	23,26,27	0.46	0	32,38,41	0.45	0
3	PSU	L5	3639	3	18,21,22	1.13	1 (5%)	21,30,33	1.93	5 (23%)
3	5MC	L5	4447	3,88	19,22,23	0.67	0	26,32,35	0.62	0
3	UR3	L5	4530	3	19,22,23	2.78	7 (36%)	26,32,35	1.57	3 (11%)
3	A2M	L5	400	3	22,25,26	1.27	1 (4%)	30,36,39	1.56	7 (23%)
3	PSU	L5	1536	3	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
51	PSU	S2	1232	51	18,21,22	1.15	1 (5%)	21,30,33	1.91	5 (23%)
3	OMG	L5	4494	3	23,26,27	0.47	0	32,38,41	0.51	0
3	OMU	L5	4620	3	19,22,23	3.34	7 (36%)	25,31,34	1.66	4 (16%)
51	MA6	S2	1850	51	23,26,27	1.27	2 (8%)	33,38,41	3.14	11 (33%)
51	PSU	S2	1056	51	18,21,22	1.14	1 (5%)	21,30,33	1.93	6 (28%)
51	OMC	S2	462	51	19,22,23	0.50	0	25,31,34	0.69	0
3	OMC	L5	3887	3	19,22,23	0.51	0	25,31,34	0.67	0
51	A2M	S2	159	51	22,25,26	1.20	1 (4%)	30,36,39	1.52	5 (16%)
51	OMU	S2	428	51	19,22,23	3.33	7 (36%)	25,31,34	1.77	5 (20%)
51	OMG	S2	683	51	23,26,27	0.49	0	32,38,41	0.49	0
51	OMC	S2	1272	51	19,22,23	0.56	0	25,31,34	0.91	2 (8%)
3	OMG	L5	1625	3,88	23,26,27	0.47	0	32,38,41	0.48	0
3	OMG	L5	3627	3	23,26,27	0.46	0	32,38,41	0.56	0
51	PSU	S2	406	51	18,21,22	1.14	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L5	1782	3	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
51	OMU	S2	1442	51	19,22,23	3.40	7 (36%)	25,31,34	1.77	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMG	L5	4392	3	23,26,27	0.44	0	32,38,41	0.50	0
3	PSU	L5	4500	3	18,21,22	1.16	1 (5%)	21,30,33	1.87	4 (19%)
5	PSU	L8	69	5	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)
51	OMG	S2	1490	51	23,26,27	0.50	0	32,38,41	0.53	0
3	PSU	L5	3637	3,88	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
51	A2M	S2	484	51	22,25,26	1.24	2 (9%)	30,36,39	1.51	7 (23%)
3	PSU	L5	4493	3,88	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
3	A2M	L5	2401	3	22,25,26	1.25	1 (4%)	30,36,39	1.61	6 (20%)
3	OMC	L5	2824	3	19,22,23	0.50	0	25,31,34	0.68	0
51	OMC	S2	1703	51	19,22,23	0.50	0	25,31,34	0.51	0
3	A2M	L5	2363	85,3	22,25,26	1.18	1 (4%)	30,36,39	1.48	6 (20%)
51	PSU	S2	1046	51	18,21,22	1.13	1 (5%)	21,30,33	1.80	5 (23%)
51	PSU	S2	649	51	18,21,22	1.13	1 (5%)	21,30,33	1.91	5 (23%)
51	PSU	S2	1004	51	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
3	OMC	L5	1340	3	19,22,23	0.52	0	25,31,34	0.76	0
51	OMU	S2	121	51	19,22,23	3.33	7 (36%)	25,31,34	1.67	5 (20%)
3	A2M	L5	4523	85,3	22,25,26	1.26	1 (4%)	30,36,39	1.54	6 (20%)
51	PSU	S2	966	85,51	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
3	OMC	L5	3808	3	19,22,23	0.52	0	25,31,34	0.79	1 (4%)
51	A2M	S2	27	51	22,25,26	1.25	2 (9%)	30,36,39	1.40	4 (13%)
51	OMC	S2	517	51	19,22,23	0.49	0	25,31,34	0.70	0
3	OMU	L5	4227	3	19,22,23	3.39	7 (36%)	25,31,34	1.79	4 (16%)
3	PSU	L5	4673	85,3	18,21,22	1.13	1 (5%)	21,30,33	1.88	5 (23%)
51	A2M	S2	166	51	22,25,26	1.27	2 (9%)	30,36,39	1.48	4 (13%)
3	PSU	L5	4576	3	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
3	PSU	L5	4579	3	18,21,22	1.11	1 (5%)	21,30,33	1.90	5 (23%)
3	OMG	L5	1522	3	23,26,27	0.48	0	32,38,41	0.62	0
51	A2M	S2	1383	51	22,25,26	1.25	1 (4%)	30,36,39	1.61	6 (20%)
51	PSU	S2	866	51	18,21,22	1.13	1 (5%)	21,30,33	1.92	5 (23%)
51	OMU	S2	354	51	19,22,23	3.33	7 (36%)	25,31,34	1.78	5 (20%)
51	OMU	S2	627	51	19,22,23	3.39	7 (36%)	25,31,34	1.80	5 (20%)
51	OMU	S2	799	51	19,22,23	3.44	7 (36%)	25,31,34	1.79	5 (20%)
51	OMG	S2	644	51	23,26,27	0.45	0	32,38,41	0.50	0
3	OMG	L5	4370	3	23,26,27	0.47	0	32,38,41	0.52	0
3	OMC	L5	2351	3	19,22,23	0.53	0	25,31,34	0.88	1 (4%)
3	A2M	L5	3825	3	22,25,26	1.24	1 (4%)	30,36,39	1.57	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	L5	2839	3	18,21,22	1.13	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L5	3920	85,3	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
51	PSU	S2	1081	51	18,21,22	1.13	1 (5%)	21,30,33	1.75	5 (23%)
3	OMG	L5	4637	3,88	23,26,27	0.47	0	32,38,41	0.49	0
3	PSU	L5	1860	3	18,21,22	1.12	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L5	2365	85,3	19,22,23	0.49	0	25,31,34	0.59	0
3	PSU	L5	4296	3	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
51	4AC	S2	1337	51	21,24,25	0.38	0	28,34,37	0.56	0
51	PSU	S2	863	51	18,21,22	1.11	1 (5%)	21,30,33	1.80	4 (19%)
3	A2M	L5	1323	3	22,25,26	1.23	2 (9%)	30,36,39	1.46	5 (16%)
3	PSU	L5	4636	3	18,21,22	1.14	1 (5%)	21,30,33	2.02	6 (28%)
3	A2M	L5	2787	3	22,25,26	1.24	1 (4%)	30,36,39	1.52	7 (23%)
3	PSU	L5	4353	3	18,21,22	1.13	1 (5%)	21,30,33	1.93	6 (28%)
3	PSU	L5	3884	3	18,21,22	1.15	1 (5%)	21,30,33	1.92	5 (23%)
51	A2M	S2	576	51	22,25,26	1.25	2 (9%)	30,36,39	1.53	5 (16%)
51	OMG	S2	601	51	23,26,27	0.45	0	32,38,41	0.46	0
51	PSU	S2	1367	51	18,21,22	1.13	1 (5%)	21,30,33	1.88	5 (23%)
3	OMG	L5	4228	3	23,26,27	0.48	0	32,38,41	0.62	0
3	OMC	L5	2422	85,3	19,22,23	0.50	0	25,31,34	0.64	0
3	OMU	L5	4498	3,88	19,22,23	3.32	7 (36%)	25,31,34	1.77	5 (20%)
51	A2M	S2	1031	51	22,25,26	1.21	2 (9%)	30,36,39	1.46	4 (13%)
3	OMG	L5	4196	50,3	23,26,27	0.47	0	32,38,41	0.47	0
3	OMG	L5	3899	3	23,26,27	0.50	0	32,38,41	0.54	0
3	PSU	L5	1792	3	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.30	2 (9%)	30,36,39	1.53	6 (20%)
3	OMC	L5	2804	3	19,22,23	0.49	0	25,31,34	0.72	0
51	PSU	S2	801	51	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
3	OMU	L5	4306	3	19,22,23	3.32	7 (36%)	25,31,34	1.79	4 (16%)
3	PSU	L5	4431	3	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
3	OMC	L5	3701	3,88	19,22,23	0.58	0	25,31,34	1.52	4 (16%)
3	PSU	L5	4457	3	18,21,22	1.12	1 (5%)	21,30,33	1.84	5 (23%)
3	OMC	L5	4536	3	19,22,23	0.53	0	25,31,34	0.70	0
3	A2M	L5	3718	3	22,25,26	1.20	2 (9%)	30,36,39	1.48	4 (13%)
51	A2M	S2	99	85,51	22,25,26	1.25	2 (9%)	30,36,39	1.41	4 (13%)
51	OMU	S2	116	51	19,22,23	3.33	7 (36%)	25,31,34	1.67	5 (20%)
3	PSU	L5	1781	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L5	4972	3	18,21,22	1.13	1 (5%)	21,30,33	1.89	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	OMG	L8	75	5	23,26,27	0.46	0	32,38,41	0.47	0
3	A2M	L5	4590	3	22,25,26	1.22	1 (4%)	30,36,39	1.53	6 (20%)
51	A2M	S2	468	51	22,25,26	1.26	1 (4%)	30,36,39	1.57	6 (20%)
51	PSU	S2	681	51	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	1744	85,3	18,21,22	1.13	1 (5%)	21,30,33	1.91	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3695	3,88	-	0/7/25/26	0/2/2/2
51	6MZ	S2	1832	85,51	-	5/12/28/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1534	85,3	-	1/9/27/28	0/3/3/3
51	OMU	S2	1326	51	-	0/9/27/28	0/2/2/2
51	PSU	S2	1174	51	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
51	OMU	S2	1288	51	-	2/9/27/28	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
51	PSU	S2	93	51	-	0/7/25/26	0/2/2/2
51	OMG	S2	436	51	-	0/9/27/28	0/3/3/3
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	2364	85,3	-	3/9/27/28	0/3/3/3
51	MA6	S2	1851	51	-	1/11/29/30	0/3/3/3
3	6MZ	L5	4220	3	-	1/12/28/28	0/3/3/3
51	A2M	S2	668	85,51	-	3/9/27/28	0/3/3/3
51	4AC	S2	1842	51	-	0/11/29/30	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
51	PSU	S2	651	51	-	0/7/25/26	0/2/2/2
51	PSU	S2	1045	51	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	85,3,88	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4403	3,88	-	0/7/25/26	0/2/2/2
51	PSU	S2	686	51	-	0/7/25/26	0/2/2/2
51	OMG	S2	867	51	-	3/9/27/28	0/3/3/3
51	PSU	S2	109	51	-	0/7/25/26	0/2/2/2
51	OMU	S2	172	51	-	0/9/27/28	0/2/2/2
3	A2M	L5	1871	85,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
51	PSU	S2	105	51	-	0/7/25/26	0/2/2/2
3	1MA	L5	1322	85,3	-	0/7/25/26	0/3/3/3
3	PSU	L5	1683	3,88	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	85,3,88	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
51	PSU	S2	1177	51	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
3	UY1	L5	3818	3,88	-	3/9/27/28	0/2/2/2
51	OMC	S2	1391	51	-	1/9/27/28	0/2/2/2
3	A2M	L5	2815	3	-	1/9/27/28	0/3/3/3
51	OMC	S2	174	51	-	0/9/27/28	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	85,3	-	0/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
51	OMG	S2	509	51	-	0/9/27/28	0/3/3/3
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
51	OMG	S2	1328	51	-	1/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	B8N	S2	1248	51	-	4/16/34/35	0/2/2/2
51	PSU	S2	1244	51	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
51	G7M	S2	1639	50,51	-	2/7/25/26	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
51	PSU	S2	814	51	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3,88	-	4/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
51	PSU	S2	1232	51	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2
51	MA6	S2	1850	51	-	1/11/29/30	0/3/3/3
51	PSU	S2	1056	51	-	0/7/25/26	0/2/2/2
51	OMC	S2	462	51	-	0/9/27/28	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
51	A2M	S2	159	51	-	1/9/27/28	0/3/3/3
51	OMU	S2	428	51	-	4/9/27/28	0/2/2/2
51	OMG	S2	683	51	-	0/9/27/28	0/3/3/3
51	OMC	S2	1272	51	-	4/9/27/28	0/2/2/2
3	OMG	L5	1625	3,88	-	2/9/27/28	0/3/3/3
3	OMG	L5	3627	3	-	1/9/27/28	0/3/3/3
51	PSU	S2	406	51	-	0/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
51	OMU	S2	1442	51	-	2/9/27/28	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	4/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
51	OMG	S2	1490	51	-	2/9/27/28	0/3/3/3
3	PSU	L5	3637	3,88	-	0/7/25/26	0/2/2/2
51	A2M	S2	484	51	-	0/9/27/28	0/3/3/3
3	PSU	L5	4493	3,88	-	0/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
51	OMC	S2	1703	51	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	2363	85,3	-	0/9/27/28	0/3/3/3
51	PSU	S2	1046	51	-	0/7/25/26	0/2/2/2
51	PSU	S2	649	51	-	0/7/25/26	0/2/2/2
51	PSU	S2	1004	51	-	0/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
51	OMU	S2	121	51	-	0/9/27/28	0/2/2/2
3	A2M	L5	4523	85,3	-	0/9/27/28	0/3/3/3
51	PSU	S2	966	85,51	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
51	A2M	S2	27	51	-	1/9/27/28	0/3/3/3
51	OMC	S2	517	51	-	0/9/27/28	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4673	85,3	-	0/7/25/26	0/2/2/2
51	A2M	S2	166	51	-	0/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
51	A2M	S2	1383	51	-	3/9/27/28	0/3/3/3
51	PSU	S2	866	51	-	0/7/25/26	0/2/2/2
51	OMU	S2	354	51	-	1/9/27/28	0/2/2/2
51	OMU	S2	627	51	-	6/9/27/28	0/2/2/2
51	OMU	S2	799	51	-	0/9/27/28	0/2/2/2
51	OMG	S2	644	51	-	4/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2351	3	-	3/9/27/28	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	85,3	-	0/7/25/26	0/2/2/2
51	PSU	S2	1081	51	-	1/7/25/26	0/2/2/2
3	OMG	L5	4637	3,88	-	2/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	85,3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4296	3	-	1/7/25/26	0/2/2/2
51	4AC	S2	1337	51	-	1/11/29/30	0/2/2/2
51	PSU	S2	863	51	-	2/7/25/26	0/2/2/2
3	A2M	L5	1323	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A2M	S2	576	51	-	3/9/27/28	0/3/3/3
51	OMG	S2	601	51	-	1/9/27/28	0/3/3/3
51	PSU	S2	1367	51	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2422	85,3	-	2/9/27/28	0/2/2/2
3	OMU	L5	4498	3,88	-	0/9/27/28	0/2/2/2
51	A2M	S2	1031	51	-	0/9/27/28	0/3/3/3
3	OMG	L5	4196	50,3	-	1/9/27/28	0/3/3/3
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
51	PSU	S2	801	51	-	1/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	3,88	-	6/9/27/28	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
51	A2M	S2	99	85,51	-	1/9/27/28	0/3/3/3
51	OMU	S2	116	51	-	1/9/27/28	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	5	-	1/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	3/9/27/28	0/3/3/3
51	A2M	S2	468	51	-	1/9/27/28	0/3/3/3
51	PSU	S2	681	51	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	85,3	-	0/7/25/26	0/2/2/2

The worst 5 of 274 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C6-C5	12.88	1.49	1.35
51	S2	1832	6MZ	C6-N6	12.60	1.48	1.34
3	L5	4220	6MZ	C6-N6	12.45	1.48	1.34
3	L5	3818	UY1	C2-N1	11.74	1.52	1.36
51	S2	799	OMU	C2-N1	8.65	1.52	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S2	1851	MA6	N1-C6-N6	-11.22	103.19	116.86
51	S2	1850	MA6	N1-C6-N6	-10.69	103.84	116.86
51	S2	1832	6MZ	OP3-P-O5'	7.75	126.89	106.67
51	S2	1639	G7M	C1'-N9-C4	7.73	149.31	126.49
51	S2	1639	G7M	C1'-N9-C8	-7.65	100.91	126.74

There are no chirality outliers.

5 of 139 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L8	75	OMG	C1'-C2'-O2'-CM2
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1340	OMC	C1'-C2'-O2'-CM2
3	L5	1625	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

82 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	S2	1832	6MZ	2	0
3	L5	1534	A2M	2	0
51	S2	1288	OMU	1	0
3	L5	5001	PSU	1	0
3	L5	3867	A2M	4	0
3	L5	4456	OMC	1	0
3	L5	4220	6MZ	4	0
3	L5	4689	PSU	1	0
3	L5	3869	OMC	1	0
3	L5	4293	PSU	1	0
51	S2	867	OMG	1	0
3	L5	1871	A2M	1	0
3	L5	3841	OMC	1	0
3	L5	1683	PSU	3	0
3	L5	4442	PSU	1	0
3	L5	4521	PSU	1	0
3	L5	4571	A2M	2	0
3	L5	1326	A2M	3	0
51	S2	1177	PSU	1	0
3	L5	2861	OMC	1	0
3	L5	3818	UY1	1	0
51	S2	1391	OMC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2815	A2M	3	0
3	L5	3785	A2M	1	0
3	L5	3925	OMU	1	0
51	S2	509	OMG	6	0
3	L5	4618	OMG	1	0
3	L5	2876	OMG	2	0
51	S2	1328	OMG	1	0
3	L5	2632	PSU	1	0
3	L5	2424	OMG	1	0
3	L5	4447	5MC	1	0
3	L5	400	A2M	1	0
51	S2	1232	PSU	2	0
3	L5	4620	OMU	4	0
51	S2	1850	MA6	3	0
51	S2	462	OMC	3	0
51	S2	159	A2M	2	0
51	S2	1272	OMC	1	0
3	L5	1625	OMG	1	0
3	L5	4500	PSU	1	0
51	S2	1490	OMG	1	0
3	L5	3637	PSU	1	0
51	S2	484	A2M	2	0
51	S2	1703	OMC	1	0
3	L5	2363	A2M	1	0
51	S2	649	PSU	1	0
3	L5	1340	OMC	2	0
51	S2	121	OMU	4	0
3	L5	4523	A2M	1	0
51	S2	27	A2M	2	0
3	L5	4227	OMU	1	0
51	S2	166	A2M	1	0
3	L5	4579	PSU	2	0
51	S2	1383	A2M	1	0
51	S2	354	OMU	1	0
51	S2	644	OMG	1	0
3	L5	2351	OMC	2	0
3	L5	3825	A2M	1	0
3	L5	3920	PSU	1	0
3	L5	4637	OMG	1	0
51	S2	1337	4AC	3	0
3	L5	4636	PSU	1	0
51	S2	576	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	S2	601	OMG	2	0
51	S2	1367	PSU	1	0
51	S2	1031	A2M	1	0
3	L5	4196	OMG	1	0
3	L5	2804	OMC	1	0
3	L5	4306	OMU	1	0
3	L5	4431	PSU	1	0
3	L5	3701	OMC	1	0
3	L5	4457	PSU	1	0
3	L5	4536	OMC	1	0
3	L5	3718	A2M	5	0
51	S2	99	A2M	3	0
51	S2	116	OMU	4	0
3	L5	1781	PSU	1	0
5	L8	75	OMG	1	0
3	L5	4590	A2M	1	0
51	S2	468	A2M	1	0
51	S2	681	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 328 ligands modelled in this entry, 307 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	SPM	L5	5291	-	13,13,13	0.35	0	12,12,12	0.74	0
87	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.85	0
86	SPM	L5	5259	-	13,13,13	0.36	0	12,12,12	0.95	0
86	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.95	0
87	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.77	0
86	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.83	0
87	SPD	S2	1931	-	9,9,9	0.32	0	8,8,8	0.77	0
87	SPD	L5	5283	85	9,9,9	0.32	0	8,8,8	0.85	0
86	SPM	L5	5267	-	13,13,13	0.35	0	12,12,12	0.97	0
87	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.86	0
87	SPD	S2	1930	-	9,9,9	0.31	0	8,8,8	0.83	0
86	SPM	L5	5264	-	13,13,13	0.34	0	12,12,12	0.98	0
87	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.75	0
87	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.84	0
87	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.85	0
90	PUT	S2	1932	-	5,5,5	0.24	0	4,4,4	0.52	0
87	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.68	0
87	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.94	0
86	SPM	S2	1929	-	13,13,13	0.35	0	12,12,12	1.02	0
86	SPM	L5	5288	-	13,13,13	0.36	0	12,12,12	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPM	L5	5291	-	-	2/11/11/11	-
87	SPD	L5	5287	-	-	1/7/7/7	-
86	SPM	L5	5259	-	-	1/11/11/11	-
86	SPM	L5	5263	-	-	4/11/11/11	-
87	SPD	L5	5285	-	-	4/7/7/7	-
87	SPD	L5	5284	-	-	2/7/7/7	-
86	SPM	L5	5292	-	-	3/11/11/11	-
87	SPD	S2	1931	-	-	4/7/7/7	-
87	SPD	L5	5283	85	-	1/7/7/7	-
86	SPM	L5	5267	-	-	4/11/11/11	-
87	SPD	L8	202	-	-	2/7/7/7	-
87	SPD	S2	1930	-	-	2/7/7/7	-
86	SPM	L5	5264	-	-	3/11/11/11	-
87	SPD	LN	301	-	-	1/7/7/7	-
87	SPD	L5	5286	-	-	2/7/7/7	-
87	SPD	L5	5289	-	-	1/7/7/7	-
90	PUT	S2	1932	-	-	0/3/3/3	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	L5	5290	-	-	3/7/7/7	-
87	SPD	L5	5261	-	-	0/7/7/7	-
86	SPM	S2	1929	-	-	5/11/11/11	-
86	SPM	L5	5288	-	-	6/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

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

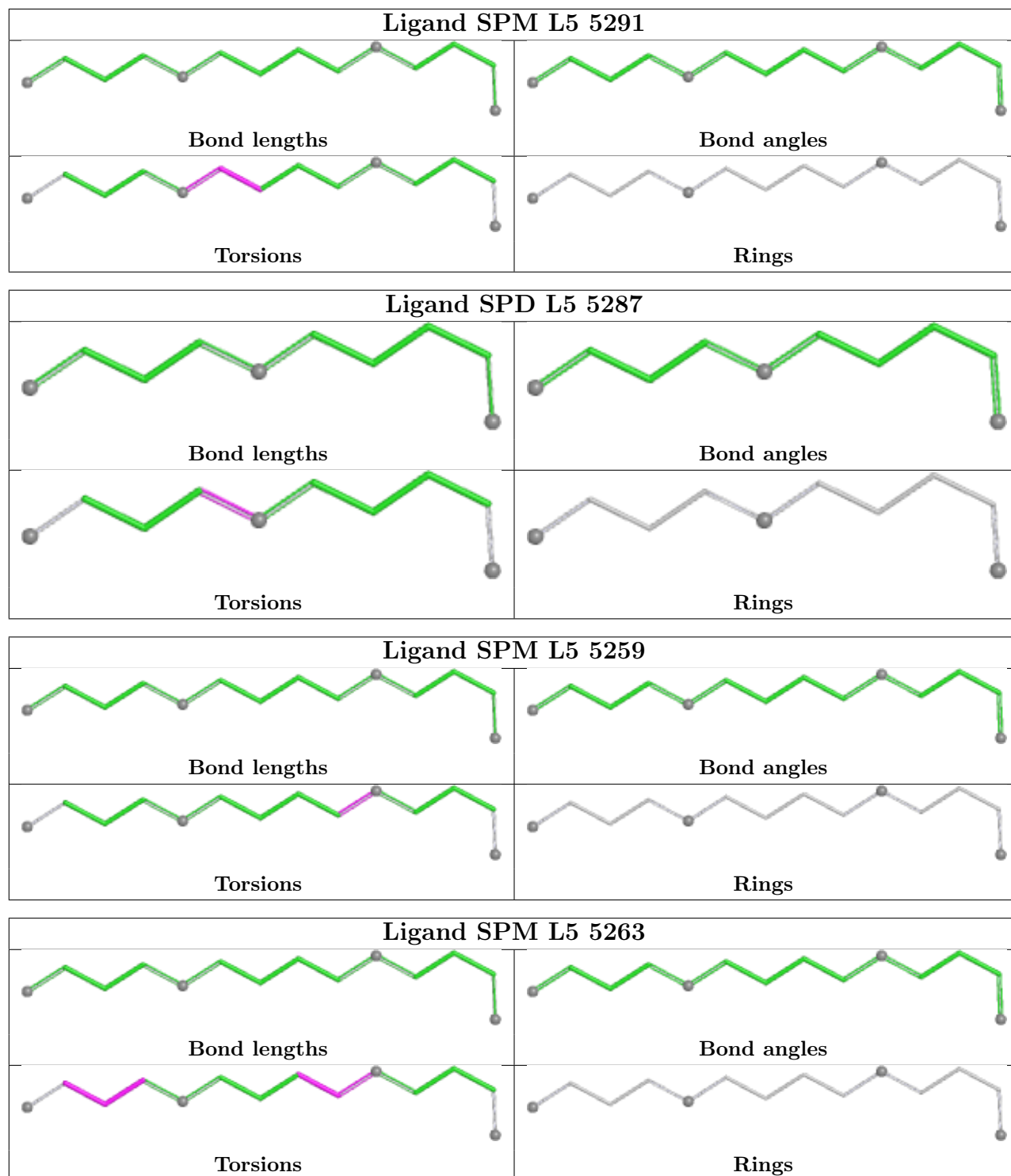
There are no ring outliers.

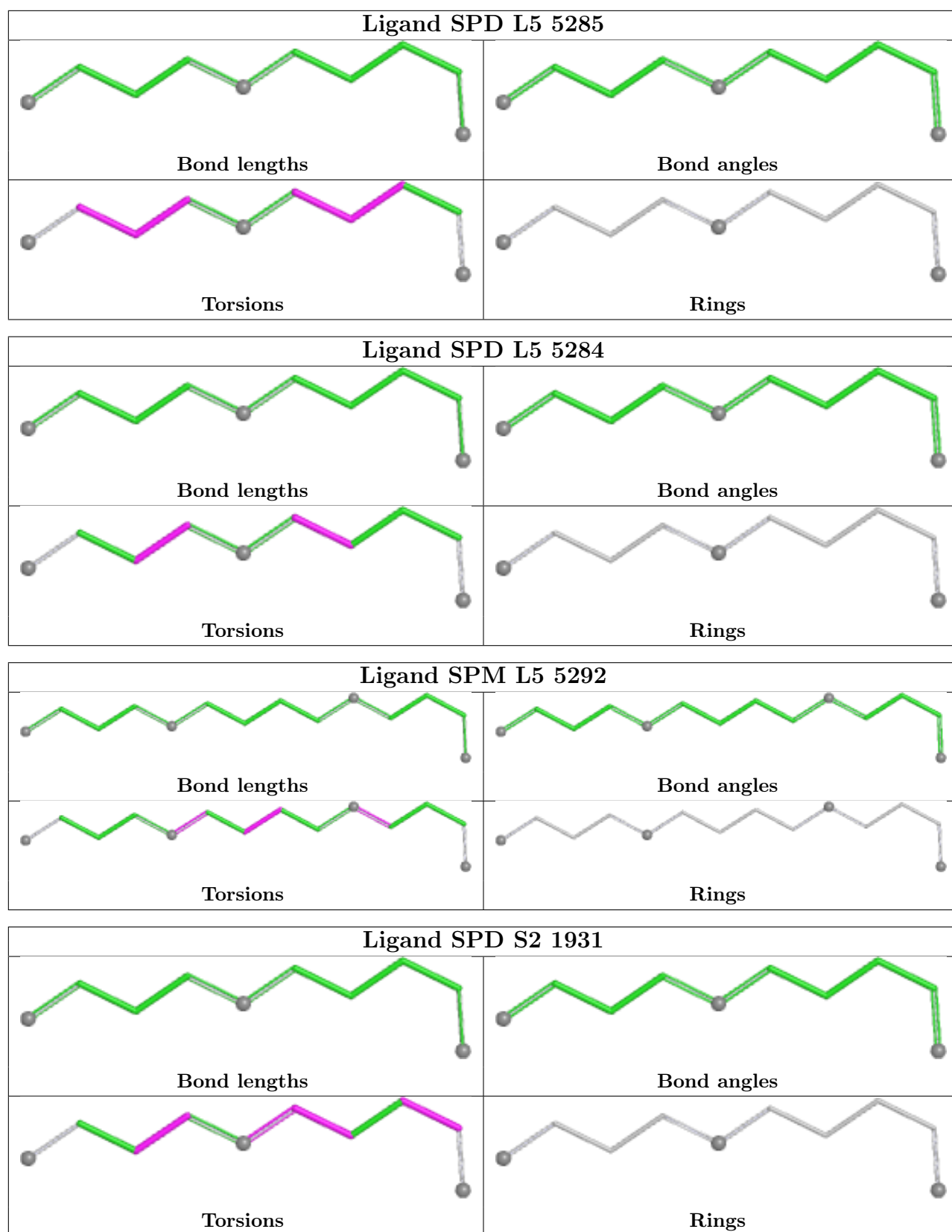
9 monomers are involved in 15 short contacts:

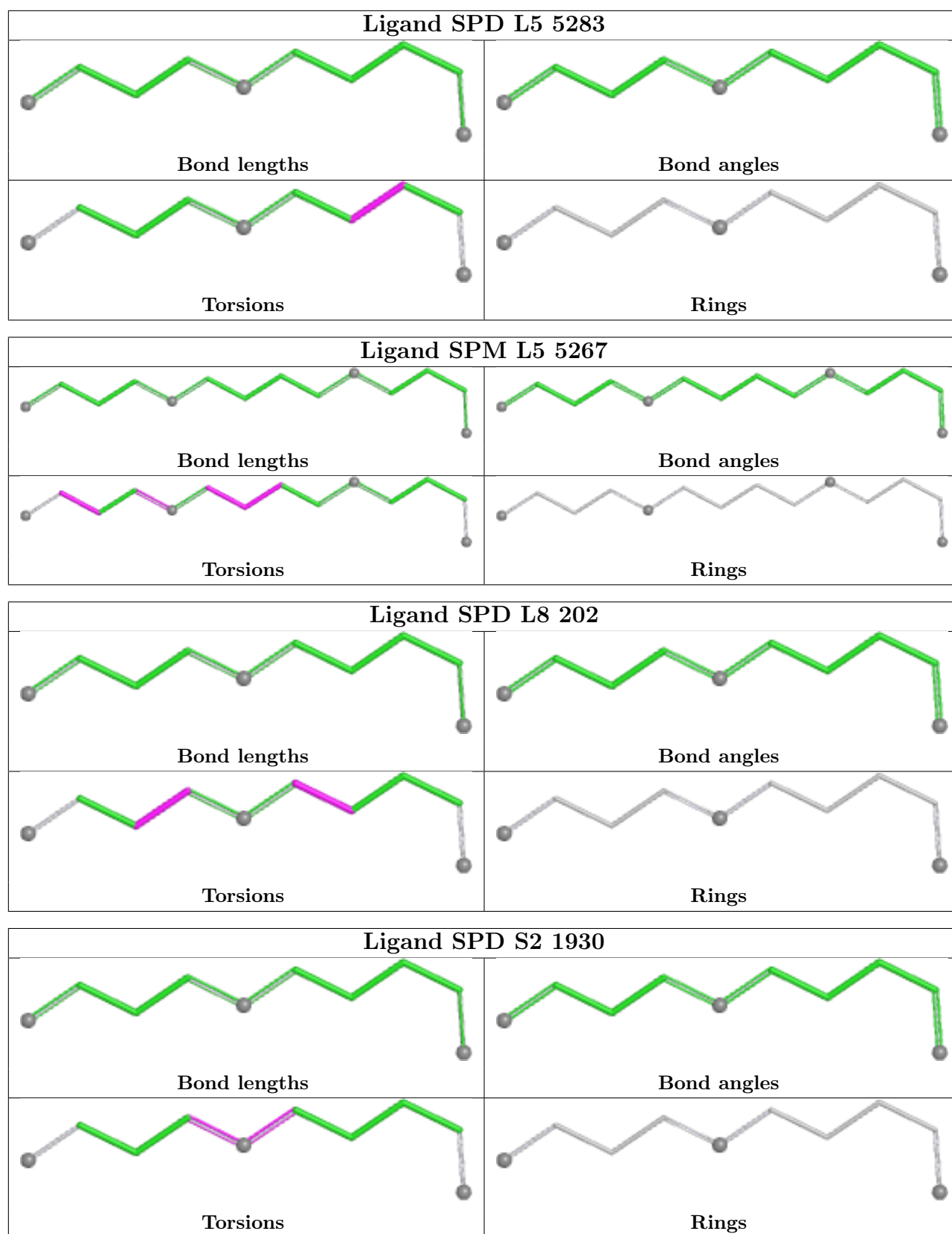
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5291	SPM	1	0
86	L5	5259	SPM	2	0
87	L5	5284	SPD	1	0
86	L5	5292	SPM	4	0
86	L5	5264	SPM	2	0
87	L5	5290	SPD	1	0
87	L5	5261	SPD	1	0
86	S2	1929	SPM	2	0
86	L5	5288	SPM	1	0

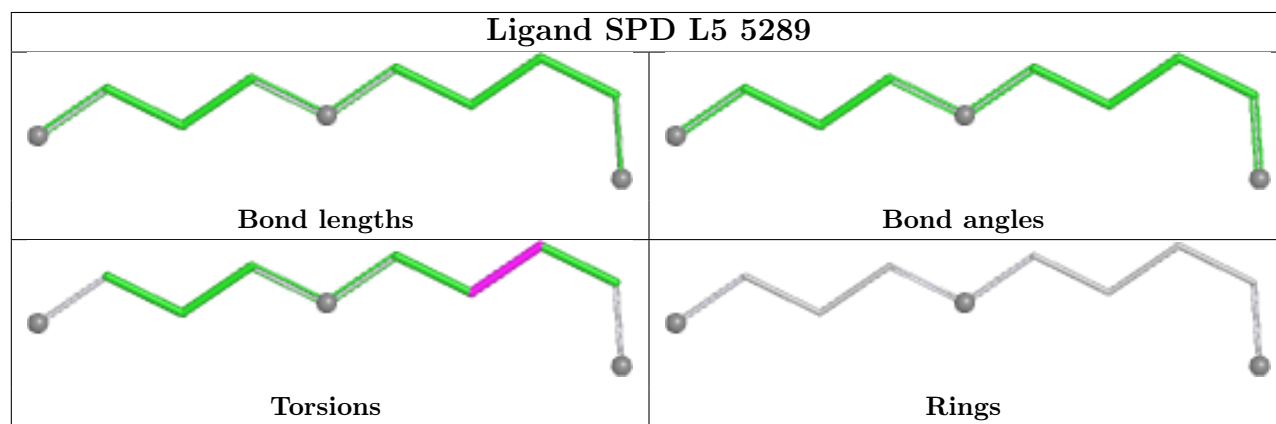
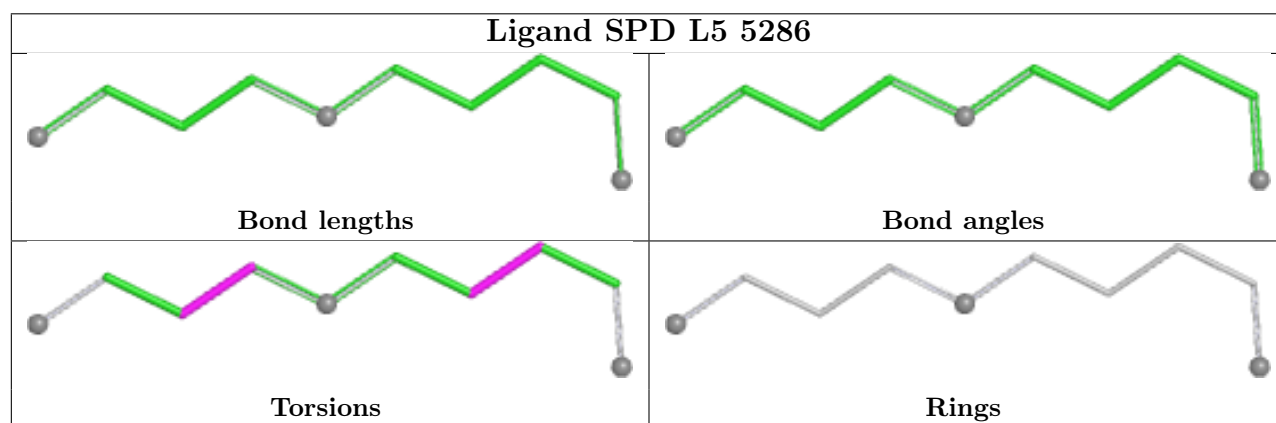
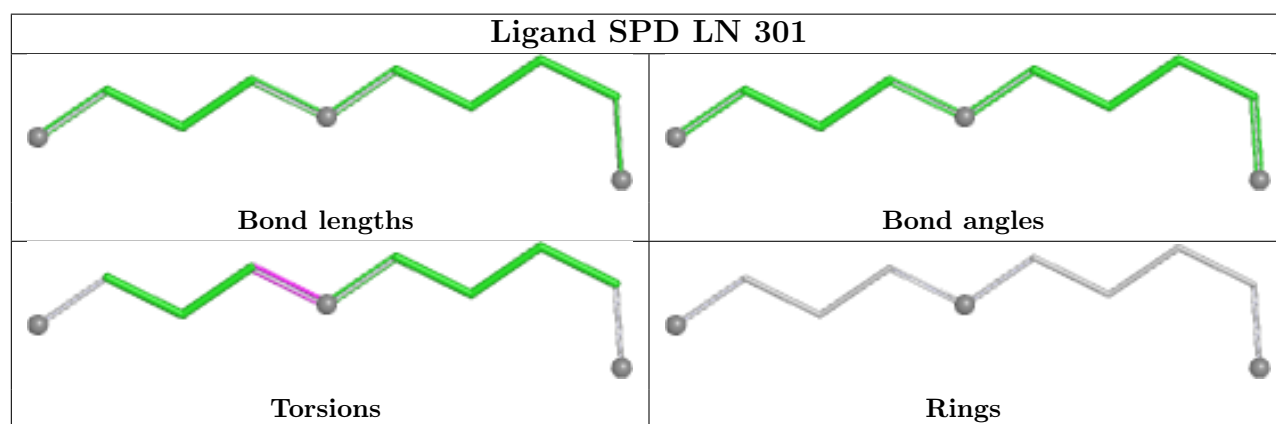
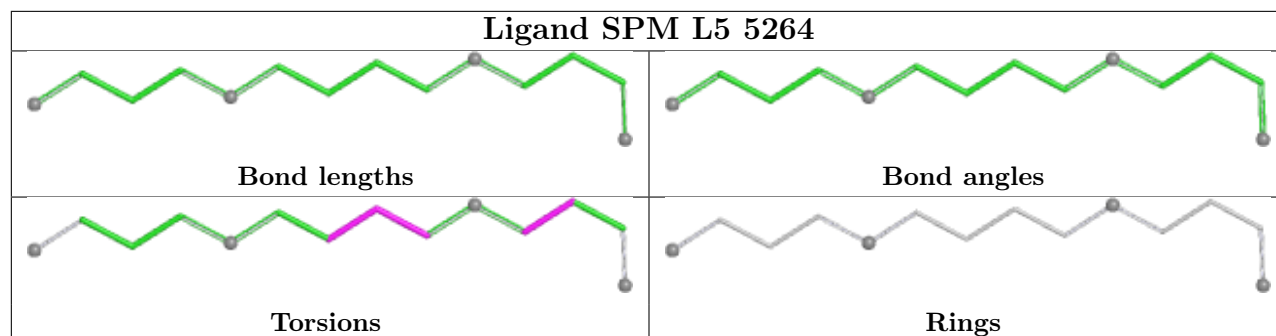
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

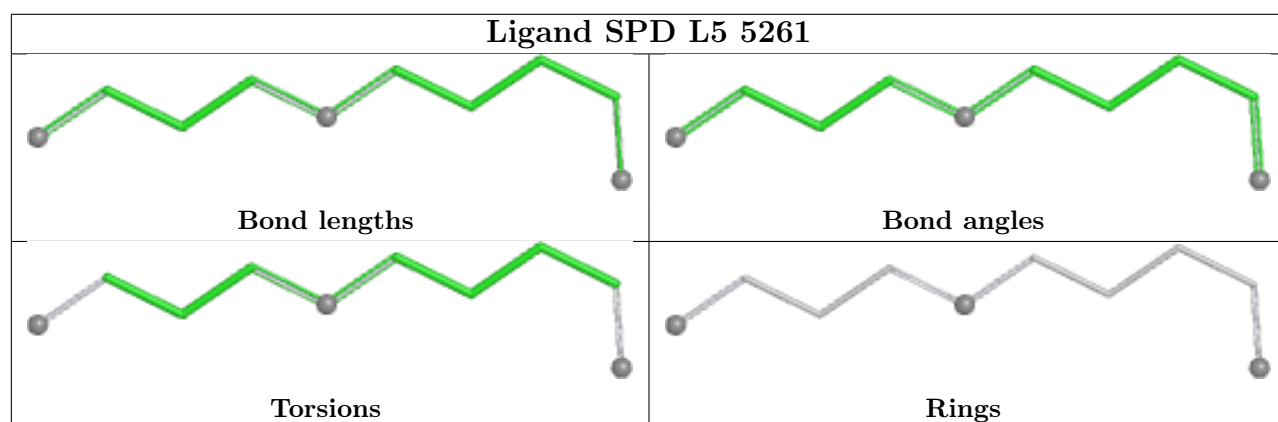
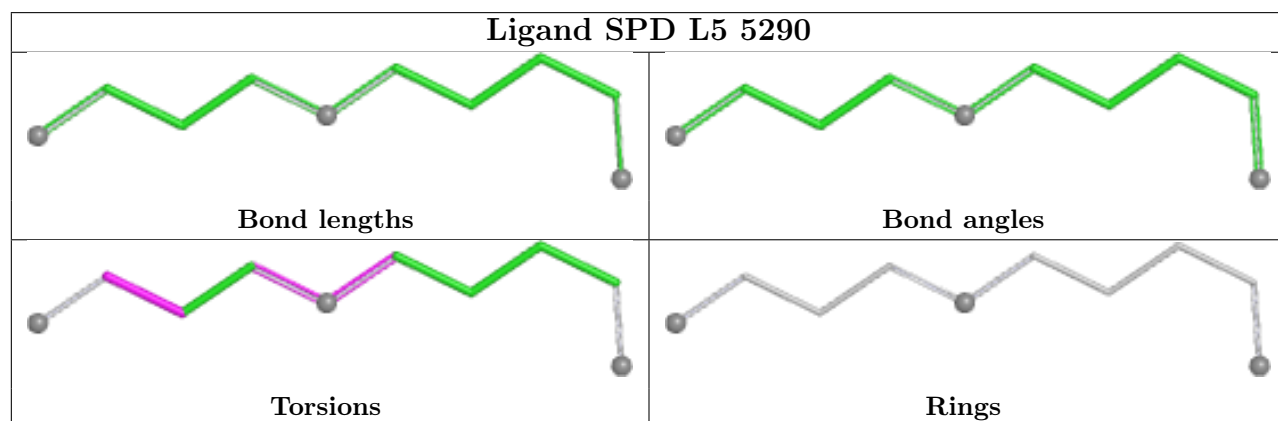
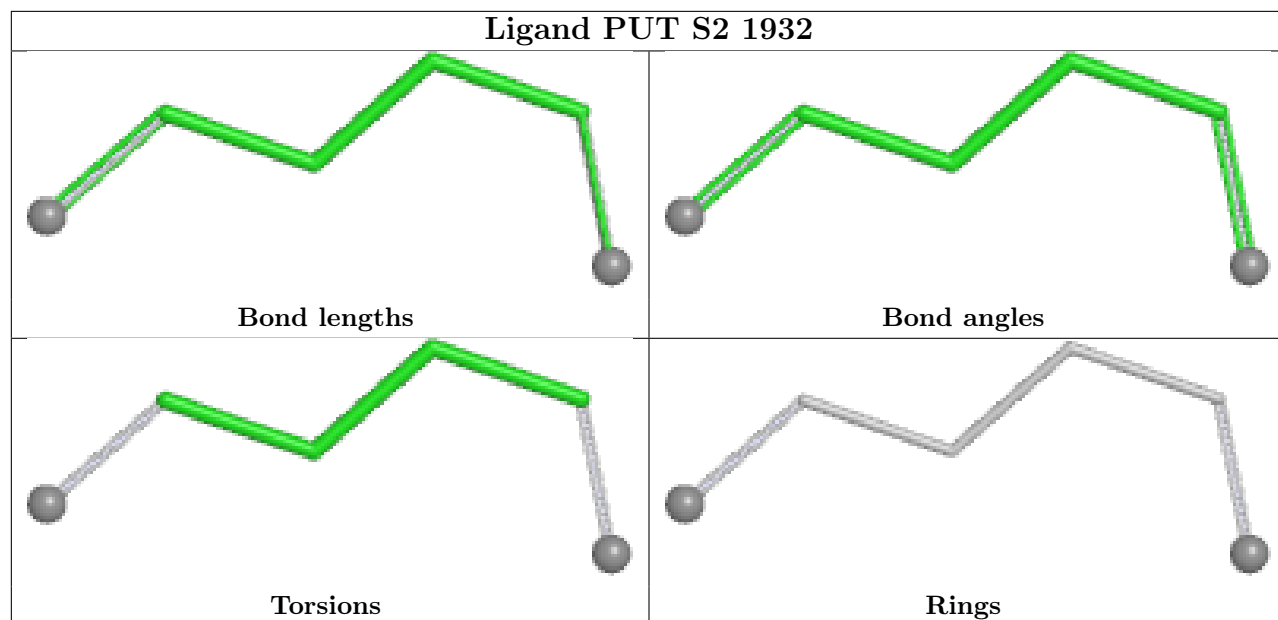
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

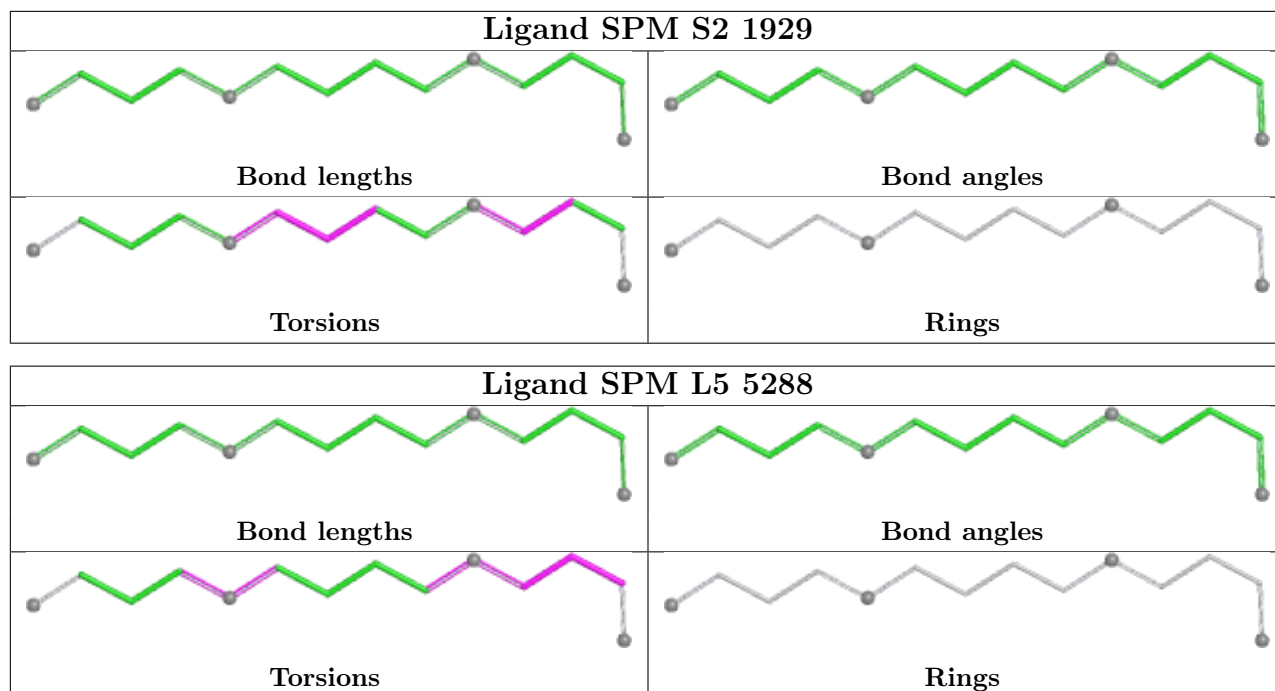












## 5.7 Other polymers [i](#)

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
51	S2	5
1	CD	1
32	Lb	1
49	Lt	1
59	SH	1
50	Pt	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	37:LYS	C	389:ALA	N	174.73
1	Lb	76:VAL	C	89:VAL	N	35.22
1	S2	753:C	O3'	785:C	P	28.37
1	S2	739:C	O3'	746:C	P	13.09
1	S2	698:G	O3'	730:C	P	12.71

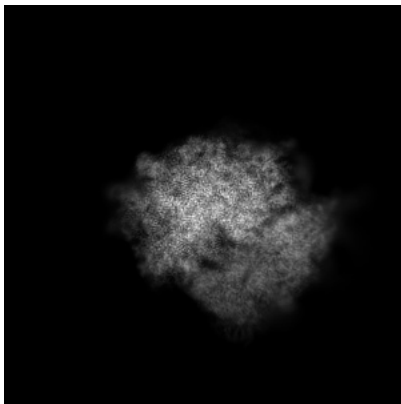
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71477. These allow visual inspection of the internal detail of the map and identification of artifacts.

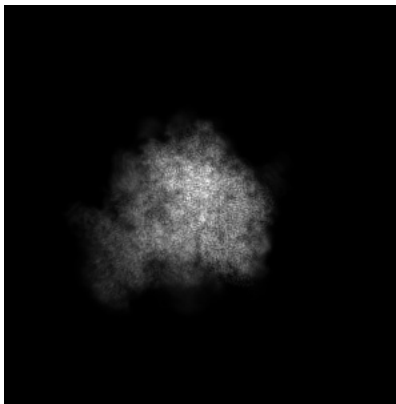
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

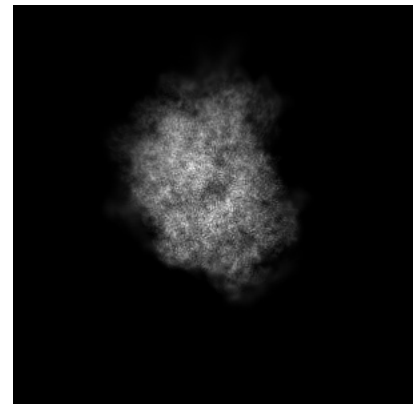
#### 6.1.1 Primary map



X

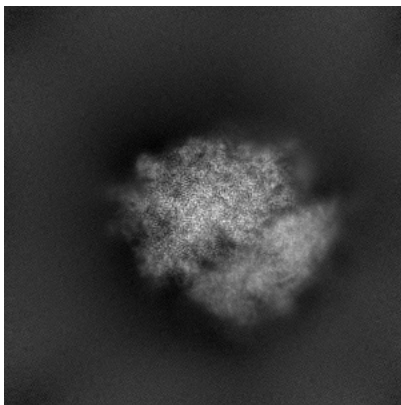


Y

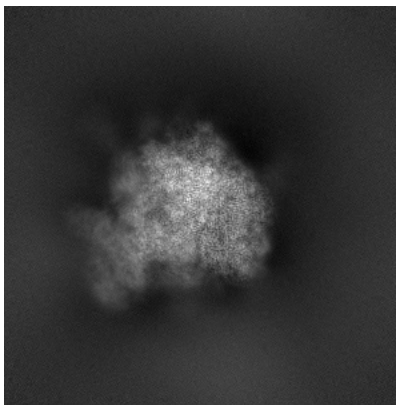


Z

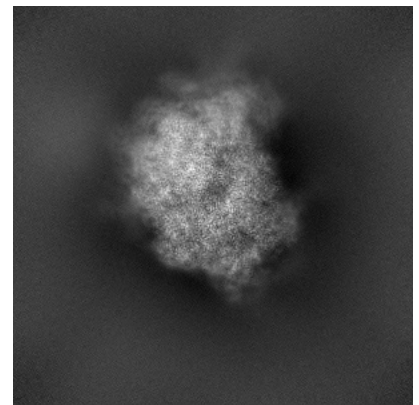
#### 6.1.2 Raw map



X



Y

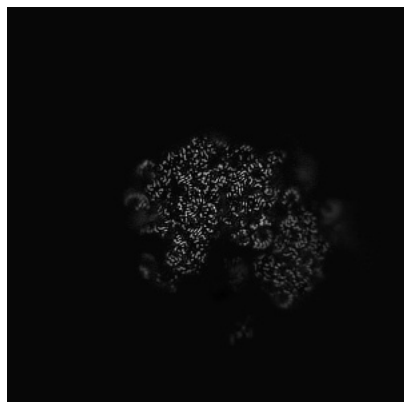


Z

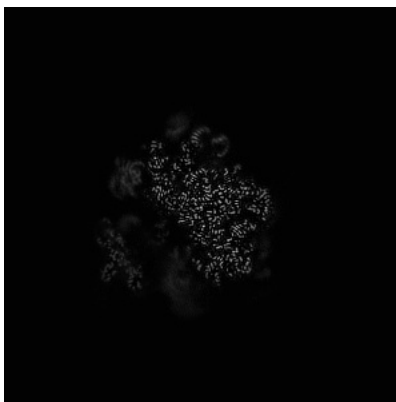
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

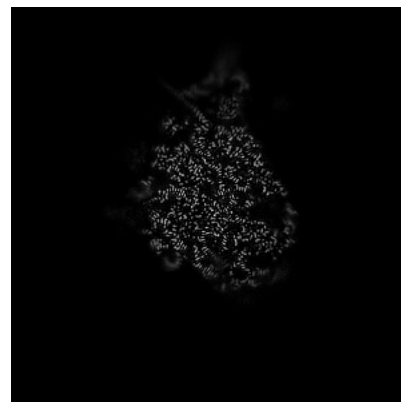
### 6.2.1 Primary map



X Index: 288

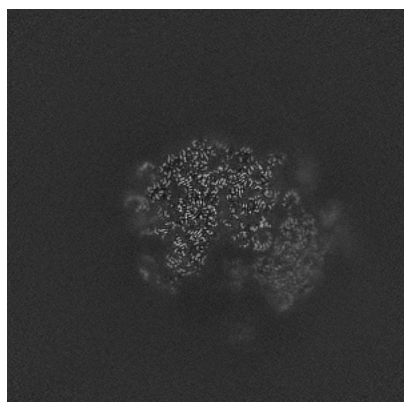


Y Index: 288

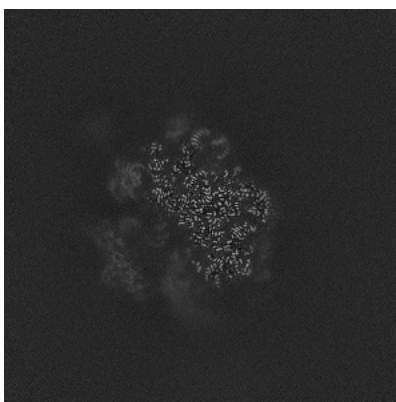


Z Index: 288

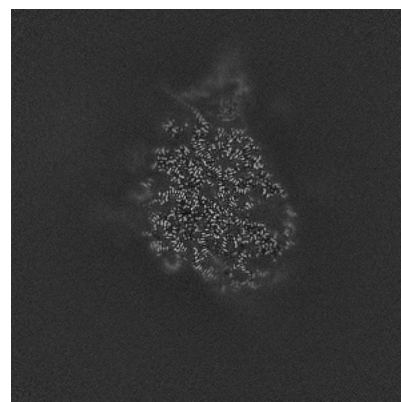
### 6.2.2 Raw map



X Index: 288



Y Index: 288

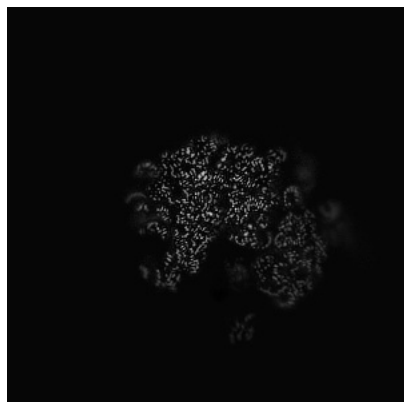


Z Index: 288

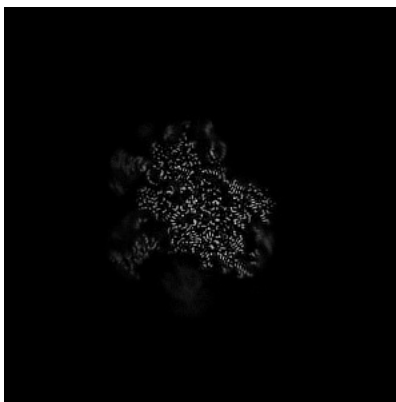
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

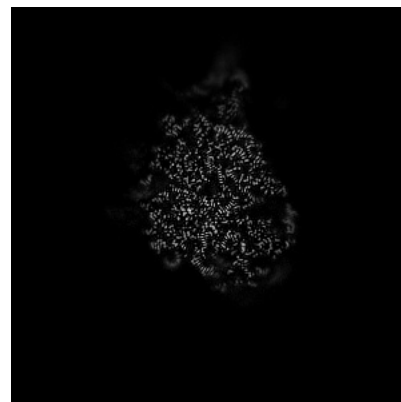
### 6.3.1 Primary map



X Index: 285

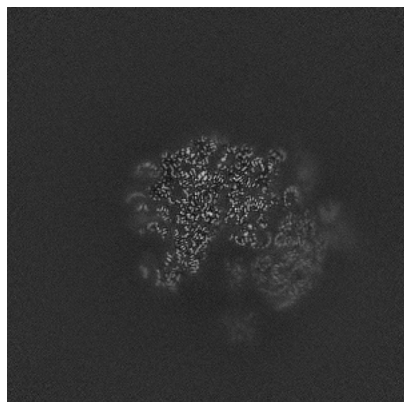


Y Index: 272

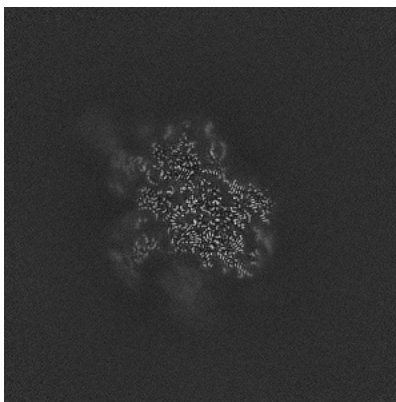


Z Index: 290

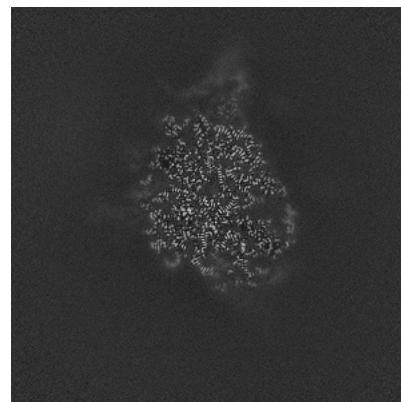
### 6.3.2 Raw map



X Index: 285



Y Index: 272

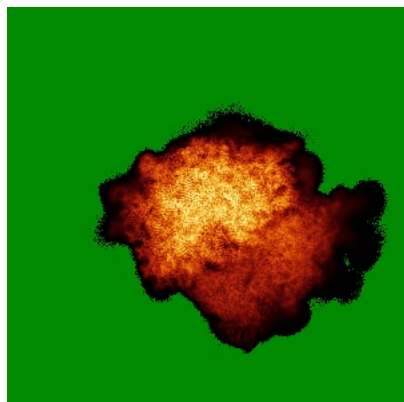


Z Index: 290

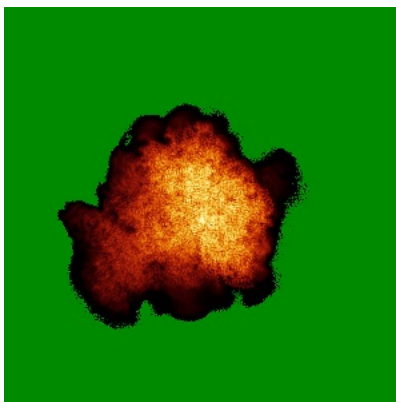
The images above show the largest variance slices of the map in three orthogonal directions.

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

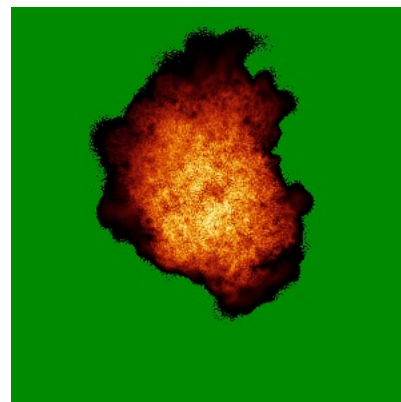
### 6.4.1 Primary map



X

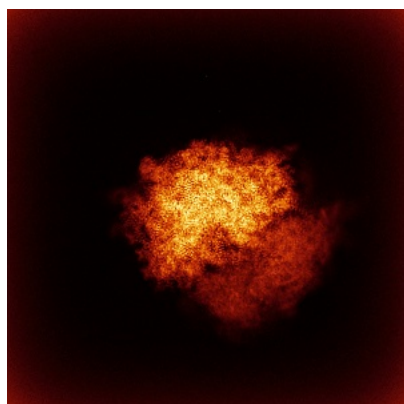


Y

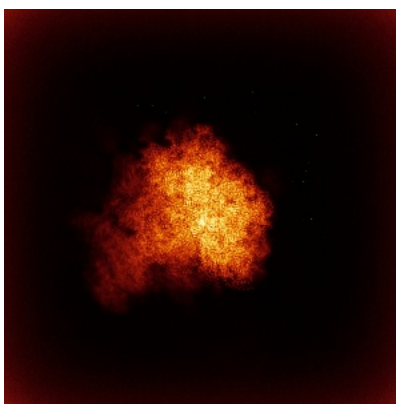


Z

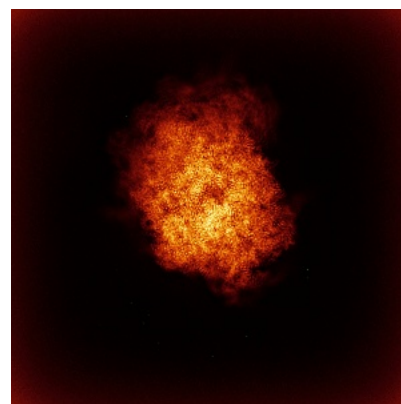
### 6.4.2 Raw map



X



Y

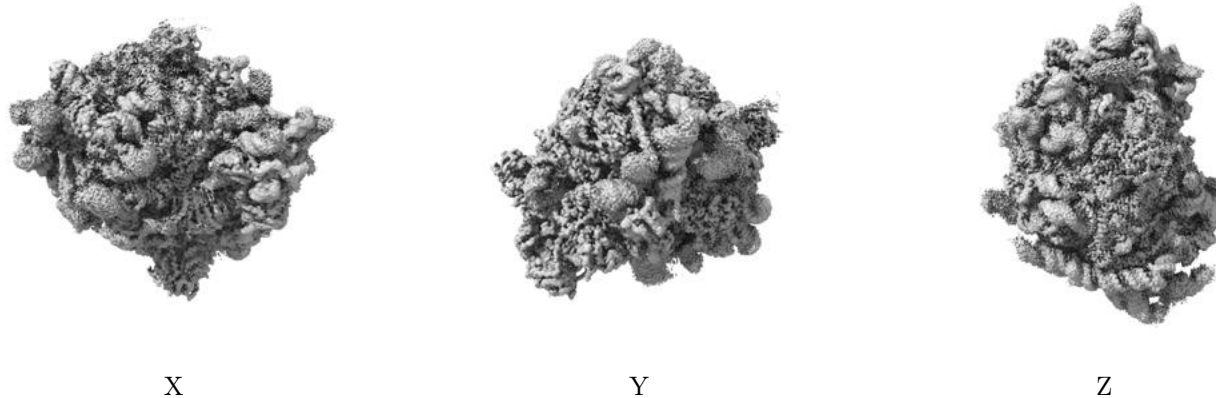


Z

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.

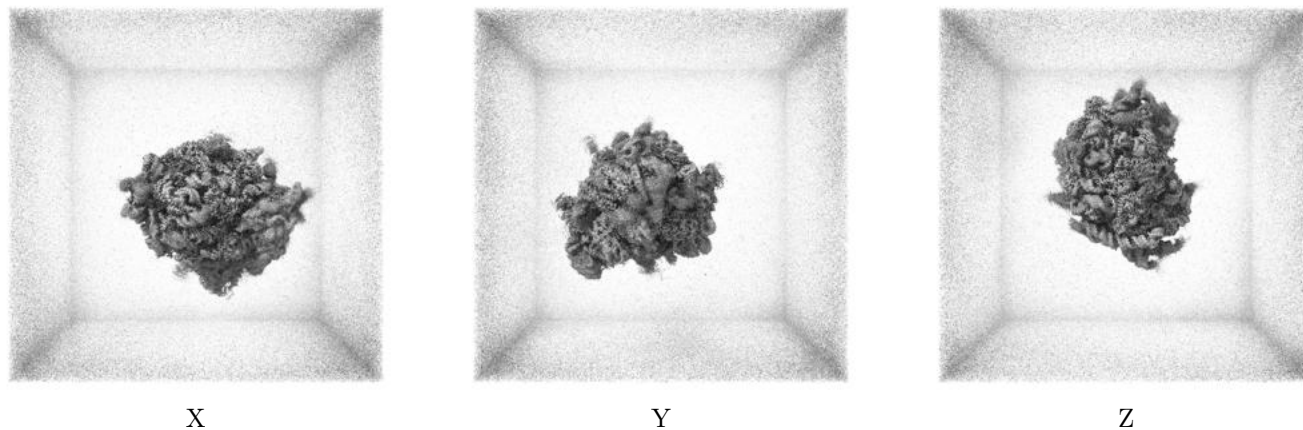
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0169. 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.

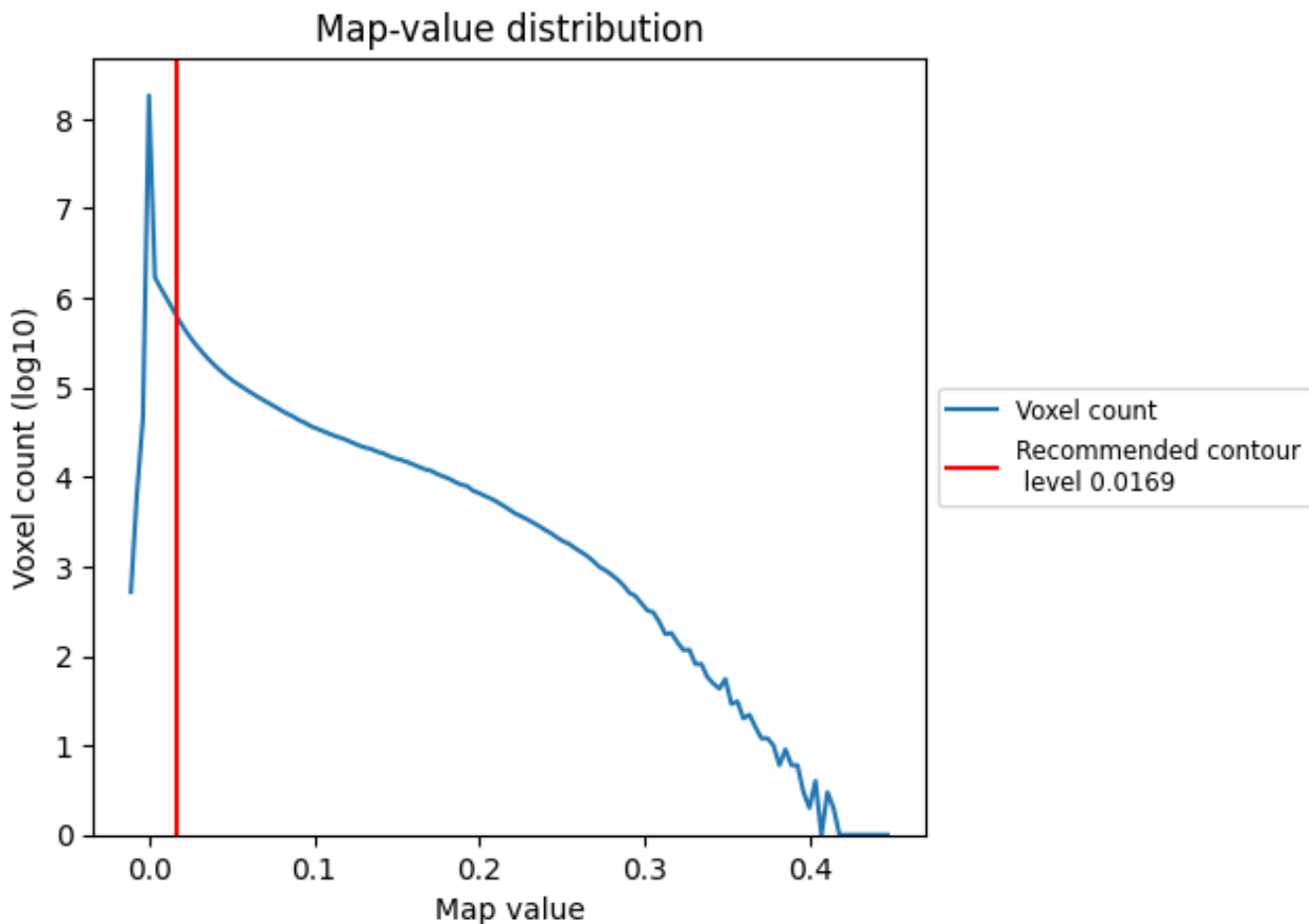
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

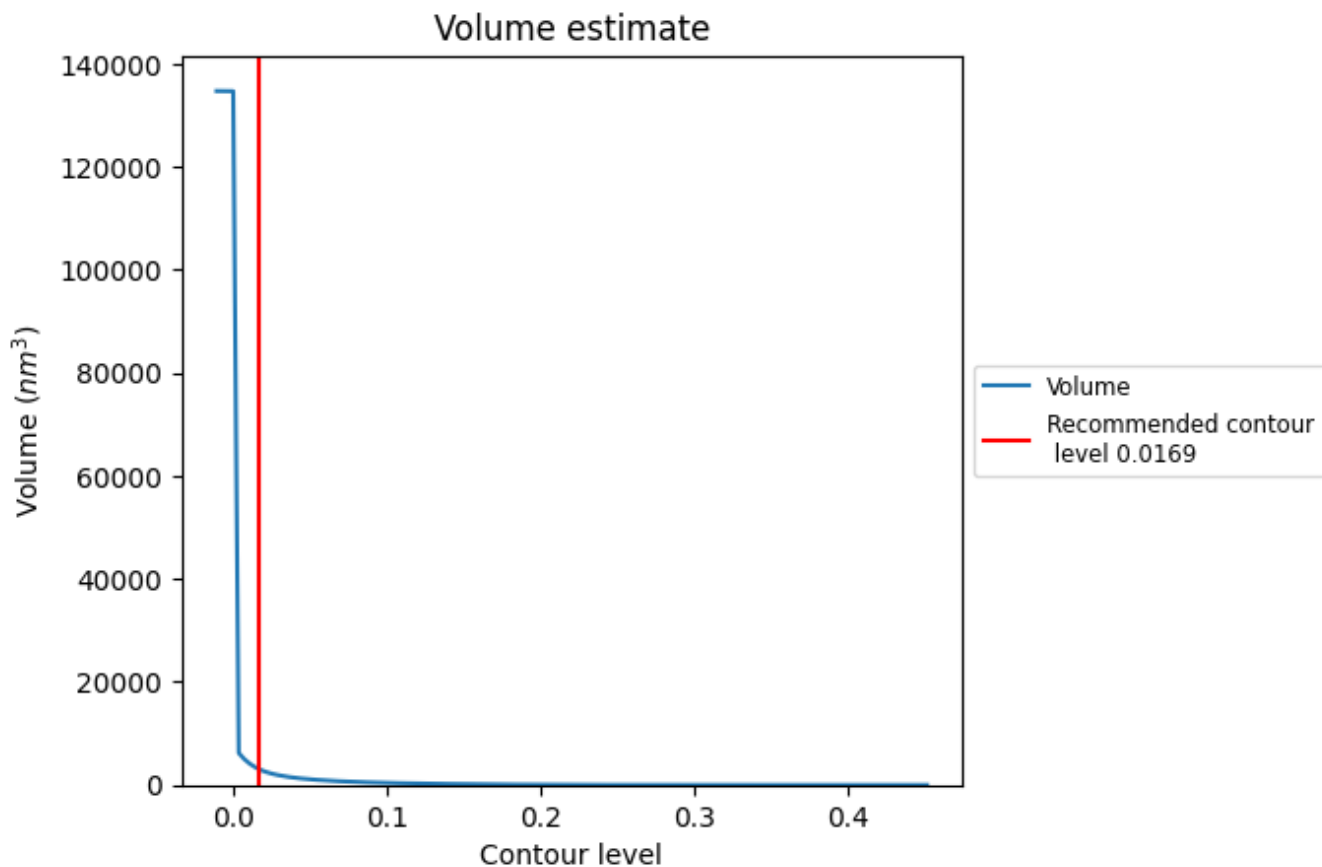
This section contains the results of statistical analysis of the map.

### 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.

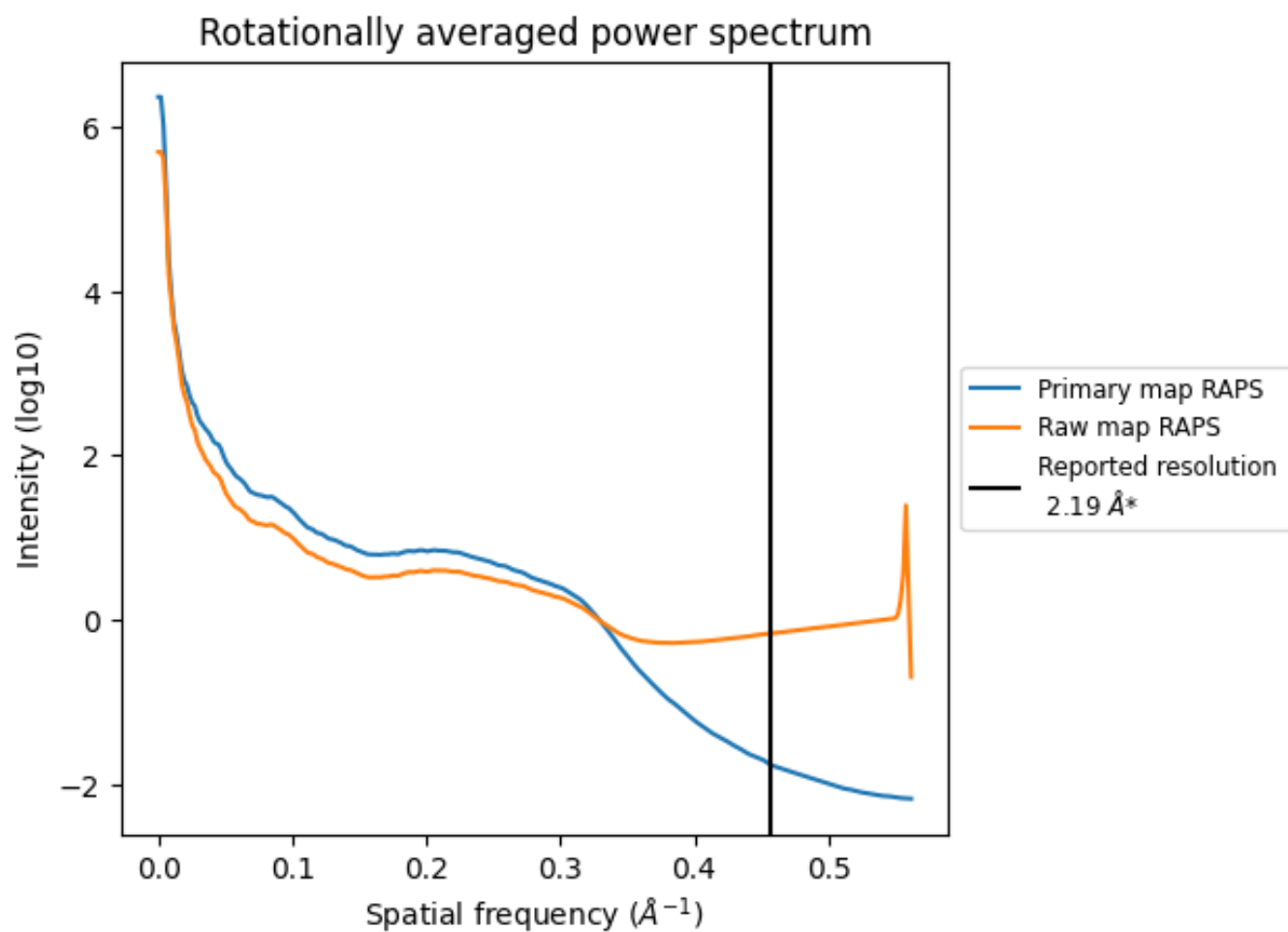
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3024  $\text{nm}^3$ ; this corresponds to an approximate mass of 2732 kDa.

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

### 7.3 Rotationally averaged power spectrum i

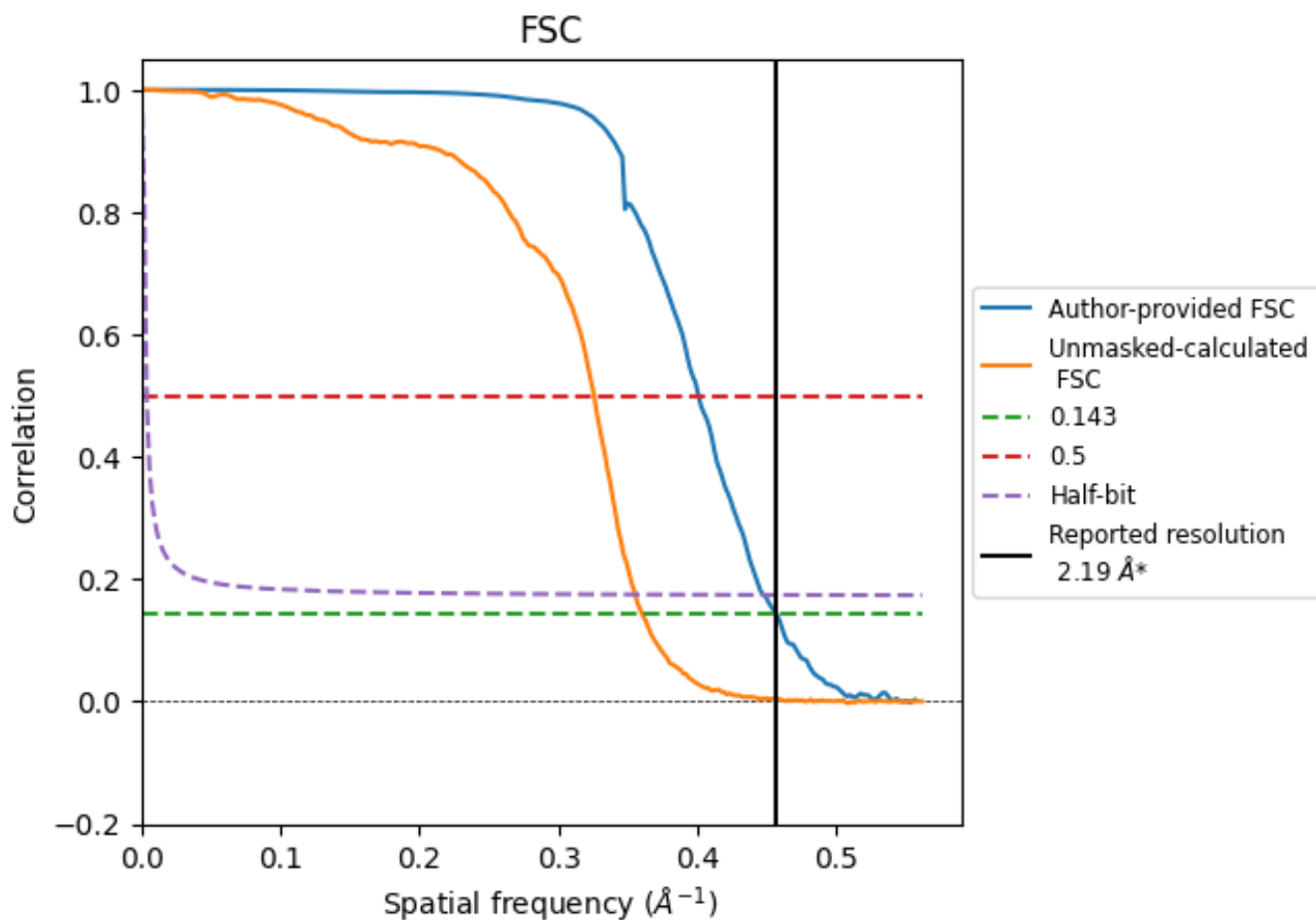


\*Reported resolution corresponds to spatial frequency of  $0.457 \text{ \AA}^{-1}$

## 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 0.457 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

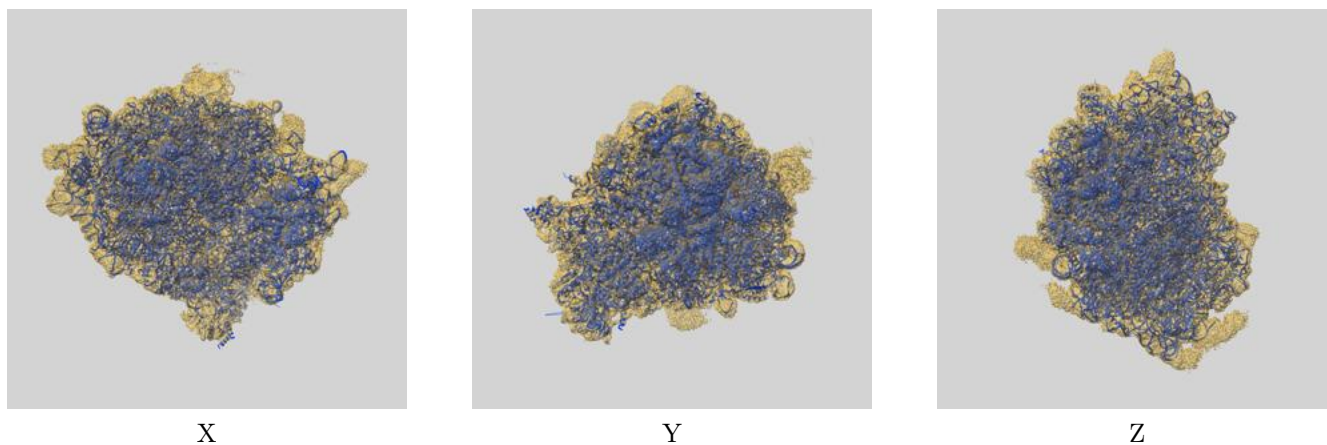
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.19	2.49	2.23
Unmasked-calculated*	2.77	3.07	2.81

\*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 2.77 differs from the reported value 2.19 by more than 10 %

## 9 Map-model fit [i](#)

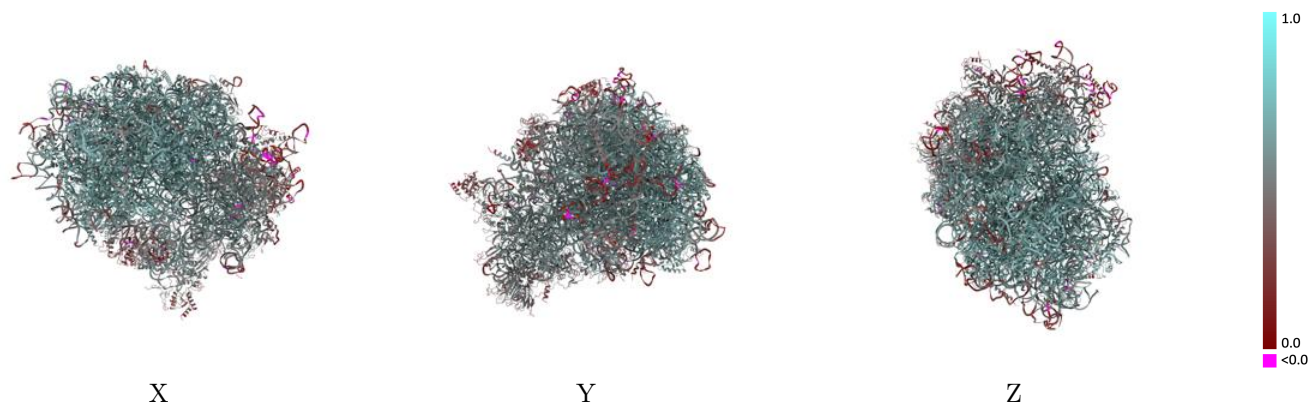
This section contains information regarding the fit between EMDB map EMD-71477 and PDB model 9PBE. Per-residue inclusion information can be found in section 3 on page 27.

### 9.1 Map-model overlay [i](#)



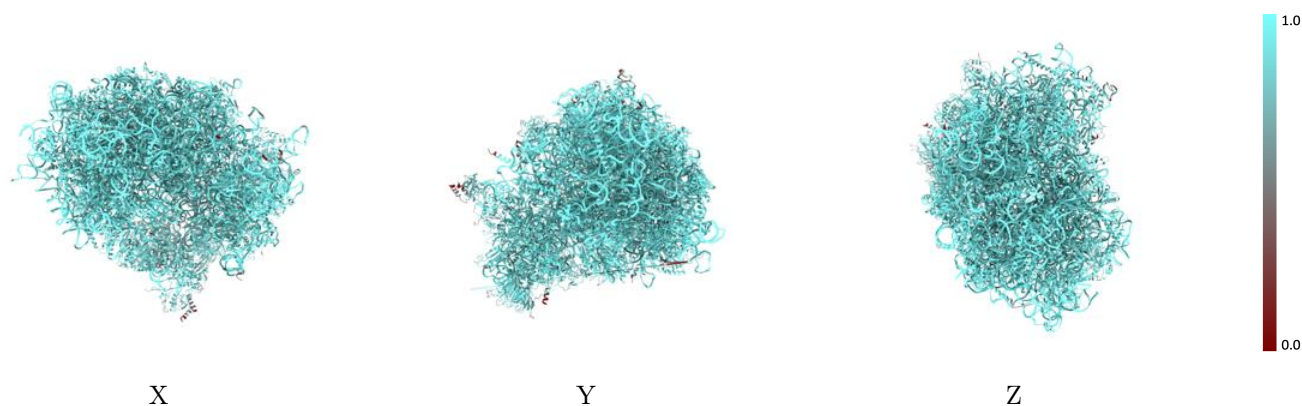
The images above show the 3D surface view of the map at the recommended contour level 0.0169 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



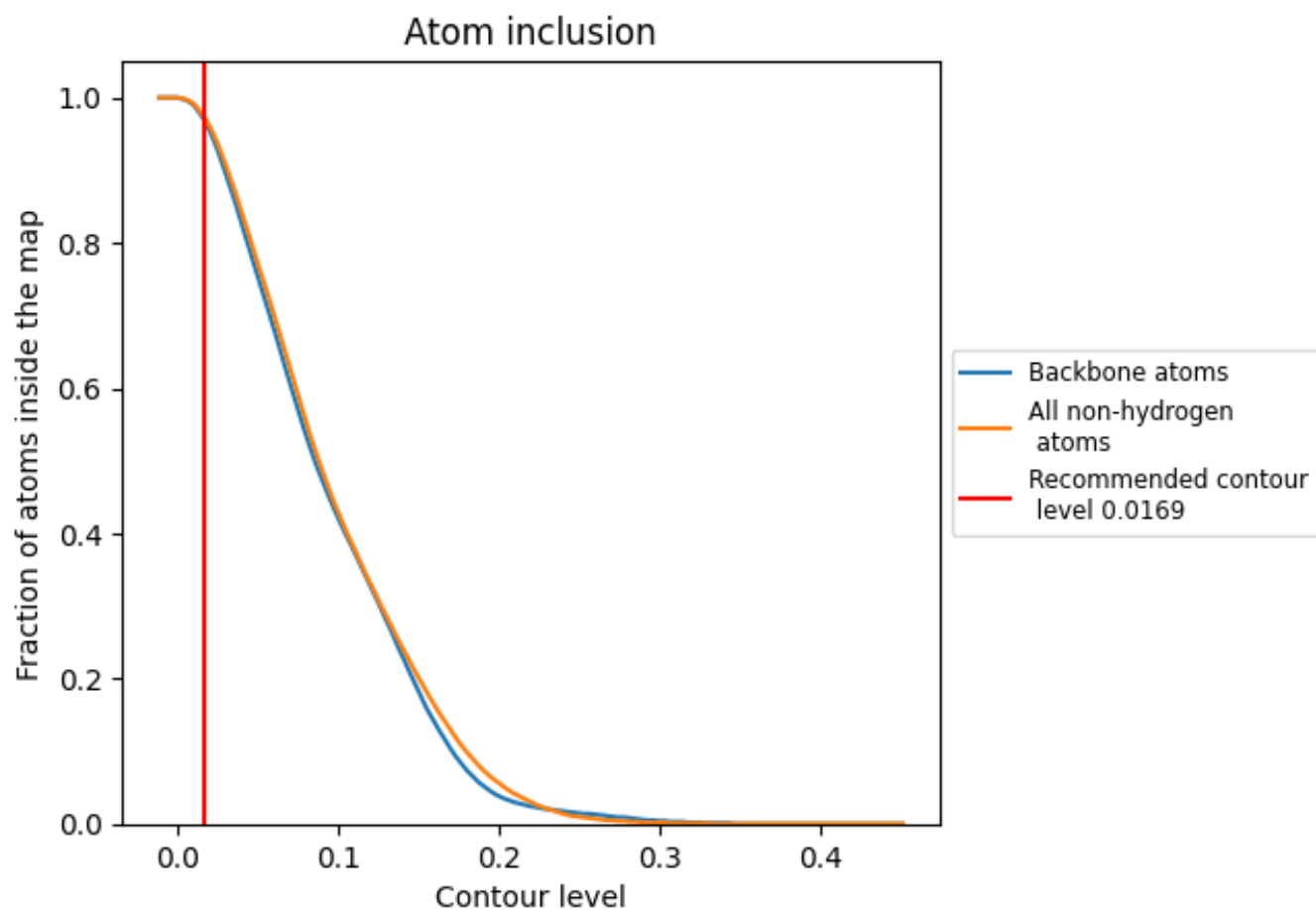
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0169).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.0169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9730	 0.5610
CD	 0.7750	 0.4390
CI	 0.8790	 0.5010
L5	 0.9930	 0.5880
L7	 0.9990	 0.6310
L8	 0.9930	 0.6090
LA	 0.9960	 0.6450
LB	 0.9790	 0.6300
LC	 0.9810	 0.6330
LD	 0.9780	 0.5910
LE	 0.9680	 0.5670
LF	 0.9930	 0.6440
LG	 0.9540	 0.5700
LH	 0.9850	 0.6140
LI	 0.9820	 0.6330
LJ	 0.9540	 0.5250
LL	 0.9550	 0.6060
LM	 0.9890	 0.6140
LN	 0.9990	 0.6680
LO	 0.9880	 0.6430
LP	 0.9910	 0.6490
LQ	 0.9970	 0.6620
LR	 0.9420	 0.5670
LS	 0.9970	 0.6520
LT	 0.9800	 0.6180
LU	 0.9580	 0.5330
LV	 0.9950	 0.6310
LW	 0.9070	 0.4430
LX	 0.9820	 0.6180
LY	 0.9840	 0.6210
LZ	 0.9960	 0.6070
La	 0.9940	 0.6650
Lb	 0.9450	 0.5620
Lc	 0.9730	 0.5780
Ld	 0.9770	 0.6140



















*Continued on next page...*

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Chain	Atom inclusion	Q-score
Le	 0.9940	 0.6570
Lf	 0.9930	 0.6610
Lg	 0.9840	 0.6280
Lh	 0.9800	 0.6150
Li	 0.9840	 0.6170
Lj	 0.9910	 0.6560
Lk	 0.9460	 0.5430
Ll	 0.9910	 0.6340
Lm	 0.9810	 0.6330
Ln	 0.9900	 0.6100
Lo	 0.9830	 0.6350
Lp	 0.9770	 0.6200
Lr	 0.9890	 0.6390
Ls	 0.8640	 0.3570
Lt	 0.7400	 0.1680
Pt	 0.9240	 0.5090
S2	 0.9920	 0.5210
SA	 0.9210	 0.4930
SB	 0.9570	 0.5170
SC	 0.9700	 0.5430
SD	 0.9200	 0.4860
SE	 0.9580	 0.5070
SF	 0.9230	 0.4920
SG	 0.9230	 0.4200
SH	 0.8900	 0.4190
SI	 0.9530	 0.4950
SJ	 0.9350	 0.5060
SK	 0.9170	 0.4950
SL	 0.9220	 0.5150
SM	 0.6260	 0.3050
SN	 0.9810	 0.5400
SO	 0.9470	 0.5330
SP	 0.9450	 0.4860
SQ	 0.9250	 0.4980
SR	 0.8890	 0.4510
SS	 0.9330	 0.4610
ST	 0.9310	 0.4960
SU	 0.8910	 0.4570
SV	 0.9660	 0.5230
SW	 0.9760	 0.5490
SX	 0.9720	 0.5620
SY	 0.8960	 0.4350

*Continued on next page...*

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Chain	Atom inclusion	Q-score
SZ	 0.8870	 0.4590
Sa	 0.9440	 0.5300
Sb	 0.9470	 0.4970
Sc	 0.8850	 0.4290
Sd	 0.9750	 0.5580
Se	 0.8600	 0.4240
Sf	 0.8310	 0.3930
Sg	 0.8860	 0.4470