



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 05:02 am BST

PDB ID : 7O7Z / pdb_00007o7z
EMDB ID : EMD-12757
Title : Rabbit 80S ribosome stalled close to the mutated SARS-CoV-2 slippery site
by a pseudoknot (classified for pseudoknot)
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.
Deposited on : 2021-04-14
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

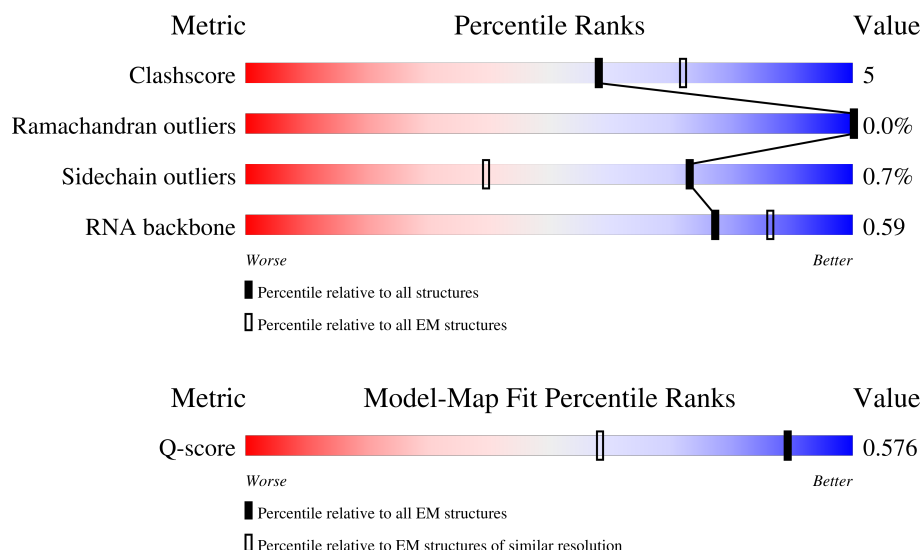
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	A2	1870	<div> <div>6%</div> <div>63%</div> <div>27%</div> <div>5%</div> <div>5%</div> </div>
2	AA	84	<div> <div>7%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
3	AB	69	<div> <div>7%</div> <div>77%</div> <div>14%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	
9	AH	220	
10	AI	76	
11	AT	76	
12	AZ	295	
13	Aa	264	
14	Ab	293	
15	Ac	281	
16	Ad	263	
17	Ae	204	
18	Af	249	
19	Ag	432	
20	Ah	208	
21	Ai	194	
22	Aj	165	
23	Ak	158	
24	Al	132	
25	Am	151	
26	An	151	
27	Ao	145	
28	Ap	172	



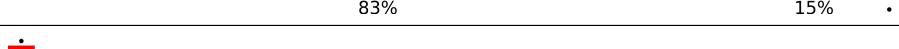
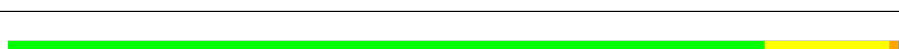

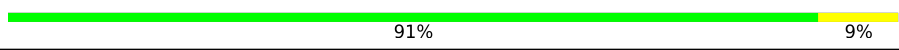

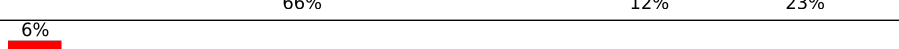



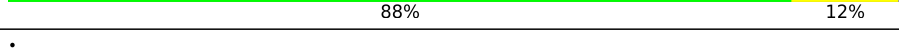

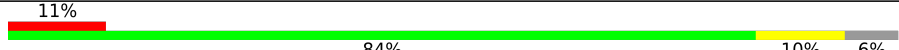


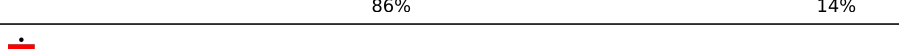







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Mol	Chain	Length	Quality of chain
29	Aq	135	
30	Ar	152	
31	As	145	
32	At	119	
33	Au	83	
34	Av	130	
35	Aw	143	
36	Ax	130	
37	Ay	124	
38	Az	25	
39	B5	4808	
40	B7	120	
41	B8	158	
42	BA	257	
43	BB	403	
44	BC	413	
45	BD	297	
46	BE	291	
47	BF	247	
48	BG	266	
49	BH	192	
50	BI	214	
51	BJ	178	
52	BK	1071	
53	BL	211	




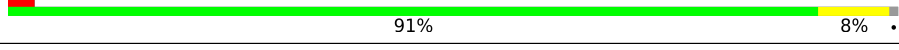

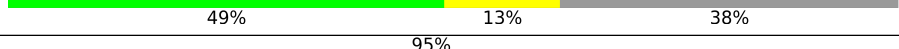
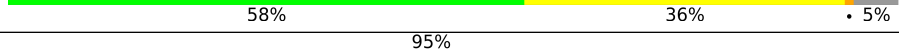
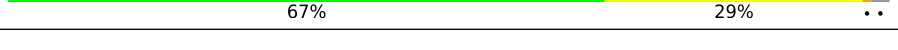
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Mol	Chain	Length	Quality of chain
54	BM	218	
55	BN	204	
56	BO	203	
57	BP	184	
58	BQ	188	
59	BR	196	
60	BS	176	
61	BT	160	
62	BU	128	
63	BV	140	
64	BW	157	
65	BX	156	
66	BY	145	
67	BZ	136	
68	Ba	148	
69	Bb	245	
70	Bc	115	
71	Bd	125	
72	Be	135	
73	Bf	110	
74	Bg	117	
75	Bh	123	
76	Bi	105	
77	Bj	97	
78	Bk	70	

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Mol	Chain	Length	Quality of chain
79	Bl	51	
80	Bm	128	
81	Bo	106	
82	Bp	92	
83	Br	137	
84	Bs	318	
85	Bt	165	
86	Bv	217	

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 229742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A2	1770	Total	C	N	O	P	0	0
			37833	16911	6781	12371	1770		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 2 is a protein called 40S ribosomal protein S27.

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

- Molecule 3 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 4 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AC	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 5 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AD	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 6 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 7 is a protein called RACK1.

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

- Molecule 8 is a protein called uS14.

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

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	95	Total	C	N	O	P	0	0
			2018	901	349	673	95		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AI	76	Total	C	N	O	P	0	0
			939	393	11	459	76		

- Molecule 11 is a RNA chain called P-site Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 13 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Aa	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 14 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

- Molecule 15 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ac	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 16 is a protein called Ribosomal protein eS4.

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

- Molecule 17 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 18 is a protein called 40S ribosomal protein S6.

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

- Molecule 19 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 20 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 21 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 22 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Aj	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 23 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 25 is a protein called uS15.

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

- Molecule 26 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	An	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 27 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 28 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ap	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 29 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 30 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 31 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	As	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 32 is a protein called 40S ribosomal protein uS10.

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

- Molecule 33 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Au	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 34 is a protein called Ribosomal protein S15a.

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

- Molecule 35 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Aw	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 36 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ay	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 38 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Az	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B5	3764	Total	C	N	O	P	0	0
			80772	36003	14762	26243	3764		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 40 is a RNA chain called 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 42 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BA	253	Total	C	N	O	S	0	0
			1940	1214	396	324	6		

- Molecule 43 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BB	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BC	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 45 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BD	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 46 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BE	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 47 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BF	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

- Molecule 48 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BG	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BH	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 50 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BI	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 51 is a protein called Ribosomal protein L11.

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

- Molecule 52 is a protein called Replicase polyprotein 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BK	35	Total	C	N	O	S	0	0
			265	163	45	51	6		

- Molecule 53 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BL	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 54 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BM	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 55 is a protein called Ribosomal protein L15.

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

- Molecule 56 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BO	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 57 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BP	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 58 is a protein called Ribosomal Protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BQ	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 59 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BR	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 60 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BS	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 61 is a protein called eL21.

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

- Molecule 62 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BU	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

- Molecule 63 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BV	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 64 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 65 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 66 is a protein called Ribosomal protein L26.

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

- Molecule 67 is a protein called 60S ribosomal protein L27.

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

- Molecule 68 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 69 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 70 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 71 is a protein called eL31.

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

- Molecule 72 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 73 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 74 is a protein called 60S ribosomal protein L34.

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

- Molecule 75 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bh	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 76 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bi	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 77 is a protein called Ribosomal protein L37.

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

- Molecule 78 is a protein called eL38.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 79 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bl	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 80 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 81 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bo	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 82 is a protein called eL43.

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

- Molecule 83 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Br	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bs	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

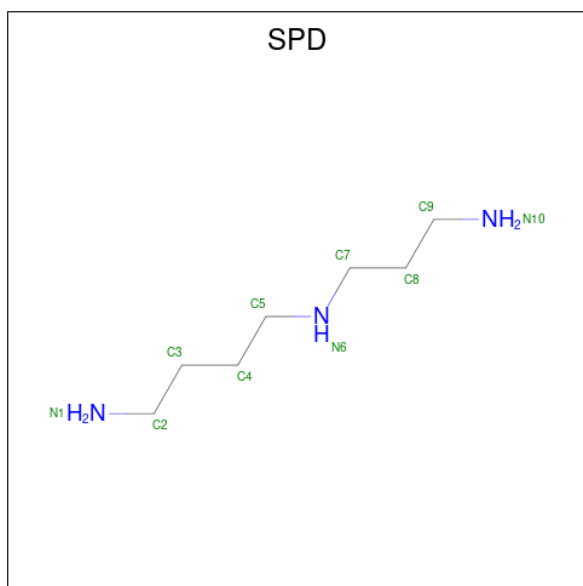
- Molecule 85 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Bt	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 86 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Bv	212	Total	C	N	O	S	0	0
			1707	1092	308	299	8		

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	

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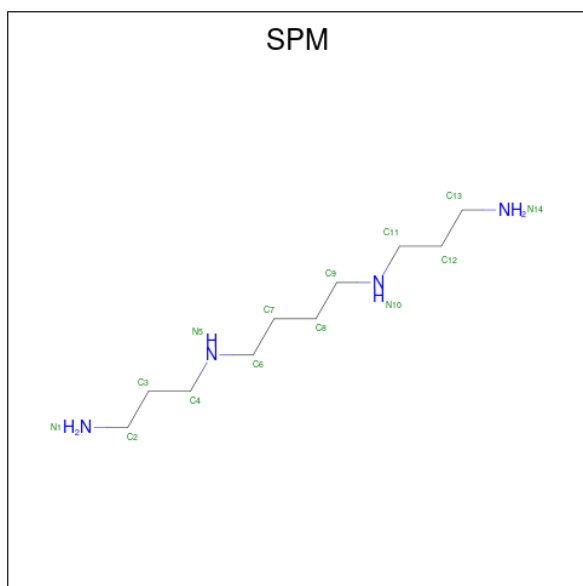
[illegible]

WORLDWIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms			AltConf
87	B5	1	Total	C	N	0
			10	7	3	

- Molecule 88 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
88	A2	1	Total	C	N	0
			14	10	4	
88	B5	1	Total	C	N	0
			14	10	4	
88	B5	1	Total	C	N	0
			14	10	4	

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	A2	109	Total	Mg	0
			109	109	
89	AH	1	Total	Mg	0
			1	1	
89	AT	3	Total	Mg	0
			3	3	
89	Af	1	Total	Mg	0
			1	1	
89	B5	284	Total	Mg	0
			284	284	

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Mol	Chain	Residues	Atoms		AltConf
89	B7	9	Total 9	Mg 9	0
89	B8	9	Total 9	Mg 9	0
89	BP	1	Total 1	Mg 1	0
89	BR	1	Total 1	Mg 1	0
89	BV	1	Total 1	Mg 1	0
89	Ba	1	Total 1	Mg 1	0

- Molecule 90 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
90	A2	60	Total 60	X 60	0
90	AT	4	Total 4	X 4	0
90	Ae	1	Total 1	X 1	0
90	An	1	Total 1	X 1	0
90	Ar	1	Total 1	X 1	0
90	As	1	Total 1	X 1	0
90	B5	225	Total 225	X 225	0
90	B7	6	Total 6	X 6	0
90	B8	8	Total 8	X 8	0
90	BA	3	Total 3	X 3	0
90	BB	4	Total 4	X 4	0
90	BC	1	Total 1	X 1	0
90	BH	1	Total 1	X 1	0

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Mol	Chain	Residues	Atoms		AltConf
90	BI	1	Total 1	X 1	0
90	BL	1	Total 1	X 1	0
90	BN	1	Total 1	X 1	0
90	BQ	2	Total 2	X 2	0
90	BT	2	Total 2	X 2	0
90	Bb	1	Total 1	X 1	0
90	Be	1	Total 1	X 1	0
90	Bf	1	Total 1	X 1	0
90	Bg	1	Total 1	X 1	0
90	Bl	1	Total 1	X 1	0
90	Bo	1	Total 1	X 1	0

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	AC	1	Total 1	Zn 1	0
91	AE	1	Total 1	Zn 1	0
91	AG	1	Total 1	Zn 1	0
91	Bg	1	Total 1	Zn 1	0
91	Bj	1	Total 1	Zn 1	0
91	Bm	1	Total 1	Zn 1	0
91	Bo	1	Total 1	Zn 1	0
91	Bp	1	Total 1	Zn 1	0

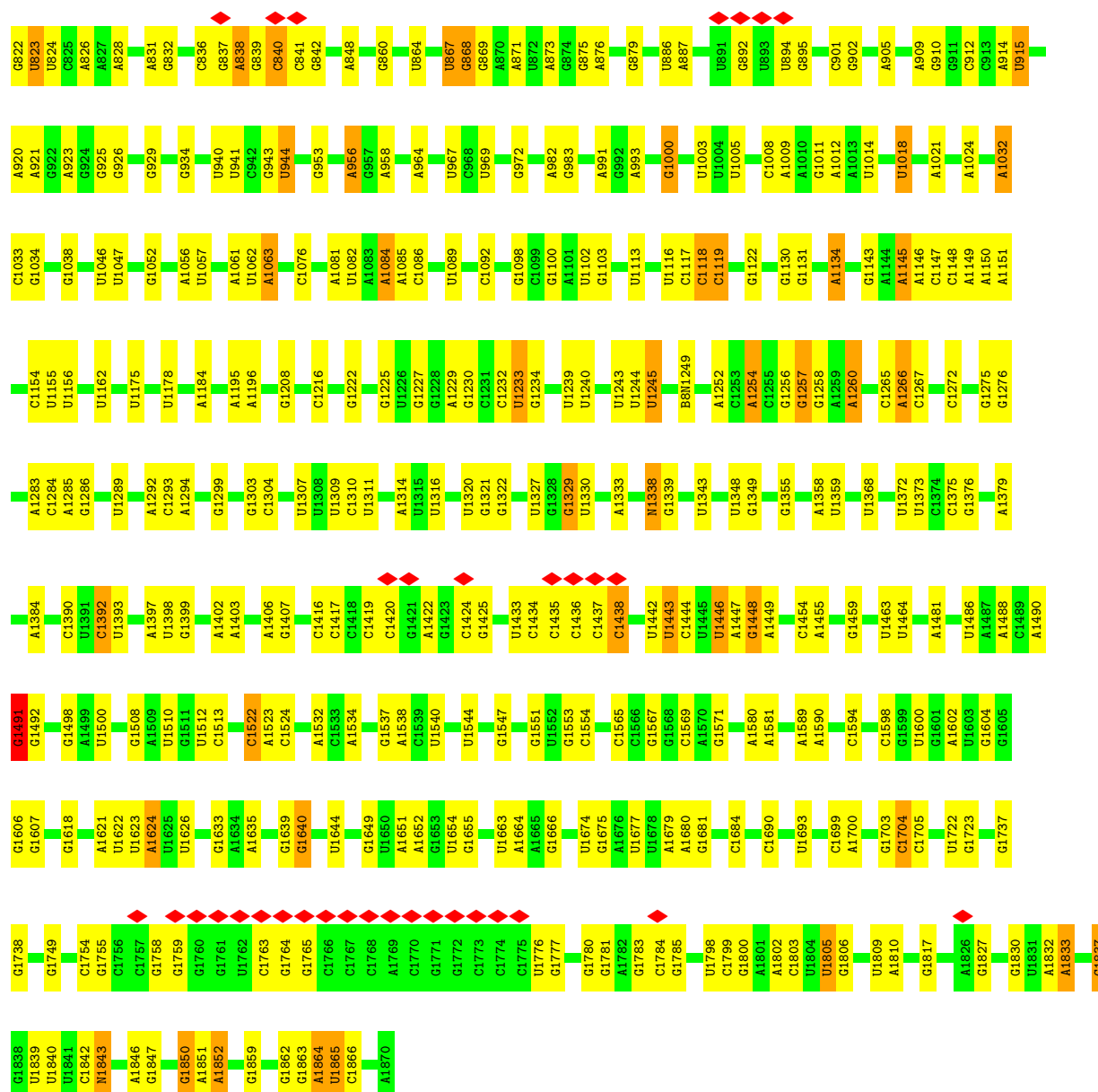
- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	A2	526	Total 526	O 526	0
92	AH	9	Total 9	O 9	0
92	AI	1	Total 1	O 1	0
92	AT	12	Total 12	O 12	0
92	Aa	1	Total 1	O 1	0
92	Ac	1	Total 1	O 1	0
92	Af	3	Total 3	O 3	0
92	Ak	1	Total 1	O 1	0
92	Am	1	Total 1	O 1	0
92	An	2	Total 2	O 2	0
92	Ap	3	Total 3	O 3	0
92	As	2	Total 2	O 2	0
92	At	1	Total 1	O 1	0
92	Aw	3	Total 3	O 3	0
92	B5	1391	Total 1391	O 1391	0
92	B7	45	Total 45	O 45	0
92	B8	50	Total 50	O 50	0
92	BA	10	Total 10	O 10	0
92	BB	5	Total 5	O 5	0
92	BC	7	Total 7	O 7	0
92	BD	1	Total 1	O 1	0

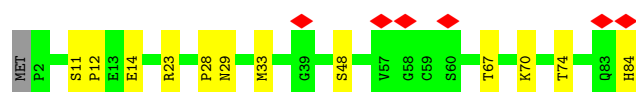
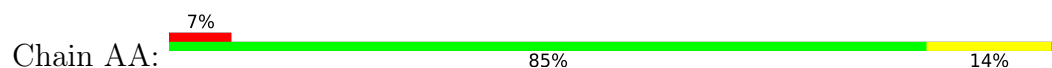
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Mol	Chain	Residues	Atoms		AltConf
92	BF	1	Total 1	O 1	0
92	BH	1	Total 1	O 1	0
92	BI	4	Total 4	O 4	0
92	BL	3	Total 3	O 3	0
92	BN	3	Total 3	O 3	0
92	BO	1	Total 1	O 1	0
92	BP	2	Total 2	O 2	0
92	BR	5	Total 5	O 5	0
92	BV	2	Total 2	O 2	0
92	BX	2	Total 2	O 2	0
92	Ba	6	Total 6	O 6	0
92	Bd	1	Total 1	O 1	0
92	Be	4	Total 4	O 4	0
92	Bg	2	Total 2	O 2	0
92	Bj	3	Total 3	O 3	0
92	Bl	1	Total 1	O 1	0
92	Bo	1	Total 1	O 1	0



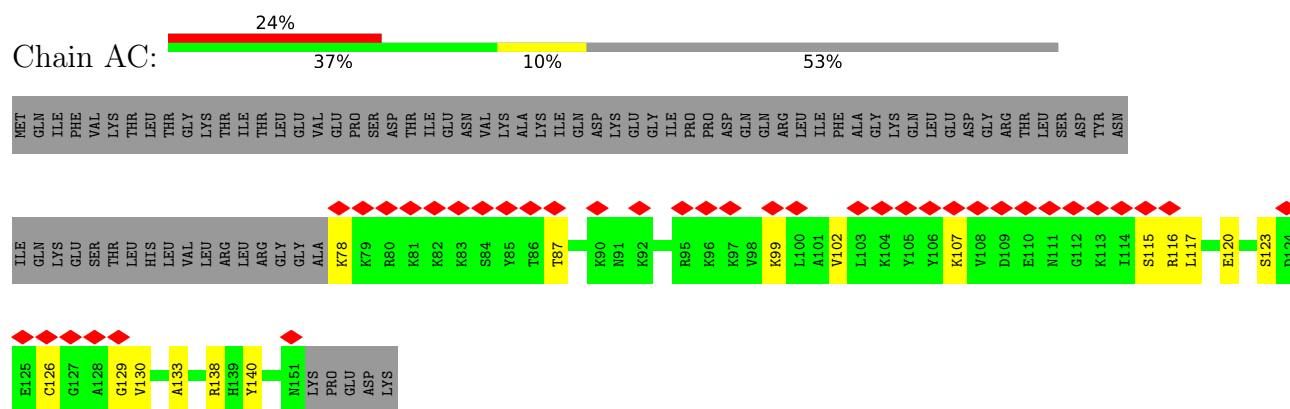
• Molecule 2: 40S ribosomal protein S27



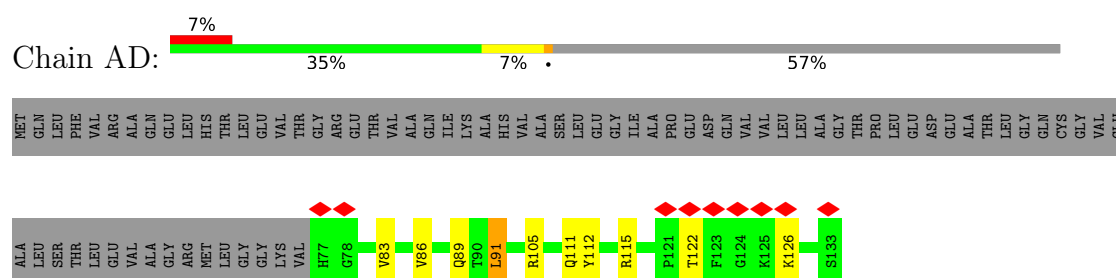
• Molecule 3: Ribosomal protein S28



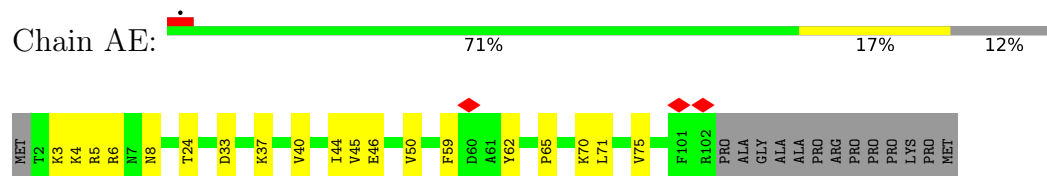
- Molecule 4: Ribosomal protein S27a



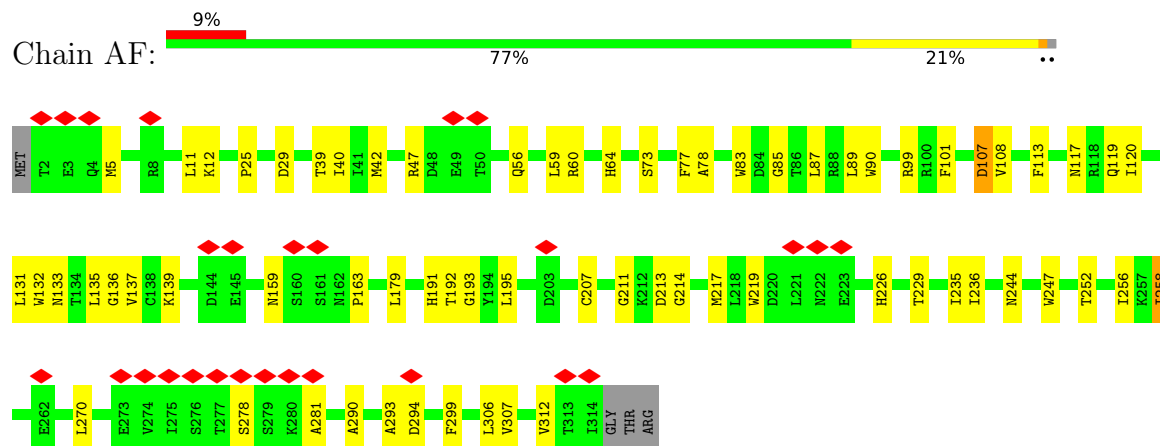
- Molecule 5: 40S ribosomal protein S30



- Molecule 6: Ribosomal protein eS26

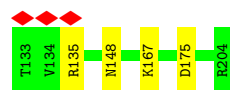


- Molecule 7: RACK1

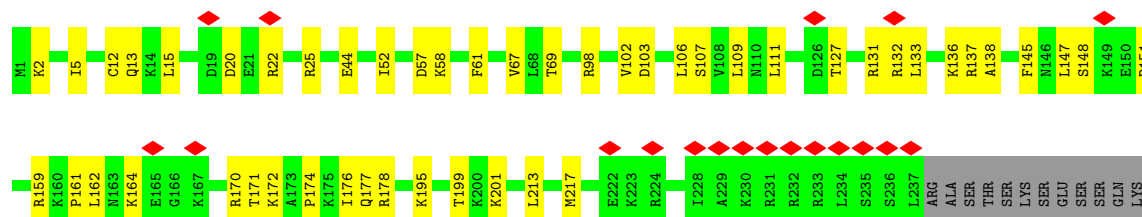
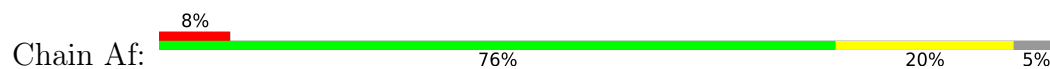


- Molecule 8: uS14

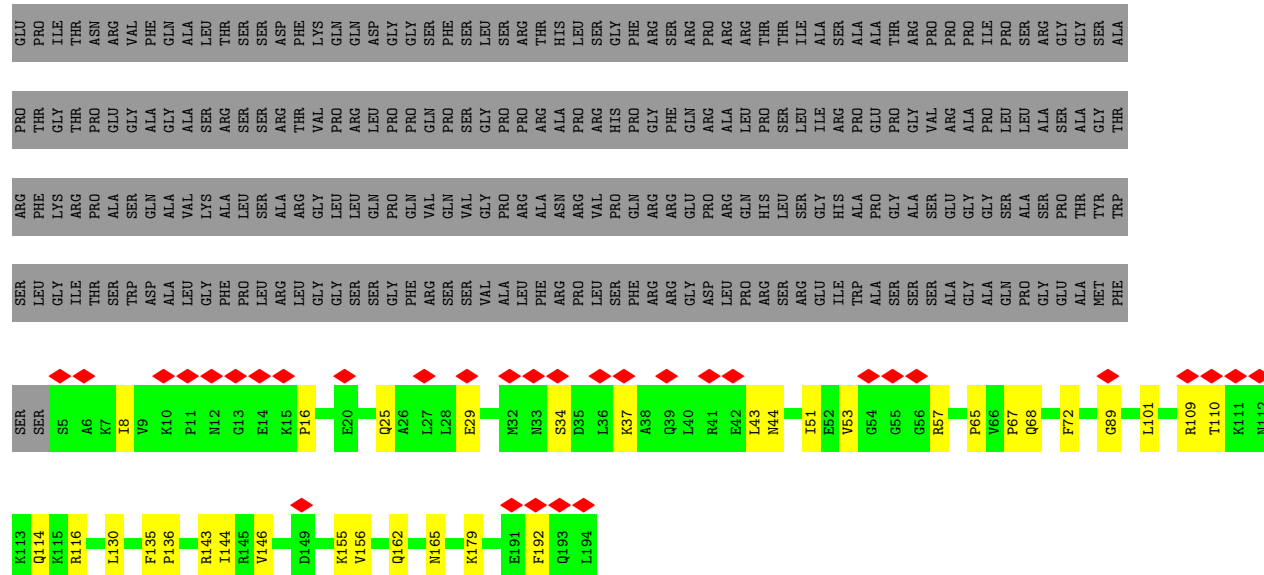
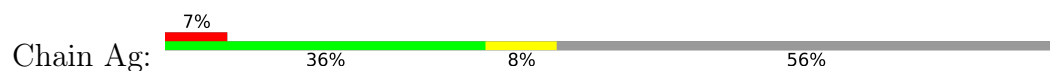




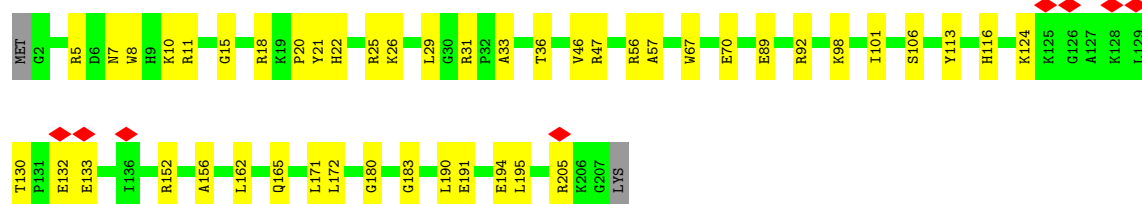
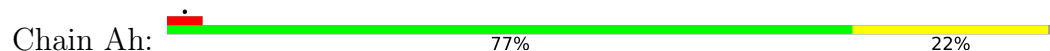
• Molecule 18: 40S ribosomal protein S6



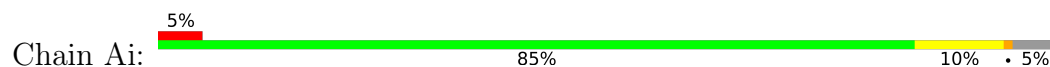
• Molecule 19: 40S ribosomal protein S7



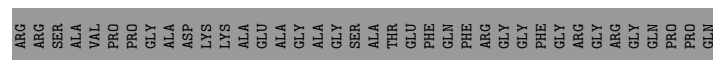
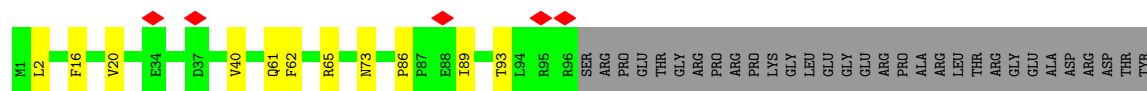
• Molecule 20: 40S ribosomal protein S8



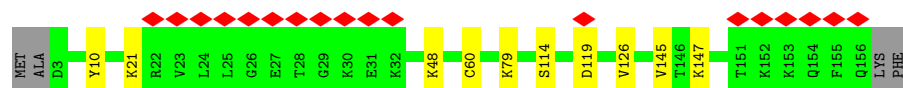
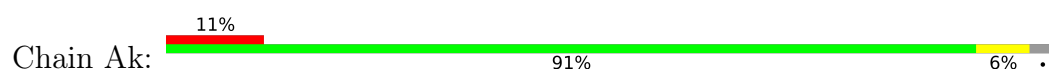
• Molecule 21: Ribosomal protein S9 (Predicted)



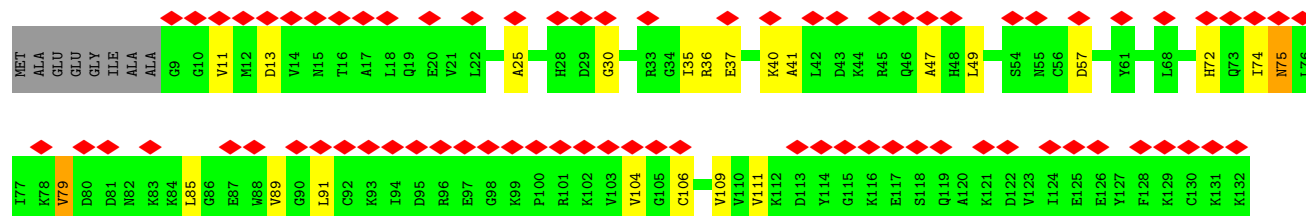
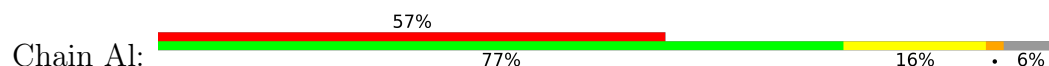
- Molecule 22: eS10



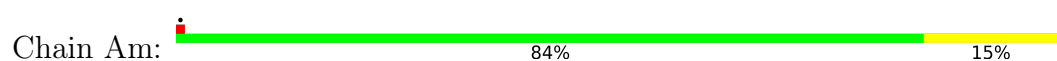
- Molecule 23: 40S ribosomal protein S11



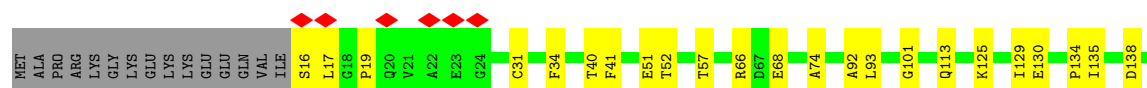
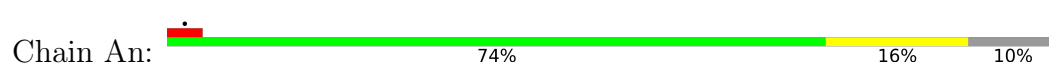
- Molecule 24: 40S ribosomal protein S12




- Molecule 25: uS15



- Molecule 26: 40S ribosomal protein uS11



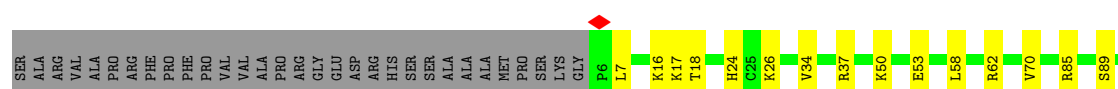
- Molecule 27: 40S ribosomal protein uS19

Chain Ao: 




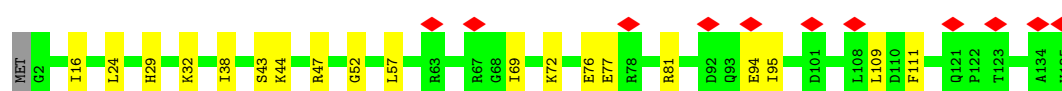
- Molecule 28: uS9

Chain Ap: 




- Molecule 29: 40S ribosomal protein eS17

Chain Aq: 

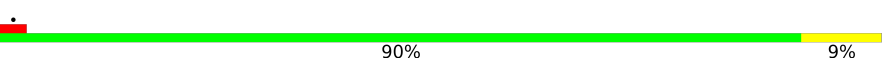


- Molecule 30: 40S ribosomal protein S18

Chain Ar: 




- Molecule 31: Ribosomal protein eS19

Chain As: 




- Molecule 32: 40S ribosomal protein uS10

Chain At: 




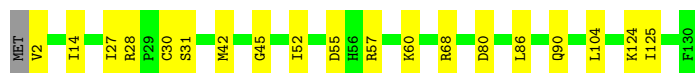
- Molecule 33: Ribosomal protein eS21

Chain Au:  87% 12%



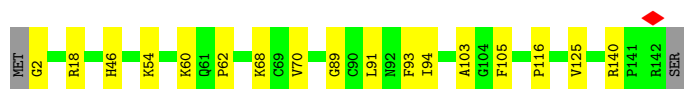
- Molecule 34: Ribosomal protein S15a

Chain Av:  85% 15%




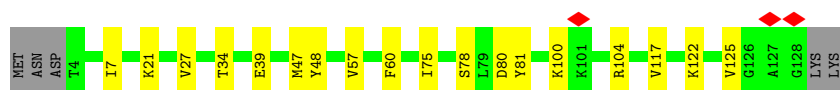
- Molecule 35: 40S ribosomal protein S23

Chain Aw:  87% 12%



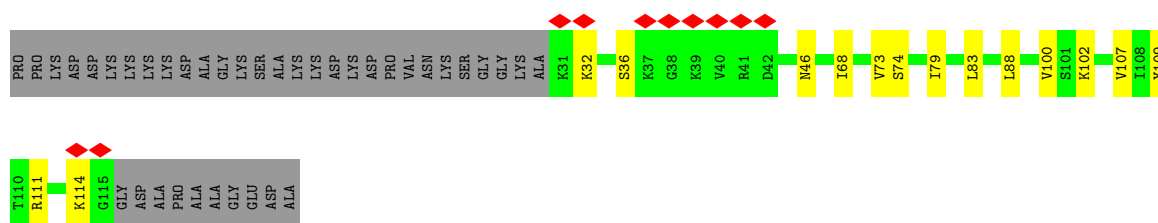
- Molecule 36: 40S ribosomal protein S24

Chain Ax:  82% 14%




- Molecule 37: 40S ribosomal protein S25

Chain Ay:  8% 56% 12% 31%



- Molecule 38: 60s ribosomal protein l41

Chain Az:  84% 16%



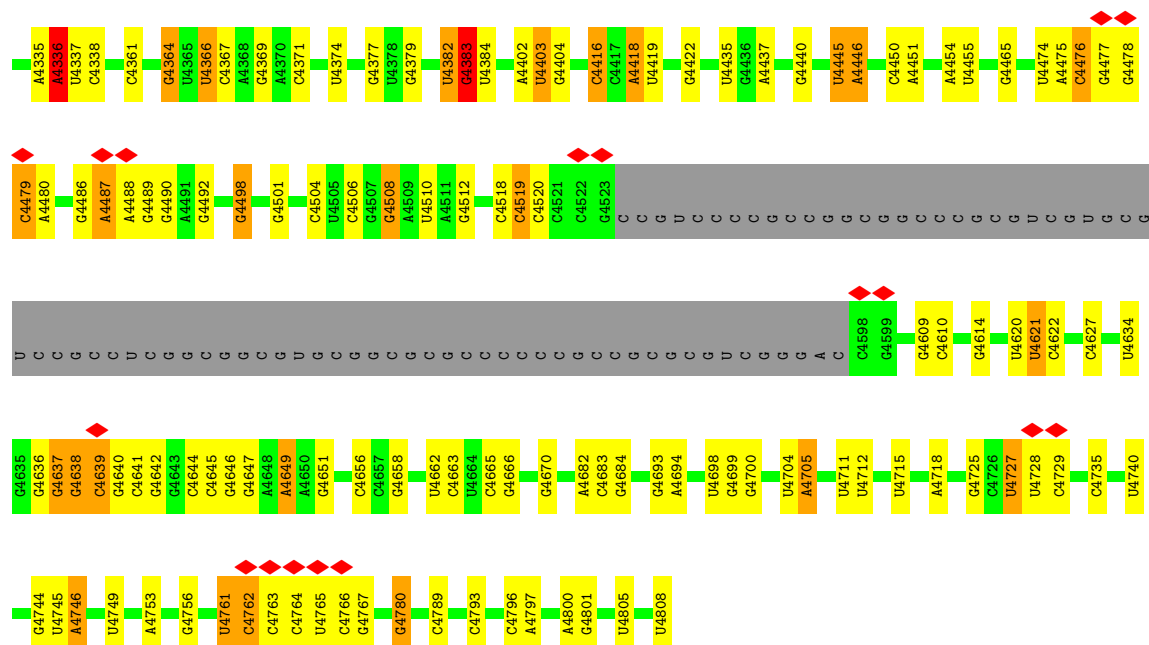
- Molecule 39: 28S rRNA

Chain B5:  5% 54% 21% 22%

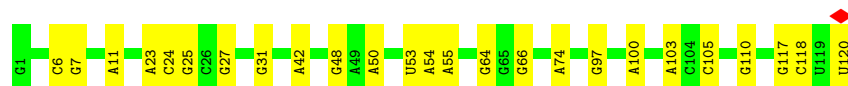
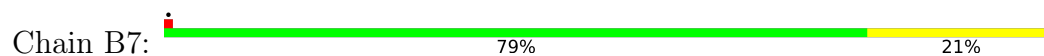




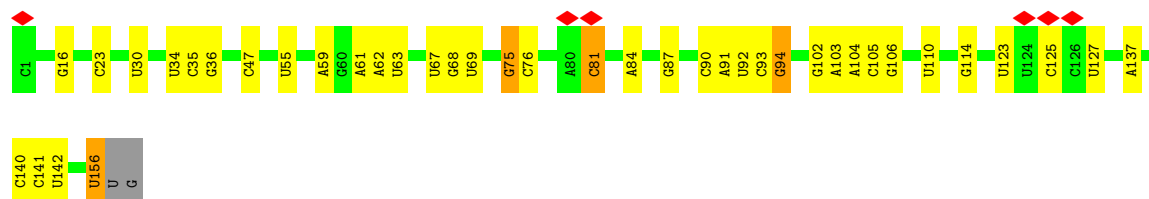




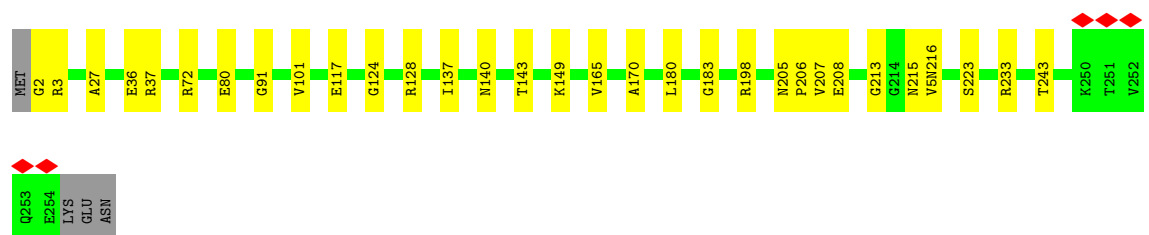
- Molecule 40: 5S




- Molecule 41: 5.8S rRNA

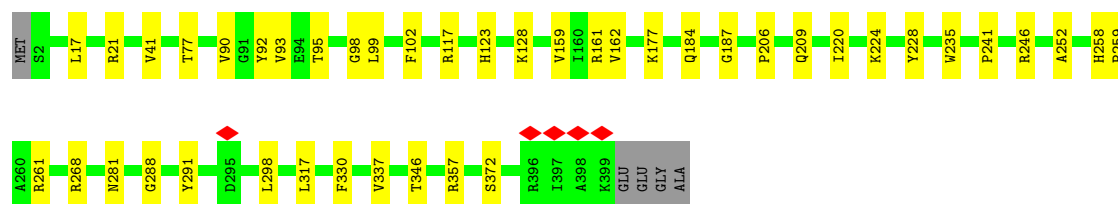


- Molecule 42: Ribosomal protein uL2




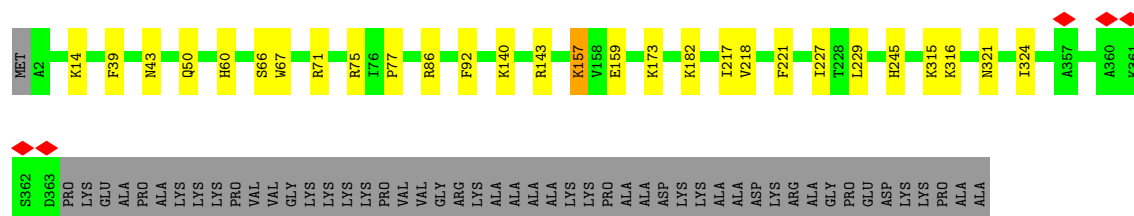
- Molecule 43: Ribosomal protein L3

Chain BB:  88% 11% .



- Molecule 44: 60S ribosomal protein L4

Chain BC:  81% 7% 12%



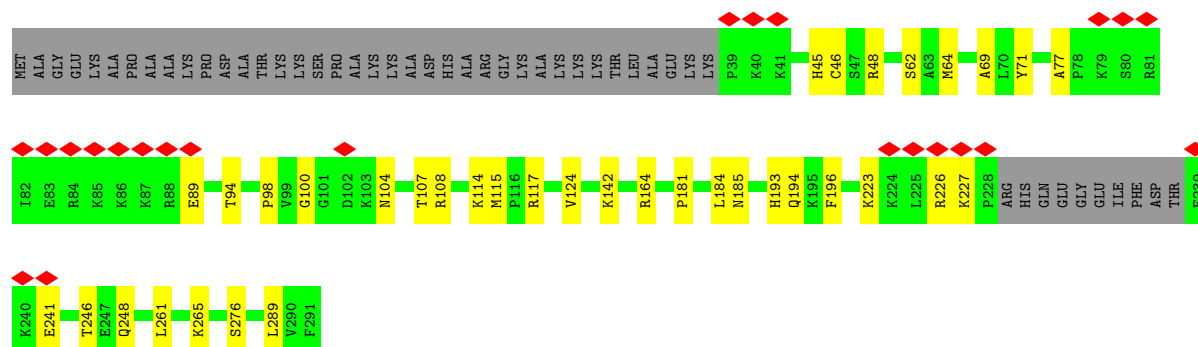
- Molecule 45: Ribosomal_L18_c domain-containing protein

Chain BD:  88% 11% .




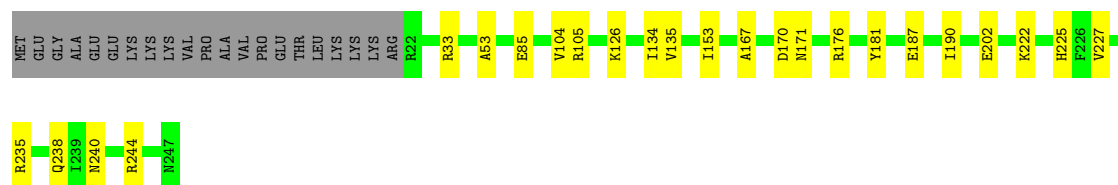
- Molecule 46: 60S ribosomal protein L6

Chain BE:  8% 71% 13% 16%

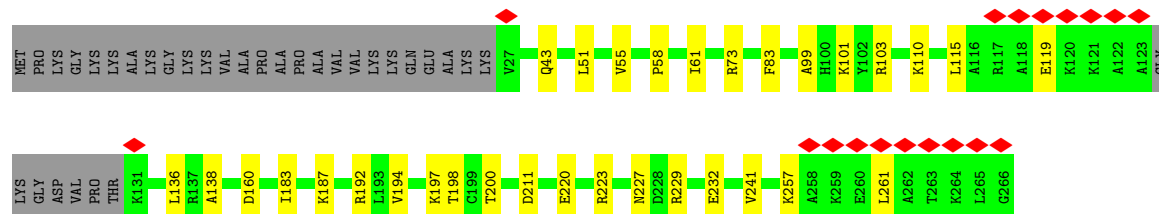
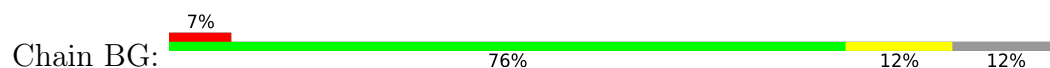


- Molecule 47: Ribosomal Protein uL30

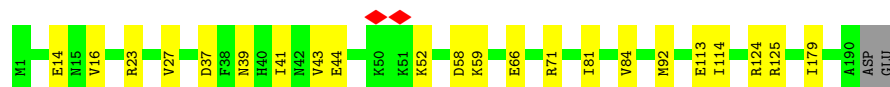
Chain BF:  82% 10% 9%



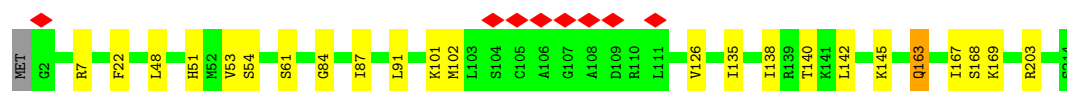
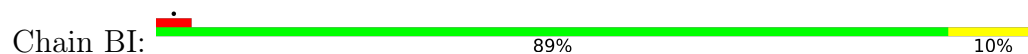
- Molecule 48: Ribosomal protein eL8



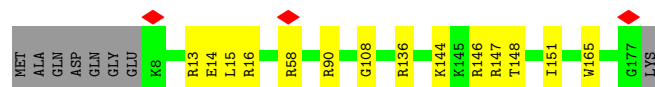
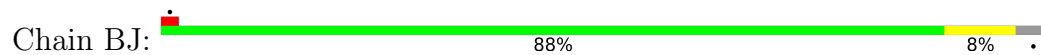
- Molecule 49: 60S ribosomal protein L9



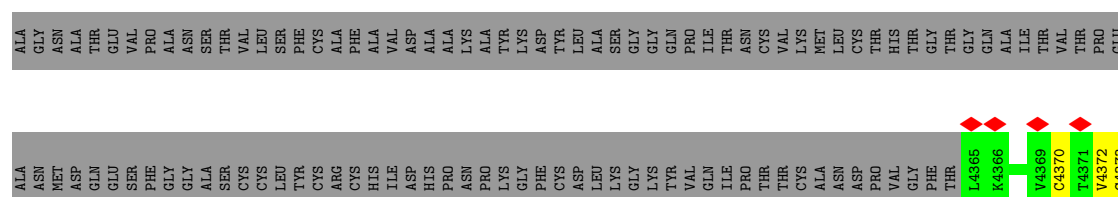
- Molecule 50: 60S ribosomal protein L10



- Molecule 51: Ribosomal protein L11



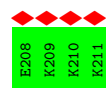
- Molecule 52: Replicase polypeptide 1ab



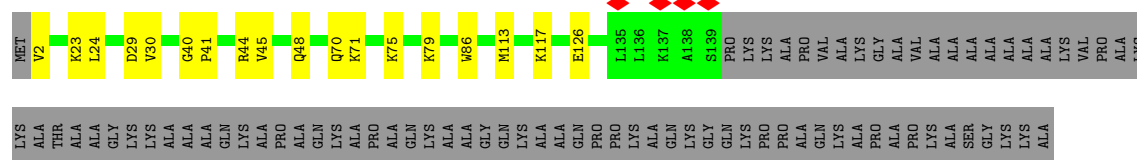


Frequency	Percentage
Daily	85%
Occasionally	14%





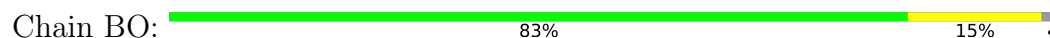
• Molecule 54: Ribosomal protein L14



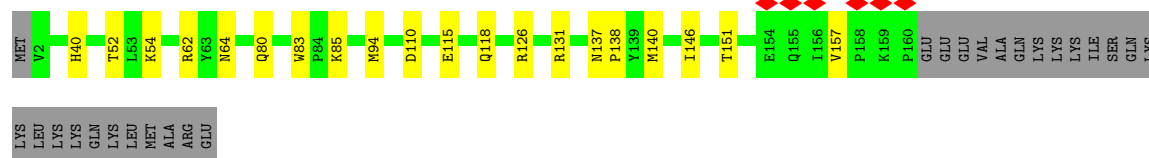
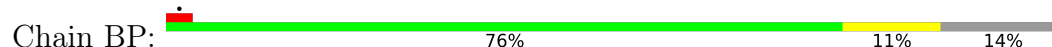
• Molecule 55: Ribosomal protein L15



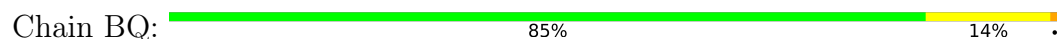
• Molecule 56: Ribosomal protein uL13




• Molecule 57: uL22

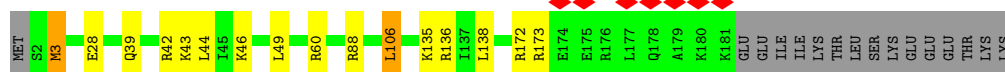


• Molecule 58: Ribosomal Protein eL18



• Molecule 59: 60S ribosomal protein L19

Chain BR:  84% 7% 8%




- Molecule 60: Ribosomal protein eL20

Chain BS:  91% 9%



- Molecule 61: eL21

Chain BT:  88% 12%



- Molecule 62: Ribosomal protein eL22

Chain BU:  66% 12% 23%




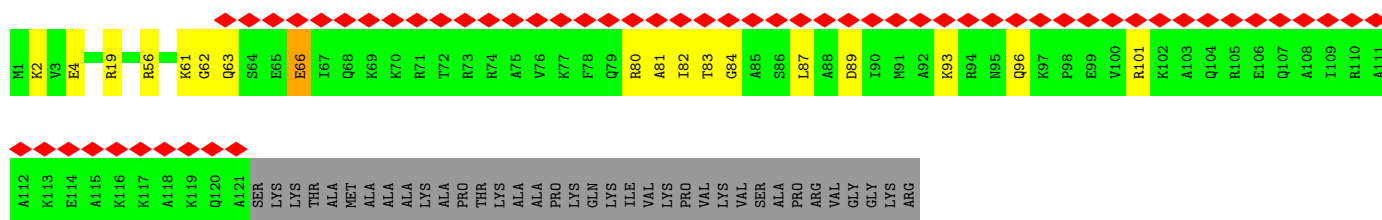
- Molecule 63: Ribosomal protein L23

Chain BV:  6% 91% 9%




- Molecule 64: eL24

Chain BW:  38% 66% 11% 23%

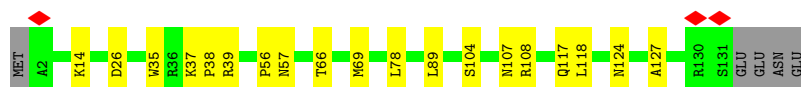
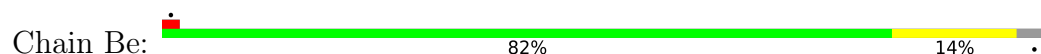


- Molecule 65: uL23

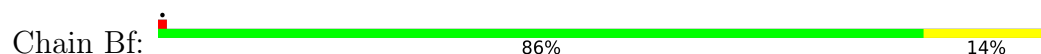
Chain BX:  72% 24%



- Molecule 72: eL32



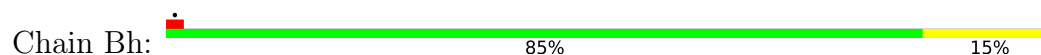
- Molecule 73: eL33



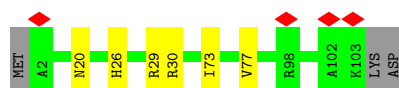
- Molecule 74: 60S ribosomal protein L34



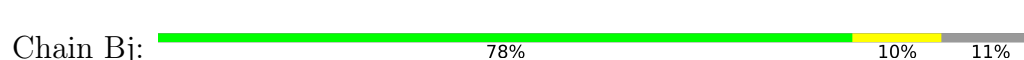
- Molecule 75: uL29




- Molecule 76: 60S ribosomal protein L36



- Molecule 77: Ribosomal protein L37




- Molecule 78: eL38

Chain Bk:  87% 10% ..



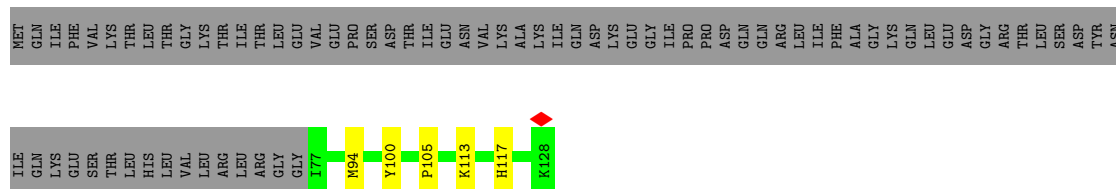
- Molecule 79: eL39

Chain Bl:  78% 18% ..



- Molecule 80: 60S ribosomal protein L40

Chain Bm:  37% 59%



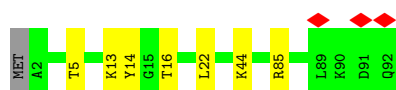
- Molecule 81: eL42

Chain Bo:  88% 11% .




- Molecule 82: eL43

Chain Bp:  91% 8% .



- Molecule 83: Ribosomal protein eL28

Chain Br:  84% 8% 8%



- Molecule 84: 60S acidic ribosomal protein P0

Chain Bs:  62% 49% 13% 38%

N182	I183	H184	L185	A186	V187	N188	F189	L190	V191	S192	L193	L194	K195	K196	N197	W198	Q199	N200	V201	R202	A203	L204	Y205	L206	K207	S208	T209	M210	G211	K212	P213	Q214	R215	L216	Y217
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	171706	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.454	Depositor
Minimum map value	-18.107	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.952	Depositor
Recommended contour level	5	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, AYA, MLZ, UNX, UY1, ZN, OMG, AME, M2G, UR3, SPM, H2U, 4AC, MG, 1MA, G7M, MA6, PSU, AAC, 5MC, NMM, 6MZ, OMU, HY3, SPD, GTP, 2MG, OMC, M3L, B8N, YYG, V5N, HIC, A2M, SAC

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	A2	0.15	0/40342	0.17	0/62877
2	AA	0.10	0/665	0.27	0/891
3	AB	0.10	0/497	0.23	0/666
4	AC	0.08	0/622	0.24	0/822
5	AD	0.10	0/462	0.25	0/607
6	AE	0.11	0/828	0.23	0/1109
7	AF	0.09	0/2493	0.24	0/3394
8	AG	0.11	0/470	0.26	0/623
9	AH	0.06	0/2253	0.13	0/3508
10	AI	0.15	0/68	0.23	0/103
11	AT	0.16	0/1440	0.14	0/2242
12	AZ	0.10	0/1771	0.23	0/2406
13	Aa	0.11	0/1841	0.24	0/2459
14	Ab	0.11	0/1742	0.26	0/2354
15	Ac	0.10	0/1779	0.24	0/2395
16	Ad	0.11	0/2118	0.26	0/2849
17	Ae	0.10	0/1531	0.27	0/2059
18	Af	0.09	0/1946	0.24	0/2590
19	Ag	0.09	0/1552	0.24	0/2079
20	Ah	0.10	0/1715	0.25	0/2287
21	Ai	0.09	0/1550	0.22	0/2069
22	Aj	0.10	0/834	0.26	0/1125
23	Ak	0.11	0/1284	0.24	0/1717
24	Al	0.08	0/968	0.25	0/1296
25	Am	0.11	0/1232	0.25	0/1656
26	An	0.12	0/1029	0.31	0/1380
27	Ao	0.11	0/1069	0.26	0/1429
28	Ap	0.10	0/1142	0.28	0/1528
29	Aq	0.09	0/1094	0.23	0/1469
30	Ar	0.08	0/1226	0.22	0/1643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	As	0.10	0/1119	0.24	0/1498
32	At	0.11	0/831	0.24	0/1115
33	Au	0.10	0/636	0.24	0/852
34	Av	0.12	0/1051	0.25	0/1406
35	Aw	0.10	0/1107	0.25	0/1475
36	Ax	0.09	0/1032	0.22	0/1371
37	Ay	0.09	0/691	0.22	0/922
38	Az	0.10	0/240	0.21	0/305
39	B5	0.14	2/87403 (0.0%)	0.18	0/136359
40	B7	0.11	0/2835	0.16	0/4418
41	B8	0.11	0/3635	0.17	0/5661
42	BA	0.13	0/1965	0.29	0/2633
43	BB	0.12	0/3261	0.26	0/4364
44	BC	0.11	0/2932	0.24	0/3939
45	BD	0.11	0/2437	0.24	0/3264
46	BE	0.10	0/1998	0.23	0/2673
47	BF	0.11	0/1922	0.25	0/2563
48	BG	0.11	0/1908	0.24	0/2566
49	BH	0.11	0/1535	0.25	0/2063
50	BI	0.11	0/1756	0.24	0/2346
51	BJ	0.10	0/1385	0.24	0/1852
52	BK	0.10	0/269	0.28	0/361
53	BL	0.11	0/1733	0.23	0/2316
54	BM	0.10	0/1158	0.23	0/1547
55	BN	0.12	0/1746	0.24	0/2338
56	BO	0.12	0/1662	0.23	0/2222
57	BP	0.11	0/1317	0.25	0/1768
58	BQ	0.12	0/1539	0.26	0/2054
59	BR	0.09	0/1524	0.23	0/2013
60	BS	0.12	0/1497	0.24	0/2008
61	BT	0.11	0/1326	0.24	0/1770
62	BU	0.09	0/820	0.24	0/1100
63	BV	0.12	0/1048	0.26	0/1402
64	BW	0.09	0/1006	0.23	0/1334
65	BX	0.10	0/984	0.23	0/1323
66	BY	0.10	0/1132	0.23	0/1504
67	BZ	0.10	0/1130	0.23	0/1507
68	Ba	0.11	0/1179	0.25	0/1572
69	Bb	0.10	0/884	0.27	0/1169
70	Bc	0.10	0/847	0.21	0/1134
71	Bd	0.12	0/903	0.24	0/1216
72	Be	0.11	0/1088	0.25	0/1451
73	Bf	0.12	0/903	0.26	0/1208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Bg	0.11	0/916	0.25	0/1220
75	Bh	0.09	0/1021	0.21	0/1348
76	Bi	0.09	0/841	0.24	0/1112
77	Bj	0.12	0/720	0.28	0/952
78	Bk	0.09	0/575	0.21	0/761
79	Bl	0.12	0/459	0.25	0/608
80	Bm	0.10	0/426	0.27	0/564
81	Bo	0.12	0/866	0.26	0/1141
82	Bp	0.11	0/718	0.27	0/953
83	Br	0.11	0/1020	0.25	0/1366
84	Bs	0.08	0/1530	0.23	0/2064
85	Bt	0.08	0/1193	0.25	0/1609
86	Bv	0.09	0/1735	0.30	0/2328
All	All	0.13	2/236957 (0.0%)	0.21	0/347620

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
81	Bo	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4761	U	C4-O4	5.13	1.33	1.23
39	B5	4269	A2M	O3'-P	5.00	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
81	Bo	53	MLZ	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	37833	0	19167	300	0
2	AA	651	0	672	9	0
3	AB	495	0	523	6	0
4	AC	610	0	634	16	0
5	AD	457	0	502	11	0
6	AE	814	0	863	13	0
7	AF	2436	0	2393	43	0
8	AG	459	0	448	7	0
9	AH	2018	0	1018	14	0
10	AI	939	0	618	4	0
11	AT	1652	0	859	12	0
12	AZ	1743	0	1748	22	0
13	Aa	1815	0	1908	24	0
14	Ab	1706	0	1796	16	0
15	Ac	1751	0	1846	23	0
16	Ad	2076	0	2177	18	0
17	Ae	1509	0	1563	21	0
18	Af	1923	0	2089	39	0
19	Ag	1529	0	1627	20	0
20	Ah	1686	0	1772	32	0
21	Ai	1525	0	1640	15	0
22	Aj	810	0	836	9	0
23	Ak	1262	0	1335	7	0
24	Al	958	0	993	18	0
25	Am	1208	0	1293	16	0
26	An	1016	0	1039	18	0
27	Ao	1048	0	1093	10	0
28	Ap	1124	0	1193	19	0
29	Aq	1080	0	1135	13	0
30	Ar	1217	0	1279	18	0
31	As	1113	0	1145	12	0
32	At	821	0	883	8	0
33	Au	640	0	633	7	0
34	Av	1034	0	1080	16	0
35	Aw	1099	0	1162	11	0
36	Ax	1015	0	1086	13	0
37	Ay	683	0	761	10	0
38	Az	239	0	289	5	0
39	B5	80772	0	40876	563	0
40	B7	2570	0	1294	14	0
41	B8	3319	0	1684	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BA	1940	0	2029	20	0
43	BB	3206	0	3353	30	0
44	BC	2886	0	3057	20	0
45	BD	2398	0	2430	23	0
46	BE	1960	0	2153	24	0
47	BF	1886	0	2008	17	0
48	BG	1877	0	2023	18	0
49	BH	1516	0	1597	14	0
50	BI	1717	0	1763	15	0
51	BJ	1362	0	1399	8	0
52	BK	265	0	254	5	0
53	BL	1702	0	1820	21	0
54	BM	1137	0	1211	14	0
55	BN	1701	0	1749	19	0
56	BO	1630	0	1777	22	0
57	BP	1289	0	1329	15	0
58	BQ	1515	0	1634	21	0
59	BR	1508	0	1664	14	0
60	BS	1457	0	1492	10	0
61	BT	1298	0	1366	16	0
62	BU	806	0	827	9	0
63	BV	1034	0	1097	10	0
64	BW	991	0	1048	12	0
65	BX	967	0	1040	3	0
66	BY	1115	0	1205	13	0
67	BZ	1107	0	1182	11	0
68	Ba	1163	0	1202	16	0
69	Bb	881	0	957	11	0
70	Bc	836	0	888	6	0
71	Bd	888	0	930	11	0
72	Be	1070	0	1165	17	0
73	Bf	884	0	923	11	0
74	Bg	906	0	998	5	0
75	Bh	1013	0	1147	14	0
76	Bi	830	0	916	4	0
77	Bj	705	0	737	8	0
78	Bk	569	0	637	6	0
79	Bl	447	0	479	8	0
80	Bm	432	0	470	3	0
81	Bo	863	0	929	8	0
82	Bp	708	0	756	6	0
83	Br	1014	0	1083	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Bs	1507	0	1564	29	0
85	Bt	1178	0	1235	38	0
86	Bv	1707	0	1815	43	0
87	A2	80	0	152	6	0
87	B5	220	0	418	18	0
88	A2	14	0	26	2	0
88	B5	28	0	52	3	0
89	A2	109	0	0	0	0
89	AH	1	0	0	0	0
89	AT	3	0	0	0	0
89	Af	1	0	0	0	0
89	B5	284	0	0	0	0
89	B7	9	0	0	0	0
89	B8	9	0	0	0	0
89	BP	1	0	0	0	0
89	BR	1	0	0	0	0
89	BV	1	0	0	0	0
89	Ba	1	0	0	0	0
90	A2	60	0	0	0	0
90	AT	4	0	0	0	0
90	Ae	1	0	0	0	0
90	An	1	0	0	0	0
90	Ar	1	0	0	0	0
90	As	1	0	0	0	0
90	B5	225	0	0	0	0
90	B7	6	0	0	0	0
90	B8	8	0	0	0	0
90	BA	3	0	0	0	0
90	BB	4	0	0	0	0
90	BC	1	0	0	0	0
90	BH	1	0	0	0	0
90	BI	1	0	0	0	0
90	BL	1	0	0	0	0
90	BN	1	0	0	0	0
90	BQ	2	0	0	0	0
90	BT	2	0	0	0	0
90	Bb	1	0	0	0	0
90	Be	1	0	0	0	0
90	Bf	1	0	0	0	0
90	Bg	1	0	0	0	0
90	Bl	1	0	0	0	0
90	Bo	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	AC	1	0	0	0	0
91	AE	1	0	0	0	0
91	AG	1	0	0	0	0
91	Bg	1	0	0	0	0
91	Bj	1	0	0	0	0
91	Bm	1	0	0	0	0
91	Bo	1	0	0	0	0
91	Bp	1	0	0	0	0
92	A2	526	0	0	9	0
92	AH	9	0	0	0	0
92	AI	1	0	0	1	0
92	AT	12	0	0	0	0
92	Aa	1	0	0	0	0
92	Ac	1	0	0	0	0
92	Af	3	0	0	0	0
92	Ak	1	0	0	0	0
92	Am	1	0	0	0	0
92	An	2	0	0	1	0
92	Ap	3	0	0	0	0
92	As	2	0	0	0	0
92	At	1	0	0	0	0
92	Aw	3	0	0	0	0
92	B5	1391	0	0	11	0
92	B7	45	0	0	2	0
92	B8	50	0	0	0	0
92	BA	10	0	0	1	0
92	BB	5	0	0	0	0
92	BC	7	0	0	0	0
92	BD	1	0	0	0	0
92	BF	1	0	0	0	0
92	BH	1	0	0	0	0
92	BI	4	0	0	0	0
92	BL	3	0	0	0	0
92	BN	3	0	0	0	0
92	BO	1	0	0	0	0
92	BP	2	0	0	0	0
92	BR	5	0	0	0	0
92	BV	2	0	0	1	0
92	BX	2	0	0	0	0
92	Ba	6	0	0	0	0
92	Bd	1	0	0	0	0
92	Be	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	Bg	2	0	0	0	0
92	Bj	3	0	0	0	0
92	Bl	1	0	0	0	0
92	Bo	1	0	0	0	0
All	All	229742	0	168938	1699	0

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

The worst 5 of 1699 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)
1:A2:1092:C:HO2'	34:Av:2:VAL:N	1.56	1.03
41:B8:81:C:HO2'	75:Bh:2:ALA:N	1.64	0.94
39:B5:1:C:H42	41:B8:156:U:H3	1.25	0.82
1:A2:929:G:H1	1:A2:1014:U:H3	1.33	0.77
63:BV:50:ASN:ND2	92:BV:301:HOH:O	2.16	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	70 (97%)	2 (3%)	0	100	100
5	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
6	AE	99/115 (86%)	99 (100%)	0	0	100	100
7	AF	311/317 (98%)	302 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
12	AZ	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
13	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
14	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
15	Ac	223/281 (79%)	222 (100%)	1 (0%)	0	100	100
16	Ad	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
17	Ae	189/204 (93%)	186 (98%)	3 (2%)	0	100	100
18	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
19	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100
20	Ah	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
21	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
22	Aj	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
23	Ak	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
24	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
25	Am	148/151 (98%)	148 (100%)	0	0	100	100
26	An	134/151 (89%)	131 (98%)	3 (2%)	0	100	100
27	Ao	126/145 (87%)	125 (99%)	0	1 (1%)	16	25
28	Ap	139/172 (81%)	135 (97%)	3 (2%)	1 (1%)	18	28
29	Aq	132/135 (98%)	132 (100%)	0	0	100	100
30	Ar	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
31	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
32	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
33	Au	81/83 (98%)	81 (100%)	0	0	100	100
34	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
35	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
36	Ax	123/130 (95%)	123 (100%)	0	0	100	100
37	Ay	83/124 (67%)	81 (98%)	2 (2%)	0	100	100
38	Az	23/25 (92%)	23 (100%)	0	0	100	100
42	BA	250/257 (97%)	242 (97%)	8 (3%)	0	100	100
43	BB	395/403 (98%)	391 (99%)	4 (1%)	0	100	100
44	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BD	291/297 (98%)	289 (99%)	2 (1%)	0	100	100
46	BE	239/291 (82%)	233 (98%)	6 (2%)	0	100	100
47	BF	224/247 (91%)	218 (97%)	6 (3%)	0	100	100
48	BG	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
49	BH	188/192 (98%)	188 (100%)	0	0	100	100
50	BI	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
51	BJ	168/178 (94%)	168 (100%)	0	0	100	100
52	BK	33/1071 (3%)	33 (100%)	0	0	100	100
53	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
54	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
55	BN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
56	BO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
57	BP	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
58	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
59	BR	178/196 (91%)	178 (100%)	0	0	100	100
60	BS	174/176 (99%)	174 (100%)	0	0	100	100
61	BT	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
62	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
63	BV	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
64	BW	119/157 (76%)	119 (100%)	0	0	100	100
65	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
66	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
67	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
68	Ba	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	28
69	Bb	103/245 (42%)	99 (96%)	4 (4%)	0	100	100
70	Bc	106/115 (92%)	106 (100%)	0	0	100	100
71	Bd	105/125 (84%)	105 (100%)	0	0	100	100
72	Be	128/135 (95%)	128 (100%)	0	0	100	100
73	Bf	108/110 (98%)	108 (100%)	0	0	100	100
74	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
75	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
77	Bj	84/97 (87%)	84 (100%)	0	0	100	100
78	Bk	67/70 (96%)	67 (100%)	0	0	100	100
79	Bl	48/51 (94%)	48 (100%)	0	0	100	100
80	Bm	49/128 (38%)	49 (100%)	0	0	100	100
81	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
82	Bp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
83	Br	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
84	Bs	194/318 (61%)	189 (97%)	5 (3%)	0	100	100
85	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
86	Bv	210/217 (97%)	197 (94%)	13 (6%)	0	100	100
All	All	11943/14908 (80%)	11780 (99%)	160 (1%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	Ao	137	HIS
28	Ap	100	VAL
68	Ba	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	61	80
3	AB	56/62 (90%)	55 (98%)	1 (2%)	51	73
4	AC	67/140 (48%)	67 (100%)	0	100	100
5	AD	47/106 (44%)	46 (98%)	1 (2%)	47	69
6	AE	88/98 (90%)	86 (98%)	2 (2%)	44	66
7	AF	272/275 (99%)	268 (98%)	4 (2%)	57	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AG	48/49 (98%)	48 (100%)	0	100	100
12	AZ	182/243 (75%)	175 (96%)	7 (4%)	29	49
13	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	84
14	Ab	185/223 (83%)	184 (100%)	1 (0%)	81	91
15	Ac	189/232 (82%)	185 (98%)	4 (2%)	47	69
16	Ad	224/225 (100%)	224 (100%)	0	100	100
17	Ae	161/170 (95%)	160 (99%)	1 (1%)	78	89
18	Af	207/218 (95%)	206 (100%)	1 (0%)	81	91
19	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	89
20	Ah	178/180 (99%)	177 (99%)	1 (1%)	78	89
21	Ai	161/168 (96%)	160 (99%)	1 (1%)	78	89
22	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	82
23	Ak	139/142 (98%)	139 (100%)	0	100	100
24	Al	104/108 (96%)	101 (97%)	3 (3%)	37	60
25	Am	130/131 (99%)	130 (100%)	0	100	100
26	An	106/119 (89%)	105 (99%)	1 (1%)	70	85
27	Ao	114/130 (88%)	113 (99%)	1 (1%)	70	85
28	Ap	117/140 (84%)	117 (100%)	0	100	100
29	Aq	120/121 (99%)	120 (100%)	0	100	100
30	Ar	127/131 (97%)	124 (98%)	3 (2%)	43	65
31	As	112/114 (98%)	112 (100%)	0	100	100
32	At	94/107 (88%)	92 (98%)	2 (2%)	47	69
33	Au	67/67 (100%)	65 (97%)	2 (3%)	36	58
34	Av	112/113 (99%)	112 (100%)	0	100	100
35	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	73
36	Ax	107/112 (96%)	107 (100%)	0	100	100
37	Ay	75/102 (74%)	75 (100%)	0	100	100
38	Az	24/24 (100%)	24 (100%)	0	100	100
42	BA	194/198 (98%)	193 (100%)	1 (0%)	81	91
43	BB	344/347 (99%)	342 (99%)	2 (1%)	78	89
44	BC	302/337 (90%)	301 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BD	247/250 (99%)	247 (100%)	0	100	100
46	BE	216/251 (86%)	214 (99%)	2 (1%)	70	85
47	BF	197/215 (92%)	197 (100%)	0	100	100
48	BG	199/223 (89%)	198 (100%)	1 (0%)	81	91
49	BH	169/171 (99%)	169 (100%)	0	100	100
50	BI	180/181 (99%)	179 (99%)	1 (1%)	78	89
51	BJ	143/149 (96%)	143 (100%)	0	100	100
52	BK	30/936 (3%)	30 (100%)	0	100	100
53	BL	175/176 (99%)	173 (99%)	2 (1%)	65	82
54	BM	117/161 (73%)	117 (100%)	0	100	100
55	BN	171/172 (99%)	171 (100%)	0	100	100
56	BO	171/173 (99%)	171 (100%)	0	100	100
57	BP	140/163 (86%)	140 (100%)	0	100	100
58	BQ	164/165 (99%)	161 (98%)	3 (2%)	51	73
59	BR	159/175 (91%)	157 (99%)	2 (1%)	61	80
60	BS	154/154 (100%)	154 (100%)	0	100	100
61	BT	139/140 (99%)	138 (99%)	1 (1%)	76	88
62	BU	88/113 (78%)	88 (100%)	0	100	100
63	BV	106/107 (99%)	106 (100%)	0	100	100
64	BW	100/126 (79%)	99 (99%)	1 (1%)	68	84
65	BX	106/134 (79%)	106 (100%)	0	100	100
66	BY	124/135 (92%)	124 (100%)	0	100	100
67	BZ	117/118 (99%)	117 (100%)	0	100	100
68	Ba	118/119 (99%)	118 (100%)	0	100	100
69	Bb	87/183 (48%)	87 (100%)	0	100	100
70	Bc	92/98 (94%)	91 (99%)	1 (1%)	65	82
71	Bd	98/110 (89%)	98 (100%)	0	100	100
72	Be	116/121 (96%)	116 (100%)	0	100	100
73	Bf	89/89 (100%)	89 (100%)	0	100	100
74	Bg	98/100 (98%)	98 (100%)	0	100	100
75	Bh	109/110 (99%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	Bi	86/89 (97%)	86 (100%)	0	100	100
77	Bj	73/80 (91%)	73 (100%)	0	100	100
78	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	76
79	Bl	47/48 (98%)	45 (96%)	2 (4%)	26	44
80	Bm	47/115 (41%)	47 (100%)	0	100	100
81	Bo	92/93 (99%)	92 (100%)	0	100	100
82	Bp	74/75 (99%)	74 (100%)	0	100	100
83	Br	109/120 (91%)	109 (100%)	0	100	100
84	Bs	164/258 (64%)	161 (98%)	3 (2%)	51	73
85	Bt	128/137 (93%)	124 (97%)	4 (3%)	35	57
86	Bv	191/195 (98%)	186 (97%)	5 (3%)	40	63
All	All	10394/12642 (82%)	10318 (99%)	76 (1%)	73	88

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	BR	106	LEU
86	Bv	58	THR
64	BW	66	GLU
84	Bs	78	LEU
86	Bv	159	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
47	BF	115	GLN
57	BP	97	ASN
83	Br	6	GLN
48	BG	38	ASN
50	BI	73	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1764/1870 (94%)	226 (12%)	0
10	AI	2/76 (2%)	1 (50%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AT	75/76 (98%)	10 (13%)	0
39	B5	3752/4808 (78%)	489 (13%)	3 (0%)
40	B7	118/120 (98%)	8 (6%)	0
41	B8	155/158 (98%)	17 (10%)	0
9	AH	94/220 (42%)	29 (30%)	0
All	All	5960/7328 (81%)	780 (13%)	3 (0%)

5 of 780 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	C
1	A2	4	C
1	A2	33	G
1	A2	41	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	B5	1545	C
39	B5	1588	G
39	B5	4445	U

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

239 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	$\# Z > 2$
1	PSU	A2	1005	1	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	A2	684	1	23,26,27	1.19	3 (13%)	33,38,41	1.96	6 (18%)
1	OMU	A2	1443	1,89	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
39	PSU	B5	4107	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	AME	Au	1	33	9,10,11	0.47	0	9,11,13	0.88	1 (11%)
39	OMG	B5	3676	39	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
39	PSU	B5	1720	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A2	1032	1	22,25,26	1.43	4 (18%)	31,36,39	2.17	10 (32%)
1	OMC	A2	1704	1	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
1	OMU	A2	429	1	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
39	A2M	B5	1479	39	22,25,26	1.44	4 (18%)	31,36,39	2.10	10 (32%)
1	PSU	A2	1446	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	A2	1679	1	22,25,26	1.45	4 (18%)	31,36,39	2.16	10 (32%)
83	SAC	Br	2	83	7,8,9	0.51	0	8,9,11	0.86	1 (12%)
1	OMG	A2	1491	1,89	23,26,27	1.19	3 (13%)	33,38,41	1.97	7 (21%)
1	PSU	A2	823	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	573	1	18,21,22	1.33	2 (11%)	22,30,33	1.91	4 (18%)
39	OMC	B5	4282	89,39	19,22,23	0.82	0	26,31,34	0.83	0
39	A2M	B5	1489	89,39	22,25,26	1.46	4 (18%)	31,36,39	2.07	9 (29%)
1	MA6	A2	1852	1	23,26,27	1.53	5 (21%)	34,38,41	2.16	11 (32%)
39	OMG	B5	1580	39	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	A2	463	1	19,22,23	0.81	0	26,31,34	0.81	0
1	OMC	A2	518	1	19,22,23	0.81	0	26,31,34	0.80	0
39	PSU	B5	3496	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
39	OMC	B5	4202	39	19,22,23	0.81	0	26,31,34	0.80	0
41	PSU	B8	55	41	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
39	PSU	B5	1683	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
39	OMC	B5	1820	89,39	19,22,23	0.81	0	26,31,34	0.84	0
39	PSU	B5	4045	39	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4188	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	4177	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
41	OMG	B8	75	41	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
39	OMG	B5	4364	39	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	A2M	A2	159	1	22,25,26	1.46	4 (18%)	31,36,39	2.16	10 (32%)
39	OMU	B5	4366	39	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
39	PSU	B5	4169	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4435	39	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	1718	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
11	2MG	AT	10	11	23,26,27	1.26	4 (17%)	32,38,41	2.17	6 (18%)
1	PSU	A2	1348	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	OMC	B5	2208	89,39	19,22,23	0.79	0	26,31,34	0.78	0
39	OMC	B5	3433	39	19,22,23	0.79	0	26,31,34	0.76	0
39	PSU	B5	4039	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	G7M	A2	1640	1,11	23,26,27	2.32	5 (21%)	35,39,42	2.92	10 (28%)
39	UR3	B5	4276	39	19,22,23	0.99	1 (5%)	26,32,35	1.42	1 (3%)
39	PSU	B5	4217	39	18,21,22	1.39	2 (11%)	22,30,33	1.87	3 (13%)
44	AYA	BC	2	44	6,7,8	0.75	0	5,8,10	0.24	0
39	PSU	B5	1801	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	A2	34	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
39	PSU	B5	4298	39	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
39	OMG	B5	3359	39	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
39	PSU	B5	4749	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	218	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
39	OMC	B5	3573	39	19,22,23	0.81	0	26,31,34	0.87	1 (3%)
39	OMG	B5	3942	11,39	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
39	A2M	B5	3517	39	22,25,26	1.41	4 (18%)	31,36,39	2.24	11 (35%)
39	OMU	B5	3973	39	19,22,23	1.24	3 (15%)	26,31,34	1.69	4 (15%)
39	A2M	B5	3492	1,39	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
39	PSU	B5	2351	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
39	A2M	B5	3599	39	22,25,26	1.46	4 (18%)	31,36,39	2.09	10 (32%)
39	OMC	B5	2667	39	19,22,23	0.81	0	26,31,34	0.82	1 (3%)
39	PSU	B5	3554	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
39	6MZ	B5	3966	39	22,25,26	1.42	4 (18%)	30,36,39	2.19	9 (30%)
39	PSU	B5	3616	39	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	A2	121	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
1	A2M	A2	591	1	22,25,26	1.46	4 (18%)	31,36,39	2.18	7 (22%)
39	PSU	B5	3462	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	4374	39	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
35	HY3	Aw	62	35	6,8,9	1.90	1 (16%)	5,10,12	1.13	1 (20%)
39	PSU	B5	3447	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	A2	815	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	816	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
39	PSU	B5	4149	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
39	PSU	B5	4419	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	OMG	A2	437	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	A2	577	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
11	H2U	AT	17	11	18,21,22	1.00	2 (11%)	21,30,33	1.72	2 (9%)
11	PSU	AT	28	11	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
68	V5N	Ba	39	68	9,11,12	2.14	2 (22%)	9,14,16	1.70	2 (22%)
39	OMU	B5	3657	39	19,22,23	1.24	2 (10%)	26,31,34	1.76	5 (19%)
1	PSU	A2	867	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
39	PSU	B5	3502	39	18,21,22	1.37	2 (11%)	22,30,33	1.95	4 (18%)
1	OMU	A2	172	1	19,22,23	1.20	3 (15%)	26,31,34	1.72	4 (15%)
39	OMG	B5	1260	39	23,26,27	1.20	3 (13%)	33,38,41	1.98	6 (18%)
39	PSU	B5	4325	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
1	OMU	A2	1289	1	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)
39	PSU	B5	3371	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	OMC	B5	2265	89,39	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
30	SAC	Ar	2	30	7,8,9	0.53	0	8,9,11	0.89	1 (12%)
39	PSU	B5	4246	39	18,21,22	1.35	2 (11%)	22,30,33	1.93	3 (13%)
1	PSU	A2	1368	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
39	A2M	B5	1810	89,39	22,25,26	1.45	4 (18%)	31,36,39	2.17	10 (32%)
39	OMG	B5	3974	39	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
11	PSU	AT	27	11	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	A2	1047	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	OMG	B5	2267	39	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
1	4AC	A2	1843	1	21,24,25	1.01	1 (4%)	29,34,37	1.04	3 (10%)
11	1MA	AT	58	11	21,25,26	1.38	4 (19%)	31,37,40	1.69	5 (16%)
1	B8N	A2	1249	1	24,29,30	1.29	3 (12%)	29,42,45	1.26	3 (10%)
11	OMC	AT	32	11	19,22,23	0.81	0	26,31,34	0.80	0
39	5MC	B5	4193	39	18,22,23	1.00	2 (11%)	26,32,35	1.24	2 (7%)
1	PSU	A2	105	1	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	1491	39	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
39	PSU	B5	4058	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
81	MLZ	Bo	53	81	8,9,10	0.48	0	4,9,11	0.10	0
39	PSU	B5	4740	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	650	1	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
39	PSU	B5	1537	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
80	M3L	Bm	98	80	10,11,12	0.82	0	9,14,16	0.50	0
39	OMG	B5	4369	39	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	A2M	B5	4336	39	22,25,26	1.46	4 (18%)	31,36,39	2.16	10 (32%)
39	PSU	B5	1731	39	18,21,22	1.35	2 (11%)	22,30,33	1.85	4 (18%)
11	H2U	AT	16	11	18,21,22	0.99	2 (11%)	21,30,33	1.38	2 (9%)
39	PSU	B5	3466	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
39	OMC	B5	3619	39	19,22,23	0.81	0	26,31,34	0.84	0
39	PSU	B5	3427	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
39	A2M	B5	3450	39	22,25,26	1.44	4 (18%)	31,36,39	2.09	9 (29%)
39	PSU	B5	1799	39	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	1638	39	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	2475	39	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
39	PSU	B5	4042	39	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
39	A2M	B5	398	39	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)
39	PSU	B5	3576	39	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
11	YYG	AT	37	11	37,42,43	1.86	7 (18%)	45,62,65	1.94	10 (22%)
39	OMU	B5	2680	39	19,22,23	1.22	2 (10%)	26,31,34	1.74	5 (19%)
11	G7M	AT	46	11	23,26,27	2.31	5 (21%)	35,39,42	2.95	10 (28%)
1	OMU	A2	1327	1,89	19,22,23	1.19	2 (10%)	26,31,34	1.71	5 (19%)
39	PSU	B5	1721	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
39	OMC	B5	2194	89,39	19,22,23	0.81	0	26,31,34	0.94	2 (7%)
1	A2M	A2	166	1	22,25,26	1.47	4 (18%)	31,36,39	2.16	10 (32%)
1	PSU	A2	1178	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
39	PSU	B5	3490	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	4 (18%)
40	GTP	B7	1	40	30,34,34	0.50	0	46,54,54	0.58	0
1	PSU	A2	864	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	1626	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
12	SAC	AZ	2	12	7,8,9	0.52	0	8,9,11	0.86	1 (12%)
39	PSU	B5	3585	89,39	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
39	OMC	B5	2647	39	19,22,23	0.81	0	26,31,34	0.82	0
1	PSU	A2	610	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	A2M	B5	2658	89,39	22,25,26	1.44	4 (18%)	31,36,39	2.10	8 (25%)
1	OMC	A2	1392	1	19,22,23	0.84	0	26,31,34	0.95	1 (3%)
1	PSU	A2	1644	1,89	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	OMG	B5	2207	39	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
11	OMG	AT	34	9,11	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
42	V5N	BA	216	42	9,11,12	2.13	2 (22%)	9,14,16	1.74	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A2	687	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	A2	27	1,89	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
1	OMG	A2	645	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
39	A2M	B5	4269	89,39	22,25,26	1.45	4 (18%)	31,36,39	2.17	10 (32%)
1	OMU	A2	628	1	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)
1	4AC	A2	1338	1	21,24,25	1.09	2 (9%)	29,34,37	1.31	3 (10%)
11	5MU	AT	54	11	19,22,23	1.41	6 (31%)	28,32,35	2.05	7 (25%)
39	OMU	B5	2258	39	19,22,23	1.22	2 (10%)	26,31,34	1.68	4 (15%)
31	NMM	As	67	31	9,11,12	0.59	0	6,12,14	0.46	0
39	PSU	B5	4099	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
1	OMU	A2	116	1	19,22,23	1.21	3 (15%)	26,31,34	1.69	5 (19%)
39	A2M	B5	3557	39	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)
39	OMC	B5	3540	39	19,22,23	0.79	0	26,31,34	0.77	0
39	PSU	B5	1632	39	18,21,22	1.38	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	A2	1175	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
11	1MA	AT	14	11	21,25,26	1.37	4 (19%)	31,37,40	1.68	6 (19%)
1	PSU	A2	407	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	3494	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	485	1	22,25,26	1.45	4 (18%)	31,36,39	2.12	9 (29%)
39	OMC	B5	2704	39	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
39	PSU	B5	3652	89,39	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	967	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	3631	39	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	A2	682	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
39	A2M	B5	2206	89,39	22,25,26	1.44	4 (18%)	31,36,39	2.05	9 (29%)
39	OMU	B5	4244	39	19,22,23	1.21	2 (10%)	26,31,34	1.70	4 (15%)
39	OMC	B5	1284	39	19,22,23	0.80	0	26,31,34	0.77	0
39	PSU	B5	4278	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	A2M	B5	1270	39	22,25,26	1.44	4 (18%)	31,36,39	2.10	9 (29%)
11	PSU	AT	39	11	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	OMG	B5	4383	39	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	OMG	A2	602	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	MA6	A2	1851	1	23,26,27	1.53	5 (21%)	34,38,41	2.19	12 (35%)
1	PSU	A2	1239	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
1	A2M	A2	99	1,89	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	B5	4322	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	3476	39	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A2	119	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
39	UY1	B5	3550	39	19,22,23	1.31	3 (15%)	22,31,34	2.02	5 (22%)
39	OMG	B5	2719	39	23,26,27	1.21	3 (13%)	33,38,41	1.98	6 (18%)
39	A2M	B5	4317	39	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
1	PSU	A2	652	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	1046	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	1233	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	OMU	A2	1805	1	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
39	PSU	B5	3583	39	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
39	OMU	B5	4052	39	19,22,23	1.23	3 (15%)	26,31,34	1.71	5 (19%)
39	PSU	B5	4267	89,39	18,21,22	1.37	2 (11%)	22,30,33	1.89	5 (22%)
39	OMG	B5	4245	39	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
43	HIC	BB	245	43	10,11,12	0.59	0	8,14,16	0.44	0
1	PSU	A2	1245	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
39	OMG	B5	4138	39	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
11	PSU	AT	55	11	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	A2M	A2	1384	1	22,25,26	1.46	4 (18%)	31,36,39	2.09	10 (32%)
1	PSU	A2	1082	1	18,21,22	1.39	3 (16%)	22,30,33	1.85	3 (13%)
39	OMG	B5	1477	39	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
39	A2M	B5	400	39	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
39	A2M	B5	3562	39	22,25,26	1.45	4 (18%)	31,36,39	2.14	10 (32%)
39	1MA	B5	1266	89,39	21,25,26	1.36	4 (19%)	31,37,40	1.68	4 (12%)
39	OMC	B5	3601	39	19,22,23	0.81	0	26,31,34	0.80	0
39	OMG	B5	4116	39	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
39	PSU	B5	4203	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
41	PSU	B8	69	41	18,21,22	1.38	2 (11%)	22,30,33	1.93	4 (18%)
39	A2M	B5	2630	89,39	22,25,26	1.44	4 (18%)	31,36,39	2.07	8 (25%)
1	PSU	A2	802	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	A2	868	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	A2	1329	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
39	A2M	B5	2244	89,39	22,25,26	1.45	4 (18%)	31,36,39	2.12	10 (32%)
39	PSU	B5	3369	39	18,21,22	1.38	3 (16%)	22,30,33	1.94	4 (18%)
39	PSU	B5	3500	39	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	5MC	B5	3514	89,39	18,22,23	0.94	2 (11%)	26,32,35	1.18	3 (11%)
39	PSU	B5	4382	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	A2	109	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4166	39	18,21,22	1.37	2 (11%)	22,30,33	1.86	4 (18%)
69	MLZ	Bb	5	69	8,9,10	0.48	0	4,9,11	0.07	0
1	A2M	A2	513	1	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)
1	PSU	A2	1693	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
11	M2G	AT	26	11	24,27,28	1.29	4 (16%)	35,40,43	1.82	6 (17%)
39	OMG	B5	3524	39	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	1057	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	A2	1448	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
39	PSU	B5	4711	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
1	OMC	A2	174	1,89	19,22,23	0.80	0	26,31,34	0.78	0
1	A2M	A2	669	1,89	22,25,26	1.44	5 (22%)	31,36,39	2.05	9 (29%)
1	PSU	A2	36	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	210	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMU	A2	355	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	4 (15%)
1	A2M	A2	469	1	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
39	A2M	B5	3456	39	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
39	OMG	B5	4240	39	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
11	5MC	AT	49	11	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
1	6MZ	A2	1833	1,89	22,25,26	1.43	4 (18%)	30,36,39	2.13	8 (26%)
1	OMG	A2	510	1,89	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A2	93	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)

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
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	684	1	-	4/9/27/28	0/3/3/3
1	OMU	A2	1443	1,89	-	1/9/27/28	0/2/2/2
39	PSU	B5	4107	39	-	0/7/25/26	0/2/2/2
33	AME	Au	1	33	-	2/9/10/12	-
39	OMG	B5	3676	39	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	1720	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	1032	1	-	0/9/27/28	0/3/3/3
1	OMC	A2	1704	1	-	2/9/27/28	0/2/2/2
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
39	A2M	B5	1479	39	-	0/9/27/28	0/3/3/3
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	1679	1	-	0/9/27/28	0/3/3/3
83	SAC	Br	2	83	-	0/7/8/10	-
1	OMG	A2	1491	1,89	-	2/9/27/28	0/3/3/3
1	PSU	A2	823	1	-	1/7/25/26	0/2/2/2
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	4282	89,39	-	0/9/27/28	0/2/2/2
39	A2M	B5	1489	89,39	-	1/9/27/28	0/3/3/3
1	MA6	A2	1852	1	-	2/11/29/30	0/3/3/3
39	OMG	B5	1580	39	-	0/9/27/28	0/3/3/3
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	3496	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	4202	39	-	1/9/27/28	0/2/2/2
41	PSU	B8	55	41	-	0/7/25/26	0/2/2/2
39	PSU	B5	1683	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	1820	89,39	-	1/9/27/28	0/2/2/2
39	PSU	B5	4045	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4188	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4177	39	-	0/7/25/26	0/2/2/2
41	OMG	B8	75	41	-	0/9/27/28	0/3/3/3
39	OMG	B5	4364	39	-	0/9/27/28	0/3/3/3
1	A2M	A2	159	1	-	0/9/27/28	0/3/3/3
39	OMU	B5	4366	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4169	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4435	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1718	39	-	0/7/25/26	0/2/2/2
11	2MG	AT	10	11	-	0/9/27/28	0/3/3/3
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	2208	89,39	-	0/9/27/28	0/2/2/2
39	OMC	B5	3433	39	-	4/9/27/28	0/2/2/2
39	PSU	B5	4039	39	-	0/7/25/26	0/2/2/2
1	G7M	A2	1640	1,11	-	0/7/25/26	0/3/3/3
39	UR3	B5	4276	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4217	39	-	0/7/25/26	0/2/2/2
44	AYA	BC	2	44	-	0/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	1801	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4298	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3359	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	4749	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3573	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	3942	11,39	-	0/9/27/28	0/3/3/3
39	A2M	B5	3517	39	-	2/9/27/28	0/3/3/3
39	OMU	B5	3973	39	-	1/9/27/28	0/2/2/2
39	A2M	B5	3492	1,39	-	3/9/27/28	0/3/3/3
39	PSU	B5	2351	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3599	39	-	2/9/27/28	0/3/3/3
39	OMC	B5	2667	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	3554	39	-	0/7/25/26	0/2/2/2
39	6MZ	B5	3966	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	3616	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	121	1	-	1/9/27/28	0/2/2/2
1	A2M	A2	591	1	-	3/9/27/28	0/3/3/3
39	PSU	B5	3462	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4374	39	-	0/7/25/26	0/2/2/2
35	HY3	Aw	62	35	-	0/1/12/14	0/1/1/1
39	PSU	B5	3447	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4149	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4419	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	437	1	-	0/9/27/28	0/3/3/3
1	A2M	A2	577	1	-	2/9/27/28	0/3/3/3
11	H2U	AT	17	11	-	6/7/38/39	0/2/2/2
11	PSU	AT	28	11	-	0/7/25/26	0/2/2/2
68	V5N	Ba	39	68	-	1/9/10/12	0/1/1/1
39	OMU	B5	3657	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3502	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
39	OMG	B5	1260	39	-	1/9/27/28	0/3/3/3
39	PSU	B5	4325	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	1289	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	3371	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2265	89,39	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SAC	Ar	2	30	-	0/7/8/10	-
39	PSU	B5	4246	39	-	1/7/25/26	0/2/2/2
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	1810	89,39	-	0/9/27/28	0/3/3/3
39	OMG	B5	3974	39	-	0/9/27/28	0/3/3/3
11	PSU	AT	27	11	-	0/7/25/26	0/2/2/2
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	2267	39	-	0/9/27/28	0/3/3/3
1	4AC	A2	1843	1	-	2/11/29/30	0/2/2/2
11	1MA	AT	58	11	-	0/7/25/26	0/3/3/3
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
11	OMC	AT	32	11	-	0/9/27/28	0/2/2/2
39	5MC	B5	4193	39	-	4/7/25/26	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1491	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4058	39	-	0/7/25/26	0/2/2/2
81	MLZ	Bo	53	81	-	0/7/8/10	-
39	PSU	B5	4740	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1537	39	-	0/7/25/26	0/2/2/2
80	M3L	Bm	98	80	-	0/9/10/12	-
39	OMG	B5	4369	39	-	1/9/27/28	0/3/3/3
39	A2M	B5	4336	39	-	1/9/27/28	0/3/3/3
39	PSU	B5	1731	39	-	0/7/25/26	0/2/2/2
11	H2U	AT	16	11	-	1/7/38/39	0/2/2/2
39	PSU	B5	3466	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	3619	39	-	2/9/27/28	0/2/2/2
39	PSU	B5	3427	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3450	39	-	1/9/27/28	0/3/3/3
39	PSU	B5	1799	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1638	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	2475	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4042	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	398	39	-	2/9/27/28	0/3/3/3
39	PSU	B5	3576	39	-	1/7/25/26	0/2/2/2
11	YYG	AT	37	11	-	0/24/42/43	0/4/4/4
39	OMU	B5	2680	39	-	1/9/27/28	0/2/2/2
11	G7M	AT	46	11	-	1/7/25/26	0/3/3/3
1	OMU	A2	1327	1,89	-	0/9/27/28	0/2/2/2
39	PSU	B5	1721	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2194	89,39	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	A2	166	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3490	39	-	0/7/25/26	0/2/2/2
40	GTP	B7	1	40	-	0/22/38/38	0/3/3/3
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
12	SAC	AZ	2	12	-	2/7/8/10	-
39	PSU	B5	3585	89,39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2647	39	-	1/9/27/28	0/2/2/2
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	2658	89,39	-	0/9/27/28	0/3/3/3
1	OMC	A2	1392	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	1644	1,89	-	0/7/25/26	0/2/2/2
39	OMG	B5	2207	39	-	2/9/27/28	0/3/3/3
11	OMG	AT	34	9,11	-	0/9/27/28	0/3/3/3
42	V5N	BA	216	42	-	1/9/10/12	0/1/1/1
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	27	1,89	-	2/9/27/28	0/3/3/3
1	OMG	A2	645	1	-	4/9/27/28	0/3/3/3
39	A2M	B5	4269	89,39	-	0/9/27/28	0/3/3/3
1	OMU	A2	628	1	-	2/9/27/28	0/2/2/2
1	4AC	A2	1338	1	-	4/11/29/30	0/2/2/2
11	5MU	AT	54	11	-	0/7/25/26	0/2/2/2
39	OMU	B5	2258	39	-	0/9/27/28	0/2/2/2
31	NMM	As	67	31	-	1/9/11/13	-
39	PSU	B5	4099	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
39	A2M	B5	3557	39	-	1/9/27/28	0/3/3/3
39	OMC	B5	3540	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	1632	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
11	1MA	AT	14	11	-	0/7/25/26	0/3/3/3
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3494	39	-	1/7/25/26	0/2/2/2
1	A2M	A2	485	1	-	0/9/27/28	0/3/3/3
39	OMC	B5	2704	39	-	1/9/27/28	0/2/2/2
39	PSU	B5	3652	89,39	-	0/7/25/26	0/2/2/2
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	3631	39	-	0/9/27/28	0/3/3/3
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	2206	89,39	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	OMU	B5	4244	39	-	0/9/27/28	0/2/2/2
39	OMC	B5	1284	39	-	2/9/27/28	0/2/2/2
39	PSU	B5	4278	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	1270	39	-	0/9/27/28	0/3/3/3
11	PSU	AT	39	11	-	0/7/25/26	0/2/2/2
39	OMG	B5	4383	39	-	0/9/27/28	0/3/3/3
1	OMG	A2	602	1	-	0/9/27/28	0/3/3/3
1	MA6	A2	1851	1	-	0/11/29/30	0/3/3/3
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	99	1,89	-	2/9/27/28	0/3/3/3
39	PSU	B5	4322	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3476	39	-	0/9/27/28	0/3/3/3
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
39	UY1	B5	3550	39	-	4/9/27/28	0/2/2/2
39	OMG	B5	2719	39	-	0/9/27/28	0/3/3/3
39	A2M	B5	4317	39	-	0/9/27/28	0/3/3/3
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	1805	1	-	2/9/27/28	0/2/2/2
39	PSU	B5	3583	39	-	1/7/25/26	0/2/2/2
39	OMU	B5	4052	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4267	89,39	-	0/7/25/26	0/2/2/2
39	OMG	B5	4245	39	-	0/9/27/28	0/3/3/3
43	HIC	BB	245	43	-	0/5/6/8	0/1/1/1
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4138	39	-	0/9/27/28	0/3/3/3
11	PSU	AT	55	11	-	0/7/25/26	0/2/2/2
1	A2M	A2	1384	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	1082	1	-	1/7/25/26	0/2/2/2
39	OMG	B5	1477	39	-	1/9/27/28	0/3/3/3
39	A2M	B5	400	39	-	0/9/27/28	0/3/3/3
39	A2M	B5	3562	39	-	0/9/27/28	0/3/3/3
39	1MA	B5	1266	89,39	-	1/7/25/26	0/3/3/3
39	OMC	B5	3601	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	4116	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	4203	39	-	0/7/25/26	0/2/2/2
41	PSU	B8	69	41	-	0/7/25/26	0/2/2/2
39	A2M	B5	2630	89,39	-	3/9/27/28	0/3/3/3
1	PSU	A2	802	1	-	2/7/25/26	0/2/2/2
1	OMG	A2	868	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A2	1329	1	-	1/9/27/28	0/3/3/3
39	A2M	B5	2244	89,39	-	0/9/27/28	0/3/3/3
39	PSU	B5	3369	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3500	39	-	0/7/25/26	0/2/2/2
39	5MC	B5	3514	89,39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4382	39	-	3/7/25/26	0/2/2/2
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4166	39	-	0/7/25/26	0/2/2/2
69	MLZ	Bb	5	69	-	2/7/8/10	-
1	A2M	A2	513	1	-	4/9/27/28	0/3/3/3
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
11	M2G	AT	26	11	-	0/11/29/30	0/3/3/3
39	OMG	B5	3524	39	-	1/9/27/28	0/3/3/3
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	1448	1	-	2/9/27/28	0/3/3/3
39	PSU	B5	4711	39	-	0/7/25/26	0/2/2/2
1	OMC	A2	174	1,89	-	0/9/27/28	0/2/2/2
1	A2M	A2	669	1,89	-	2/9/27/28	0/3/3/3
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	469	1	-	1/9/27/28	0/3/3/3
39	A2M	B5	3456	39	-	0/9/27/28	0/3/3/3
39	OMG	B5	4240	39	-	0/9/27/28	0/3/3/3
11	5MC	AT	49	11	-	0/7/25/26	0/2/2/2
1	6MZ	A2	1833	1,89	-	2/9/27/28	0/3/3/3
1	OMG	A2	510	1,89	-	0/9/27/28	0/3/3/3
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2

The worst 5 of 558 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AT	46	G7M	C8-N7	7.32	1.46	1.33
1	A2	1640	G7M	C8-N7	7.30	1.46	1.33
11	AT	37	YYG	O23-C21	6.57	1.45	1.34
11	AT	37	YYG	O18-C16	5.16	1.45	1.33
68	Ba	39	V5N	CG-ND1	-5.08	1.32	1.37

The worst 5 of 1054 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AT	46	G7M	CN7-N7-C8	-7.83	112.76	124.84
1	A2	1640	G7M	CN7-N7-C8	-7.73	112.92	124.84
11	AT	10	2MG	C2-N3-C4	7.16	120.91	112.04
11	AT	17	H2U	C4-N3-C2	-7.02	119.97	125.79
1	A2	591	A2M	C5-C4-N3	-6.82	117.86	126.75

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	C2'-C1'-N1-C2
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	645	OMG	C3'-C4'-C5'-O5'
1	A2	1833	6MZ	N1-C6-N6-C9

There are no ring outliers.

88 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A2	1443	OMU	1	0
33	Au	1	AME	2	0
39	B5	3676	OMG	1	0
39	B5	1720	PSU	1	0
1	A2	1032	A2M	1	0
1	A2	1704	OMC	2	0
1	A2	1446	PSU	1	0
1	A2	1491	OMG	1	0
39	B5	4282	OMC	1	0
39	B5	1489	A2M	1	0
1	A2	463	OMC	1	0
1	A2	518	OMC	1	0
39	B5	4202	OMC	2	0
41	B8	75	OMG	2	0
39	B5	4364	OMG	1	0
39	B5	4366	OMU	2	0
39	B5	1718	PSU	1	0
39	B5	4039	PSU	1	0
1	A2	1640	G7M	1	0
39	B5	3942	OMG	1	0
39	B5	3517	A2M	1	0
39	B5	3599	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	B5	3616	PSU	1	0
1	A2	121	OMU	1	0
1	A2	437	OMG	1	0
1	A2	577	A2M	1	0
11	AT	17	H2U	1	0
1	A2	867	PSU	1	0
1	A2	172	OMU	2	0
39	B5	1260	OMG	1	0
39	B5	4325	PSU	2	0
39	B5	1810	A2M	2	0
39	B5	3974	OMG	1	0
39	B5	2267	OMG	2	0
1	A2	1843	4AC	1	0
11	AT	58	1MA	1	0
11	AT	32	OMC	1	0
39	B5	4193	5MC	1	0
39	B5	4336	A2M	1	0
39	B5	3466	PSU	1	0
39	B5	3619	OMC	2	0
39	B5	3450	A2M	2	0
39	B5	1638	PSU	1	0
39	B5	398	A2M	1	0
11	AT	37	YYG	1	0
39	B5	2194	OMC	1	0
1	A2	166	A2M	2	0
1	A2	1392	OMC	1	0
11	AT	34	OMG	1	0
1	A2	27	A2M	1	0
39	B5	4269	A2M	1	0
1	A2	1338	4AC	1	0
39	B5	2258	OMU	1	0
1	A2	116	OMU	2	0
39	B5	3557	A2M	1	0
39	B5	3540	OMC	1	0
39	B5	1632	PSU	1	0
1	A2	485	A2M	3	0
39	B5	2704	OMC	1	0
39	B5	2206	A2M	1	0
39	B5	1284	OMC	3	0
39	B5	1270	A2M	1	0
39	B5	4383	OMG	1	0
1	A2	602	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A2	99	A2M	2	0
39	B5	3550	UY1	1	0
39	B5	2719	OMG	2	0
39	B5	4317	A2M	1	0
1	A2	1233	PSU	2	0
1	A2	1805	OMU	1	0
39	B5	4052	OMU	1	0
1	A2	1245	PSU	2	0
39	B5	4138	OMG	1	0
39	B5	3562	A2M	1	0
39	B5	4203	PSU	1	0
1	A2	868	OMG	1	0
1	A2	1329	OMG	1	0
39	B5	3514	5MC	2	0
39	B5	4166	PSU	1	0
1	A2	513	A2M	1	0
11	AT	26	M2G	1	0
1	A2	1448	OMG	3	0
1	A2	669	A2M	1	0
1	A2	36	PSU	2	0
1	A2	469	A2M	1	0
39	B5	3456	A2M	1	0
1	A2	1833	6MZ	1	0
1	A2	510	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 790 ligands modelled in this entry, 428 are monoatomic and 329 are unknown - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	SPD	B5	4913	-	9,9,9	0.16	0	8,8,8	0.17	0
87	SPD	A2	1906	-	9,9,9	0.16	0	8,8,8	0.18	0
88	SPM	B5	4912	-	13,13,13	0.15	0	12,12,12	0.23	0
87	SPD	B5	4902	-	9,9,9	0.15	0	8,8,8	0.23	0
87	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4901	-	9,9,9	0.14	0	8,8,8	0.15	0
87	SPD	B5	4904	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4916	-	9,9,9	0.15	0	8,8,8	0.22	0
87	SPD	B5	4903	-	9,9,9	0.16	0	8,8,8	0.20	0
87	SPD	A2	1902	-	9,9,9	0.15	0	8,8,8	0.15	0
87	SPD	B5	4923	-	9,9,9	0.15	0	8,8,8	0.20	0
87	SPD	A2	1904	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4919	-	9,9,9	0.15	0	8,8,8	0.21	0
88	SPM	B5	4915	-	13,13,13	0.16	0	12,12,12	0.22	0
87	SPD	B5	4918	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	B5	4922	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	A2	1905	-	9,9,9	0.16	0	8,8,8	0.17	0
87	SPD	B5	4908	-	9,9,9	0.16	0	8,8,8	0.16	0
87	SPD	B5	4914	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	A2	1903	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4909	-	9,9,9	0.16	0	8,8,8	0.19	0
87	SPD	B5	4921	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4907	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4911	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.20	0
87	SPD	B5	4910	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4920	-	9,9,9	0.15	0	8,8,8	0.23	0
87	SPD	B5	4924	-	9,9,9	0.16	0	8,8,8	0.14	0
87	SPD	B5	4906	-	9,9,9	0.15	0	8,8,8	0.16	0
87	SPD	B5	4905	-	9,9,9	0.16	0	8,8,8	0.21	0
87	SPD	B5	4917	-	9,9,9	0.15	0	8,8,8	0.18	0
88	SPM	A2	1909	-	13,13,13	0.14	0	12,12,12	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	B5	4913	-	-	0/7/7/7	-
87	SPD	A2	1906	-	-	1/7/7/7	-
88	SPM	B5	4912	-	-	1/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	B5	4902	-	-	1/7/7/7	-
87	SPD	A2	1907	-	-	1/7/7/7	-
87	SPD	B5	4901	-	-	1/7/7/7	-
87	SPD	B5	4904	-	-	0/7/7/7	-
87	SPD	B5	4916	-	-	0/7/7/7	-
87	SPD	B5	4903	-	-	2/7/7/7	-
87	SPD	A2	1902	-	-	0/7/7/7	-
87	SPD	B5	4923	-	-	0/7/7/7	-
87	SPD	A2	1904	-	-	0/7/7/7	-
87	SPD	B5	4919	-	-	0/7/7/7	-
88	SPM	B5	4915	-	-	0/11/11/11	-
87	SPD	B5	4918	-	-	0/7/7/7	-
87	SPD	B5	4922	-	-	1/7/7/7	-
87	SPD	A2	1905	-	-	0/7/7/7	-
87	SPD	B5	4908	-	-	0/7/7/7	-
87	SPD	B5	4914	-	-	0/7/7/7	-
87	SPD	A2	1903	-	-	0/7/7/7	-
87	SPD	A2	1901	-	-	1/7/7/7	-
87	SPD	B5	4909	-	-	0/7/7/7	-
87	SPD	B5	4921	-	-	1/7/7/7	-
87	SPD	B5	4907	-	-	0/7/7/7	-
87	SPD	B5	4911	-	-	0/7/7/7	-
87	SPD	A2	1908	-	-	0/7/7/7	-
87	SPD	B5	4910	-	-	1/7/7/7	-
87	SPD	B5	4920	-	-	0/7/7/7	-
87	SPD	B5	4924	-	-	1/7/7/7	-
87	SPD	B5	4906	-	-	1/7/7/7	-
87	SPD	B5	4905	-	-	0/7/7/7	-
87	SPD	B5	4917	-	-	0/7/7/7	-
88	SPM	A2	1909	-	-	1/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	A2	1909	SPM	C12-C11-N10-C9
87	B5	4901	SPD	C4-C5-N6-C7
87	B5	4902	SPD	C2-C3-C4-C5
87	B5	4924	SPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
87	B5	4903	SPD	C2-C3-C4-C5

There are no ring outliers.

19 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	B5	4913	SPD	2	0
87	A2	1906	SPD	1	0
88	B5	4912	SPM	2	0
87	B5	4904	SPD	1	0
87	B5	4916	SPD	1	0
87	A2	1904	SPD	1	0
87	B5	4919	SPD	1	0
88	B5	4915	SPM	1	0
87	B5	4922	SPD	1	0
87	A2	1905	SPD	1	0
87	B5	4908	SPD	1	0
87	A2	1903	SPD	2	0
87	A2	1901	SPD	1	0
87	B5	4921	SPD	1	0
87	B5	4907	SPD	1	0
87	B5	4920	SPD	2	0
87	B5	4924	SPD	3	0
87	B5	4917	SPD	4	0
88	A2	1909	SPM	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

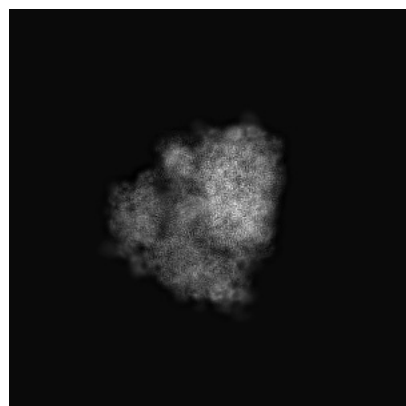
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12757. These allow visual inspection of the internal detail of the map and identification of artifacts.

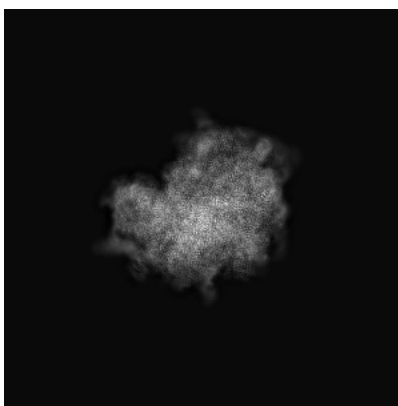
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

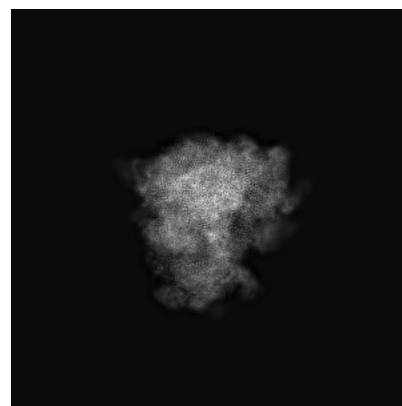
6.1.1 Primary map



X

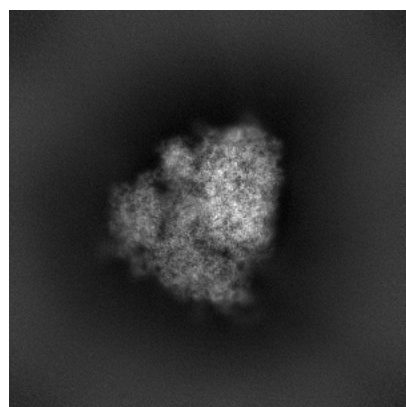


Y

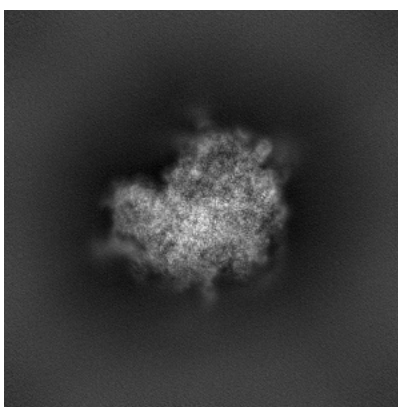


Z

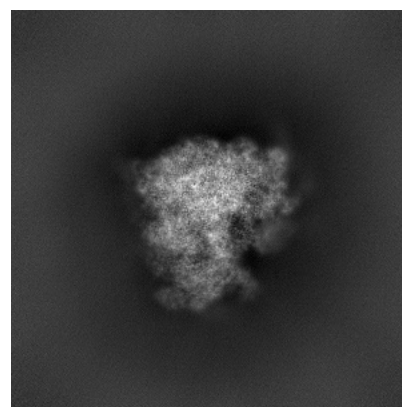
6.1.2 Raw map



X



Y

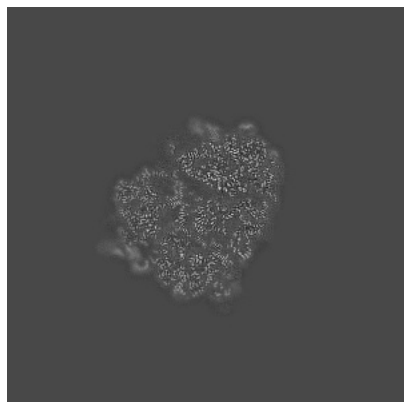


Z

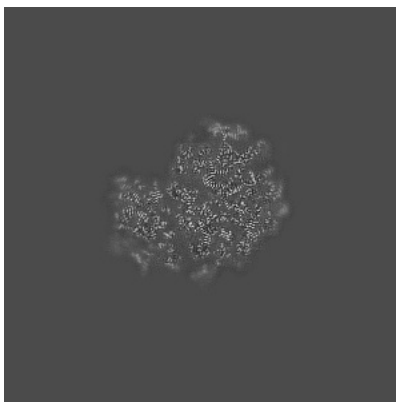
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

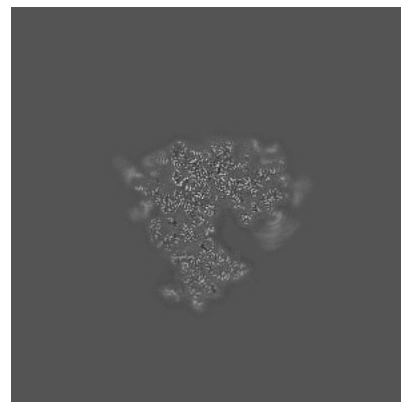
6.2.1 Primary map



X Index: 280

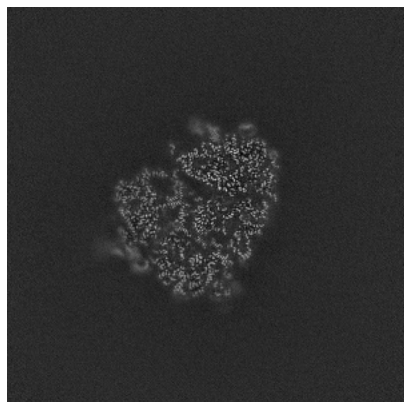


Y Index: 280

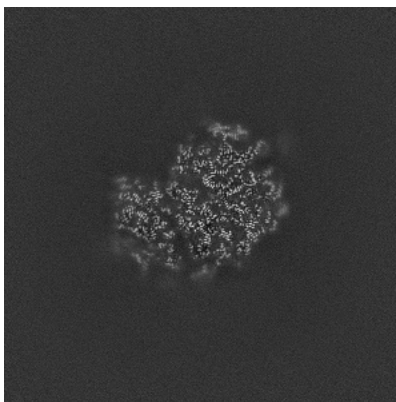


Z Index: 280

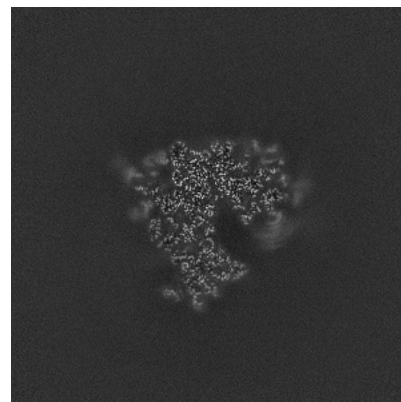
6.2.2 Raw map



X Index: 280



Y Index: 280

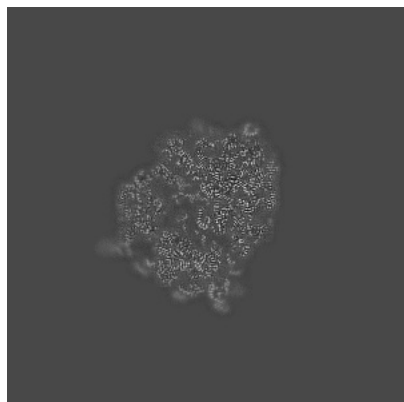


Z Index: 280

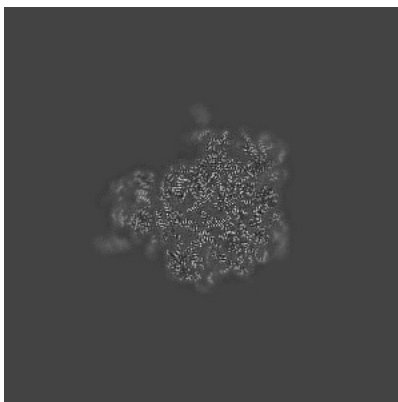
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

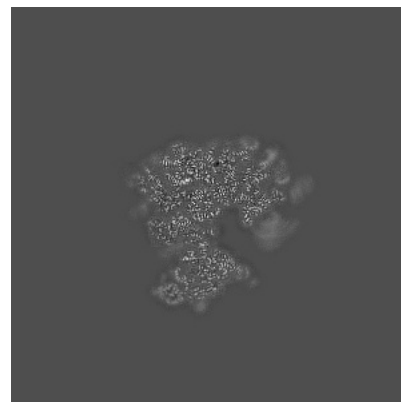
6.3.1 Primary map



X Index: 287

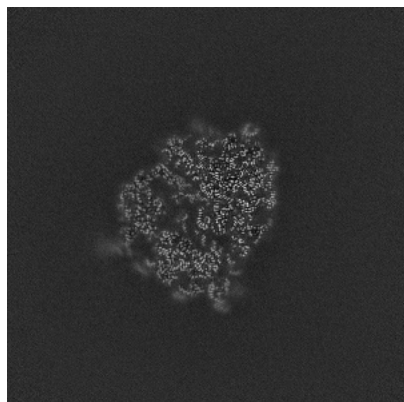


Y Index: 313

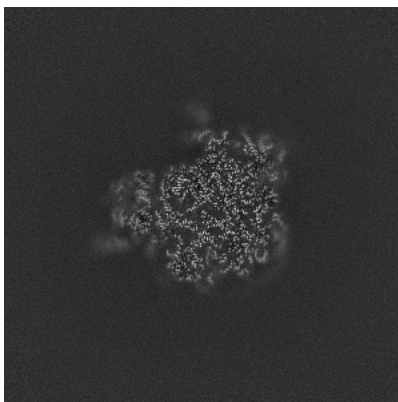


Z Index: 272

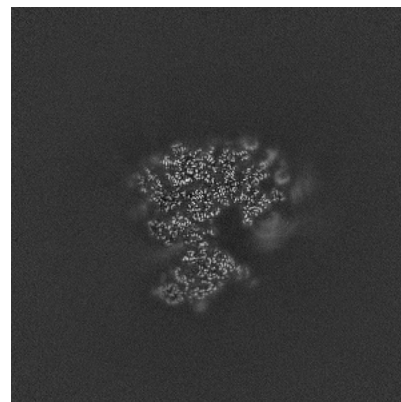
6.3.2 Raw map



X Index: 287



Y Index: 313

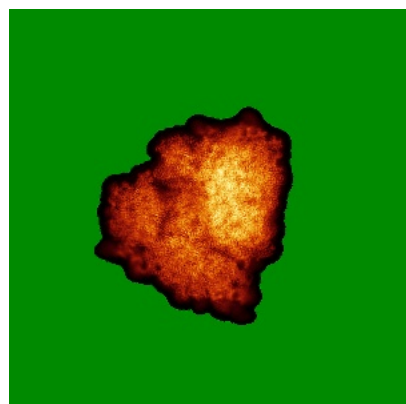


Z Index: 272

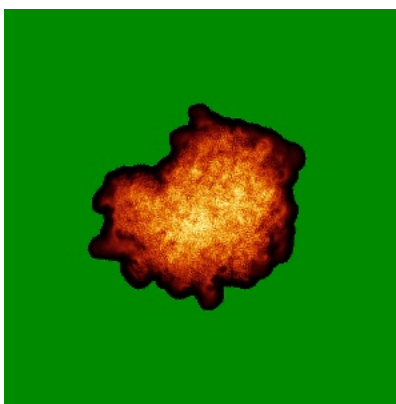
The images above show the largest variance slices of the map in three orthogonal directions.

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

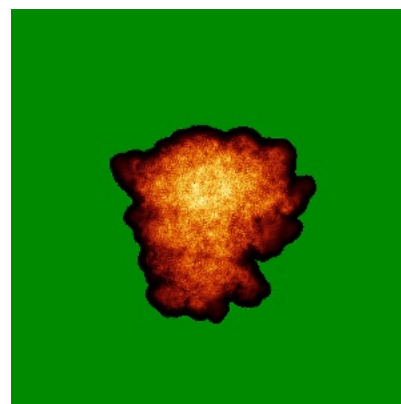
6.4.1 Primary map



X

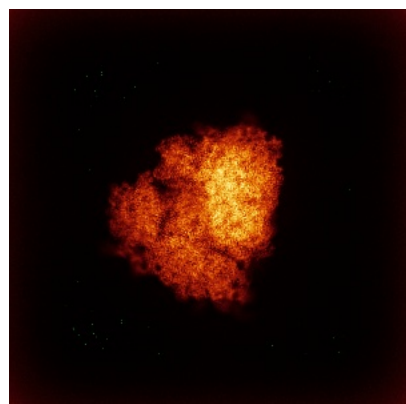


Y

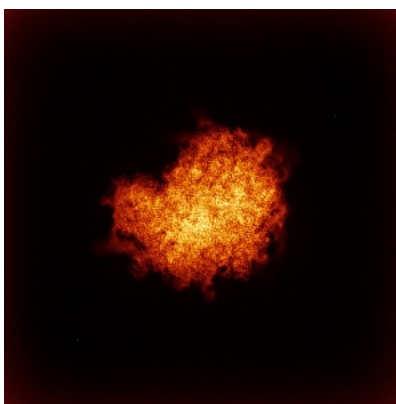


Z

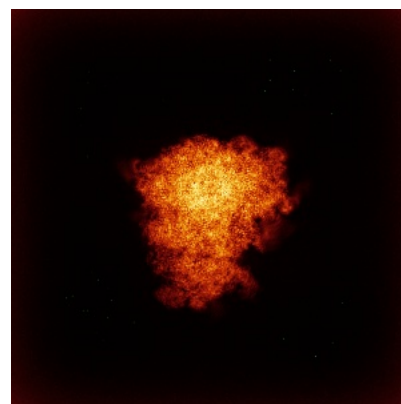
6.4.2 Raw map



X



Y

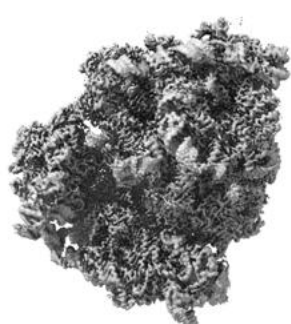


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



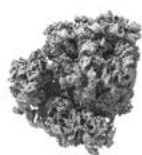
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

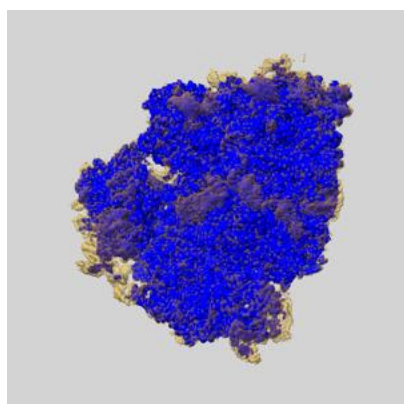
6.6 Mask visualisation [i](#)

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

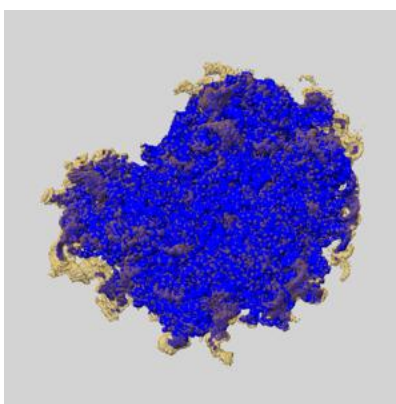
A mask typically either:

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

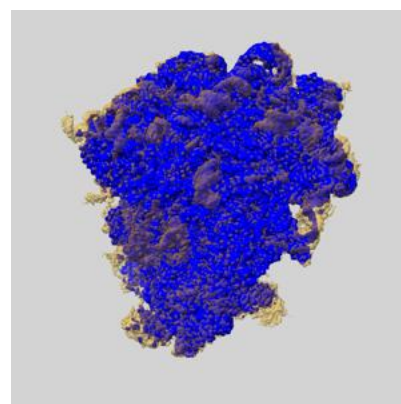
6.6.1 emd_12757_msk_1.map [i](#)



X

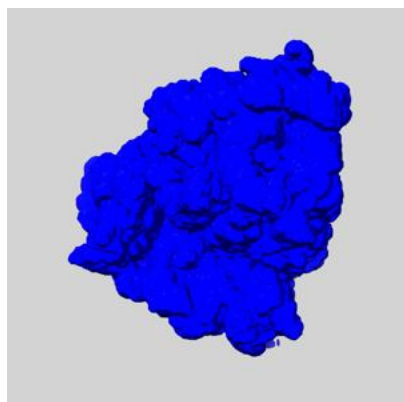


Y

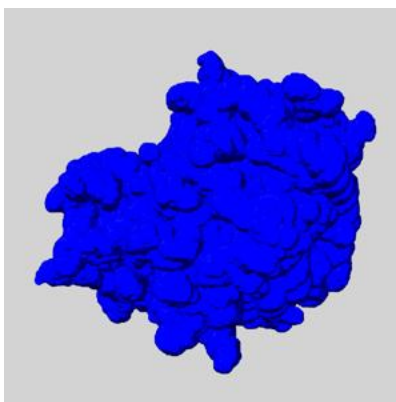


Z

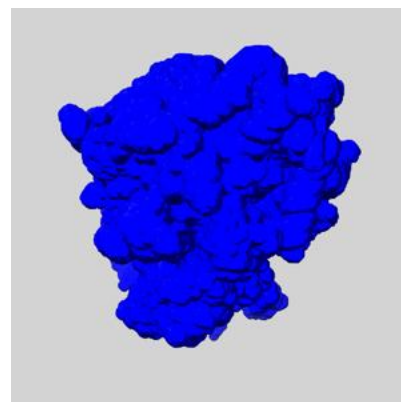
6.6.2 emd_12757_msk_2.map [i](#)



X



Y

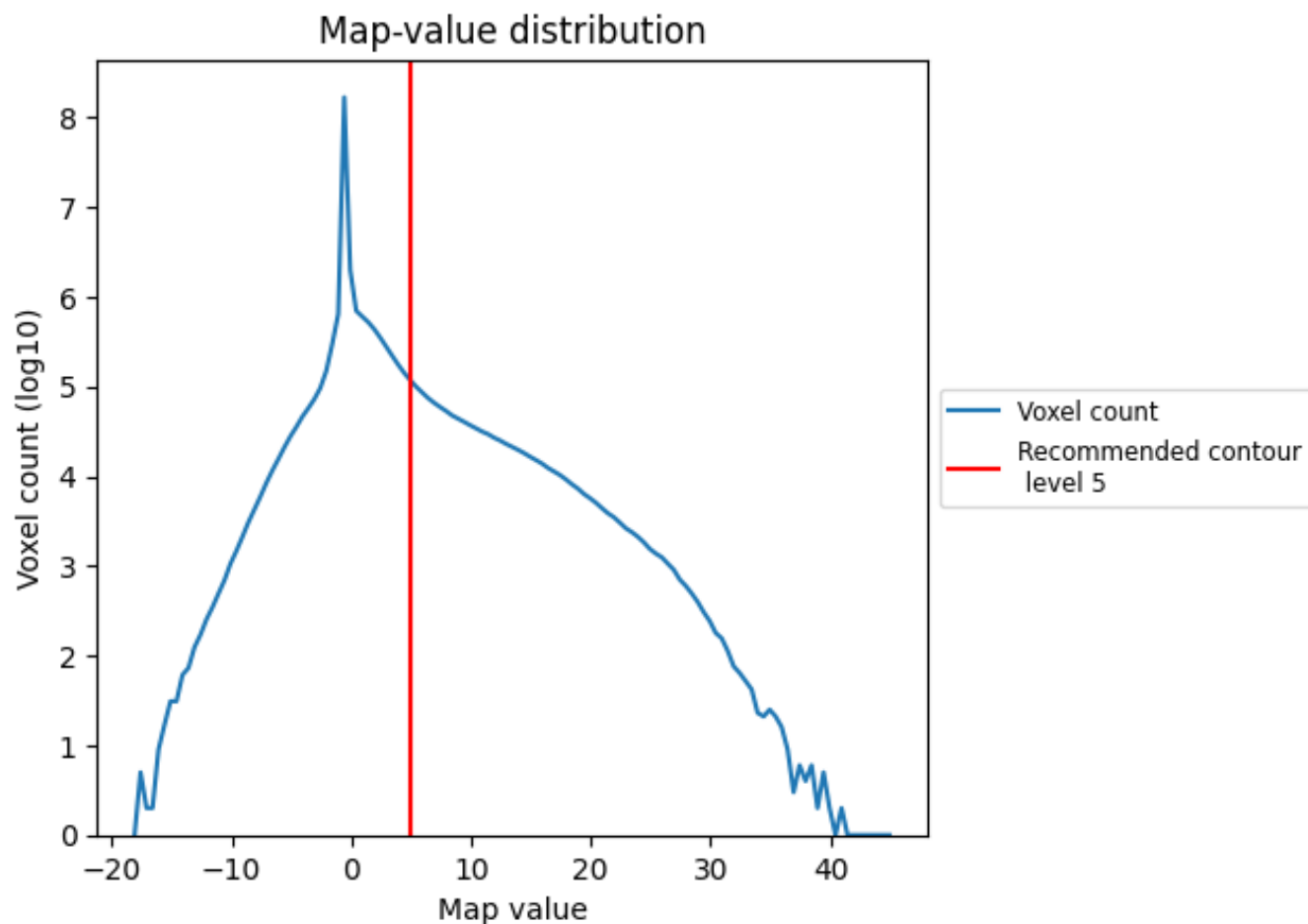


Z

7 Map analysis [i](#)

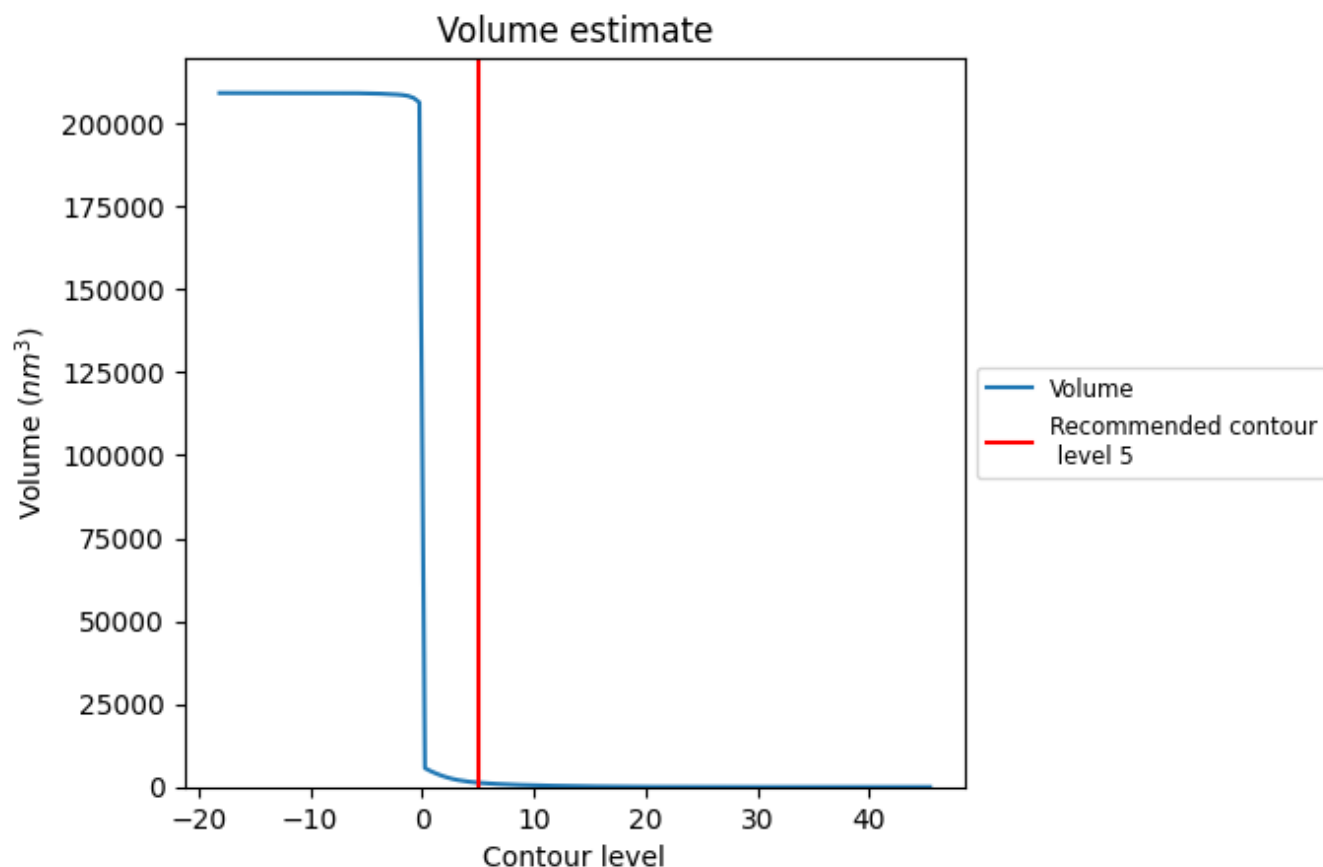
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

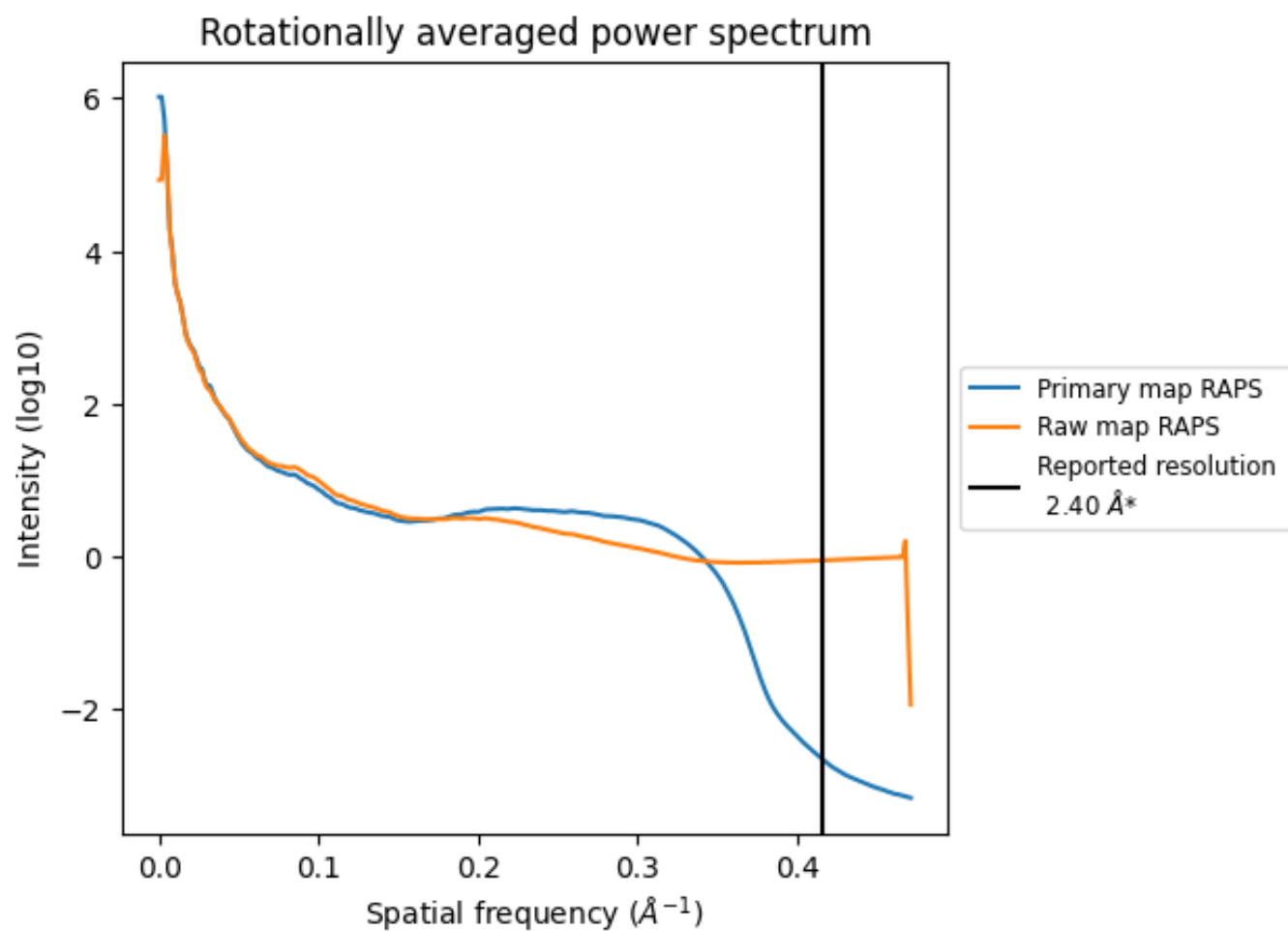
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1298 nm^3 ; this corresponds to an approximate mass of 1172 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

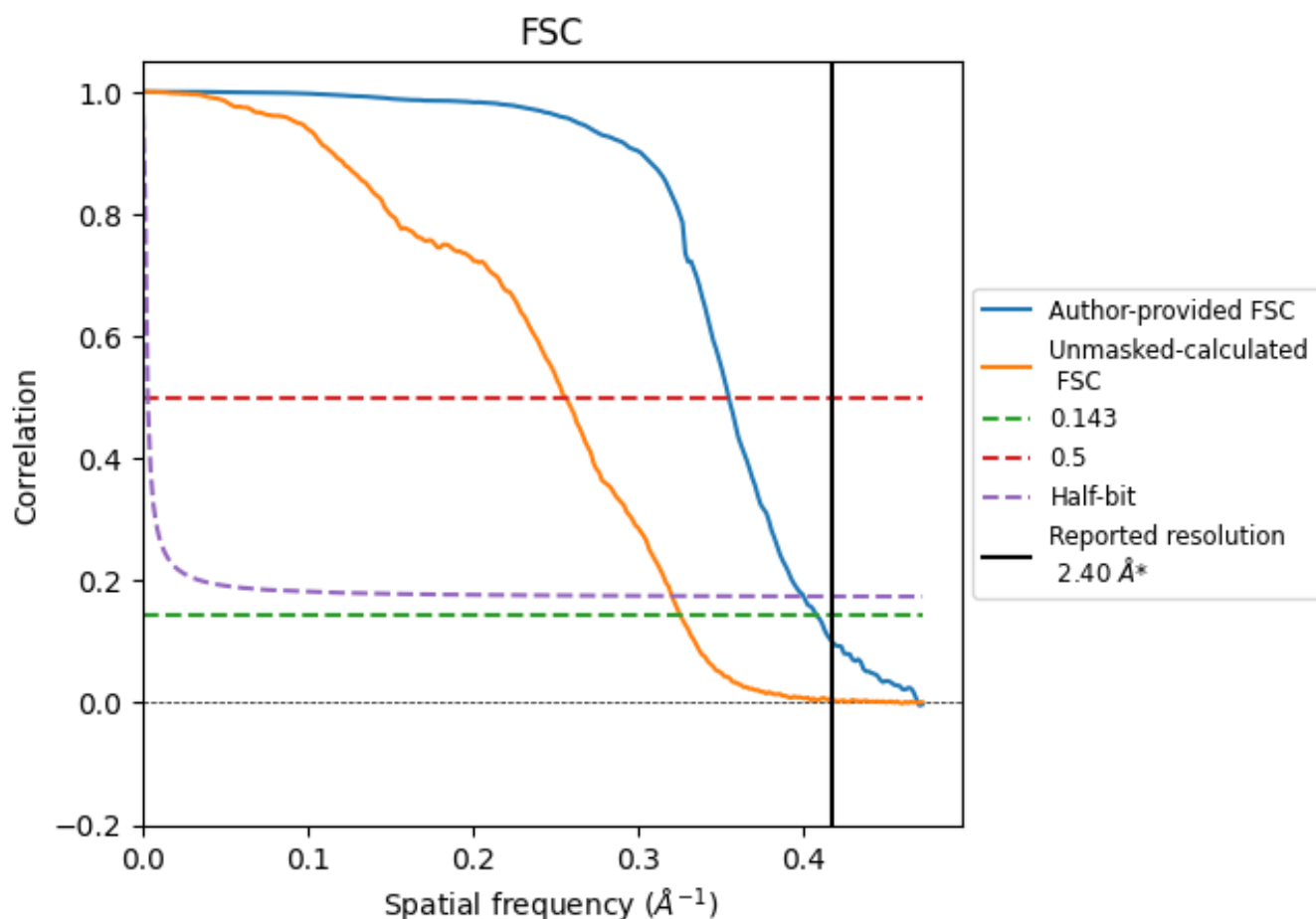


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

8.2 Resolution estimates [i](#)

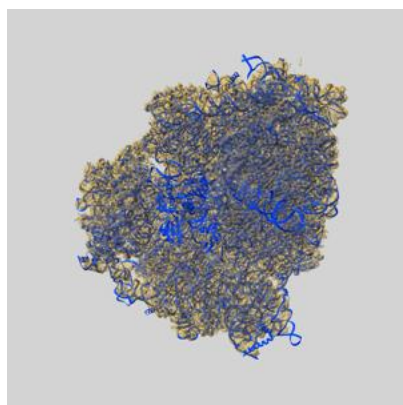
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.45	2.82	2.50
Unmasked-calculated*	3.07	3.90	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.4 by more than 10 %

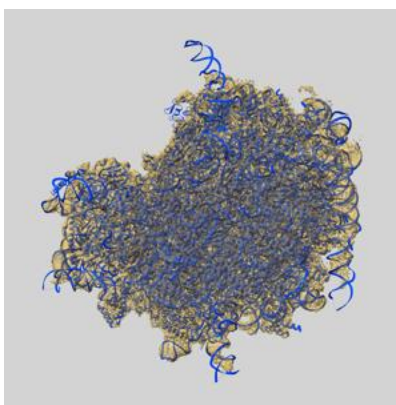
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12757 and PDB model 7O7Z. Per-residue inclusion information can be found in section [3](#) on page [27](#).

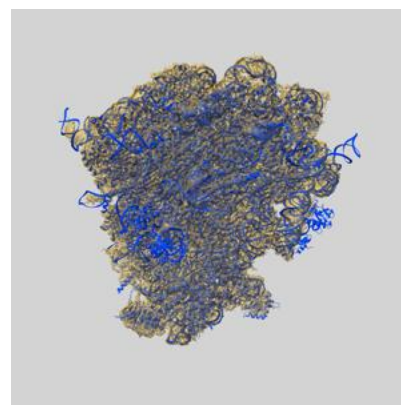
9.1 Map-model overlay [i](#)



X



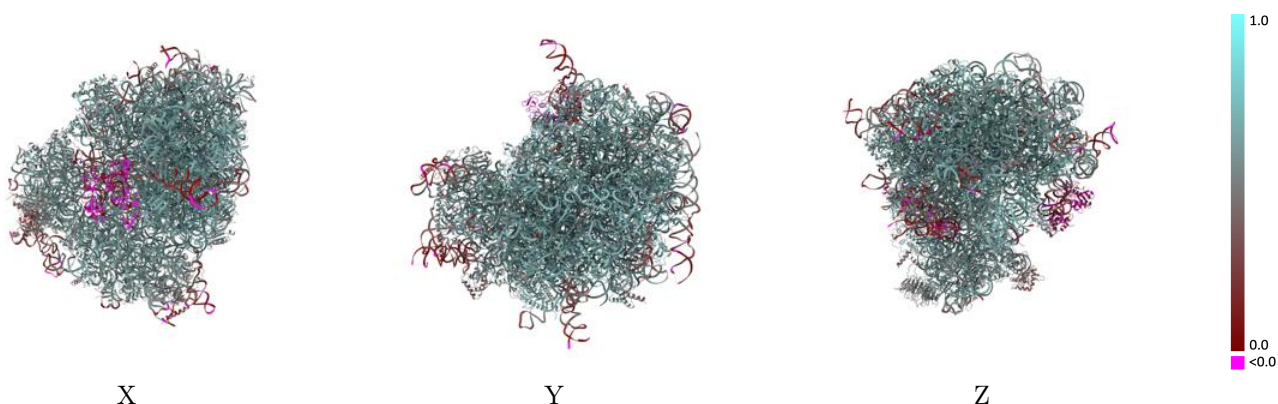
Y



Z

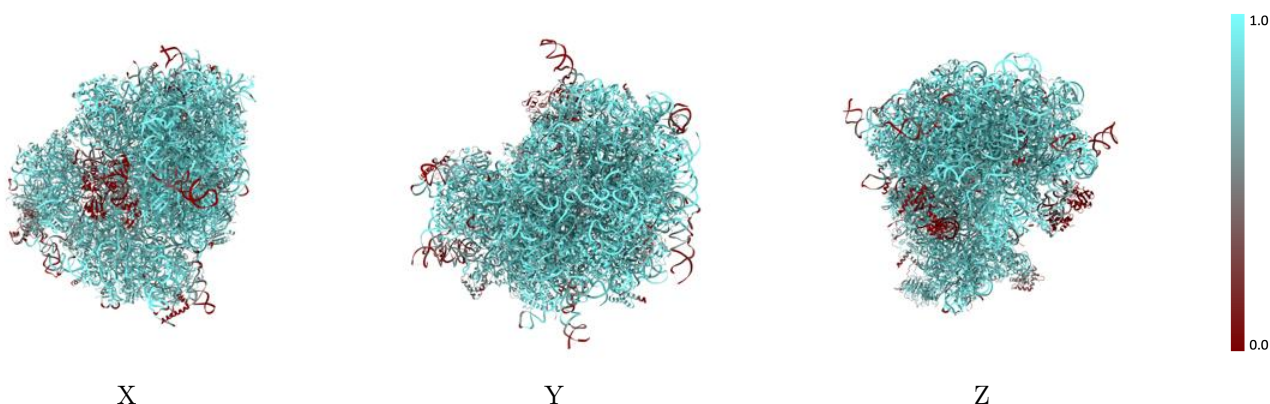
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



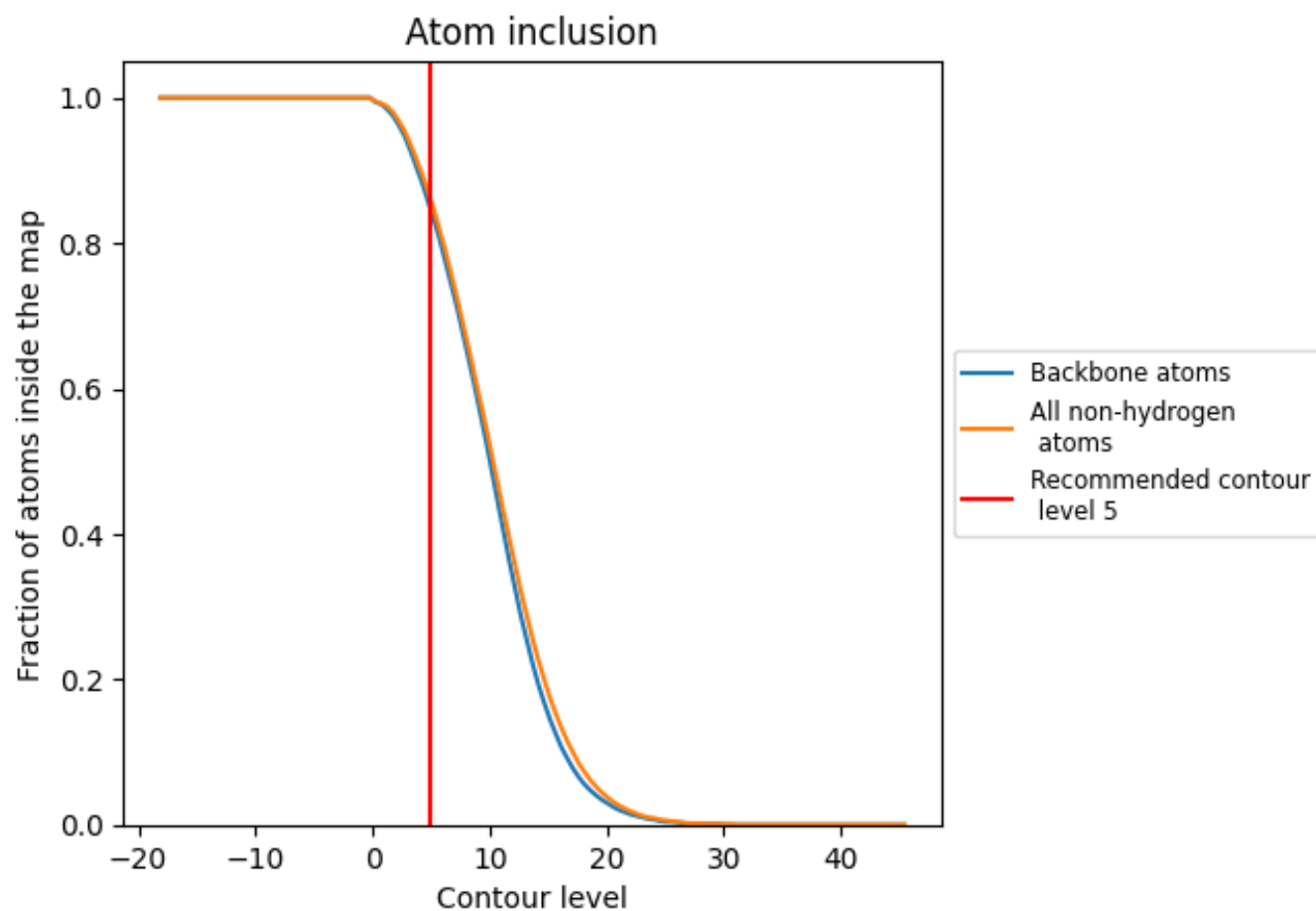
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 86% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.5760
A2	 0.9060	 0.5760
AA	 0.7930	 0.5730
AB	 0.7670	 0.5800
AC	 0.4040	 0.3600
AD	 0.7460	 0.5580
AE	 0.8720	 0.6130
AF	 0.7090	 0.4910
AG	 0.9050	 0.6280
AH	 0.4400	 0.2140
AI	 0.4400	 0.3250
AT	 0.8960	 0.6030
AZ	 0.8340	 0.6010
Aa	 0.8400	 0.6110
Ab	 0.8900	 0.6230
Ac	 0.7440	 0.5600
Ad	 0.8750	 0.5940
Ae	 0.8290	 0.6050
Af	 0.7430	 0.4900
Ag	 0.6430	 0.5080
Ah	 0.8560	 0.5960
Ai	 0.8690	 0.6040
Aj	 0.7680	 0.5230
Ak	 0.8180	 0.5960
Al	 0.3160	 0.2940
Am	 0.8860	 0.6270
An	 0.8800	 0.6310
Ao	 0.7990	 0.5420
Ap	 0.8460	 0.5760
Aq	 0.7250	 0.5510
Ar	 0.8200	 0.5640
As	 0.8520	 0.5830
At	 0.7390	 0.5270
Au	 0.8530	 0.6110
Av	 0.9430	 0.6510























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Chain	Atom inclusion	Q-score
Aw	 0.9120	 0.6380
Ax	 0.8280	 0.5500
Ay	 0.7210	 0.5460
Az	 0.8850	 0.6340
B5	 0.9010	 0.5820
B7	 0.9860	 0.6500
B8	 0.9430	 0.6250
BA	 0.9330	 0.6500
BB	 0.9210	 0.6470
BC	 0.9370	 0.6450
BD	 0.9080	 0.6190
BE	 0.8130	 0.5770
BF	 0.9430	 0.6560
BG	 0.8290	 0.5900
BH	 0.8980	 0.6340
BI	 0.8850	 0.6430
BJ	 0.8680	 0.6220
BK	 0.4100	 0.4710
BL	 0.8760	 0.6160
BM	 0.9080	 0.6220
BN	 0.9750	 0.6620
BO	 0.9420	 0.6520
BP	 0.8990	 0.6400
BQ	 0.9400	 0.6520
BR	 0.8630	 0.6040
BS	 0.9460	 0.6560
BT	 0.8890	 0.6210
BU	 0.8210	 0.5660
BV	 0.8840	 0.6410
BW	 0.5050	 0.4500
BX	 0.9030	 0.6360
BY	 0.9010	 0.6330
BZ	 0.9090	 0.6370
Ba	 0.9630	 0.6560
Bb	 0.7560	 0.5580
Bc	 0.8070	 0.5920
Bd	 0.8820	 0.6290
Be	 0.9380	 0.6460
Bf	 0.9500	 0.6570
Bg	 0.9060	 0.6290
Bh	 0.8920	 0.6290
Bi	 0.8670	 0.6150

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Chain	Atom inclusion	Q-score
Bj	 0.9640	 0.6530
Bk	 0.7850	 0.5750
Bl	 0.9280	 0.6400
Bm	 0.9240	 0.6420
Bo	 0.8970	 0.6490
Bp	 0.8950	 0.6420
Br	 0.9360	 0.6430
Bs	 0.0060	 0.0310
Bt	 0.0020	 0.0450
Bv	 0.0720	 0.1750