



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 01:58 am BST

PDB ID : 9F1C / pdb_00009f1c
EMDB ID : EMD-50125
Title : Mammalian quaternary complex of a translating 80S ribosome, NAC, MetAP1 and NatA/E
Authors : Yudin, D.; Scaiola, A.; Ban, N.
Deposited on : 2024-04-18
Resolution : 3.78 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:

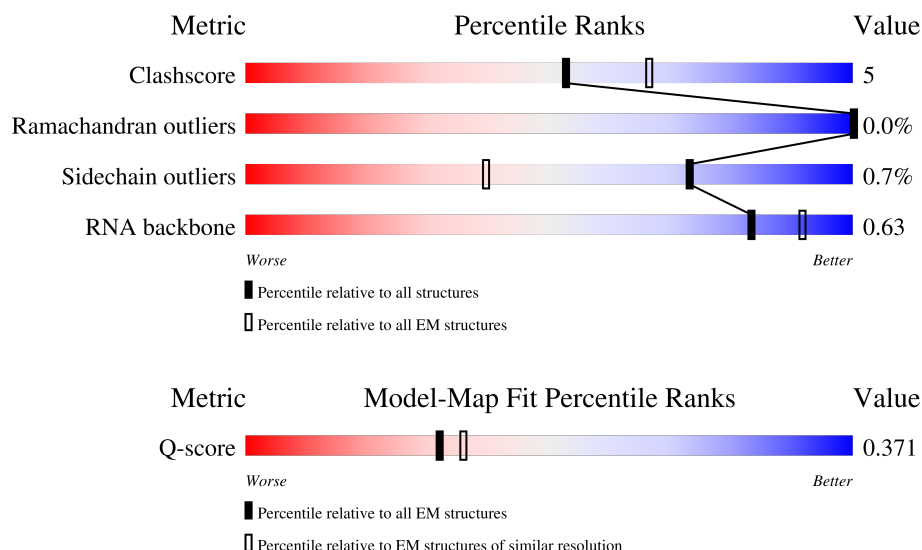
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.78 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	10074 (3.28 - 4.27)

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	AH	3	100% 100%
2	Bb	245	6% 40% 56%
3	B7	120	72% 23%

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Mol	Chain	Length	Quality of chain
4	AT	76	
5	Ar	151	
6	B8	158	
7	BU	128	
8	As	145	
9	BA	257	
10	BV	140	
11	At	119	
12	BB	403	
13	BX	156	
14	Au	83	
15	BC	412	
16	BP	184	
17	BZ	136	
18	Aw	143	
19	BE	291	
20	B5	4808	
21	BQ	188	
22	Ba	148	
23	Ax	130	
24	BF	247	
25	BY	145	
26	BW	157	
27	AZ	294	
28	Ay	124	

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Mol	Chain	Length	Quality of chain
29	BG	266	
30	Av	130	
31	BR	196	
32	Aa	264	
33	Az	25	
34	BH	192	
35	BS	176	
36	Ab	293	
37	Bc	115	
38	BI	214	
39	B	297	
40	EA	386	
41	Ac	281	
42	Bd	125	
43	BJ	178	
44	Ct	238	
45	Ad	263	
46	Be	135	
47	BK	32	
48	Cu	162	
49	Ae	204	
50	Bf	110	
51	BL	211	
52	DA	403	
53	Af	249	

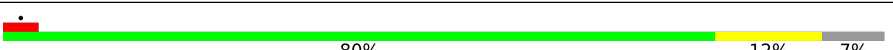
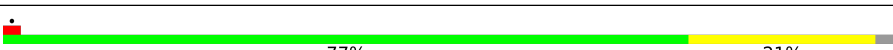
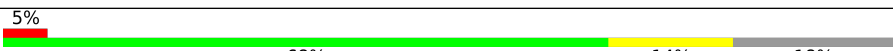
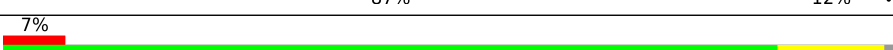
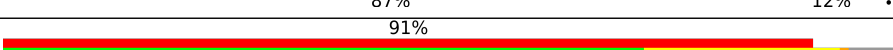
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Mol	Chain	Length	Quality of chain
54	Bg	117	
55	BM	218	
56	DB	915	
57	Ag	432	
58	Bh	123	
59	BN	204	
60	DC	235	
61	Ah	208	
62	Bi	105	
63	BO	203	
64	A2	1870	
65	Ai	194	
66	Bj	97	
67	AA	84	
68	Aj	165	
69	Bk	70	
70	AB	69	
71	Ak	158	
72	Bl	51	
73	AC	156	
74	Al	132	
75	Bm	128	
76	AD	133	
77	Am	151	
78	Bo	106	

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Mol	Chain	Length	Quality of chain
79	AE	115	
80	An	151	
81	Bp	92	
82	AF	317	
83	Ao	145	
84	Br	136	
85	AG	56	
86	Ap	172	
87	Bs	318	
88	BT	160	
89	Aq	135	
90	Bt	165	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	UNX	B5	5253	-	-	X	-
91	UNX	Be	205	-	-	X	-

2 Entry composition [i](#)

There are 98 unique types of molecules in this entry. The entry contains 236684 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 mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AH	3	Total	C	O	P	0	0
			36	15	18	3		

- Molecule 2 is a protein called 60S ribosomal protein L29.

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

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B7	119	Total	C	N	O	P	0	0
			2538	1131	451	837	119		

- Molecule 4 is a RNA chain called P-site tRNA.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 6 is a RNA chain called 5.8S rRNA.

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

- Molecule 7 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BU	102	Total	C	N	O	S	0	0
			831	531	146	152	2		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	GLY	ARG	variant	UNP G1TSG1
BU	36	ALA	GLU	variant	UNP G1TSG1
BU	39	PHE	SER	variant	UNP G1TSG1
BU	54	GLY	ARG	variant	UNP G1TSG1
BU	97	ARG	HIS	variant	UNP G1TSG1

- Molecule 8 is a protein called 40S ribosomal protein S19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
As	119	GLY	TRP	variant	UNP G1TN62
As	142	ASN	LYS	variant	UNP G1TN62

- Molecule 9 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 10 is a protein called Ribosomal protein L23.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	At	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 12 is a protein called Ribosomal protein L3.

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

- Molecule 13 is a protein called Ribosomal_L23eN domain-containing protein.

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

- Molecule 14 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 17 is a protein called 60S ribosomal protein L27.

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

- Molecule 18 is a protein called 40S ribosomal protein S23.

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

- Molecule 19 is a protein called 60S ribosomal protein L6.

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

- Molecule 20 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B5	3706	Total	C	N	O	P	0	0
			79525	35447	14532	25840	3706		

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 21 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 22 is a protein called 60S ribosomal protein L27a.

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

- Molecule 23 is a protein called 40S ribosomal protein S24.

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

- Molecule 24 is a protein called Ribosomal Protein uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	61	ARG	GLY	variant	UNP G1TUB1
BF	93	ARG	GLY	variant	UNP G1TUB1
BF	131	MET	VAL	variant	UNP G1TUB1
BF	153	ILE	VAL	variant	UNP G1TUB1

- Molecule 25 is a protein called Ribosomal protein L26.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 28 is a protein called 40S ribosomal protein S25.

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

- Molecule 29 is a protein called 60S ribosomal protein L7a.

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

- Molecule 30 is a protein called Ribosomal protein S15a.

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

- Molecule 31 is a protein called Ribosomal protein L19.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	38	ARG	CYS	variant	UNP G1TJR3
BR	64	ARG	GLN	variant	UNP G1TJR3
BR	94	THR	LYS	variant	UNP G1TJR3

- Molecule 32 is a protein called 40S ribosomal protein S3a.

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

- Molecule 33 is a protein called 60S ribosomal protein L41.

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

- Molecule 34 is a protein called 60S ribosomal protein L9.

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

- Molecule 35 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 37 is a protein called 60S ribosomal protein L30.

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

- Molecule 38 is a protein called 60S ribosomal protein L10.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B	295	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	GLY	variant	UNP G1SZF4
B	248	ARG	GLN	variant	UNP G1SZF4

- Molecule 40 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	EA	304	Total	C	N	O	S	13	0
			2445	1540	439	443	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EA	220	ASN	ASP	engineered mutation	UNP P53582

- Molecule 41 is a protein called 40S ribosomal protein S3.

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

- Molecule 42 is a protein called 60S ribosomal protein L31.

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

- Molecule 43 is a protein called 60S ribosomal protein L11.

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

- Molecule 44 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ct	116	Total	C	N	O	S	0	0
			904	566	165	169	4		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ct	-22	MET	-	initiating methionine	UNP Q13765
Ct	-21	GLY	-	expression tag	UNP Q13765
Ct	-20	SER	-	expression tag	UNP Q13765
Ct	-19	SER	-	expression tag	UNP Q13765
Ct	-18	HIS	-	expression tag	UNP Q13765
Ct	-17	HIS	-	expression tag	UNP Q13765
Ct	-16	HIS	-	expression tag	UNP Q13765
Ct	-15	HIS	-	expression tag	UNP Q13765
Ct	-14	HIS	-	expression tag	UNP Q13765
Ct	-13	HIS	-	expression tag	UNP Q13765
Ct	-12	SER	-	expression tag	UNP Q13765
Ct	-11	SER	-	expression tag	UNP Q13765
Ct	-10	GLY	-	expression tag	UNP Q13765
Ct	-9	LEU	-	expression tag	UNP Q13765
Ct	-8	GLU	-	expression tag	UNP Q13765
Ct	-7	VAL	-	expression tag	UNP Q13765
Ct	-6	LEU	-	expression tag	UNP Q13765
Ct	-5	PHE	-	expression tag	UNP Q13765
Ct	-4	GLN	-	expression tag	UNP Q13765

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Chain	Residue	Modelled	Actual	Comment	Reference
Ct	-3	GLY	-	expression tag	UNP Q13765
Ct	-2	PRO	-	expression tag	UNP Q13765
Ct	-1	SER	-	expression tag	UNP Q13765
Ct	0	GLY	-	expression tag	UNP Q13765

- Molecule 45 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ad	25	GLY	SER	variant	UNP G1TK17
Ad	51	ARG	LYS	variant	UNP G1TK17
Ad	78	THR	ALA	variant	UNP G1TK17
Ad	156	VAL	MET	variant	UNP G1TK17

- Molecule 46 is a protein called Ribosomal protein L32.

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

- Molecule 47 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	BK	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 48 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Cu	106	Total	C	N	O	S	0	0
			821	514	153	151	3		

- Molecule 49 is a protein called Ribosomal protein S5.

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

- Molecule 50 is a protein called 60S ribosomal protein L35a.

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

- Molecule 51 is a protein called Large ribosomal subunit protein eL13.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	74	ARG	HIS	variant	UNP G1TKB3
BL	190	ARG	HIS	variant	UNP G1TKB3

- Molecule 52 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,N-alpha-acetyltransferase 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	DA	155	Total	C	N	O	S	0	0
			1260	808	221	225	6		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	-15	GLY	-	linker	UNP P08515
DA	-14	SER	-	linker	UNP P08515
DA	-13	GLY	-	linker	UNP P08515
DA	-12	SER	-	linker	UNP P08515
DA	-11	GLY	-	linker	UNP P08515
DA	-10	SER	-	linker	UNP P08515
DA	-9	GLU	-	linker	UNP P08515
DA	-8	ASN	-	linker	UNP P08515
DA	-7	LEU	-	linker	UNP P08515
DA	-6	TYR	-	linker	UNP P08515
DA	-5	PHE	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	-4	GLN	-	linker	UNP P08515
DA	-3	GLY	-	linker	UNP P08515
DA	-2	ALA	-	linker	UNP P08515
DA	-1	MET	-	linker	UNP P08515
DA	0	VAL	-	linker	UNP P08515

- Molecule 53 is a protein called 40S ribosomal protein S6.

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

- Molecule 54 is a protein called 60S ribosomal protein L34.

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

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

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

- Molecule 56 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	DB	837	Total	C	N	O	S	0	0
			6900	4391	1192	1276	41		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	-48	MET	-	initiating methionine	UNP Q9BXJ9
DB	-47	GLY	-	expression tag	UNP Q9BXJ9
DB	-46	SER	-	expression tag	UNP Q9BXJ9
DB	-45	SER	-	expression tag	UNP Q9BXJ9
DB	-44	HIS	-	expression tag	UNP Q9BXJ9
DB	-43	HIS	-	expression tag	UNP Q9BXJ9
DB	-42	HIS	-	expression tag	UNP Q9BXJ9
DB	-41	HIS	-	expression tag	UNP Q9BXJ9

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	-40	HIS	-	expression tag	UNP Q9BXJ9
DB	-39	HIS	-	expression tag	UNP Q9BXJ9
DB	-38	SER	-	expression tag	UNP Q9BXJ9
DB	-37	SER	-	expression tag	UNP Q9BXJ9
DB	-36	GLY	-	expression tag	UNP Q9BXJ9
DB	-35	LEU	-	expression tag	UNP Q9BXJ9
DB	-34	VAL	-	expression tag	UNP Q9BXJ9
DB	-33	PRO	-	expression tag	UNP Q9BXJ9
DB	-32	ARG	-	expression tag	UNP Q9BXJ9
DB	-31	GLY	-	expression tag	UNP Q9BXJ9
DB	-30	SER	-	expression tag	UNP Q9BXJ9
DB	-29	HIS	-	expression tag	UNP Q9BXJ9
DB	-28	MET	-	expression tag	UNP Q9BXJ9
DB	-27	ALA	-	expression tag	UNP Q9BXJ9
DB	-26	SER	-	expression tag	UNP Q9BXJ9
DB	-25	MET	-	expression tag	UNP Q9BXJ9
DB	-24	THR	-	expression tag	UNP Q9BXJ9
DB	-23	GLY	-	expression tag	UNP Q9BXJ9
DB	-22	GLY	-	expression tag	UNP Q9BXJ9
DB	-21	GLN	-	expression tag	UNP Q9BXJ9
DB	-20	GLN	-	expression tag	UNP Q9BXJ9
DB	-19	MET	-	expression tag	UNP Q9BXJ9
DB	-18	GLY	-	expression tag	UNP Q9BXJ9
DB	-17	ARG	-	expression tag	UNP Q9BXJ9
DB	-16	ALA	-	expression tag	UNP Q9BXJ9
DB	-15	ARG	-	expression tag	UNP Q9BXJ9
DB	-14	GLY	-	expression tag	UNP Q9BXJ9
DB	-13	ILE	-	expression tag	UNP Q9BXJ9
DB	-12	GLN	-	expression tag	UNP Q9BXJ9
DB	-11	ARG	-	expression tag	UNP Q9BXJ9
DB	-10	PRO	-	expression tag	UNP Q9BXJ9
DB	-9	THR	-	expression tag	UNP Q9BXJ9
DB	-8	SER	-	expression tag	UNP Q9BXJ9
DB	-7	THR	-	expression tag	UNP Q9BXJ9
DB	-6	SER	-	expression tag	UNP Q9BXJ9
DB	-5	SER	-	expression tag	UNP Q9BXJ9
DB	-4	LEU	-	expression tag	UNP Q9BXJ9
DB	-3	VAL	-	expression tag	UNP Q9BXJ9
DB	-2	ALA	-	expression tag	UNP Q9BXJ9
DB	-1	ALA	-	expression tag	UNP Q9BXJ9
DB	0	ALA	-	expression tag	UNP Q9BXJ9

- Molecule 57 is a protein called 40S ribosomal protein S7.

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

- Molecule 58 is a protein called 60S ribosomal protein L35.

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

- Molecule 59 is a protein called Ribosomal protein L15.

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

- Molecule 60 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	DC	160	Total	C	N	O	S	0	0
			1295	815	234	235	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	24	GLN	GLU	engineered mutation	UNP P41227
DC	26	PHE	TYR	engineered mutation	UNP P41227

- Molecule 61 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	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	variant	UNP G1TJW1

- Molecule 62 is a protein called 60S ribosomal protein L36.

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

- Molecule 63 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 64 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	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 65 is a protein called 40S ribosomal protein S9.

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

- Molecule 66 is a protein called Ribosomal protein L37.

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

- Molecule 67 is a protein called 40S ribosomal protein S27.

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

- Molecule 68 is a protein called S10_ plectin domain-containing protein.

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

- Molecule 69 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	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	variant	UNP G1U001

- Molecule 70 is a protein called 40S ribosomal protein S28.

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

- Molecule 71 is a protein called 40S ribosomal protein S11.

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

- Molecule 72 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 73 is a protein called Ribosomal protein S27a.

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

- Molecule 74 is a protein called 40S ribosomal protein S12.

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

- Molecule 75 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 76 is a protein called 40S ribosomal protein S30.

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

- Molecule 77 is a protein called 40S ribosomal protein S13.

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

- Molecule 78 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 80 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	IAS	ASP	conflict	UNP A0AAA9WYR1

- Molecule 81 is a protein called 60S ribosomal protein L37a.

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

- Molecule 82 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 83 is a protein called 40S ribosomal protein uS19.

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

- Molecule 84 is a protein called Large ribosomal subunit protein eL28.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	103	ARG	HIS	conflict	UNP G1U7L1

- Molecule 85 is a protein called 40S ribosomal protein S29.

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

- Molecule 86 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 87 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 88 is a protein called 60S ribosomal protein L21.

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

- Molecule 89 is a protein called 40S ribosomal protein eS17.

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

- Molecule 90 is a protein called 60S ribosomal protein L12.

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

- Molecule 91 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
91	Bb	2	Total	X	0
			2	2	
91	B7	6	Total	X	0
			6	6	
91	AT	2	Total	X	0
			2	2	
91	Ar	1	Total	X	0
			1	1	
91	B8	6	Total	X	0
			6	6	
91	BA	3	Total	X	0
			3	3	
91	BB	1	Total	X	0
			1	1	
91	BP	1	Total	X	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
91	B5	186	Total 186	X 186	0
91	BQ	2	Total 2	X 2	0
91	BY	1	Total 1	X 1	0
91	BH	1	Total 1	X 1	0
91	BI	1	Total 1	X 1	0
91	Ad	1	Total 1	X 1	0
91	Be	4	Total 4	X 4	0
91	Bf	1	Total 1	X 1	0
91	BL	1	Total 1	X 1	0
91	BN	1	Total 1	X 1	0
91	A2	49	Total 49	X 49	0
91	Bj	1	Total 1	X 1	0
91	Ak	1	Total 1	X 1	0
91	Bo	1	Total 1	X 1	0
91	AE	1	Total 1	X 1	0
91	An	1	Total 1	X 1	0
91	BT	2	Total 2	X 2	0

- Molecule 92 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

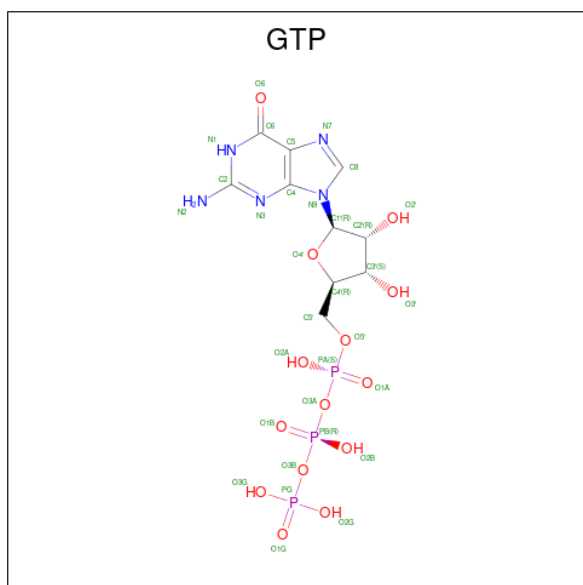
Mol	Chain	Residues	Atoms		AltConf
92	B7	9	Total 9	Mg 9	0
92	AT	2	Total 2	Mg 2	0

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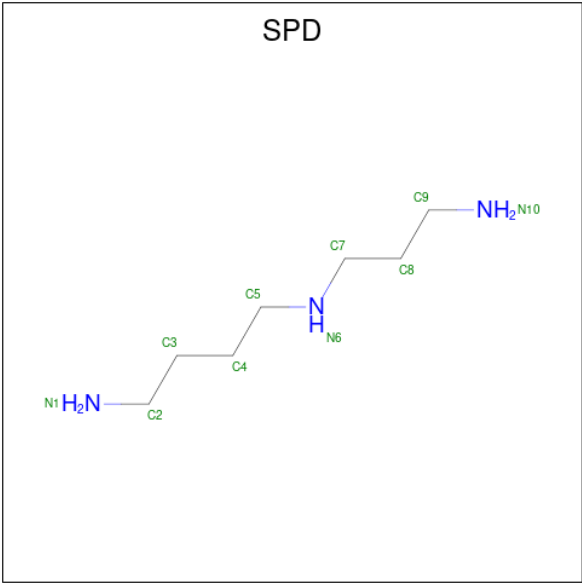
Mol	Chain	Residues	Atoms		AltConf
92	B8	8	Total 8	Mg 8	0
92	BV	1	Total 1	Mg 1	0
92	BB	1	Total 1	Mg 1	0
92	BP	1	Total 1	Mg 1	0
92	B5	282	Total 282	Mg 282	0
92	Ba	1	Total 1	Mg 1	0
92	BR	1	Total 1	Mg 1	0
92	BI	1	Total 1	Mg 1	0
92	Be	1	Total 1	Mg 1	0
92	A2	111	Total 111	Mg 111	0
92	Bj	1	Total 1	Mg 1	0

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
93	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 94 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



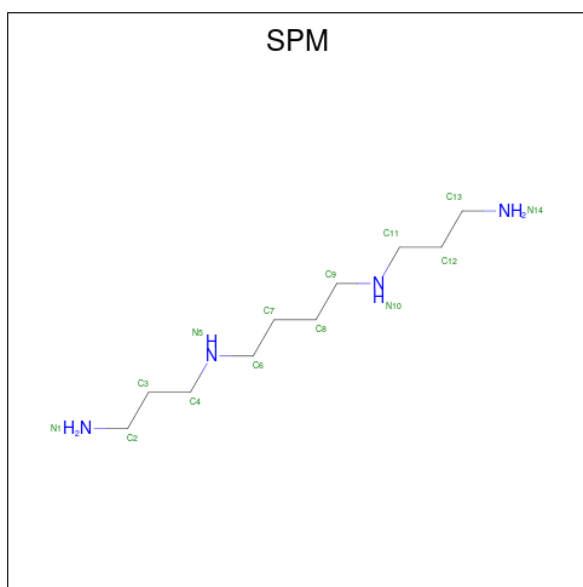
Mol	Chain	Residues	Atoms			AltConf
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N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

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Mol	Chain	Residues	Atoms			AltConf
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	B5	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	
94	A2	1	Total	C	N	0
			10	7	3	

- Molecule 95 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).

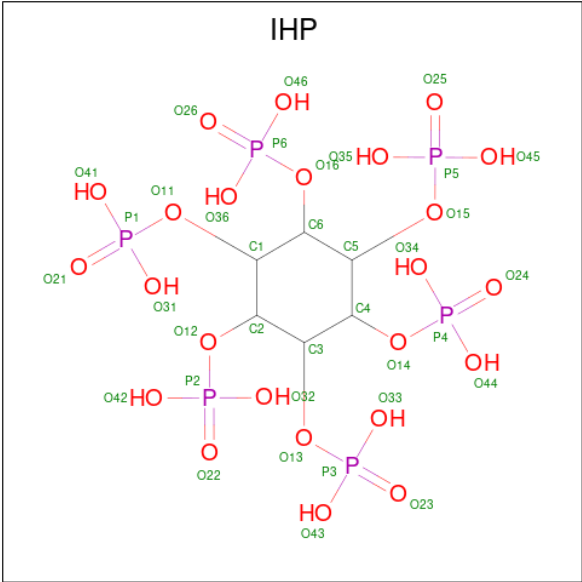


Mol	Chain	Residues	Atoms			AltConf
95	B5	1	Total	C	N	0
			14	10	4	
95	B5	1	Total	C	N	0
			14	10	4	
95	A2	1	Total	C	N	0
			14	10	4	

- Molecule 96 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 97 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
97	DB	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 98 is water.

Mol	Chain	Residues	Atoms		AltConf
98	AH	3	Total	O	0
			3	3	
98	Bb	1	Total	O	0
			1	1	
98	B7	44	Total	O	0
			44	44	
98	AT	12	Total	O	0
			12	12	
98	Ar	2	Total	O	0
			2	2	
98	B8	47	Total	O	0
			47	47	
98	As	2	Total	O	0
			2	2	
98	BA	5	Total	O	0
			5	5	
98	BV	2	Total	O	0
			2	2	
98	At	1	Total	O	0
			1	1	
98	BB	6	Total	O	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
98	BX	2	Total 2	O 2	0
98	BC	7	Total 7	O 7	0
98	BP	3	Total 3	O 3	0
98	Aw	5	Total 5	O 5	0
98	B5	1398	Total 1398	O 1398	0
98	Ba	8	Total 8	O 8	0
98	BR	5	Total 5	O 5	0
98	Aa	3	Total 3	O 3	0
98	BH	1	Total 1	O 1	0
98	Ab	1	Total 1	O 1	0
98	BI	2	Total 2	O 2	0
98	B	1	Total 1	O 1	0
98	Bd	1	Total 1	O 1	0
98	Ct	1	Total 1	O 1	0
98	Ad	1	Total 1	O 1	0
98	Be	4	Total 4	O 4	0
98	BL	2	Total 2	O 2	0
98	Af	1	Total 1	O 1	0
98	Bg	1	Total 1	O 1	0
98	BN	5	Total 5	O 5	0
98	A2	527	Total 527	O 527	0

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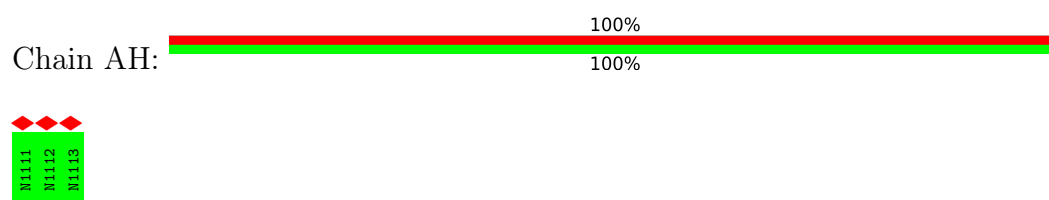
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Mol	Chain	Residues	Atoms		AltConf
98	Bj	5	Total 5	O 5	0
98	Ak	2	Total 2	O 2	0
98	Bl	2	Total 2	O 2	0
98	AE	1	Total 1	O 1	0
98	An	1	Total 1	O 1	0
98	Ap	2	Total 2	O 2	0

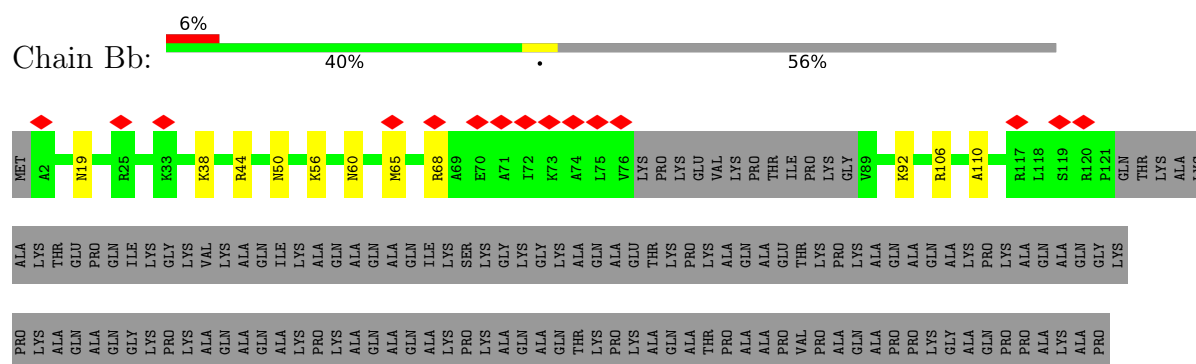
3 Residue-property plots

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

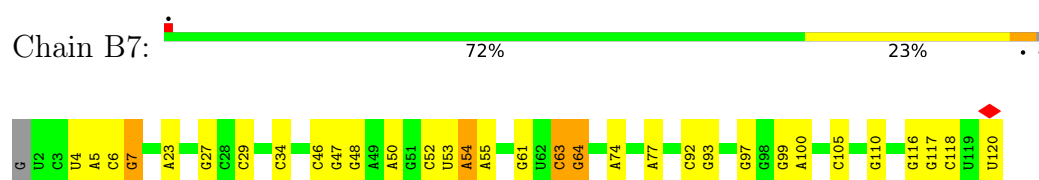
- Molecule 1: mRNA



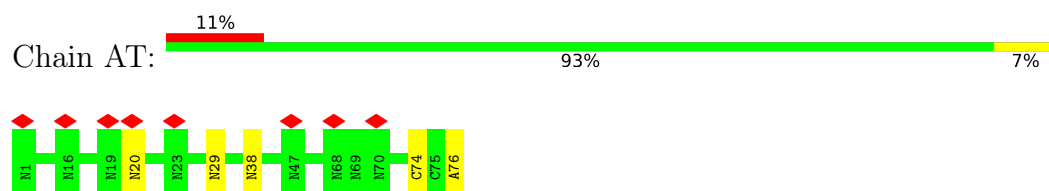
- Molecule 2: 60S ribosomal protein L29



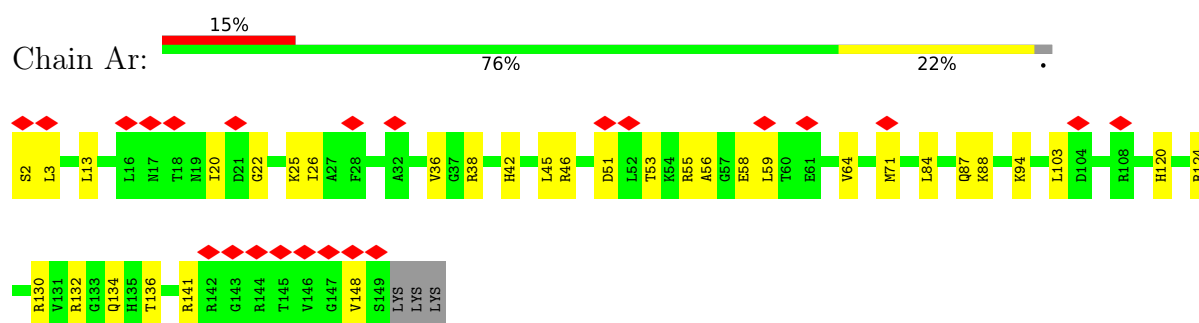
- Molecule 3: 5S rRNA



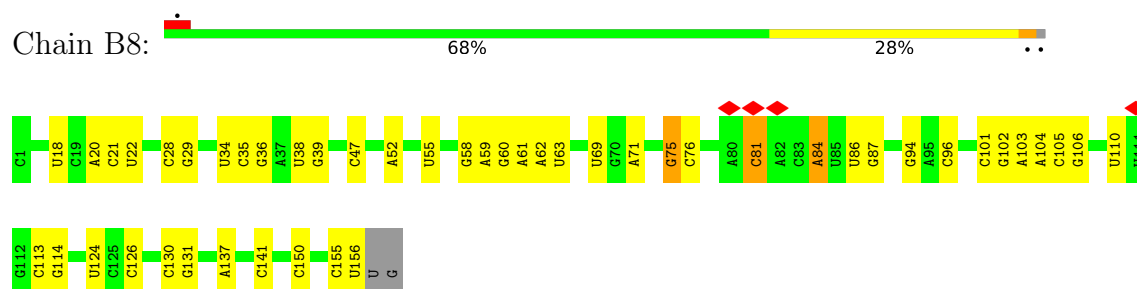
- Molecule 4: P-site tRNA



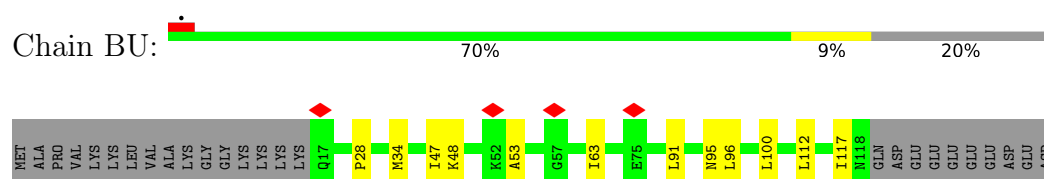
- Molecule 5: Small ribosomal subunit protein uS13



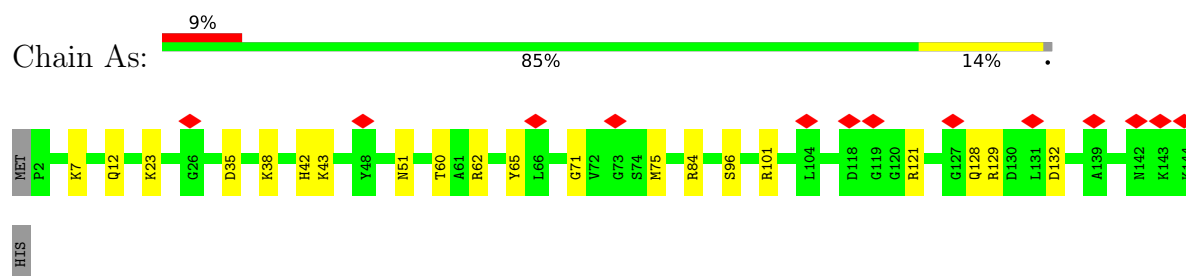
- Molecule 6: 5.8S rRNA



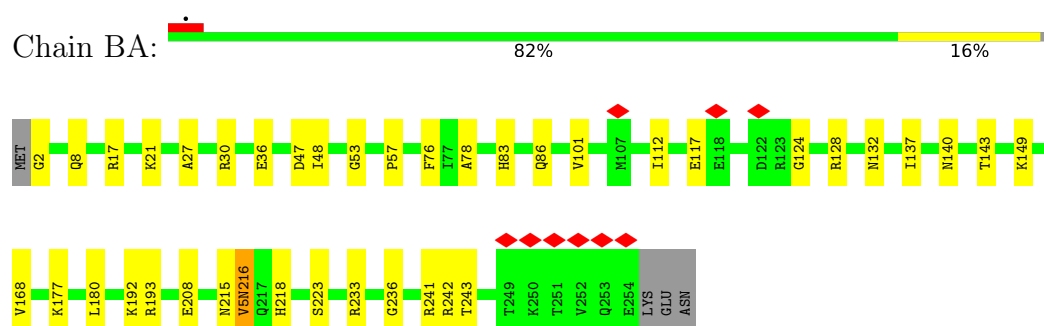
- Molecule 7: 60S ribosomal protein L22



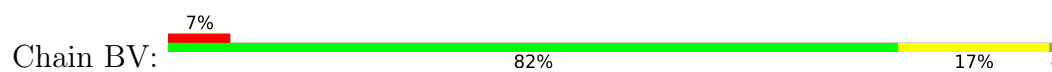
- Molecule 8: 40S ribosomal protein S19



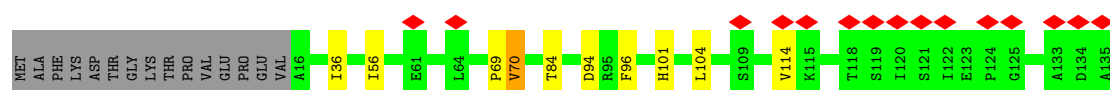
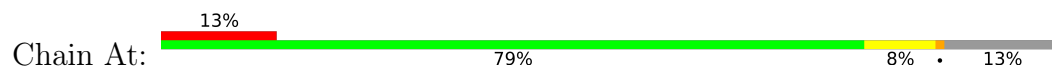
- Molecule 9: Large ribosomal subunit protein uL2



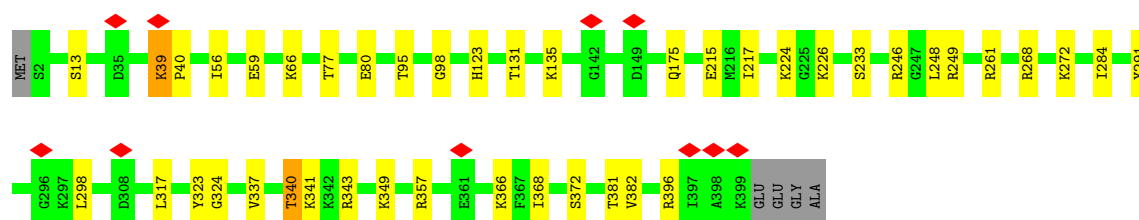
- Molecule 10: Ribosomal protein L23



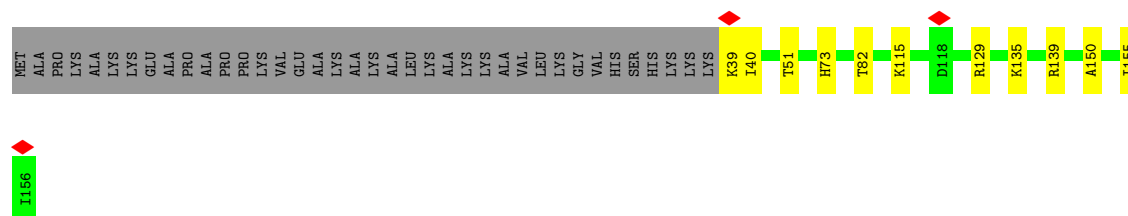
- Molecule 11: Small ribosomal subunit protein uS10



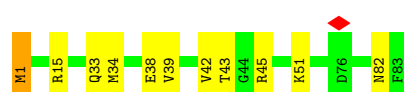
- Molecule 12: Ribosomal protein L3



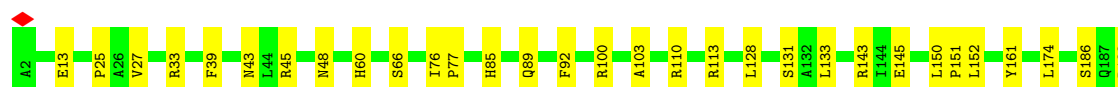
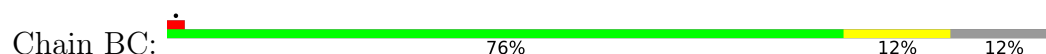
- Molecule 13: Ribosomal_L23eN domain-containing protein

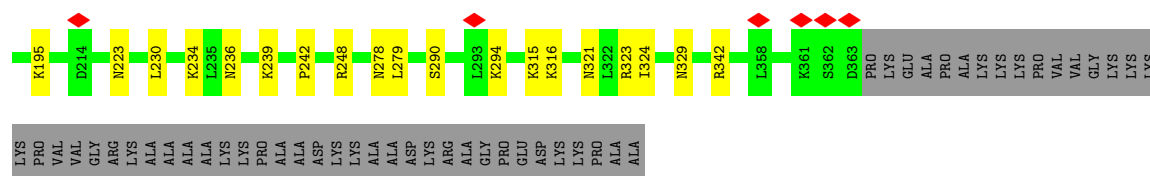


- Molecule 14: Small ribosomal subunit protein eS21

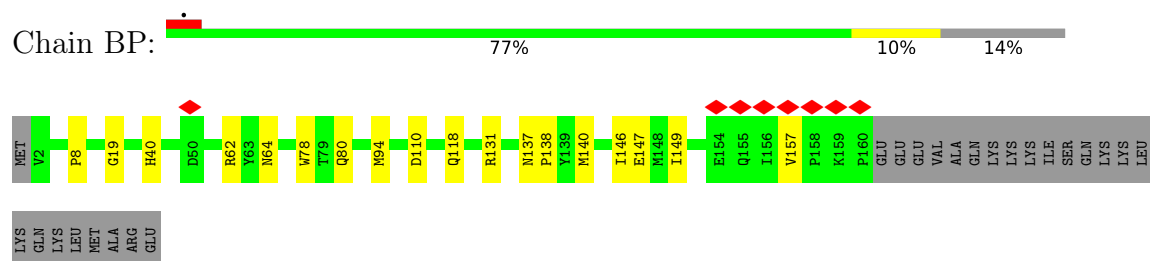


- Molecule 15: Large ribosomal subunit protein uL4

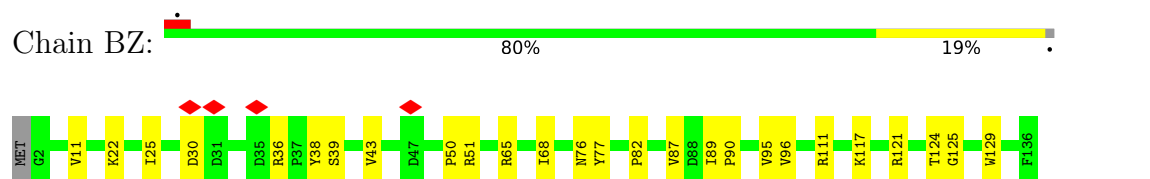




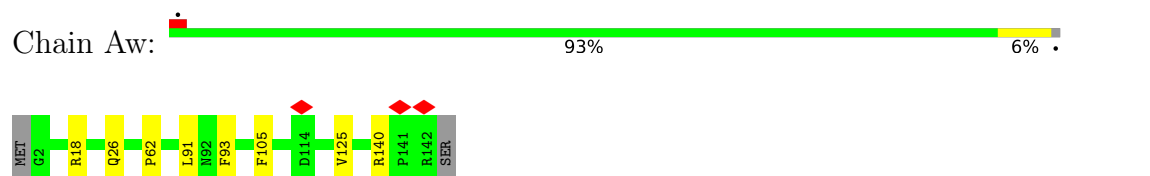
- Molecule 16: Large ribosomal subunit protein uL22



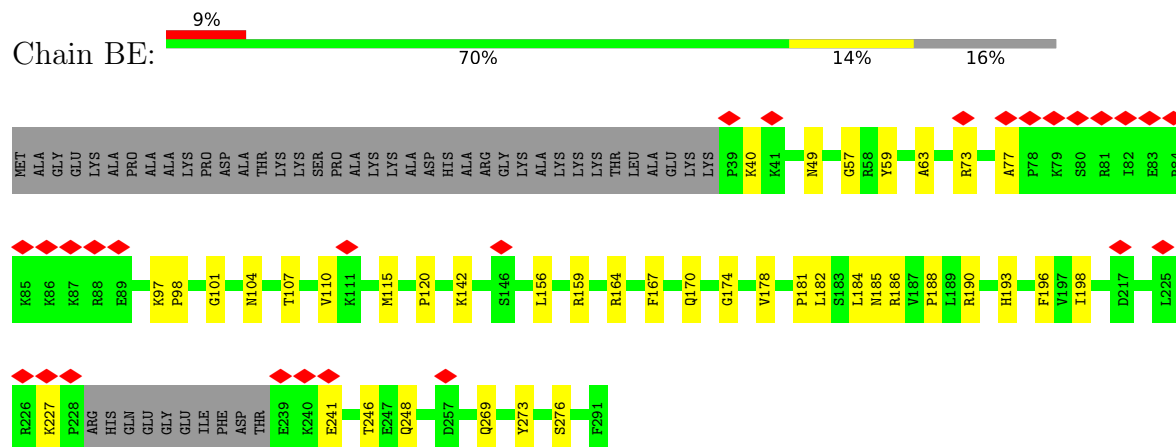
- Molecule 17: 60S ribosomal protein L27



- Molecule 18: 40S ribosomal protein S23



- Molecule 19: 60S ribosomal protein L6



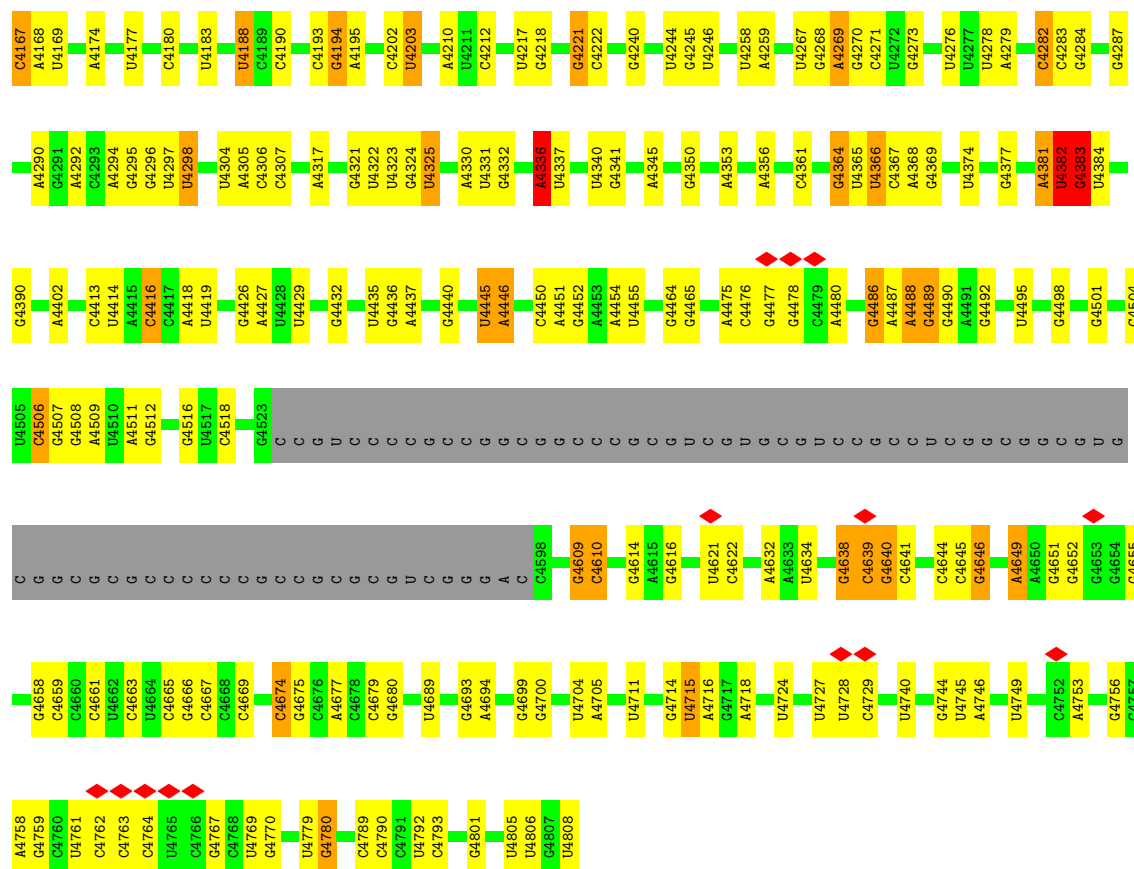
- Molecule 20: 28S rRNA











- Molecule 21: Large ribosomal subunit protein eL18

Chain BQ: 85% 15%



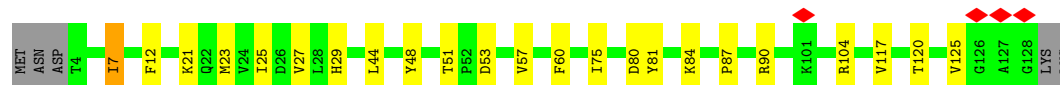
- Molecule 22: 60S ribosomal protein L27a

Chain Ba: 84% 15%



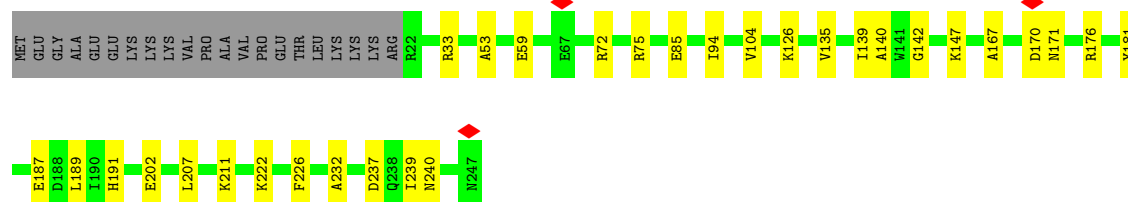
- Molecule 23: 40S ribosomal protein S24

Chain Ax: 78% 17%



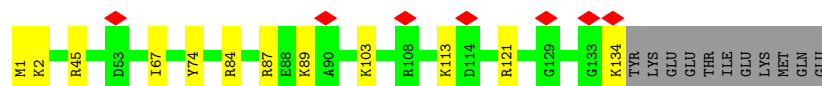
- Molecule 24: Ribosomal Protein uL30

Chain BF: 79% 13% 9%

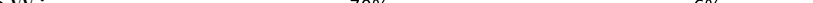


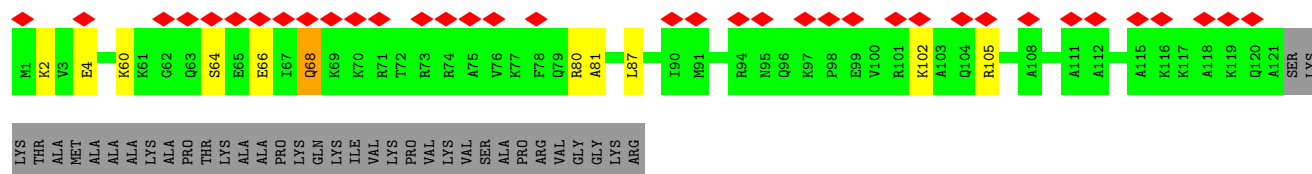
- Molecule 25: Ribosomal protein L26

Chain BY: 

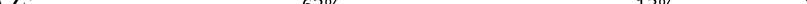


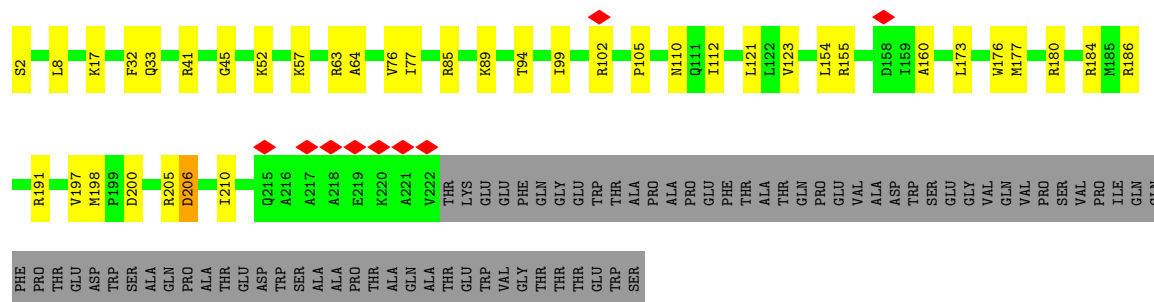
- Molecule 26: Ribosomal protein L24

Chain BW: 



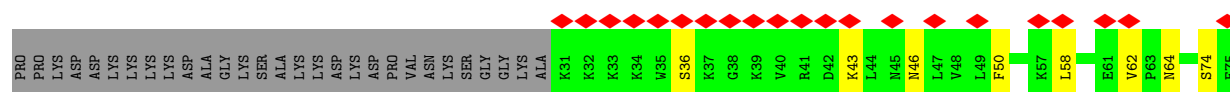
- Molecule 27: Small ribosomal subunit protein uS2

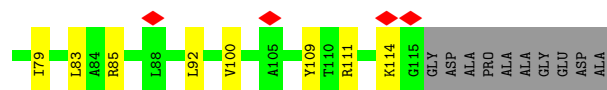
Chain AZ: 



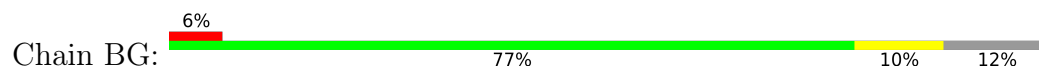
- Molecule 28: 40S ribosomal protein S25

Chain A: 20% 56% 13% 31%

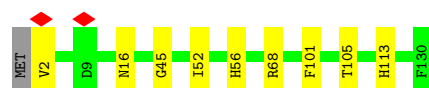




- Molecule 29: 60S ribosomal protein L7a



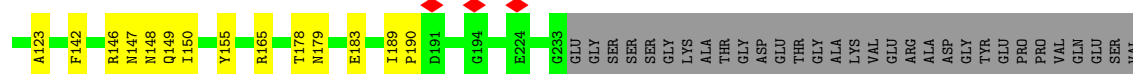
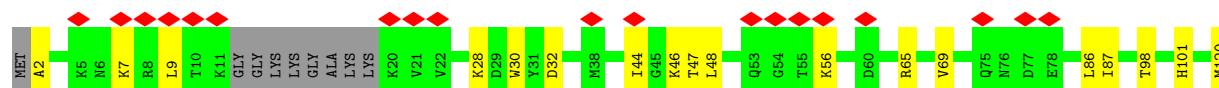
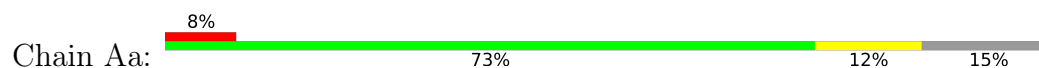
- Molecule 30: Ribosomal protein S15a



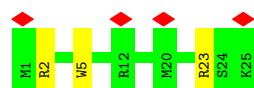
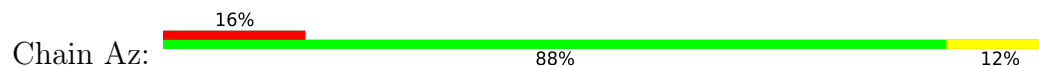
- Molecule 31: Ribosomal protein L19



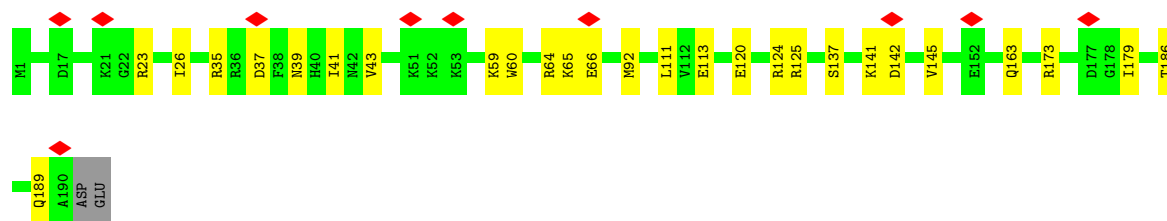
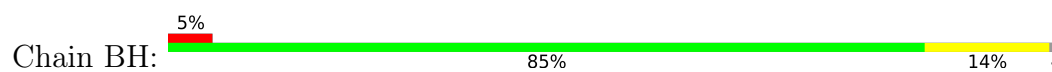
- Molecule 32: 40S ribosomal protein S3a



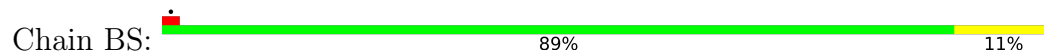
- Molecule 33: 60S ribosomal protein L41



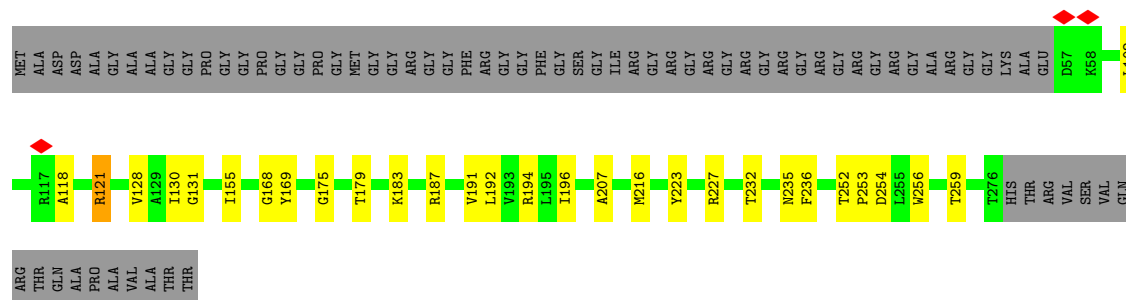
- Molecule 34: 60S ribosomal protein L9



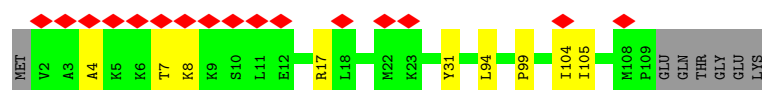
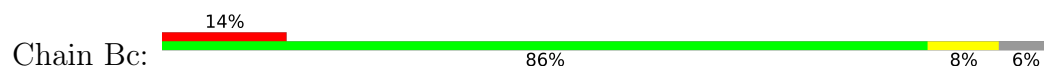
- Molecule 35: Large ribosomal subunit protein eL20



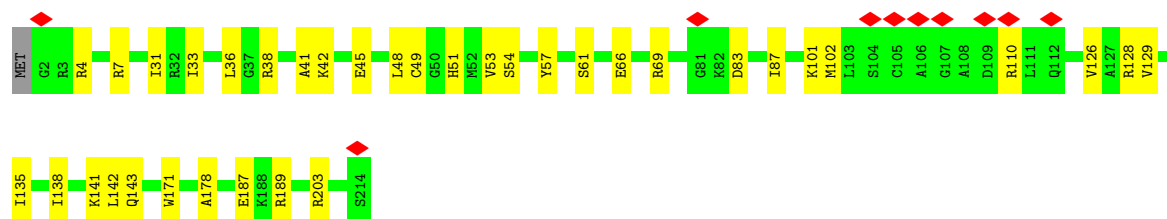
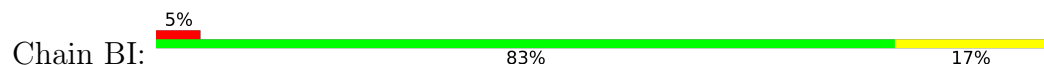
- Molecule 36: Small ribosomal subunit protein uS5



- Molecule 37: 60S ribosomal protein L30

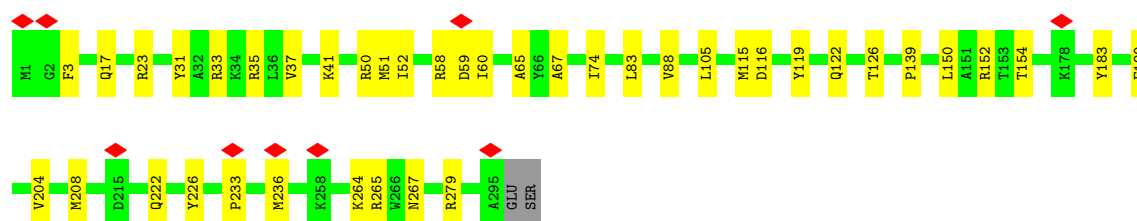


- Molecule 38: 60S ribosomal protein L10



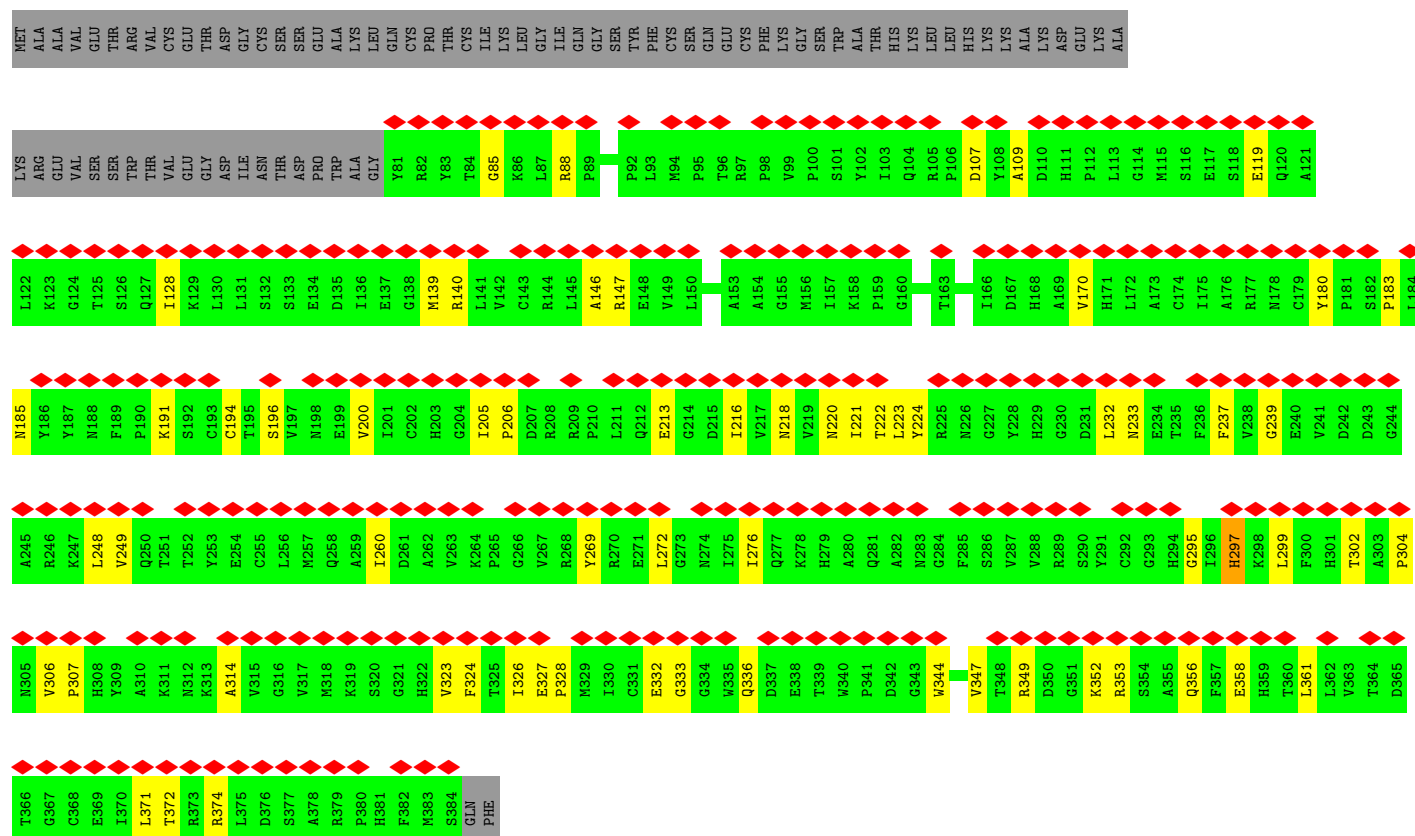
- Molecule 39: Large ribosomal subunit protein uL18

Chain B: 



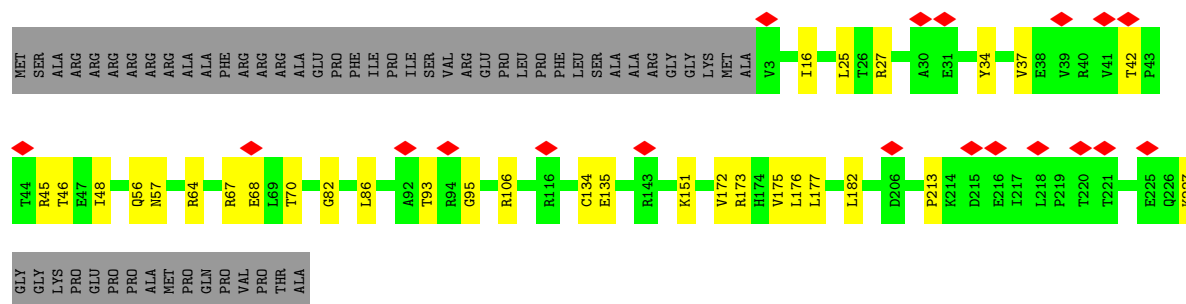
• Molecule 40: Methionine aminopeptidase 1

Chain EA: 

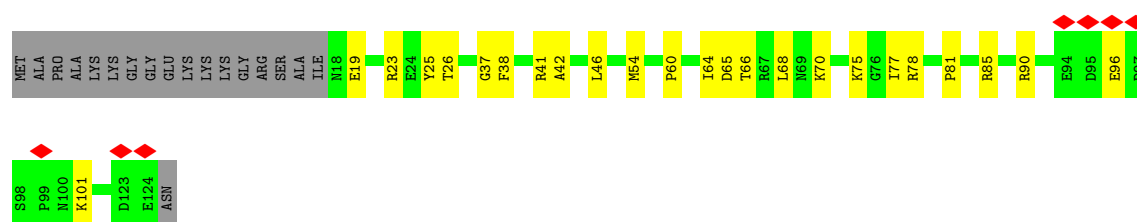


• Molecule 41: 40S ribosomal protein S3

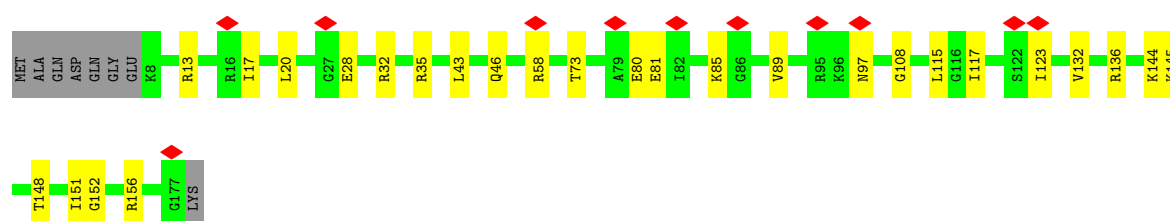
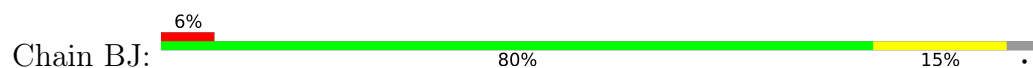
Chain Ac: 



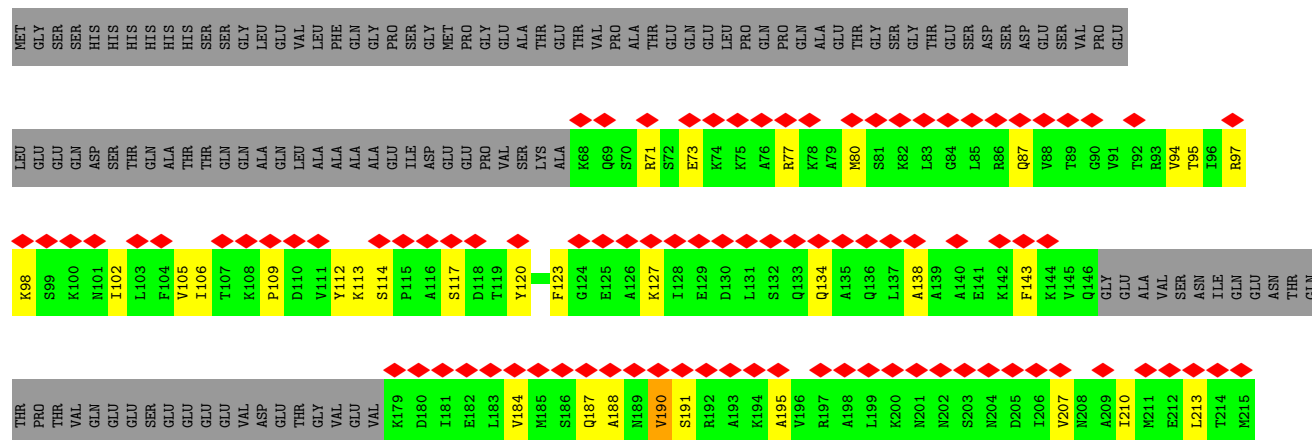
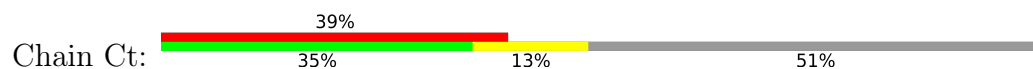
- Molecule 42: 60S ribosomal protein L31



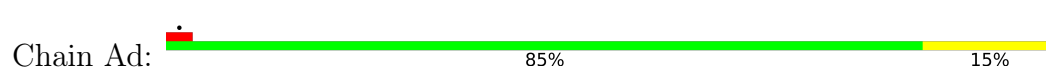
- Molecule 43: 60S ribosomal protein L11



- Molecule 44: Nascent polypeptide-associated complex subunit alpha

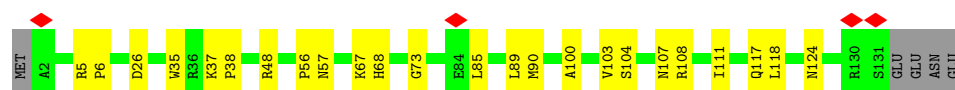


- Molecule 45: 40S ribosomal protein S4

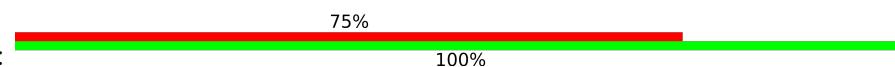


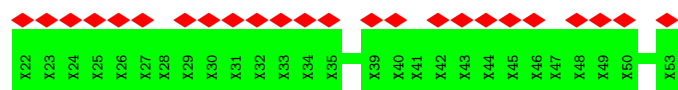
- Molecule 46: Ribosomal protein L32

Chain Be:  79% 18%



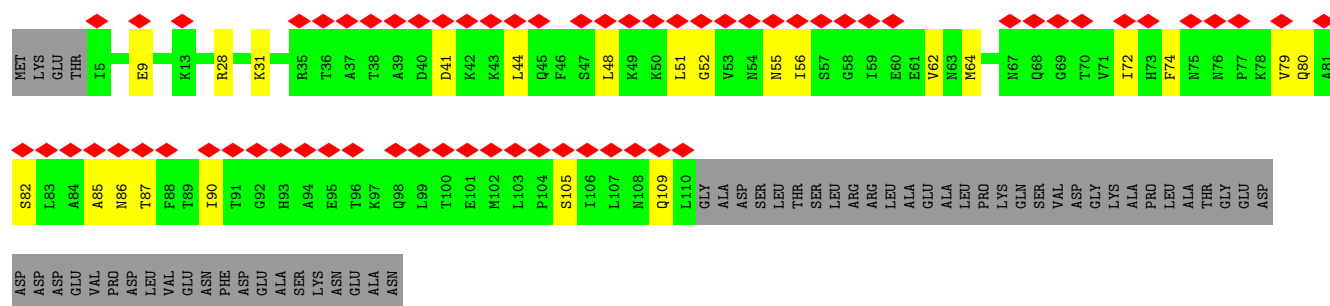
- Molecule 47: Nascent chain

Chain BK:  75% 100%



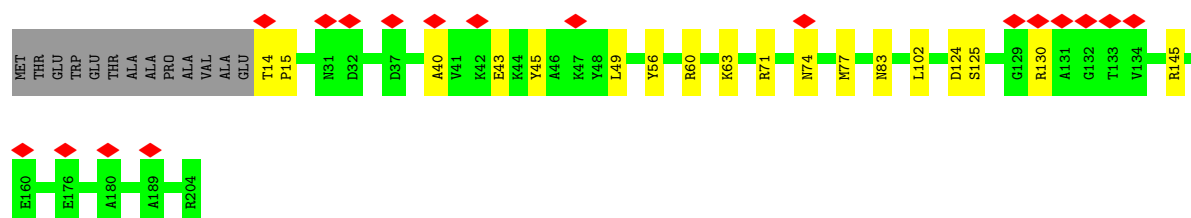
- Molecule 48: Transcription factor BTF3

Chain Cu:  41% 51% 14% 35%



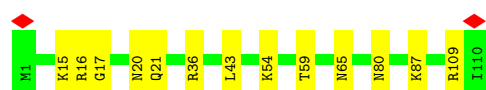
- Molecule 49: Ribosomal protein S5

Chain Ae:  9% 85% 9% 6%

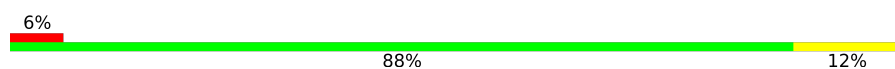


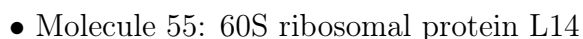
- Molecule 50: 60S ribosomal protein L35a

Chain Bf:  88% 12%

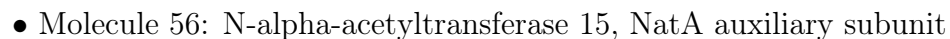


- Molecule 51: Large ribosomal subunit protein eL13

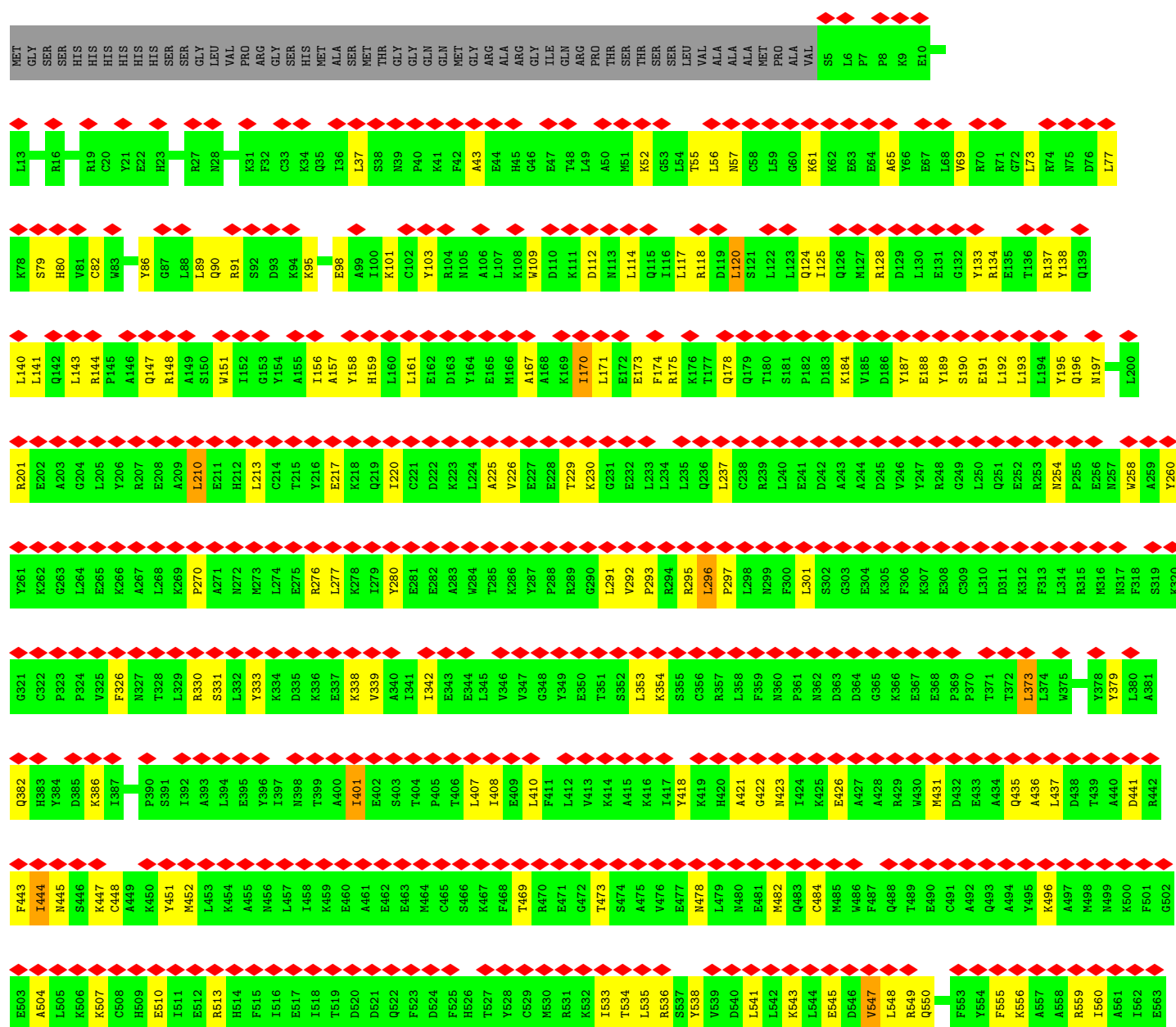
Chain BL:  6% 88% 12%



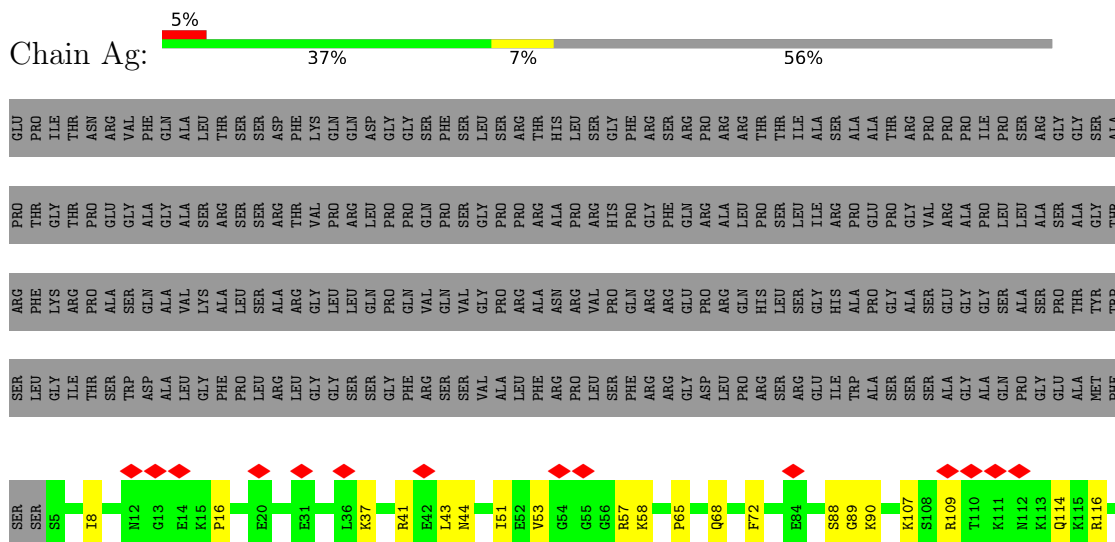
Frequency	Percentage
Daily	53%
Weekly	10%
Monthly	37%



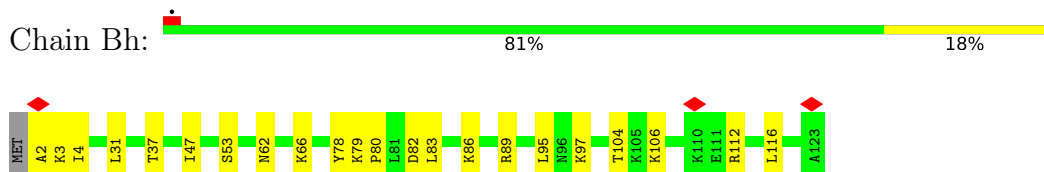
Category	Percentage
Red Bar	79%
Green Bar	68%



- Molecule 57: 40S ribosomal protein S7

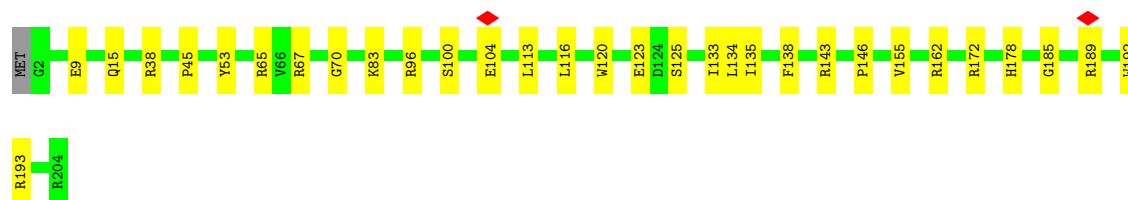


- Molecule 58: 60S ribosomal protein L35

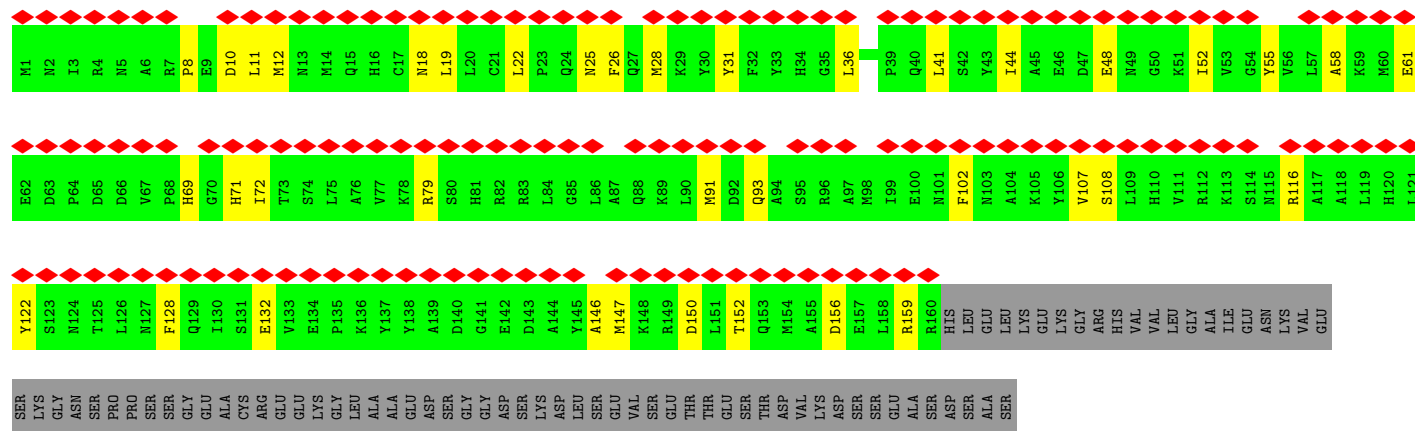


- Molecule 59: Ribosomal protein L15

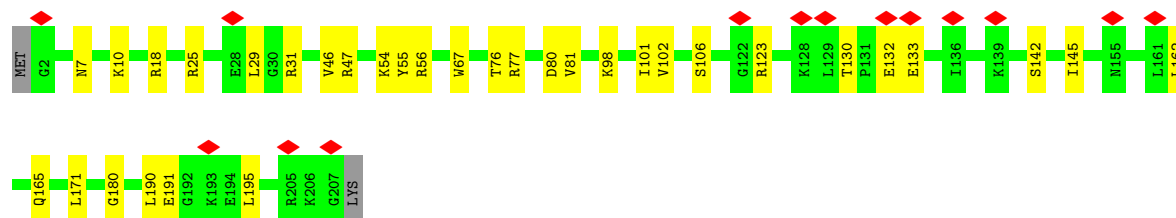
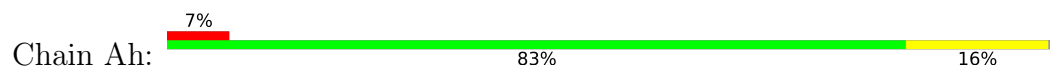




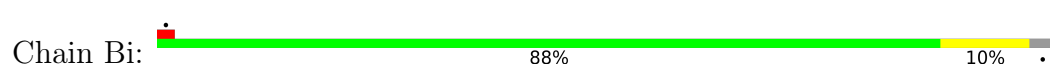
- Molecule 60: N-alpha-acetyltransferase 10



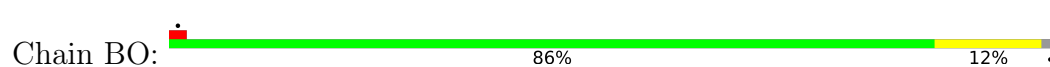
- Molecule 61: 40S ribosomal protein S8



- Molecule 62: 60S ribosomal protein L36

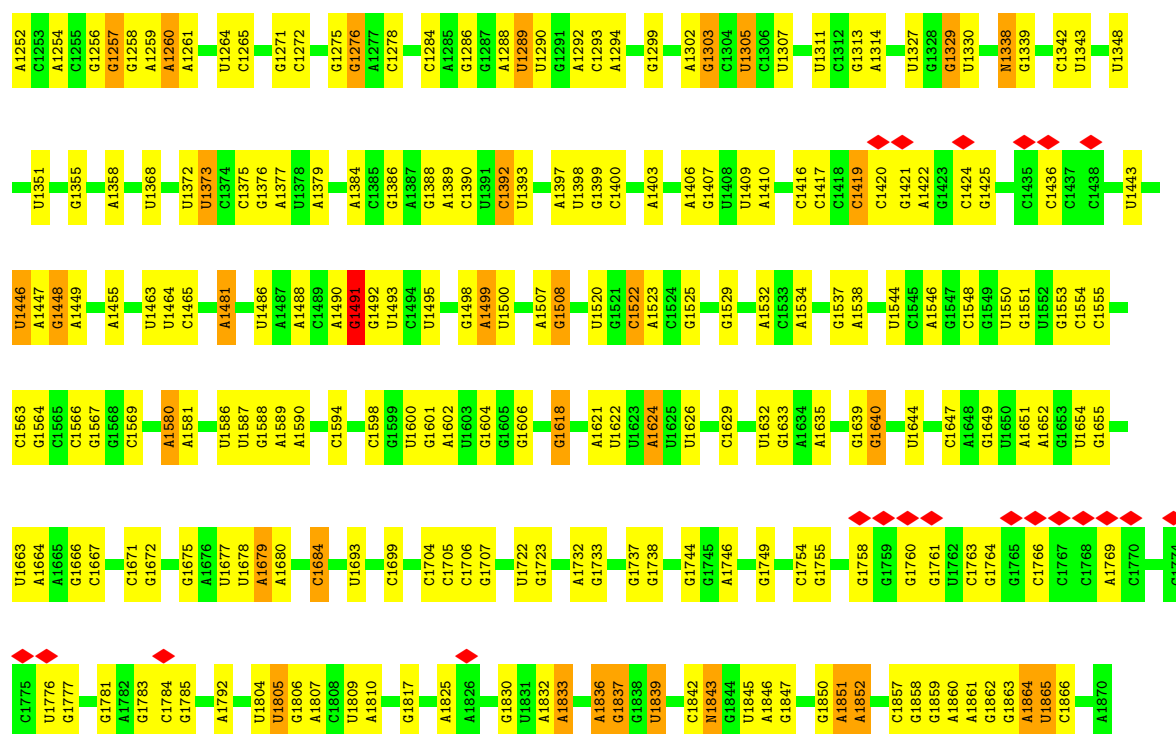


- Molecule 63: Large ribosomal subunit protein uL13

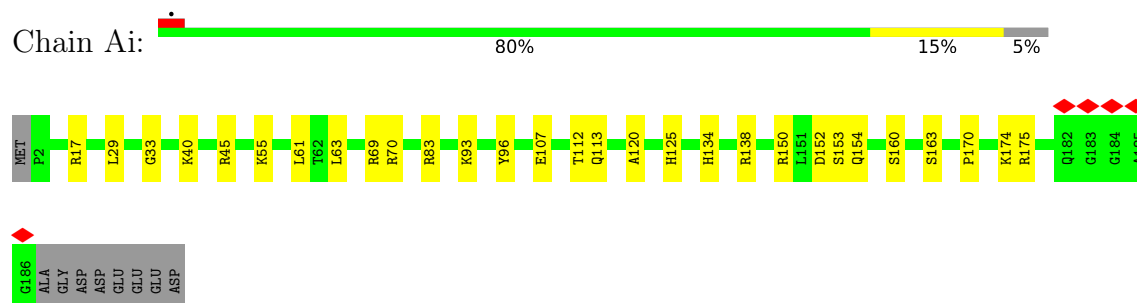


Chain A2:

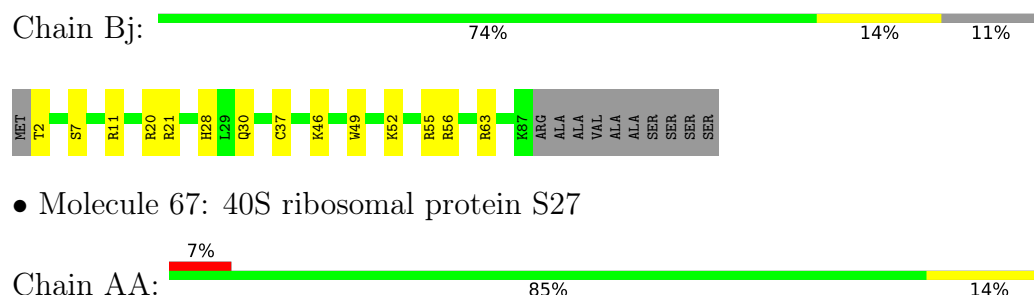




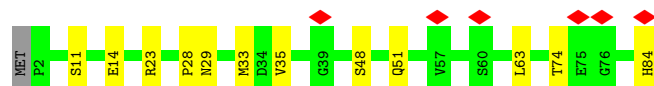
• Molecule 65: 40S ribosomal protein S9



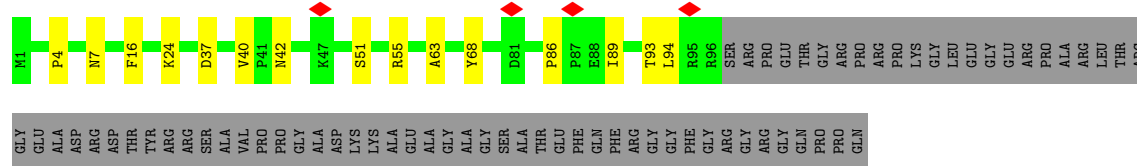
• Molecule 66: Ribosomal protein L37



• Molecule 68: S10_ plectin domain-containing protein



Chain Aj: 



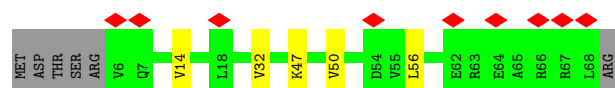
- Molecule 69: 60S ribosomal protein L38

Chain Bk: 



- Molecule 70: 40S ribosomal protein S28

Chain AB: 



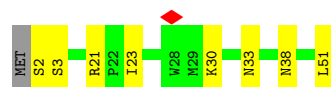
- Molecule 71: 40S ribosomal protein S11

Chain Ak: 



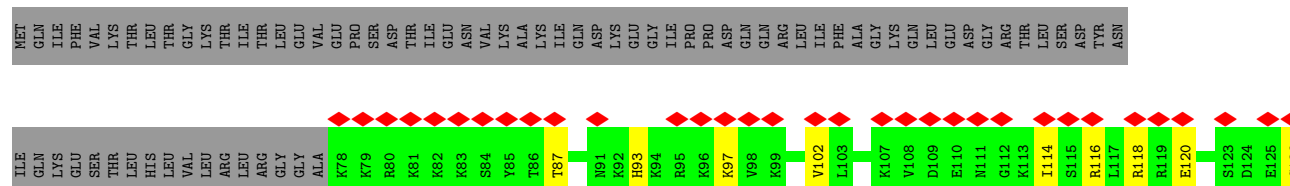
- Molecule 72: 60S ribosomal protein L39-like

Chain Bl: 



- Molecule 73: Ribosomal protein S27a

Chain AC: 



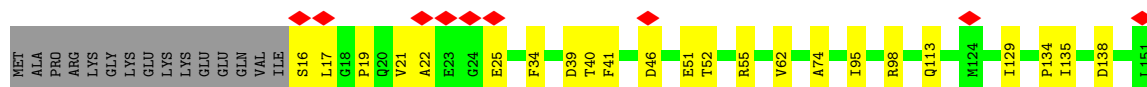
- Molecule 79: Small ribosomal subunit protein eS26

Chain AE: 

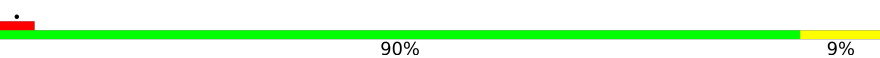


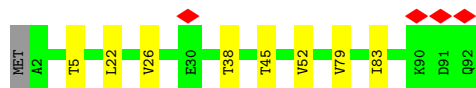
- Molecule 80: Small ribosomal subunit protein uS11

Chain An: 



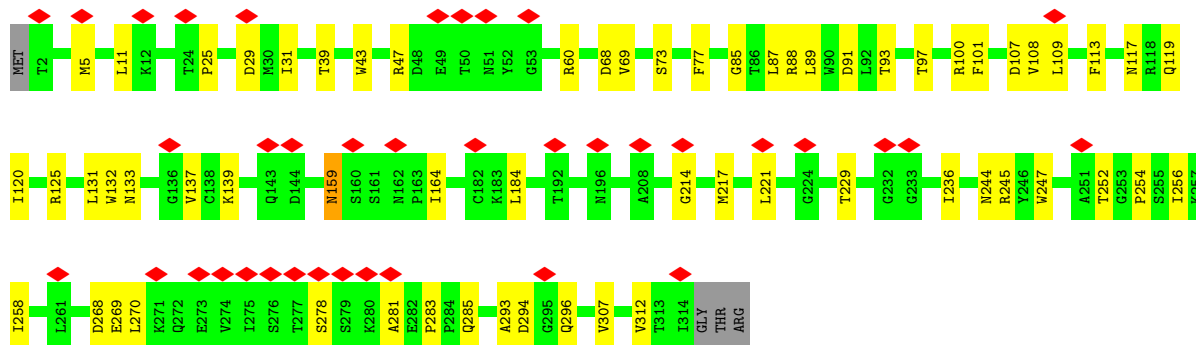
- Molecule 81: 60S ribosomal protein L37a

Chain Bp: 



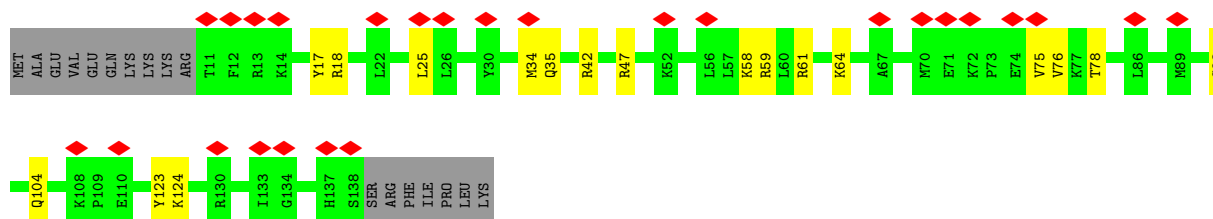
- Molecule 82: Small ribosomal subunit protein RACK1

Chain AF: 



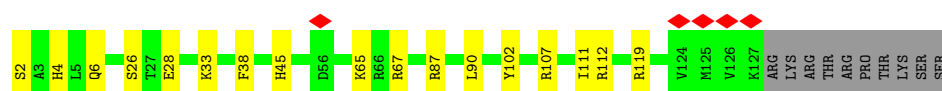
- Molecule 83: 40S ribosomal protein uS19

Chain Ao: 



- Molecule 84: Large ribosomal subunit protein eL28

Chain Br: 



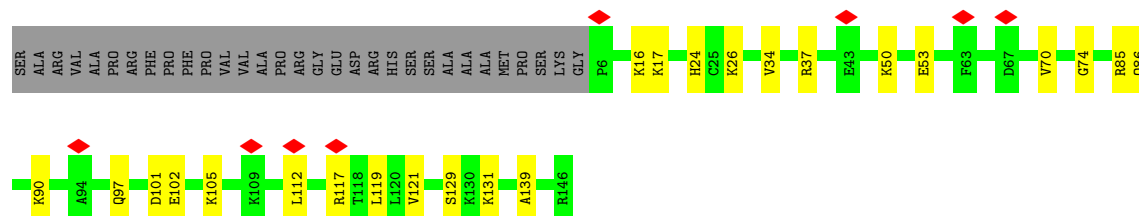
- Molecule 85: 40S ribosomal protein S29

Chain AG: 

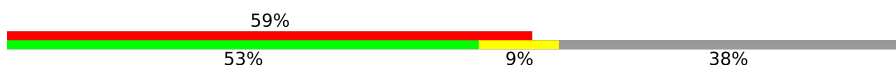


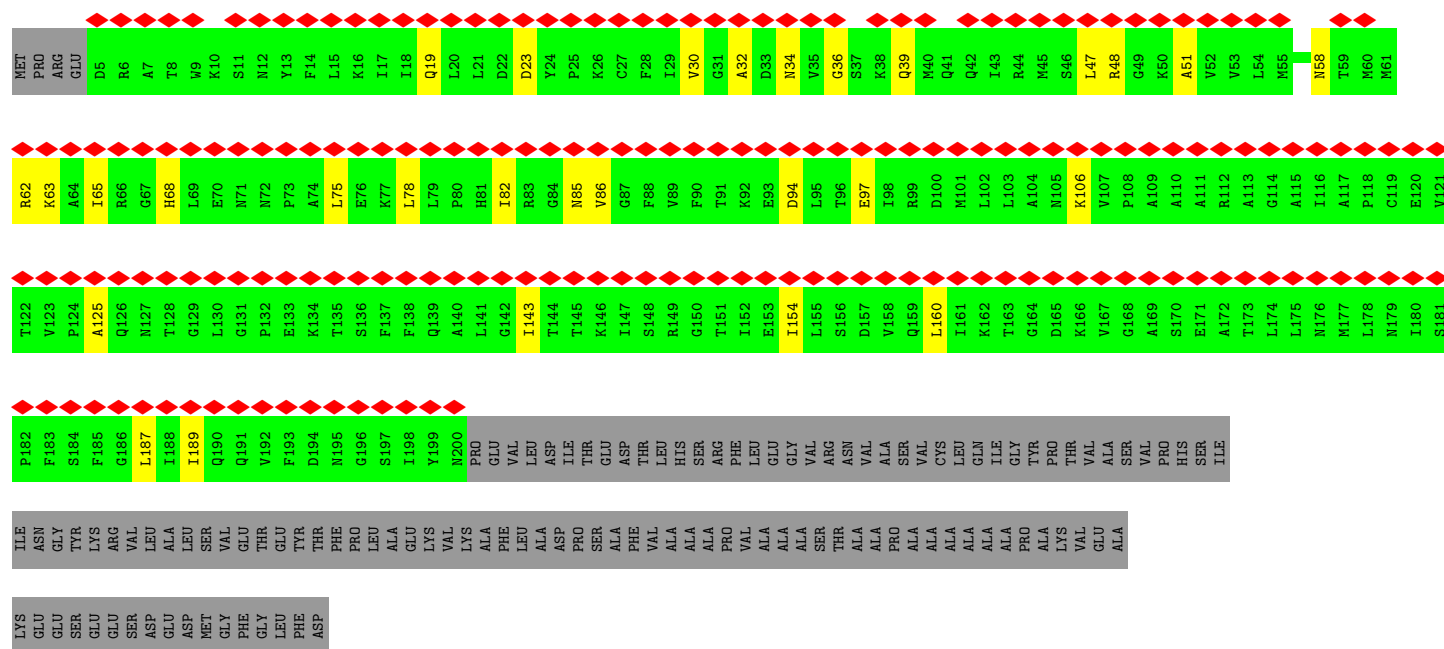
- Molecule 86: Small ribosomal subunit protein uS9

Chain Ap: 

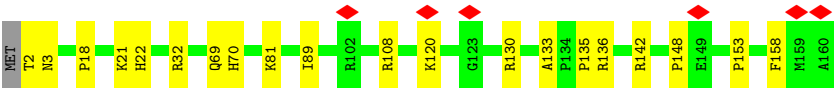
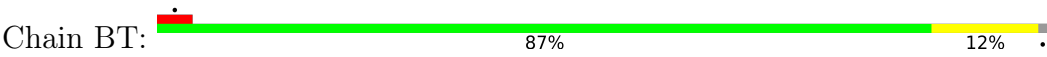


- Molecule 87: 60S acidic ribosomal protein P0

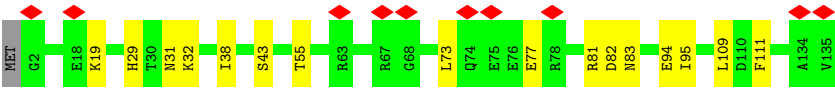
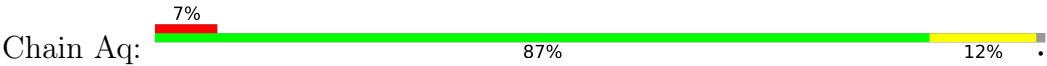
Chain Bs: 



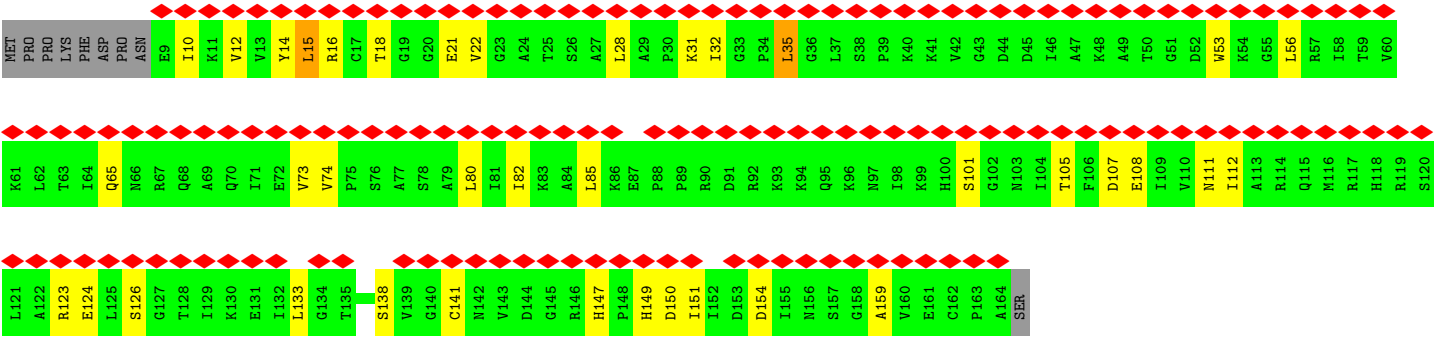
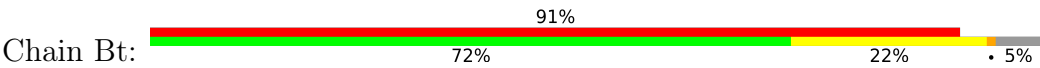
- Molecule 88: 60S ribosomal protein L21



• Molecule 89: 40S ribosomal protein eS17



• Molecule 90: 60S ribosomal protein L12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21864	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	0.906	Depositor
Minimum map value	-0.490	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.175	Depositor
Map size ($\text{\AA}$)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.065, 1.065, 1.065	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 5$
2	Bb	0.06	0/884	0.17	0/1169
3	B7	0.05	0/2835	0.08	0/4418
4	AT	0.27	0/68	0.35	0/103
5	Ar	0.06	0/1226	0.18	0/1643
6	B8	0.06	0/3635	0.11	0/5661
7	BU	0.08	0/845	0.21	0/1134
8	As	0.06	0/1119	0.18	0/1498
9	BA	0.08	0/1965	0.22	0/2633
10	BV	0.08	0/1048	0.21	0/1402
11	At	0.14	0/832	0.23	0/1117
12	BB	0.08	0/3261	0.20	0/4364
13	BX	0.07	0/984	0.19	0/1323
14	Au	0.06	0/636	0.18	0/852
15	BC	0.07	0/2932	0.18	0/3939
16	BP	0.07	0/1317	0.20	0/1768
17	BZ	0.06	0/1130	0.18	0/1507
18	Aw	0.07	0/1107	0.19	0/1475
19	BE	0.11	0/1998	0.22	0/2673
20	B5	0.10	2/86006 (0.0%)	0.12	0/134179
21	BQ	0.07	0/1539	0.20	0/2054
22	Ba	0.07	0/1179	0.18	0/1572
23	Ax	0.06	0/1032	0.17	0/1371
24	BF	0.07	0/1922	0.18	0/2563
25	BY	0.07	0/1132	0.20	0/1504
26	BW	0.06	0/1006	0.18	0/1334
27	AZ	0.07	0/1771	0.20	0/2406
28	Ay	0.07	0/691	0.19	0/922
29	BG	0.07	0/1908	0.19	0/2566
30	Av	0.08	0/1051	0.18	0/1406
31	BR	0.06	0/1524	0.16	0/2013
32	Aa	0.08	0/1841	0.20	0/2459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Az	0.05	0/240	0.13	0/305
34	BH	0.07	0/1535	0.19	0/2063
35	BS	0.08	0/1497	0.19	0/2008
36	Ab	0.07	0/1742	0.20	0/2354
37	Bc	0.06	0/847	0.17	0/1134
38	BI	0.07	0/1756	0.18	0/2346
39	B	0.08	0/2444	0.20	0/3273
40	EA	0.07	0/2561	0.21	0/3473
41	Ac	0.07	0/1779	0.19	0/2395
42	Bd	0.08	0/903	0.20	0/1216
43	BJ	0.06	0/1385	0.18	0/1852
44	Ct	0.12	0/909	0.28	0/1214
45	Ad	0.07	0/2118	0.20	0/2849
46	Be	0.07	0/1088	0.21	0/1451
48	Cu	0.16	0/829	0.31	0/1112
49	Ae	0.07	0/1531	0.22	0/2059
50	Bf	0.08	0/903	0.20	0/1208
51	BL	0.07	0/1733	0.19	0/2316
52	DA	0.07	0/1284	0.21	0/1728
53	Af	0.06	0/1946	0.18	0/2590
54	Bg	0.06	0/916	0.19	0/1220
55	BM	0.07	0/1158	0.19	0/1547
56	DB	0.14	0/7038	0.29	0/9468
57	Ag	0.07	0/1552	0.19	0/2079
58	Bh	0.06	0/1021	0.15	0/1348
59	BN	0.07	0/1746	0.18	0/2338
60	DC	0.11	0/1323	0.25	0/1783
61	Ah	0.07	0/1715	0.19	0/2287
62	Bi	0.06	0/841	0.18	0/1112
63	BO	0.08	0/1662	0.19	0/2222
64	A2	0.13	2/40342 (0.0%)	0.12	0/62877
65	Ai	0.06	0/1550	0.18	0/2069
66	Bj	0.07	0/720	0.20	0/952
67	AA	0.06	0/665	0.19	0/891
68	Aj	0.07	0/834	0.20	0/1125
69	Bk	0.07	0/575	0.18	0/761
70	AB	0.06	0/497	0.17	0/666
71	Ak	0.07	0/1284	0.19	0/1717
72	Bl	0.08	0/459	0.19	0/608
73	AC	0.06	0/622	0.19	0/822
74	Al	0.07	0/968	0.21	0/1296
75	Bm	0.07	0/426	0.21	0/564
76	AD	0.06	0/462	0.18	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	Am	0.06	0/1232	0.17	0/1656
78	Bo	0.08	0/866	0.19	0/1141
79	AE	0.17	0/828	0.23	0/1109
80	An	0.11	0/1020	0.22	0/1366
81	Bp	0.07	0/718	0.20	0/953
82	AF	0.07	0/2493	0.21	0/3394
83	Ao	0.06	0/1069	0.18	0/1429
84	Br	0.07	0/1020	0.21	0/1366
85	AG	0.06	0/470	0.18	0/623
86	Ap	0.08	0/1142	0.25	0/1528
87	Bs	0.07	0/1530	0.20	0/2064
88	BT	0.07	0/1326	0.19	0/1770
89	Aq	0.06	0/1094	0.18	0/1469
90	Bt	0.07	0/1193	0.22	0/1609
All	All	0.10	4/243831 (0.0%)	0.16	0/355810

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
78	Bo	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	1679	A2M	O3'-P	5.06	1.61	1.56
20	B5	2258	OMU	O3'-P	5.05	1.61	1.56
64	A2	485	A2M	O3'-P	5.02	1.61	1.56
20	B5	4269	A2M	O3'-P	5.01	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
78	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	AH	36	0	25	0	0
2	Bb	881	0	957	13	0
3	B7	2538	0	1283	20	0
4	AT	939	0	617	4	0
5	Ar	1217	0	1279	21	0
6	B8	3319	0	1684	28	0
7	BU	831	0	852	5	0
8	As	1113	0	1145	17	0
9	BA	1940	0	2029	32	0
10	BV	1034	0	1096	16	0
11	At	822	0	887	7	0
12	BB	3206	0	3352	34	0
13	BX	967	0	1040	8	0
14	Au	640	0	633	10	0
15	BC	2886	0	3057	36	0
16	BP	1289	0	1329	11	0
17	BZ	1107	0	1182	15	0
18	Aw	1099	0	1162	4	0
19	BE	1960	0	2153	26	0
20	B5	79525	0	40256	667	0
21	BQ	1515	0	1634	21	0
22	Ba	1163	0	1202	17	0
23	Ax	1015	0	1086	15	0
24	BF	1886	0	2008	24	0
25	BY	1115	0	1205	11	0
26	BW	991	0	1048	7	0
27	AZ	1743	0	1748	25	0
28	Ay	683	0	761	12	0
29	BG	1877	0	2023	17	0
30	Av	1034	0	1080	7	0
31	BR	1508	0	1664	8	0
32	Aa	1815	0	1908	22	0
33	Az	239	0	289	2	0
34	BH	1516	0	1597	17	0
35	BS	1457	0	1492	15	0
36	Ab	1706	0	1796	19	0
37	Bc	836	0	888	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BI	1717	0	1764	21	0
39	B	2398	0	2428	30	0
40	EA	2445	0	2407	36	0
41	Ac	1751	0	1846	22	0
42	Bd	888	0	930	14	0
43	BJ	1362	0	1399	18	0
44	Ct	904	0	968	26	0
45	Ad	2076	0	2177	25	0
46	Be	1070	0	1164	17	0
47	BK	160	0	37	0	0
48	Cu	821	0	867	18	0
49	Ae	1509	0	1563	16	0
50	Bf	884	0	922	8	0
51	BL	1702	0	1820	15	0
52	DA	1260	0	1282	19	0
53	Af	1923	0	2089	35	0
54	Bg	906	0	998	10	0
55	BM	1137	0	1211	15	0
56	DB	6900	0	6944	151	0
57	Ag	1529	0	1627	17	0
58	Bh	1013	0	1147	20	0
59	BN	1701	0	1749	23	0
60	DC	1295	0	1267	26	0
61	Ah	1686	0	1772	22	0
62	Bi	830	0	916	8	0
63	BO	1630	0	1778	19	0
64	A2	37833	0	19167	355	0
65	Ai	1525	0	1640	19	0
66	Bj	705	0	737	13	0
67	AA	651	0	672	8	0
68	Aj	810	0	836	12	0
69	Bk	569	0	637	7	0
70	AB	495	0	523	2	0
71	Ak	1262	0	1335	11	0
72	Bl	447	0	479	6	0
73	AC	610	0	634	13	0
74	Al	958	0	993	15	0
75	Bm	432	0	470	3	0
76	AD	457	0	502	9	0
77	Am	1208	0	1293	11	0
78	Bo	863	0	929	10	0
79	AE	814	0	863	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	An	1016	0	1038	16	0
81	Bp	708	0	756	6	0
82	AF	2436	0	2393	37	0
83	Ao	1048	0	1093	12	0
84	Br	1014	0	1083	12	0
85	AG	459	0	448	11	0
86	Ap	1124	0	1193	19	0
87	Bs	1507	0	1564	18	0
88	BT	1298	0	1365	21	0
89	Aq	1080	0	1135	10	0
90	Bt	1178	0	1235	22	0
91	A2	49	0	0	2	0
91	AE	1	0	0	0	0
91	AT	2	0	0	0	0
91	Ad	1	0	0	0	0
91	Ak	1	0	0	0	0
91	An	1	0	0	0	0
91	Ar	1	0	0	0	0
91	B5	186	0	0	6	0
91	B7	6	0	0	1	0
91	B8	6	0	0	0	0
91	BA	3	0	0	0	0
91	BB	1	0	0	0	0
91	BH	1	0	0	0	0
91	BI	1	0	0	0	0
91	BL	1	0	0	0	0
91	BN	1	0	0	0	0
91	BP	1	0	0	0	0
91	BQ	2	0	0	0	0
91	BT	2	0	0	0	0
91	BY	1	0	0	0	0
91	Bb	2	0	0	0	0
91	Be	4	0	0	2	0
91	Bf	1	0	0	0	0
91	Bj	1	0	0	0	0
91	Bo	1	0	0	0	0
92	A2	111	0	0	0	0
92	AT	2	0	0	0	0
92	B5	282	0	0	0	0
92	B7	9	0	0	0	0
92	B8	8	0	0	0	0
92	BB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	BI	1	0	0	0	0
92	BP	1	0	0	0	0
92	BR	1	0	0	0	0
92	BV	1	0	0	0	0
92	Ba	1	0	0	0	0
92	Be	1	0	0	0	0
92	Bj	1	0	0	0	0
93	B7	32	0	11	0	0
94	A2	80	0	152	5	0
94	B5	220	0	418	17	0
95	A2	14	0	26	4	0
95	B5	28	0	51	2	0
96	AC	1	0	0	0	0
96	AE	1	0	0	0	0
96	AG	1	0	0	0	0
96	Bg	1	0	0	0	0
96	Bj	1	0	0	0	0
96	Bm	1	0	0	0	0
96	Bo	1	0	0	0	0
96	Bp	1	0	0	0	0
97	DB	36	0	6	2	0
98	A2	527	0	0	25	0
98	AE	1	0	0	0	0
98	AH	3	0	0	0	0
98	AT	12	0	0	0	0
98	Aa	3	0	0	0	0
98	Ab	1	0	0	0	0
98	Ad	1	0	0	0	0
98	Af	1	0	0	0	0
98	Ak	2	0	0	0	0
98	An	1	0	0	0	0
98	Ap	2	0	0	0	0
98	Ar	2	0	0	0	0
98	As	2	0	0	0	0
98	At	1	0	0	0	0
98	Aw	5	0	0	1	0
98	B	1	0	0	0	0
98	B5	1398	0	0	58	0
98	B7	44	0	0	2	0
98	B8	47	0	0	1	0
98	BA	5	0	0	0	0
98	BB	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
98	BC	7	0	0	0	0
98	BH	1	0	0	0	0
98	BI	2	0	0	0	0
98	BL	2	0	0	0	0
98	BN	5	0	0	0	0
98	BP	3	0	0	0	0
98	BR	5	0	0	0	0
98	BV	2	0	0	0	0
98	BX	2	0	0	0	0
98	Ba	8	0	0	1	0
98	Bb	1	0	0	0	0
98	Bd	1	0	0	0	0
98	Be	4	0	0	0	0
98	Bg	1	0	0	0	0
98	Bj	5	0	0	0	0
98	Bl	2	0	0	0	0
98	Ct	1	0	0	0	0
All	All	236684	0	178196	2069	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 2069 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)
91:B7:210:UNX:UNK	98:B7:306:HOH:O	1.57	0.85
91:B5:5113:UNX:UNK	98:B5:5788:HOH:O	1.57	0.85
91:A2:1979:UNX:UNK	98:A2:2108:HOH:O	1.57	0.85
98:B5:6310:HOH:O	91:Be:205:UNX:UNK	1.60	0.82
30:Av:2:VAL:N	64:A2:1092:C:HO2'	1.78	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bb	103/245 (42%)	99 (96%)	4 (4%)	0	100	100
5	Ar	146/151 (97%)	144 (99%)	2 (1%)	0	100	100
7	BU	100/128 (78%)	99 (99%)	1 (1%)	0	100	100
8	As	140/145 (97%)	140 (100%)	0	0	100	100
9	BA	250/257 (97%)	241 (96%)	9 (4%)	0	100	100
10	BV	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
11	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
12	BB	395/403 (98%)	391 (99%)	4 (1%)	0	100	100
13	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
14	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
15	BC	360/412 (87%)	356 (99%)	4 (1%)	0	100	100
16	BP	157/184 (85%)	156 (99%)	1 (1%)	0	100	100
17	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
18	Aw	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
19	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
21	BQ	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
22	Ba	144/148 (97%)	139 (96%)	5 (4%)	0	100	100
23	Ax	123/130 (95%)	123 (100%)	0	0	100	100
24	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
25	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
26	BW	119/157 (76%)	119 (100%)	0	0	100	100
27	AZ	219/294 (74%)	216 (99%)	3 (1%)	0	100	100
28	Ay	83/124 (67%)	81 (98%)	2 (2%)	0	100	100
29	BG	229/266 (86%)	226 (99%)	3 (1%)	0	100	100
30	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
31	BR	178/196 (91%)	178 (100%)	0	0	100	100
32	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
33	Az	23/25 (92%)	23 (100%)	0	0	100	100
34	BH	188/192 (98%)	188 (100%)	0	0	100	100
35	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
37	Bc	106/115 (92%)	106 (100%)	0	0	100	100
38	BI	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
39	B	293/297 (99%)	289 (99%)	4 (1%)	0	100	100
40	EA	315/386 (82%)	310 (98%)	4 (1%)	1 (0%)	36	67
41	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
42	Bd	105/125 (84%)	105 (100%)	0	0	100	100
43	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
44	Ct	112/238 (47%)	108 (96%)	4 (4%)	0	100	100
45	Ad	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
46	Be	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
48	Cu	104/162 (64%)	99 (95%)	5 (5%)	0	100	100
49	Ae	189/204 (93%)	188 (100%)	1 (0%)	0	100	100
50	Bf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
51	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
52	DA	153/403 (38%)	152 (99%)	1 (1%)	0	100	100
53	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
54	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
55	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
56	DB	835/915 (91%)	821 (98%)	14 (2%)	0	100	100
57	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
58	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
59	BN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
60	DC	158/235 (67%)	156 (99%)	2 (1%)	0	100	100
61	Ah	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
62	Bi	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
63	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
65	Ai	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
66	Bj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
67	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
68	Aj	94/165 (57%)	91 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Bk	67/70 (96%)	67 (100%)	0	0	100	100
70	AB	61/69 (88%)	61 (100%)	0	0	100	100
71	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
72	Bl	48/51 (94%)	48 (100%)	0	0	100	100
73	AC	72/156 (46%)	70 (97%)	2 (3%)	0	100	100
74	Al	122/132 (92%)	120 (98%)	2 (2%)	0	100	100
75	Bm	49/128 (38%)	49 (100%)	0	0	100	100
76	AD	55/133 (41%)	55 (100%)	0	0	100	100
77	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
78	Bo	102/106 (96%)	102 (100%)	0	0	100	100
79	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
80	An	132/151 (87%)	130 (98%)	2 (2%)	0	100	100
81	Bp	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
82	AF	311/317 (98%)	305 (98%)	6 (2%)	0	100	100
83	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
84	Br	124/136 (91%)	123 (99%)	1 (1%)	0	100	100
85	AG	53/56 (95%)	53 (100%)	0	0	100	100
86	Ap	139/172 (81%)	133 (96%)	6 (4%)	0	100	100
87	Bs	194/318 (61%)	190 (98%)	4 (2%)	0	100	100
88	BT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
89	Aq	132/135 (98%)	132 (100%)	0	0	100	100
90	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
All	All	13380/15955 (84%)	13211 (99%)	168 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	EA	297	HIS

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	Bb	87/183 (48%)	87 (100%)	0	100	100
5	Ar	127/130 (98%)	125 (98%)	2 (2%)	55	68
7	BU	91/113 (80%)	89 (98%)	2 (2%)	45	63
8	As	112/114 (98%)	112 (100%)	0	100	100
9	BA	194/198 (98%)	194 (100%)	0	100	100
10	BV	106/107 (99%)	106 (100%)	0	100	100
11	At	94/107 (88%)	92 (98%)	2 (2%)	47	63
12	BB	344/347 (99%)	342 (99%)	2 (1%)	78	79
13	BX	106/134 (79%)	106 (100%)	0	100	100
14	Au	67/67 (100%)	66 (98%)	1 (2%)	57	69
15	BC	302/336 (90%)	302 (100%)	0	100	100
16	BP	140/163 (86%)	140 (100%)	0	100	100
17	BZ	117/118 (99%)	117 (100%)	0	100	100
18	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	66
19	BE	216/251 (86%)	216 (100%)	0	100	100
21	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	71
22	Ba	118/119 (99%)	118 (100%)	0	100	100
23	Ax	107/112 (96%)	106 (99%)	1 (1%)	70	74
24	BF	197/215 (92%)	197 (100%)	0	100	100
25	BY	124/135 (92%)	124 (100%)	0	100	100
26	BW	100/126 (79%)	99 (99%)	1 (1%)	68	74
27	AZ	182/242 (75%)	179 (98%)	3 (2%)	55	68
28	Ay	75/102 (74%)	75 (100%)	0	100	100
29	BG	199/223 (89%)	196 (98%)	3 (2%)	57	69
30	Av	112/113 (99%)	111 (99%)	1 (1%)	70	74
31	BR	159/175 (91%)	159 (100%)	0	100	100
32	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	74
33	Az	24/24 (100%)	24 (100%)	0	100	100
34	BH	169/171 (99%)	169 (100%)	0	100	100
35	BS	154/154 (100%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Ab	185/223 (83%)	184 (100%)	1 (0%)	81	81
37	Bc	92/98 (94%)	91 (99%)	1 (1%)	65	73
38	BI	180/181 (99%)	178 (99%)	2 (1%)	65	73
39	B	247/250 (99%)	247 (100%)	0	100	100
40	EA	274/330 (83%)	274 (100%)	0	100	100
41	Ac	189/232 (82%)	188 (100%)	1 (0%)	81	81
42	Bd	98/110 (89%)	98 (100%)	0	100	100
43	BJ	143/149 (96%)	143 (100%)	0	100	100
44	Ct	100/202 (50%)	99 (99%)	1 (1%)	68	74
45	Ad	224/225 (100%)	224 (100%)	0	100	100
46	Be	116/121 (96%)	116 (100%)	0	100	100
48	Cu	90/136 (66%)	89 (99%)	1 (1%)	65	73
49	Ae	161/170 (95%)	161 (100%)	0	100	100
50	Bf	89/89 (100%)	89 (100%)	0	100	100
51	BL	175/176 (99%)	174 (99%)	1 (1%)	78	79
52	DA	137/355 (39%)	135 (98%)	2 (2%)	57	69
53	Af	207/218 (95%)	206 (100%)	1 (0%)	81	81
54	Bg	98/100 (98%)	98 (100%)	0	100	100
55	BM	117/161 (73%)	117 (100%)	0	100	100
56	DB	746/806 (93%)	731 (98%)	15 (2%)	48	64
57	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	79
58	Bh	109/110 (99%)	109 (100%)	0	100	100
59	BN	171/172 (99%)	171 (100%)	0	100	100
60	DC	136/202 (67%)	134 (98%)	2 (2%)	57	69
61	Ah	178/180 (99%)	176 (99%)	2 (1%)	65	73
62	Bi	86/89 (97%)	86 (100%)	0	100	100
63	BO	171/173 (99%)	169 (99%)	2 (1%)	63	71
65	Ai	161/168 (96%)	160 (99%)	1 (1%)	78	79
66	Bj	73/80 (91%)	73 (100%)	0	100	100
67	AA	75/76 (99%)	74 (99%)	1 (1%)	61	71
68	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	68
70	AB	56/62 (90%)	54 (96%)	2 (4%)	31	53
71	Ak	139/142 (98%)	138 (99%)	1 (1%)	76	77
72	Bl	47/48 (98%)	47 (100%)	0	100	100
73	AC	67/140 (48%)	67 (100%)	0	100	100
74	Al	104/108 (96%)	102 (98%)	2 (2%)	50	65
75	Bm	47/115 (41%)	47 (100%)	0	100	100
76	AD	47/106 (44%)	47 (100%)	0	100	100
77	Am	130/131 (99%)	130 (100%)	0	100	100
78	Bo	92/93 (99%)	92 (100%)	0	100	100
79	AE	88/98 (90%)	86 (98%)	2 (2%)	44	62
80	An	105/118 (89%)	104 (99%)	1 (1%)	68	74
81	Bp	74/75 (99%)	73 (99%)	1 (1%)	59	70
82	AF	272/275 (99%)	270 (99%)	2 (1%)	76	77
83	Ao	114/130 (88%)	114 (100%)	0	100	100
84	Br	109/119 (92%)	109 (100%)	0	100	100
85	AG	48/49 (98%)	48 (100%)	0	100	100
86	Ap	117/140 (84%)	117 (100%)	0	100	100
87	Bs	164/258 (64%)	163 (99%)	1 (1%)	78	79
88	BT	139/140 (99%)	139 (100%)	0	100	100
89	Aq	120/121 (99%)	118 (98%)	2 (2%)	53	67
90	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	47
All	All	11658/13537 (86%)	11577 (99%)	81 (1%)	73	77

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
65	Ai	55	LYS
82	AF	159	ASN
68	Aj	40	VAL
74	Al	104	VAL
90	Bt	12	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
60	DC	153	GLN
85	AG	3	HIS
63	BO	180	GLN
72	Bl	25	GLN
87	Bs	39	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AH	0/3	-	-
20	B5	3694/4808 (76%)	433 (11%)	2 (0%)
3	B7	118/120 (98%)	7 (5%)	0
4	AT	2/76 (2%)	1 (50%)	0
6	B8	155/158 (98%)	16 (10%)	0
64	A2	1764/1870 (94%)	211 (11%)	0
All	All	5733/7035 (81%)	668 (11%)	2 (0%)

5 of 668 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	B7	7	G
3	B7	53	U
3	B7	54	A
3	B7	63	C
3	B7	64	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	B5	1588	G
20	B5	4445	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

223 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
20	OMC	B5	2208	92,20	19,22,23	0.81	0	26,31,34	0.84	0
64	OMU	A2	355	64	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
64	PSU	A2	1348	64	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
64	OMC	A2	174	92,64	19,22,23	0.81	0	26,31,34	0.80	0
64	PSU	A2	1057	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	PSU	B5	4740	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
64	4AC	A2	1338	64	21,24,25	1.07	1 (4%)	29,34,37	1.15	3 (10%)
20	OMC	B5	2194	92,20	19,22,23	0.82	0	26,31,34	0.85	0
64	PSU	A2	650	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
12	HIC	BB	245	12	10,11,12	0.62	0	8,14,16	0.39	0
20	PSU	B5	4435	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	4382	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMU	B5	3973	20	19,22,23	1.21	2 (10%)	26,31,34	1.69	4 (15%)
20	PSU	B5	4166	20	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
64	PSU	A2	816	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	OMU	B5	2258	20	19,22,23	1.21	2 (10%)	26,31,34	1.67	4 (15%)
64	PSU	A2	1239	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	PSU	B5	1721	20	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
64	OMU	A2	116	64	19,22,23	1.20	2 (10%)	26,31,34	1.70	4 (15%)
20	5MC	B5	3514	92,20	18,22,23	0.97	2 (11%)	26,32,35	1.15	3 (11%)
20	UR3	B5	4276	20	19,22,23	0.99	0	26,32,35	1.42	1 (3%)
20	OMG	B5	4138	20	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
64	PSU	A2	36	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	A2M	A2	591	64	22,25,26	1.48	4 (18%)	31,36,39	2.23	7 (22%)
64	OMG	A2	1329	64	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
20	A2M	B5	3599	20	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
64	OMU	A2	1289	64	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
20	A2M	B5	4336	20	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
20	OMG	B5	3476	20	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
15	AYA	BC	2	15	6,7,8	0.70	0	5,8,10	0.39	0
20	PSU	B5	3427	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4298	20	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMG	B5	3974	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
64	OMG	A2	684	64	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
20	OMC	B5	3540	20	19,22,23	0.82	0	26,31,34	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PSU	B5	1491	20	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
20	OMG	B5	4116	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
64	PSU	A2	1233	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	2475	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
75	M3L	Bm	98	75	10,11,12	0.83	0	9,14,16	0.52	0
64	A2M	A2	166	64	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
64	OMU	A2	628	64	19,22,23	1.18	2 (10%)	26,31,34	1.73	5 (19%)
20	OMG	B5	4240	20	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
64	A2M	A2	669	92,64	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
64	A2M	A2	513	64	22,25,26	1.47	4 (18%)	31,36,39	2.14	9 (29%)
64	A2M	A2	577	64	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
20	PSU	B5	3576	20	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
64	PSU	A2	1368	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
27	SAC	AZ	2	27	7,8,9	0.54	0	8,9,11	0.87	1 (12%)
64	PSU	A2	119	64	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	4364	20	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
20	A2M	B5	1270	20	22,25,26	1.45	4 (18%)	31,36,39	2.08	9 (29%)
20	A2M	B5	3456	20	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
64	OMC	A2	463	64	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
20	A2M	B5	400	20	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
20	OMU	B5	2680	20	19,22,23	1.20	2 (10%)	26,31,34	1.70	5 (19%)
20	PSU	B5	4749	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3554	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	6MZ	B5	3966	20	22,25,26	1.45	4 (18%)	30,36,39	2.19	9 (30%)
20	PSU	B5	3585	92,20	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	OMC	B5	3601	20	19,22,23	0.81	0	26,31,34	0.81	0
64	OMU	A2	1327	92,64	19,22,23	1.19	2 (10%)	26,31,34	1.71	5 (19%)
20	PSU	B5	4217	20	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
20	A2M	B5	2244	92,20	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
20	PSU	B5	3502	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
64	OMC	A2	1392	64	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
20	PSU	B5	1537	20	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
6	OMG	B8	75	6	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
64	OMC	A2	518	64	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
20	OMG	B5	1580	20	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	V5N	Ba	39	22	9,11,12	2.06	2 (22%)	9,14,16	1.68	2 (22%)
64	PSU	A2	1046	64	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	PSU	A2	218	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	PSU	B5	3500	20	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
20	OMG	B5	3676	20	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
20	OMG	B5	3524	20	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
20	A2M	B5	3562	20	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
64	PSU	A2	109	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	OMG	B5	2267	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
20	PSU	B5	4169	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	3942	20,4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
64	PSU	A2	407	64	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
64	PSU	A2	1175	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMG	B5	1477	20	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
64	A2M	A2	469	64	22,25,26	1.47	4 (18%)	31,36,39	2.10	10 (32%)
64	PSU	A2	1446	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMG	B5	2719	20	23,26,27	1.21	3 (13%)	33,38,41	1.98	6 (18%)
64	MA6	A2	1852	64	23,26,27	2.23	5 (21%)	34,38,41	3.69	14 (41%)
64	PSU	A2	1178	64	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
8	NMM	As	67	8	9,11,12	0.59	0	6,12,14	0.45	0
64	PSU	A2	802	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMG	B5	4245	20	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
20	OMG	B5	2207	20	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
64	PSU	A2	823	64	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	OMC	B5	2265	92,20	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
20	UY1	B5	3550	20	19,22,23	1.40	3 (15%)	22,31,34	1.85	5 (22%)
78	MLZ	Bo	53	78	8,9,10	0.49	0	4,9,11	0.13	0
80	IAS	An	138	80	6,7,8	1.07	0	6,8,10	1.33	1 (16%)
20	OMC	B5	2647	20	19,22,23	0.83	0	26,31,34	0.84	0
20	PSU	B5	3490	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	OMU	B5	4366	20	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
64	OMG	A2	645	64	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
20	PSU	B5	4058	20	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
64	PSU	A2	1005	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	5MC	B5	4193	20	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OMC	B5	1284	20	19,22,23	0.82	0	26,31,34	0.82	0
20	OMG	B5	4369	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
64	PSU	A2	687	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
64	A2M	A2	1032	64	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
20	A2M	B5	3517	20	22,25,26	1.44	4 (18%)	31,36,39	2.17	11 (35%)
20	PSU	B5	4107	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	3492	20,64	22,25,26	1.47	4 (18%)	31,36,39	2.17	10 (32%)
20	PSU	B5	4322	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4045	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	1632	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	4 (18%)
64	A2M	A2	485	64	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
20	PSU	B5	4419	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4325	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
5	SAC	Ar	2	5	7,8,9	0.52	0	8,9,11	0.90	1 (12%)
20	1MA	B5	1266	92,20	21,25,26	1.39	4 (19%)	31,37,40	1.71	5 (16%)
20	A2M	B5	2206	92,20	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
20	OMC	B5	4282	92,20	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
20	PSU	B5	4177	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4099	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
64	PSU	A2	864	64	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	OMC	B5	3573	20	19,22,23	0.81	0	26,31,34	0.87	1 (3%)
64	OMU	A2	121	64	19,22,23	1.21	3 (15%)	26,31,34	1.69	4 (15%)
64	4AC	A2	1843	64	21,24,25	1.09	2 (9%)	29,34,37	1.23	3 (10%)
20	A2M	B5	4317	20	22,25,26	1.47	4 (18%)	31,36,39	2.15	9 (29%)
20	PSU	B5	4042	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	OMU	A2	172	64	19,22,23	1.20	3 (15%)	26,31,34	1.70	4 (15%)
64	PSU	A2	1082	64	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3466	20	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	3616	20	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
64	OMG	A2	1448	64	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
20	PSU	B5	4149	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	1479	20	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
20	OMU	B5	4052	20	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
18	HY3	Aw	62	18	6,8,9	1.99	1 (16%)	5,10,12	1.10	1 (20%)
20	PSU	B5	1720	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OMC	B5	1820	92,20	19,22,23	0.80	0	26,31,34	0.79	0
64	PSU	A2	610	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
64	A2M	A2	159	64	22,25,26	1.47	4 (18%)	31,36,39	2.15	9 (29%)
64	OMG	A2	868	64	23,26,27	1.18	3 (13%)	33,38,41	1.92	5 (15%)
64	PSU	A2	682	64	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
20	OMU	B5	3657	20	19,22,23	1.21	2 (10%)	26,31,34	1.71	5 (19%)
20	PSU	B5	3462	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	3494	20	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
20	PSU	B5	4278	20	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	1489	92,20	22,25,26	1.45	4 (18%)	31,36,39	2.10	9 (29%)
20	OMG	B5	4383	20	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
64	PSU	A2	1626	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4203	20	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
20	PSU	B5	4374	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
64	A2M	A2	1384	64	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
20	A2M	B5	4269	92,20	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
64	OMU	A2	429	64	19,22,23	1.21	3 (15%)	26,31,34	1.67	4 (15%)
64	PSU	A2	867	64	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
20	OMC	B5	2667	20	19,22,23	0.81	0	26,31,34	0.82	0
64	PSU	A2	573	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
6	PSU	B8	55	6	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
20	A2M	B5	3450	20	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
64	PSU	A2	105	64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
20	OMC	B5	4202	20	19,22,23	0.82	0	26,31,34	0.81	0
20	PSU	B5	3652	92,20	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
20	OMU	B5	4244	20	19,22,23	1.20	2 (10%)	26,31,34	1.68	5 (19%)
64	PSU	A2	1047	64	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	A2M	B5	1810	92,20	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
20	PSU	B5	4267	92,20	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
64	PSU	A2	967	64	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
64	PSU	A2	93	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	A2M	B5	3557	20	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
64	OMG	A2	437	64	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
64	PSU	A2	210	64	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
64	A2M	A2	99	92,64	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PSU	B5	3447	20	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	G7M	A2	1640	64	23,26,27	3.15	9 (39%)	35,39,42	3.32	13 (37%)
20	A2M	B5	2658	92,20	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
20	PSU	B5	3496	20	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	3583	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	1683	20	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
20	OMC	B5	2704	20	19,22,23	0.82	0	26,31,34	0.82	0
64	PSU	A2	1644	92,64	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
64	6MZ	A2	1833	92,64	22,25,26	1.45	4 (18%)	30,36,39	2.17	9 (30%)
20	PSU	B5	1731	20	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
20	PSU	B5	1801	20	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
20	OMC	B5	3619	20	19,22,23	0.81	0	26,31,34	0.84	0
20	PSU	B5	4039	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
20	PSU	B5	4711	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
64	A2M	A2	27	92,64	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
64	PSU	A2	652	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
20	A2M	B5	398	20	22,25,26	1.46	4 (18%)	31,36,39	2.19	10 (32%)
20	PSU	B5	2351	20	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	3371	20	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
64	PSU	A2	815	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
6	PSU	B8	69	6	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
64	MA6	A2	1851	64	23,26,27	2.27	5 (21%)	34,38,41	3.68	14 (41%)
20	PSU	B5	1638	20	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
20	PSU	B5	1799	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
64	OMG	A2	602	64	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
64	A2M	A2	1679	64	22,25,26	1.45	4 (18%)	31,36,39	2.24	10 (32%)
64	OMG	A2	510	92,64	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
20	A2M	B5	2630	92,20	22,25,26	1.46	4 (18%)	31,36,39	2.17	9 (29%)
64	PSU	A2	1693	64	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
2	MLZ	Bb	5	2	8,9,10	0.49	0	4,9,11	0.14	0
64	B8N	A2	1249	64	24,29,30	1.33	3 (12%)	29,42,45	1.30	3 (10%)
20	OMG	B5	1260	20	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
9	V5N	BA	216	9	9,11,12	2.06	2 (22%)	9,14,16	1.72	2 (22%)
20	PSU	B5	3369	20	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
20	OMG	B5	3359	20	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
64	PSU	A2	1245	64	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
64	OMG	A2	1491	92,64	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
64	OMU	A2	1443	92,64	19,22,23	1.23	3 (15%)	26,31,34	1.69	5 (19%)
64	OMC	A2	1704	64	19,22,23	0.80	0	26,31,34	0.79	0
64	OMU	A2	1805	64	19,22,23	1.22	3 (15%)	26,31,34	1.69	5 (19%)
20	OMC	B5	3433	20	19,22,23	0.79	0	26,31,34	0.75	0
20	PSU	B5	1718	20	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
14	AME	Au	1	14	9,10,11	0.47	0	9,11,13	0.87	1 (11%)
20	PSU	B5	4246	20	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
20	OMG	B5	3631	20	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
84	SAC	Br	2	84	7,8,9	0.53	0	8,9,11	0.83	1 (12%)
64	PSU	A2	34	64	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
20	PSU	B5	4188	20	18,21,22	1.34	2 (11%)	22,30,33	1.85	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
20	OMC	B5	2208	92,20	-	0/9/27/28	0/2/2/2
64	OMU	A2	355	64	-	0/9/27/28	0/2/2/2
64	PSU	A2	1348	64	-	0/7/25/26	0/2/2/2
64	OMC	A2	174	92,64	-	0/9/27/28	0/2/2/2
64	PSU	A2	1057	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	4740	20	-	0/7/25/26	0/2/2/2
64	4AC	A2	1338	64	-	3/11/29/30	0/2/2/2
20	OMC	B5	2194	92,20	-	1/9/27/28	0/2/2/2
64	PSU	A2	650	64	-	0/7/25/26	0/2/2/2
12	HIC	BB	245	12	-	2/5/6/8	0/1/1/1
20	PSU	B5	4435	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4382	20	-	4/7/25/26	0/2/2/2
20	OMU	B5	3973	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	4166	20	-	3/7/25/26	0/2/2/2
64	PSU	A2	816	64	-	0/7/25/26	0/2/2/2
20	OMU	B5	2258	20	-	0/9/27/28	0/2/2/2
64	PSU	A2	1239	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	1721	20	-	0/7/25/26	0/2/2/2
64	OMU	A2	116	64	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	5MC	B5	3514	92,20	-	0/7/25/26	0/2/2/2
20	UR3	B5	4276	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	4138	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	36	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	591	64	-	4/9/27/28	0/3/3/3
64	OMG	A2	1329	64	-	0/9/27/28	0/3/3/3
20	A2M	B5	3599	20	-	1/9/27/28	0/3/3/3
64	OMU	A2	1289	64	-	0/9/27/28	0/2/2/2
20	A2M	B5	4336	20	-	1/9/27/28	0/3/3/3
20	OMG	B5	3476	20	-	1/9/27/28	0/3/3/3
15	AYA	BC	2	15	-	3/4/6/8	-
20	PSU	B5	3427	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4298	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	3974	20	-	0/9/27/28	0/3/3/3
64	OMG	A2	684	64	-	0/9/27/28	0/3/3/3
20	OMC	B5	3540	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	1491	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	4116	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	1233	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	2475	20	-	0/7/25/26	0/2/2/2
75	M3L	Bm	98	75	-	0/9/10/12	-
64	A2M	A2	166	64	-	0/9/27/28	0/3/3/3
64	OMU	A2	628	64	-	4/9/27/28	0/2/2/2
20	OMG	B5	4240	20	-	0/9/27/28	0/3/3/3
64	A2M	A2	669	92,64	-	2/9/27/28	0/3/3/3
64	A2M	A2	513	64	-	2/9/27/28	0/3/3/3
64	A2M	A2	577	64	-	2/9/27/28	0/3/3/3
20	PSU	B5	3576	20	-	1/7/25/26	0/2/2/2
64	PSU	A2	1368	64	-	0/7/25/26	0/2/2/2
27	SAC	AZ	2	27	-	2/7/8/10	-
64	PSU	A2	119	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	4364	20	-	1/9/27/28	0/3/3/3
20	A2M	B5	1270	20	-	0/9/27/28	0/3/3/3
20	A2M	B5	3456	20	-	0/9/27/28	0/3/3/3
64	OMC	A2	463	64	-	0/9/27/28	0/2/2/2
20	A2M	B5	400	20	-	0/9/27/28	0/3/3/3
20	OMU	B5	2680	20	-	1/9/27/28	0/2/2/2
20	PSU	B5	4749	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3554	20	-	0/7/25/26	0/2/2/2
20	6MZ	B5	3966	20	-	0/9/27/28	0/3/3/3
20	PSU	B5	3585	92,20	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OMC	B5	3601	20	-	0/9/27/28	0/2/2/2
64	OMU	A2	1327	92,64	-	0/9/27/28	0/2/2/2
20	PSU	B5	4217	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	2244	92,20	-	0/9/27/28	0/3/3/3
20	PSU	B5	3502	20	-	0/7/25/26	0/2/2/2
64	OMC	A2	1392	64	-	0/9/27/28	0/2/2/2
20	PSU	B5	1537	20	-	0/7/25/26	0/2/2/2
6	OMG	B8	75	6	-	0/9/27/28	0/3/3/3
64	OMC	A2	518	64	-	0/9/27/28	0/2/2/2
20	OMG	B5	1580	20	-	0/9/27/28	0/3/3/3
22	V5N	Ba	39	22	-	1/9/10/12	0/1/1/1
64	PSU	A2	1046	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	218	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3500	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	3676	20	-	0/9/27/28	0/3/3/3
20	OMG	B5	3524	20	-	0/9/27/28	0/3/3/3
20	A2M	B5	3562	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	109	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	2267	20	-	0/9/27/28	0/3/3/3
20	PSU	B5	4169	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	3942	20,4	-	0/9/27/28	0/3/3/3
64	PSU	A2	407	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	1175	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	1477	20	-	0/9/27/28	0/3/3/3
64	A2M	A2	469	64	-	2/9/27/28	0/3/3/3
64	PSU	A2	1446	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	2719	20	-	0/9/27/28	0/3/3/3
64	MA6	A2	1852	64	-	4/11/29/30	0/3/3/3
64	PSU	A2	1178	64	-	0/7/25/26	0/2/2/2
8	NMM	As	67	8	-	0/9/11/13	-
64	PSU	A2	802	64	-	0/7/25/26	0/2/2/2
20	OMG	B5	4245	20	-	0/9/27/28	0/3/3/3
20	OMG	B5	2207	20	-	2/9/27/28	0/3/3/3
64	PSU	A2	823	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	2265	92,20	-	0/9/27/28	0/2/2/2
20	UY1	B5	3550	20	-	1/9/27/28	0/2/2/2
78	MLZ	Bo	53	78	-	1/7/8/10	-
80	IAS	An	138	80	-	2/7/7/8	-
20	OMC	B5	2647	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	3490	20	-	0/7/25/26	0/2/2/2
20	OMU	B5	4366	20	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	OMG	A2	645	64	-	3/9/27/28	0/3/3/3
20	PSU	B5	4058	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	1005	64	-	0/7/25/26	0/2/2/2
20	5MC	B5	4193	20	-	4/7/25/26	0/2/2/2
20	OMC	B5	1284	20	-	0/9/27/28	0/2/2/2
20	OMG	B5	4369	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	687	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	1032	64	-	0/9/27/28	0/3/3/3
20	A2M	B5	3517	20	-	2/9/27/28	0/3/3/3
20	PSU	B5	4107	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	3492	20,64	-	1/9/27/28	0/3/3/3
20	PSU	B5	4322	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4045	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1632	20	-	0/7/25/26	0/2/2/2
64	A2M	A2	485	64	-	0/9/27/28	0/3/3/3
20	PSU	B5	4419	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4325	20	-	0/7/25/26	0/2/2/2
5	SAC	Ar	2	5	-	0/7/8/10	-
20	1MA	B5	1266	92,20	-	0/7/25/26	0/3/3/3
20	A2M	B5	2206	92,20	-	0/9/27/28	0/3/3/3
20	OMC	B5	4282	92,20	-	0/9/27/28	0/2/2/2
20	PSU	B5	4177	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4099	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	864	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	3573	20	-	0/9/27/28	0/2/2/2
64	OMU	A2	121	64	-	0/9/27/28	0/2/2/2
64	4AC	A2	1843	64	-	4/11/29/30	0/2/2/2
20	A2M	B5	4317	20	-	0/9/27/28	0/3/3/3
20	PSU	B5	4042	20	-	0/7/25/26	0/2/2/2
64	OMU	A2	172	64	-	0/9/27/28	0/2/2/2
64	PSU	A2	1082	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	3466	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3616	20	-	0/7/25/26	0/2/2/2
64	OMG	A2	1448	64	-	3/9/27/28	0/3/3/3
20	PSU	B5	4149	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	1479	20	-	0/9/27/28	0/3/3/3
20	OMU	B5	4052	20	-	1/9/27/28	0/2/2/2
18	HY3	Aw	62	18	-	1/1/12/14	0/1/1/1
20	PSU	B5	1720	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	1820	92,20	-	0/9/27/28	0/2/2/2
64	PSU	A2	610	64	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	A2M	A2	159	64	-	0/9/27/28	0/3/3/3
64	OMG	A2	868	64	-	1/9/27/28	0/3/3/3
64	PSU	A2	682	64	-	0/7/25/26	0/2/2/2
20	OMU	B5	3657	20	-	1/9/27/28	0/2/2/2
20	PSU	B5	3462	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3494	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4278	20	-	0/7/25/26	0/2/2/2
20	A2M	B5	1489	92,20	-	2/9/27/28	0/3/3/3
20	OMG	B5	4383	20	-	1/9/27/28	0/3/3/3
64	PSU	A2	1626	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	4203	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4374	20	-	0/7/25/26	0/2/2/2
64	A2M	A2	1384	64	-	0/9/27/28	0/3/3/3
20	A2M	B5	4269	92,20	-	0/9/27/28	0/3/3/3
64	OMU	A2	429	64	-	4/9/27/28	0/2/2/2
64	PSU	A2	867	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	2667	20	-	1/9/27/28	0/2/2/2
64	PSU	A2	573	64	-	0/7/25/26	0/2/2/2
6	PSU	B8	55	6	-	0/7/25/26	0/2/2/2
20	A2M	B5	3450	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	105	64	-	0/7/25/26	0/2/2/2
20	OMC	B5	4202	20	-	0/9/27/28	0/2/2/2
20	PSU	B5	3652	92,20	-	0/7/25/26	0/2/2/2
20	OMU	B5	4244	20	-	0/9/27/28	0/2/2/2
64	PSU	A2	1047	64	-	0/7/25/26	0/2/2/2
20	A2M	B5	1810	92,20	-	0/9/27/28	0/3/3/3
20	PSU	B5	4267	92,20	-	0/7/25/26	0/2/2/2
64	PSU	A2	967	64	-	0/7/25/26	0/2/2/2
64	PSU	A2	93	64	-	0/7/25/26	0/2/2/2
20	A2M	B5	3557	20	-	0/9/27/28	0/3/3/3
64	OMG	A2	437	64	-	0/9/27/28	0/3/3/3
64	PSU	A2	210	64	-	0/7/25/26	0/2/2/2
64	A2M	A2	99	92,64	-	1/9/27/28	0/3/3/3
20	PSU	B5	3447	20	-	0/7/25/26	0/2/2/2
64	G7M	A2	1640	64	-	2/7/25/26	0/3/3/3
20	A2M	B5	2658	92,20	-	0/9/27/28	0/3/3/3
20	PSU	B5	3496	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3583	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1683	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	2704	20	-	0/9/27/28	0/2/2/2
64	PSU	A2	1644	92,64	-	0/7/25/26	0/2/2/2
64	6MZ	A2	1833	92,64	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PSU	B5	1731	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1801	20	-	0/7/25/26	0/2/2/2
20	OMC	B5	3619	20	-	2/9/27/28	0/2/2/2
20	PSU	B5	4039	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	4711	20	-	0/7/25/26	0/2/2/2
64	A2M	A2	27	92,64	-	3/9/27/28	0/3/3/3
64	PSU	A2	652	64	-	0/7/25/26	0/2/2/2
20	A2M	B5	398	20	-	2/9/27/28	0/3/3/3
20	PSU	B5	2351	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	3371	20	-	0/7/25/26	0/2/2/2
64	PSU	A2	815	64	-	0/7/25/26	0/2/2/2
6	PSU	B8	69	6	-	0/7/25/26	0/2/2/2
64	MA6	A2	1851	64	-	3/11/29/30	0/3/3/3
20	PSU	B5	1638	20	-	0/7/25/26	0/2/2/2
20	PSU	B5	1799	20	-	0/7/25/26	0/2/2/2
64	OMG	A2	602	64	-	0/9/27/28	0/3/3/3
64	A2M	A2	1679	64	-	1/9/27/28	0/3/3/3
64	OMG	A2	510	92,64	-	1/9/27/28	0/3/3/3
20	A2M	B5	2630	92,20	-	3/9/27/28	0/3/3/3
64	PSU	A2	1693	64	-	0/7/25/26	0/2/2/2
2	MLZ	Bb	5	2	-	2/7/8/10	-
64	B8N	A2	1249	64	-	4/16/34/35	0/2/2/2
20	OMG	B5	1260	20	-	0/9/27/28	0/3/3/3
9	V5N	BA	216	9	-	3/9/10/12	0/1/1/1
20	PSU	B5	3369	20	-	0/7/25/26	0/2/2/2
20	OMG	B5	3359	20	-	0/9/27/28	0/3/3/3
64	PSU	A2	1245	64	-	0/7/25/26	0/2/2/2
64	OMG	A2	1491	92,64	-	0/9/27/28	0/3/3/3
64	OMU	A2	1443	92,64	-	0/9/27/28	0/2/2/2
64	OMC	A2	1704	64	-	1/9/27/28	0/2/2/2
64	OMU	A2	1805	64	-	0/9/27/28	0/2/2/2
20	OMC	B5	3433	20	-	4/9/27/28	0/2/2/2
20	PSU	B5	1718	20	-	0/7/25/26	0/2/2/2
14	AME	Au	1	14	-	2/9/10/12	-
20	PSU	B5	4246	20	-	2/7/25/26	0/2/2/2
20	OMG	B5	3631	20	-	1/9/27/28	0/3/3/3
84	SAC	Br	2	84	-	1/7/8/10	-
64	PSU	A2	34	64	-	0/7/25/26	0/2/2/2
20	PSU	B5	4188	20	-	0/7/25/26	0/2/2/2

The worst 5 of 506 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	A2	1640	G7M	C4-N9	7.96	1.58	1.38
64	A2	1640	G7M	O6-C6	7.64	1.38	1.23
64	A2	1851	MA6	C5-N7	6.86	1.52	1.39
64	A2	1852	MA6	C5-N7	6.68	1.51	1.39
64	A2	1640	G7M	C5-C4	6.23	1.54	1.38

The worst 5 of 960 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	A2	1851	MA6	C4-N9-C8	14.65	121.60	105.73
64	A2	1852	MA6	C4-N9-C8	14.48	121.42	105.73
64	A2	1640	G7M	C8-N7-C5	11.43	122.07	107.78
64	A2	1852	MA6	N3-C4-N9	7.10	138.77	127.08
64	A2	591	A2M	C5-C4-N3	-7.01	117.60	126.75

There are no chirality outliers.

5 of 118 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	BA	216	V5N	O-C-CA-CB
15	BC	2	AYA	C-CA-N-CT
20	B5	3433	OMC	C2'-C1'-N1-C2
20	B5	3433	OMC	C2'-C1'-N1-C6
20	B5	4166	PSU	C2'-C1'-C5-C4

There are no ring outliers.

99 monomers are involved in 139 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B5	2208	OMC	2	0
64	A2	355	OMU	1	0
64	A2	1338	4AC	2	0
20	B5	2194	OMC	2	0
20	B5	4382	PSU	2	0
20	B5	3973	OMU	1	0
20	B5	4166	PSU	3	0
20	B5	2258	OMU	1	0
64	A2	116	OMU	2	0
20	B5	4138	OMG	1	0
64	A2	36	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	A2	1329	OMG	1	0
64	A2	1289	OMU	2	0
20	B5	4336	A2M	1	0
20	B5	3476	OMG	1	0
20	B5	4298	PSU	2	0
20	B5	3540	OMC	1	0
64	A2	166	A2M	2	0
64	A2	513	A2M	1	0
64	A2	577	A2M	1	0
20	B5	4364	OMG	1	0
20	B5	3456	A2M	2	0
64	A2	463	OMC	2	0
20	B5	400	A2M	2	0
20	B5	3966	6MZ	1	0
20	B5	3585	PSU	1	0
20	B5	3601	OMC	1	0
20	B5	2244	A2M	1	0
64	A2	1392	OMC	1	0
6	B8	75	OMG	2	0
64	A2	518	OMC	1	0
20	B5	3676	OMG	2	0
20	B5	3524	OMG	1	0
20	B5	3562	A2M	2	0
20	B5	2267	OMG	1	0
20	B5	3942	OMG	2	0
64	A2	469	A2M	2	0
64	A2	1446	PSU	1	0
20	B5	2207	OMG	3	0
64	A2	823	PSU	1	0
20	B5	3550	UY1	1	0
20	B5	2647	OMC	1	0
20	B5	4366	OMU	3	0
64	A2	645	OMG	1	0
20	B5	4058	PSU	1	0
20	B5	1284	OMC	1	0
64	A2	1032	A2M	1	0
20	B5	3517	A2M	2	0
20	B5	3492	A2M	1	0
64	A2	485	A2M	1	0
20	B5	4325	PSU	1	0
20	B5	2206	A2M	2	0
20	B5	4282	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B5	4099	PSU	1	0
64	A2	121	OMU	2	0
64	A2	1843	4AC	1	0
20	B5	4042	PSU	1	0
64	A2	172	OMU	2	0
64	A2	1448	OMG	2	0
20	B5	1479	A2M	1	0
20	B5	4052	OMU	1	0
64	A2	159	A2M	1	0
64	A2	868	OMG	2	0
20	B5	1489	A2M	2	0
20	B5	4383	OMG	1	0
20	B5	4203	PSU	1	0
20	B5	4269	A2M	3	0
64	A2	867	PSU	2	0
20	B5	2667	OMC	1	0
20	B5	3450	A2M	2	0
64	A2	105	PSU	1	0
20	B5	4202	OMC	1	0
20	B5	3652	PSU	2	0
20	B5	1810	A2M	2	0
20	B5	3557	A2M	2	0
64	A2	437	OMG	2	0
64	A2	99	A2M	2	0
64	A2	1640	G7M	1	0
20	B5	2658	A2M	1	0
20	B5	2704	OMC	1	0
64	A2	1833	6MZ	1	0
20	B5	3619	OMC	1	0
20	B5	4039	PSU	1	0
64	A2	27	A2M	3	0
20	B5	398	A2M	1	0
20	B5	2351	PSU	1	0
64	A2	1851	MA6	1	0
64	A2	1679	A2M	2	0
64	A2	510	OMG	2	0
20	B5	2630	A2M	1	0
20	B5	1260	OMG	1	0
9	BA	216	V5N	1	0
64	A2	1491	OMG	1	0
64	A2	1704	OMC	1	0
64	A2	1805	OMU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B5	1718	PSU	1	0
14	Au	1	AME	1	0
20	B5	3631	OMG	1	0
20	B5	4188	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 740 ligands modelled in this entry, 277 are unknown and 428 are monoatomic - leaving 35 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	$\# Z > 2$
94	SPD	B5	4989	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	B5	5084	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	B5	5159	-	9,9,9	0.15	0	8,8,8	0.16	0
94	SPD	B5	5297	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	2056	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	2063	-	9,9,9	0.16	0	8,8,8	0.17	0
95	SPM	B5	5203	-	13,13,13	0.15	0	12,12,12	0.14	0
93	GTP	B7	212	3	30,34,34	0.50	0	46,54,54	0.54	0
94	SPD	B5	5101	-	9,9,9	0.15	0	8,8,8	0.17	0
95	SPM	A2	1939	-	13,13,13	0.14	0	12,12,12	0.17	0
94	SPD	B5	5318	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	5359	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	B5	5237	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5216	-	9,9,9	0.15	0	8,8,8	0.15	0
94	SPD	B5	5122	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5010	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	4968	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	A2	1935	-	9,9,9	0.15	0	8,8,8	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
94	SPD	B5	4926	-	9,9,9	0.15	0	8,8,8	0.18	0
97	IHP	DB	901	-	36,36,36	1.55	6 (16%)	54,60,60	1.13	4 (7%)
94	SPD	B5	5140	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5066	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5338	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5377	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	1928	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5046	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1921	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	A2	1915	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	4905	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5276	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5027	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5257	-	9,9,9	0.16	0	8,8,8	0.17	0
95	SPM	B5	4947	-	13,13,13	0.15	0	12,12,12	0.19	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
94	SPD	B5	4989	-	-	0/7/7/7	-
94	SPD	B5	5084	-	-	0/7/7/7	-
94	SPD	B5	5159	-	-	1/7/7/7	-
94	SPD	B5	5297	-	-	1/7/7/7	-
94	SPD	A2	2056	-	-	1/7/7/7	-
94	SPD	A2	2063	-	-	0/7/7/7	-
95	SPM	B5	5203	-	-	0/11/11/11	-
93	GTP	B7	212	3	-	0/22/38/38	0/3/3/3
94	SPD	B5	5101	-	-	0/7/7/7	-
95	SPM	A2	1939	-	-	1/11/11/11	-
94	SPD	B5	5318	-	-	1/7/7/7	-
94	SPD	B5	5359	-	-	0/7/7/7	-
94	SPD	B5	5237	-	-	1/7/7/7	-
94	SPD	B5	5216	-	-	1/7/7/7	-
94	SPD	B5	5122	-	-	1/7/7/7	-
94	SPD	B5	5010	-	-	0/7/7/7	-
94	SPD	B5	4968	-	-	0/7/7/7	-
94	SPD	A2	1935	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	SPD	B5	4926	-	-	0/7/7/7	-
97	IHP	DB	901	-	-	8/30/54/54	0/1/1/1
94	SPD	B5	5140	-	-	0/7/7/7	-
94	SPD	B5	5066	-	-	0/7/7/7	-
94	SPD	B5	5338	-	-	0/7/7/7	-
94	SPD	B5	5377	-	-	0/7/7/7	-
94	SPD	A2	1928	-	-	1/7/7/7	-
94	SPD	B5	5046	-	-	0/7/7/7	-
94	SPD	A2	1921	-	-	0/7/7/7	-
94	SPD	A2	1901	-	-	0/7/7/7	-
94	SPD	A2	1915	-	-	0/7/7/7	-
94	SPD	A2	1908	-	-	0/7/7/7	-
94	SPD	B5	4905	-	-	1/7/7/7	-
94	SPD	B5	5276	-	-	0/7/7/7	-
94	SPD	B5	5027	-	-	0/7/7/7	-
94	SPD	B5	5257	-	-	1/7/7/7	-
95	SPM	B5	4947	-	-	1/11/11/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	DB	901	IHP	P2-O12	3.53	1.66	1.59
97	DB	901	IHP	P5-O15	3.45	1.65	1.59
97	DB	901	IHP	P1-O11	3.25	1.65	1.59
97	DB	901	IHP	P6-O16	3.22	1.65	1.59
97	DB	901	IHP	P3-O13	3.20	1.65	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	DB	901	IHP	C6-C5-C4	4.29	119.80	110.41
97	DB	901	IHP	C5-C4-C3	3.60	118.29	110.41
97	DB	901	IHP	C5-C6-C1	3.58	118.24	110.41
97	DB	901	IHP	C4-C3-C2	2.22	115.27	110.41

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
97	DB	901	IHP	C1-C2-O12-P2
97	DB	901	IHP	C4-C5-O15-P5

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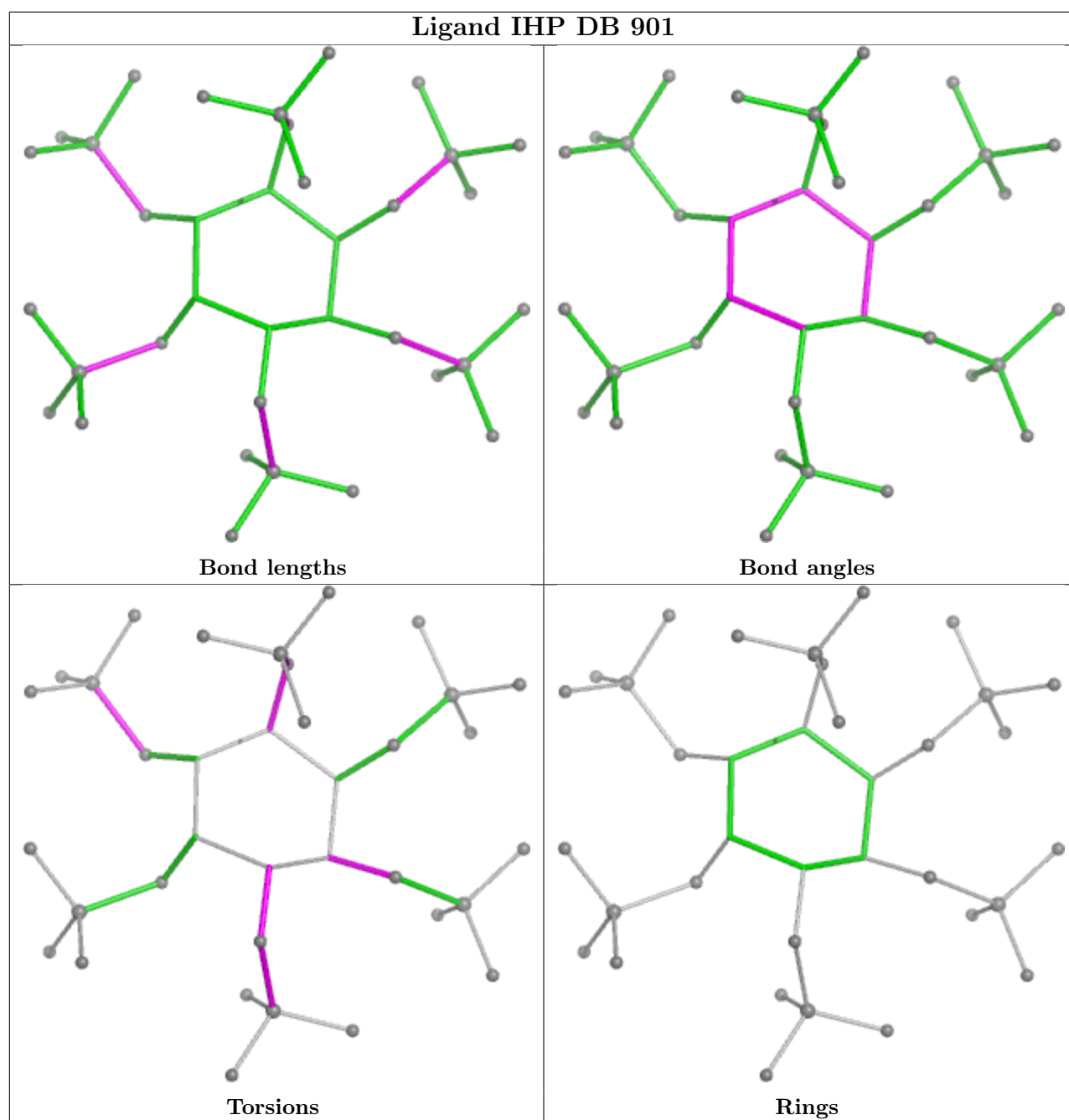
Mol	Chain	Res	Type	Atoms
97	DB	901	IHP	C4-O14-P4-O34
95	A2	1939	SPM	C8-C9-N10-C11
97	DB	901	IHP	C4-O14-P4-O24

There are no ring outliers.

16 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	B5	5159	SPD	3	0
94	B5	5297	SPD	2	0
95	A2	1939	SPM	4	0
94	B5	5318	SPD	1	0
94	B5	5359	SPD	2	0
94	B5	5010	SPD	2	0
94	A2	1935	SPD	1	0
97	DB	901	IHP	2	0
94	B5	5066	SPD	3	0
94	B5	5377	SPD	2	0
94	A2	1921	SPD	1	0
94	A2	1901	SPD	1	0
94	A2	1908	SPD	2	0
94	B5	5276	SPD	1	0
94	B5	5257	SPD	1	0
95	B5	4947	SPM	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

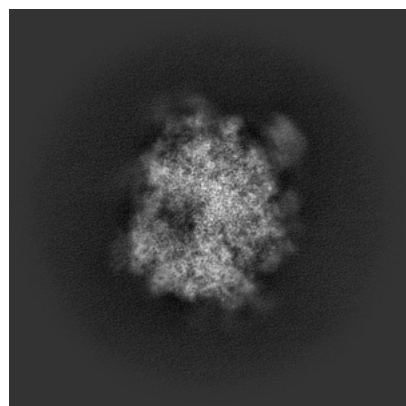
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50125. These allow visual inspection of the internal detail of the map and identification of artifacts.

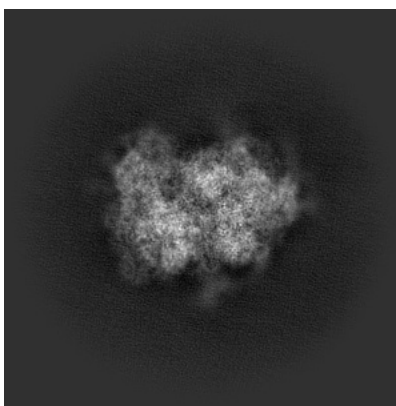
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

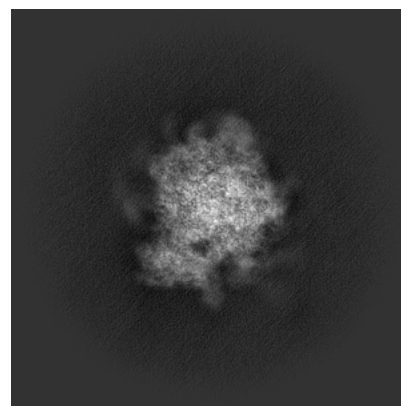
6.1.1 Primary map



X

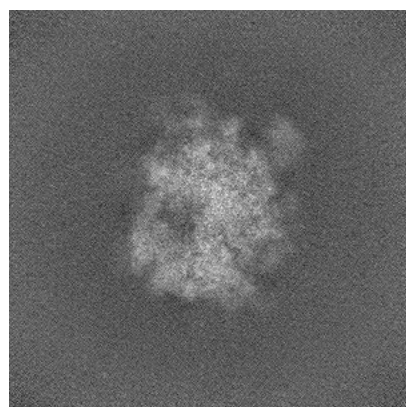


Y

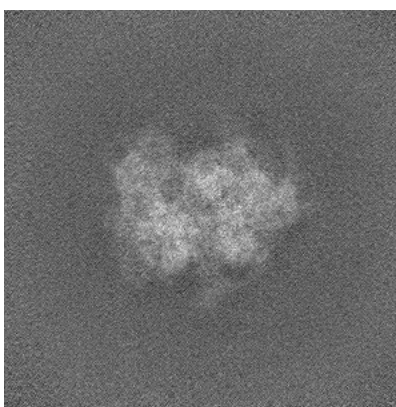


Z

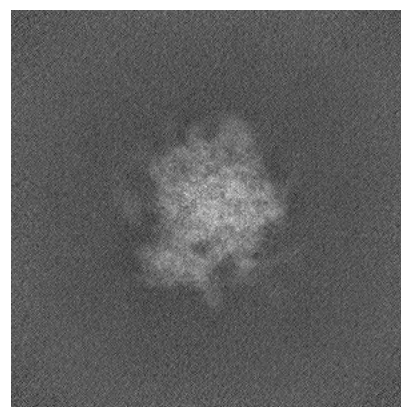
6.1.2 Raw map



X



Y

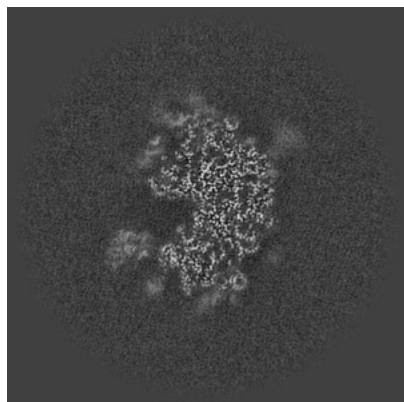


Z

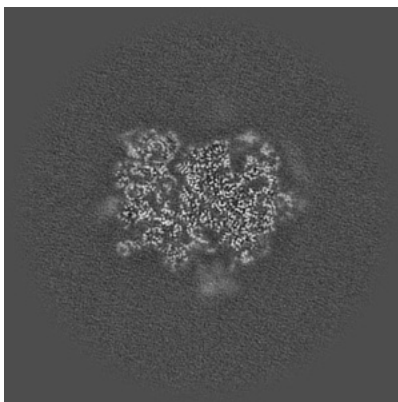
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

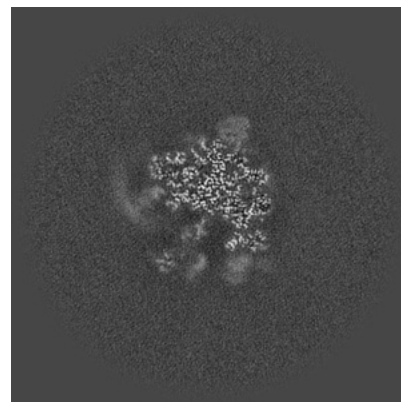
6.2.1 Primary map



X Index: 280

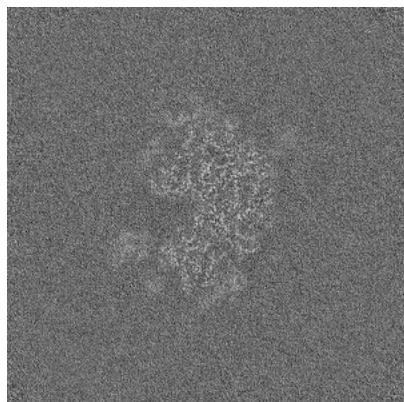


Y Index: 280

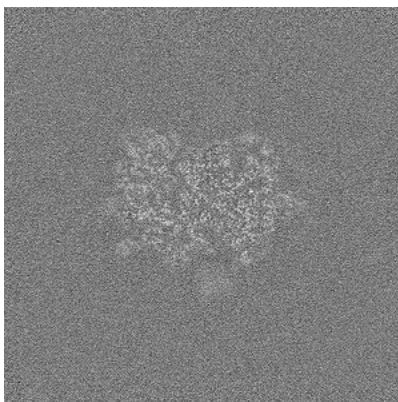


Z Index: 280

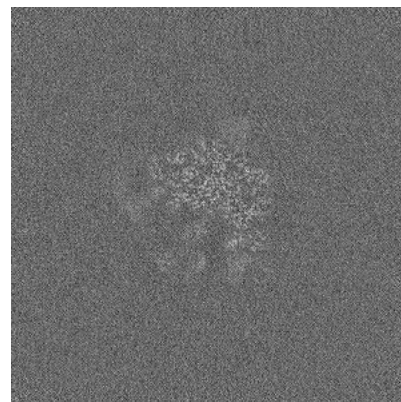
6.2.2 Raw map



X Index: 280



Y Index: 280

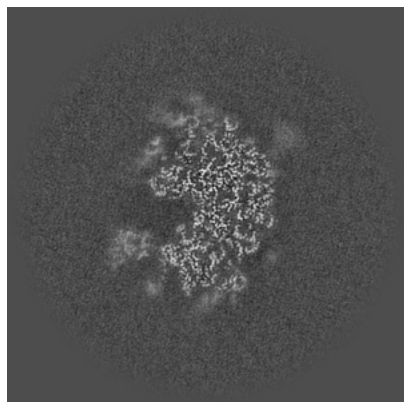


Z Index: 280

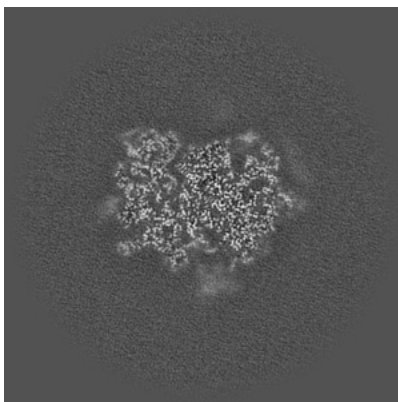
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

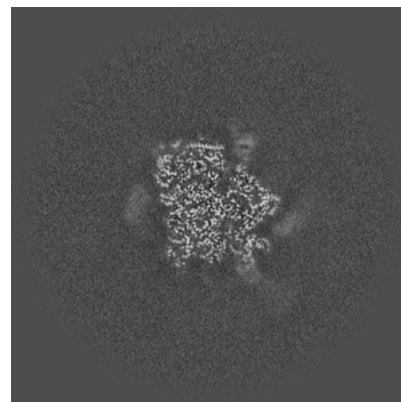
6.3.1 Primary map



X Index: 279

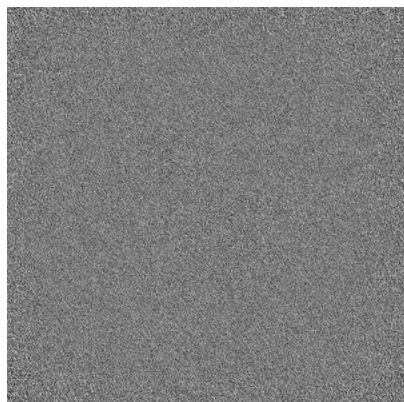


Y Index: 281

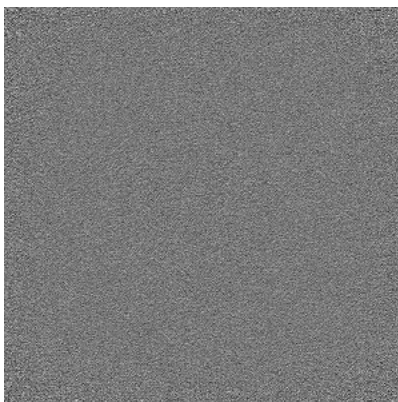


Z Index: 309

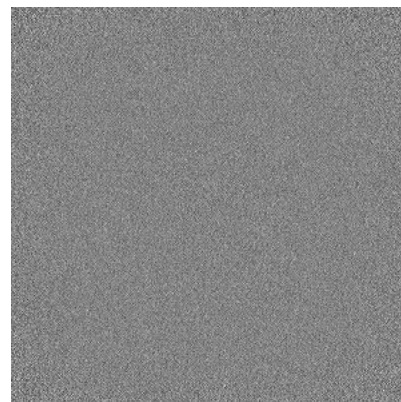
6.3.2 Raw map



X Index: 0



Y Index: 0

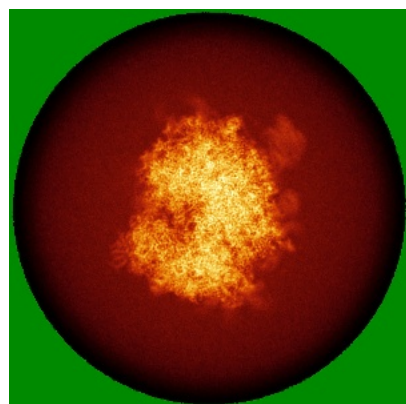


Z Index: 0

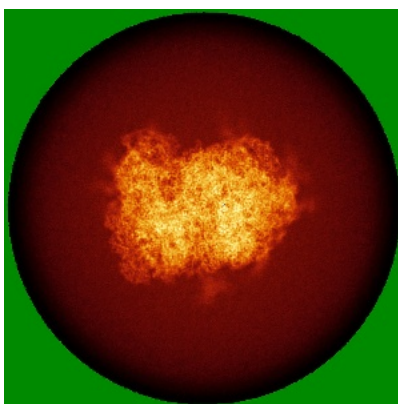
The images above show the largest variance slices of the map in three orthogonal directions.

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

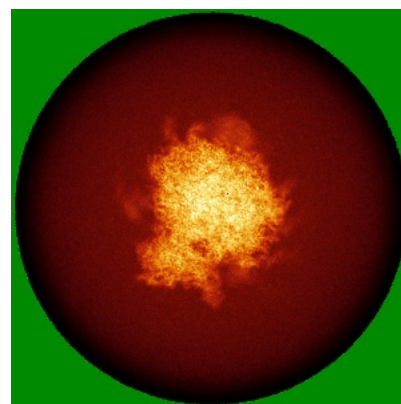
6.4.1 Primary map



X

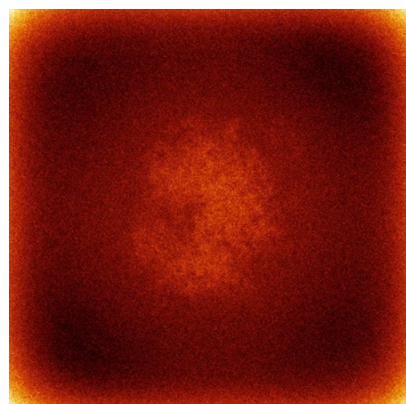


Y

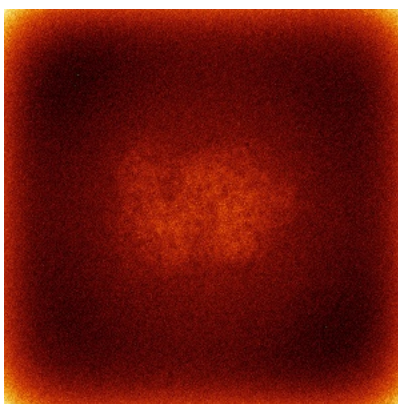


Z

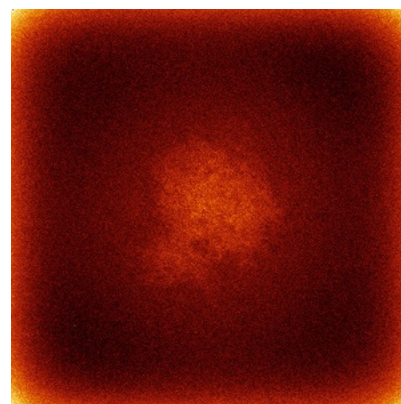
6.4.2 Raw map



X



Y

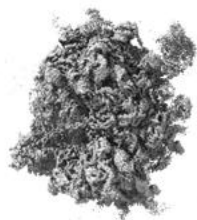


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



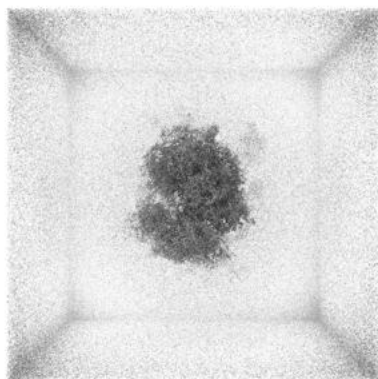
Y



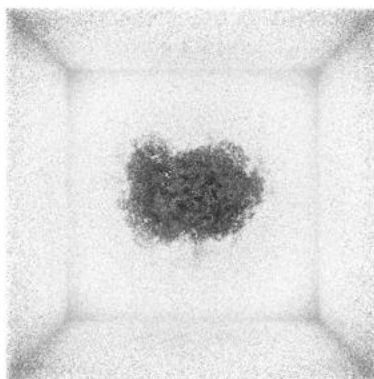
Z

The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

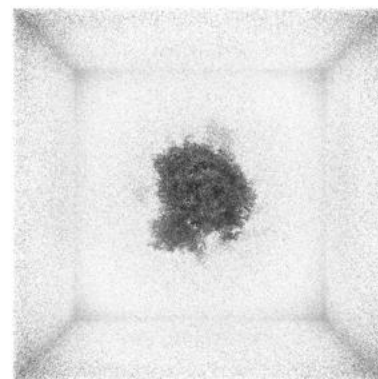
6.5.2 Raw map



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.

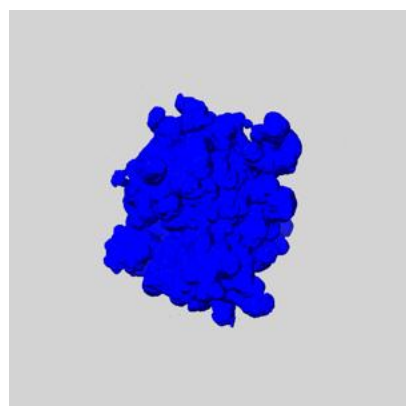
6.6 Mask visualisation [i](#)

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

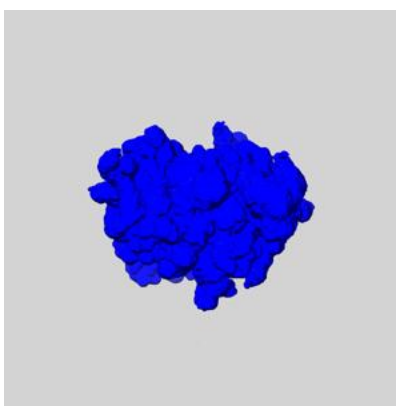
A mask typically either:

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

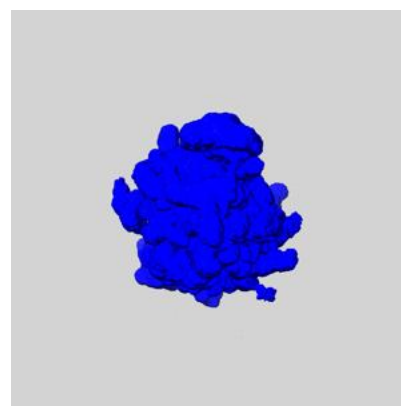
6.6.1 emd_50125_msk_1.map [i](#)



X

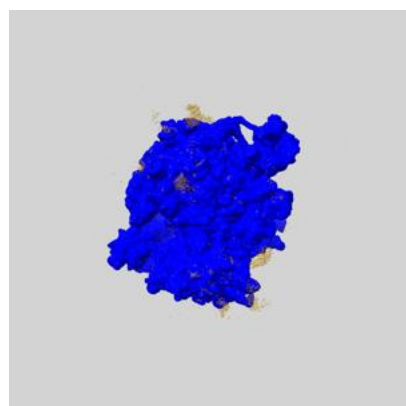


Y

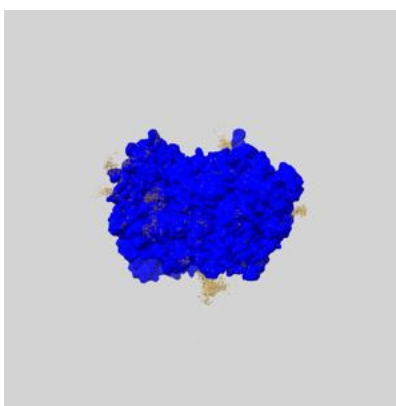


Z

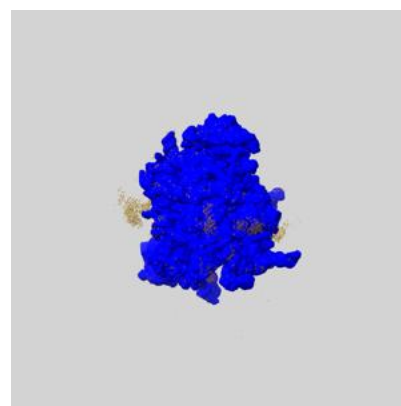
6.6.2 emd_50125_msk_2.map [i](#)



X



Y

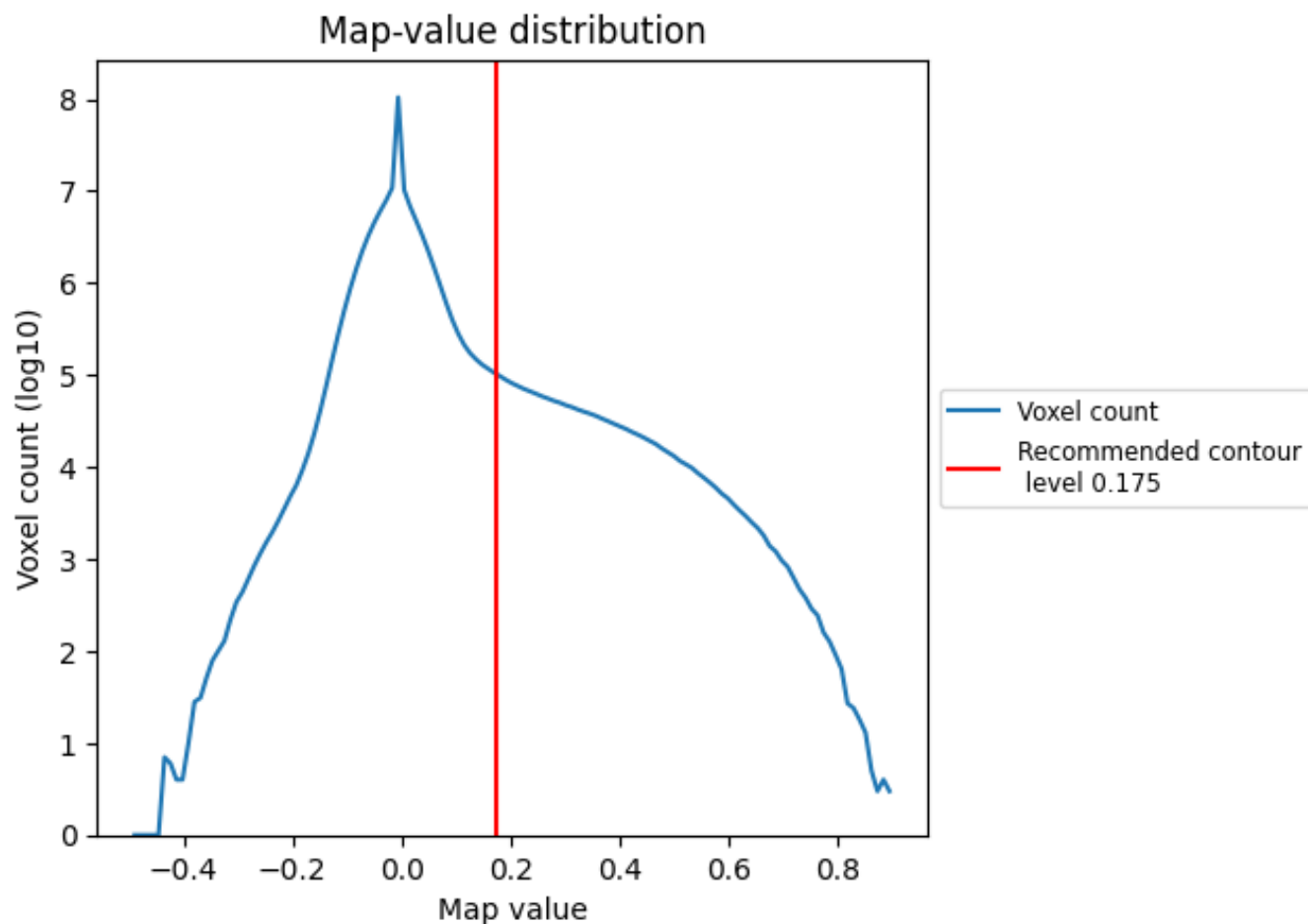


Z

7 Map analysis [i](#)

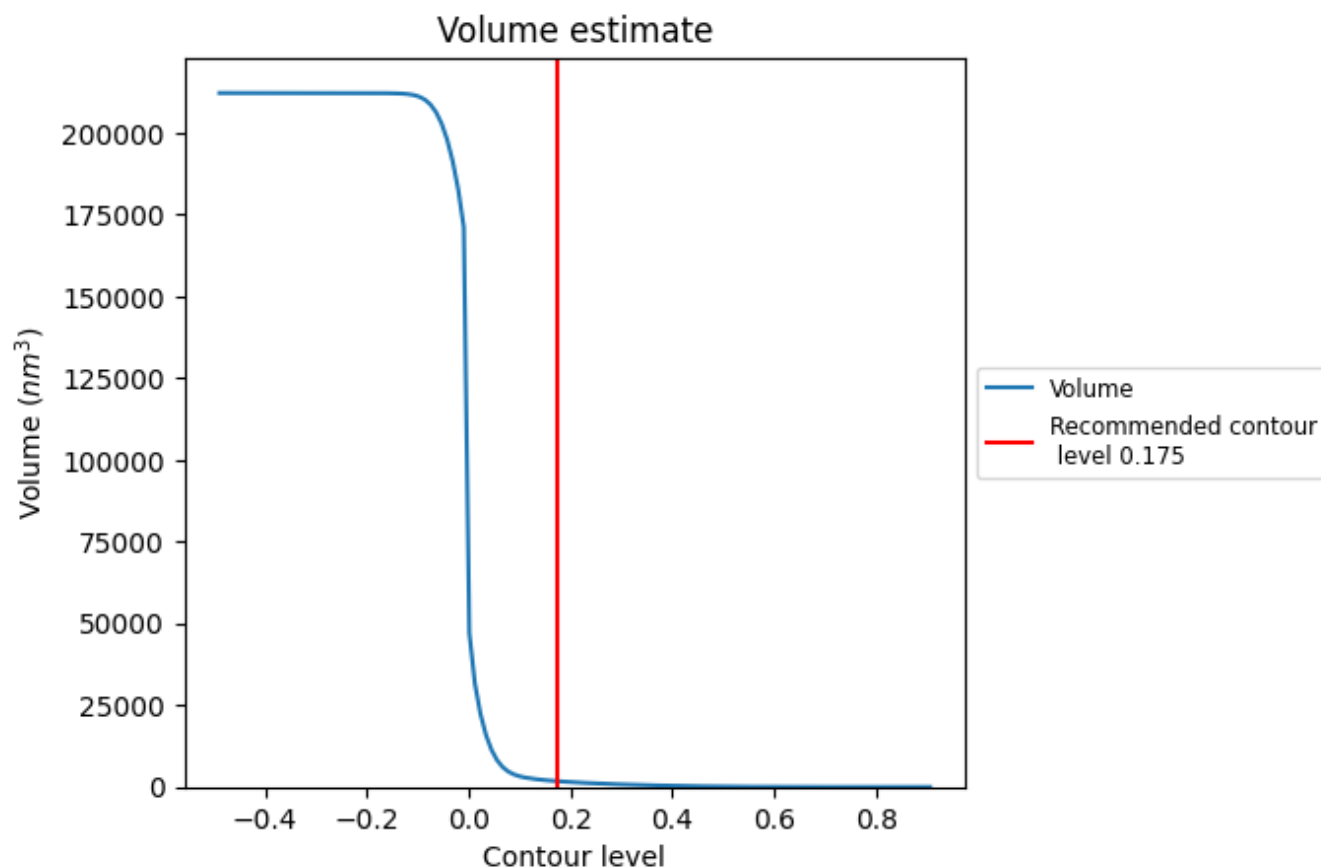
This section contains the results of statistical analysis of the map.

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.

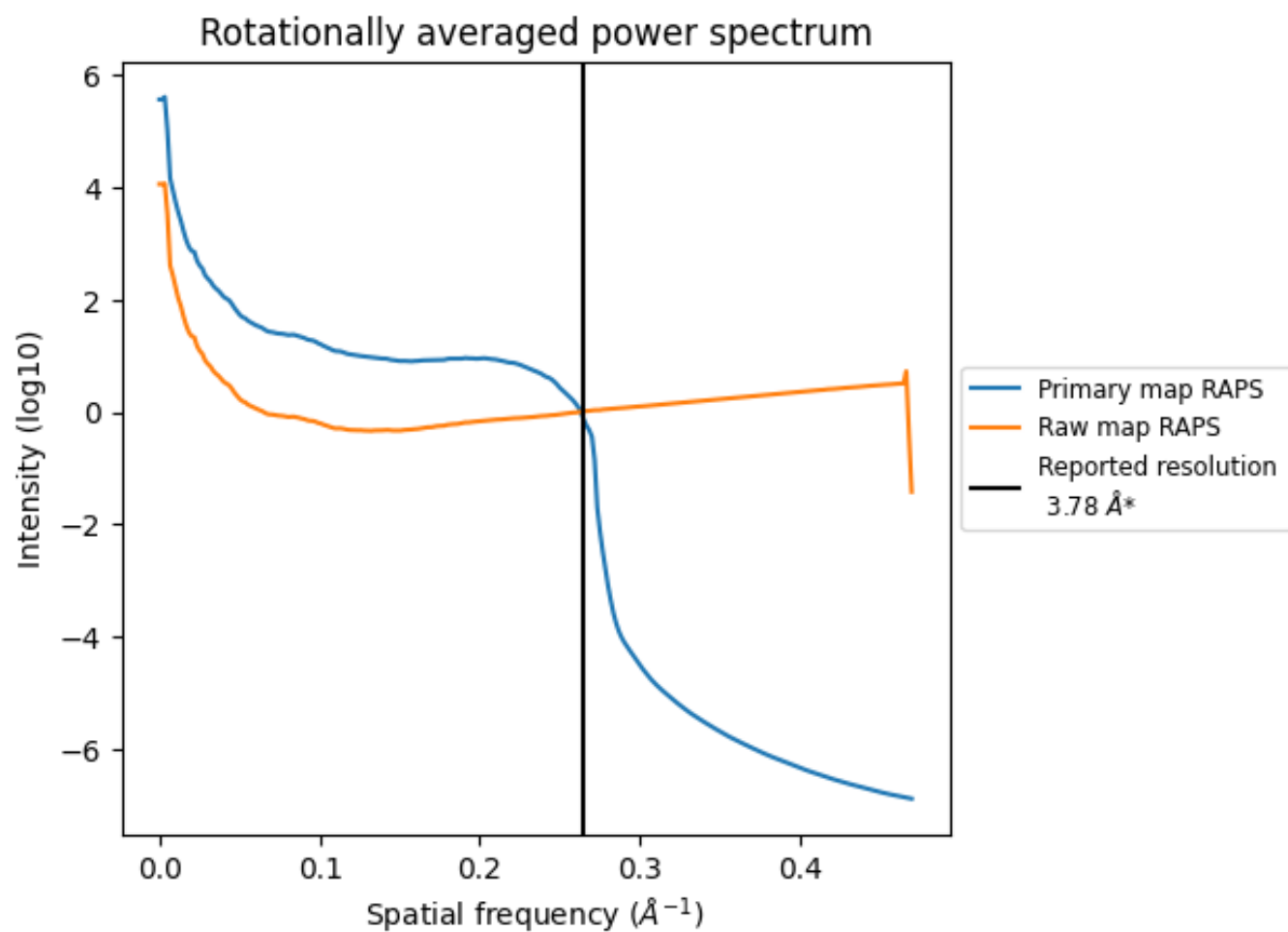
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1752 nm³; this corresponds to an approximate mass of 1582 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 ⓘ

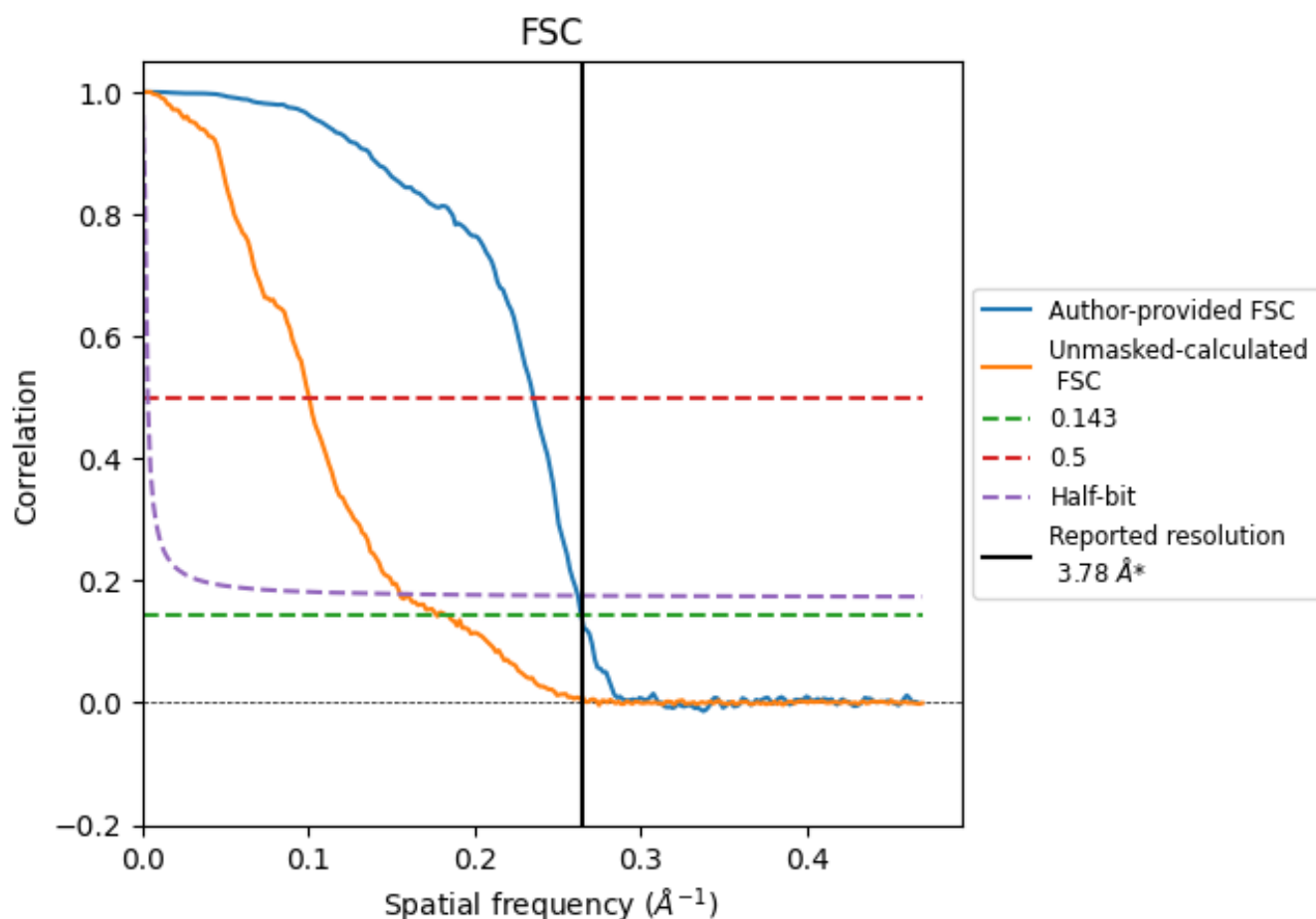


*Reported resolution corresponds to spatial frequency of 0.265 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.265 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

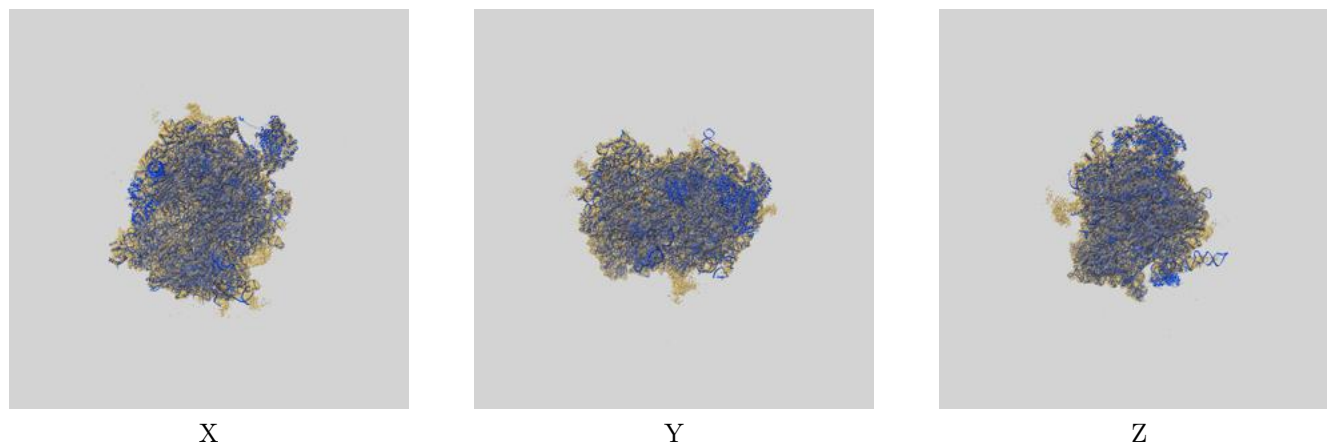
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.78	-	-
Author-provided FSC curve	3.79	4.25	3.81
Unmasked-calculated*	5.64	9.95	6.44

*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 5.64 differs from the reported value 3.78 by more than 10 %

9 Map-model fit [i](#)

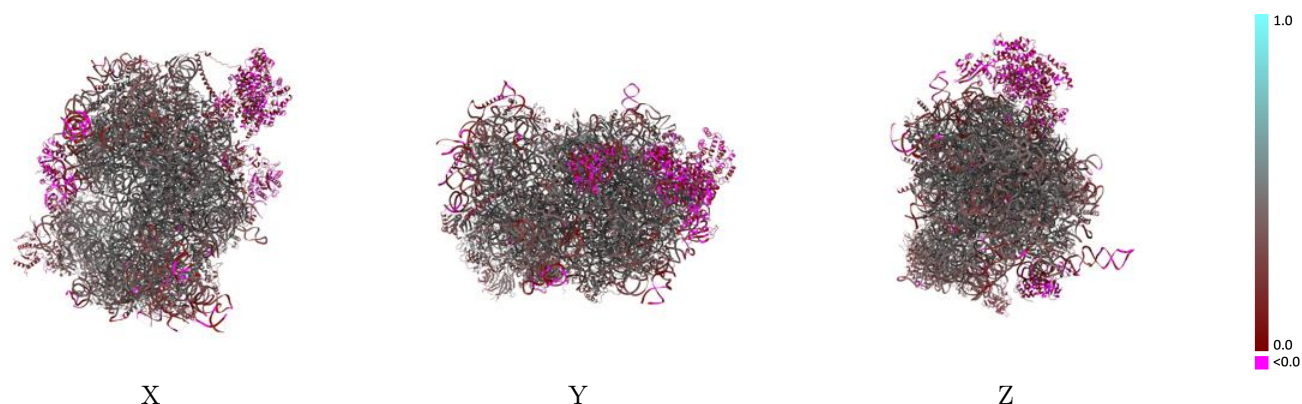
This section contains information regarding the fit between EMDB map EMD-50125 and PDB model 9F1C. Per-residue inclusion information can be found in section [3](#) on page [33](#).

9.1 Map-model overlay [i](#)



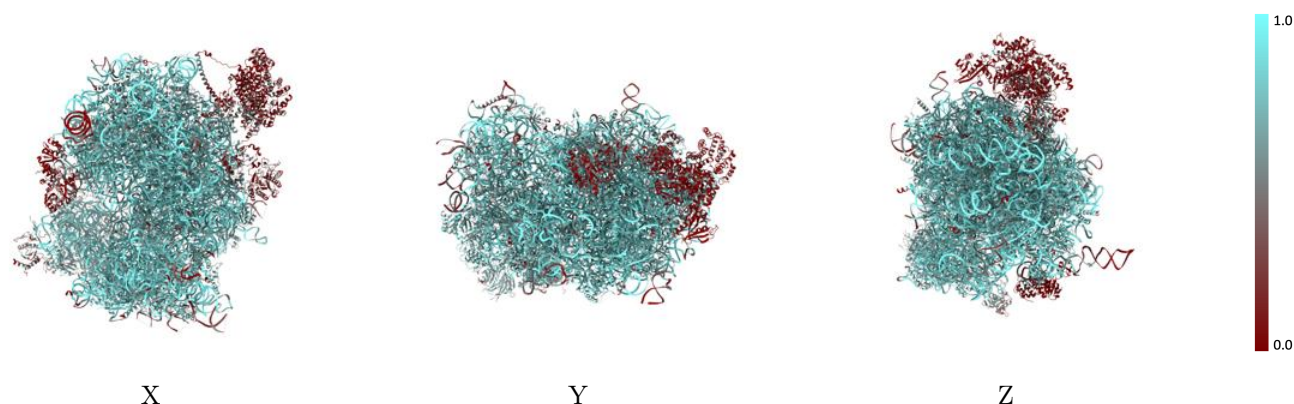
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



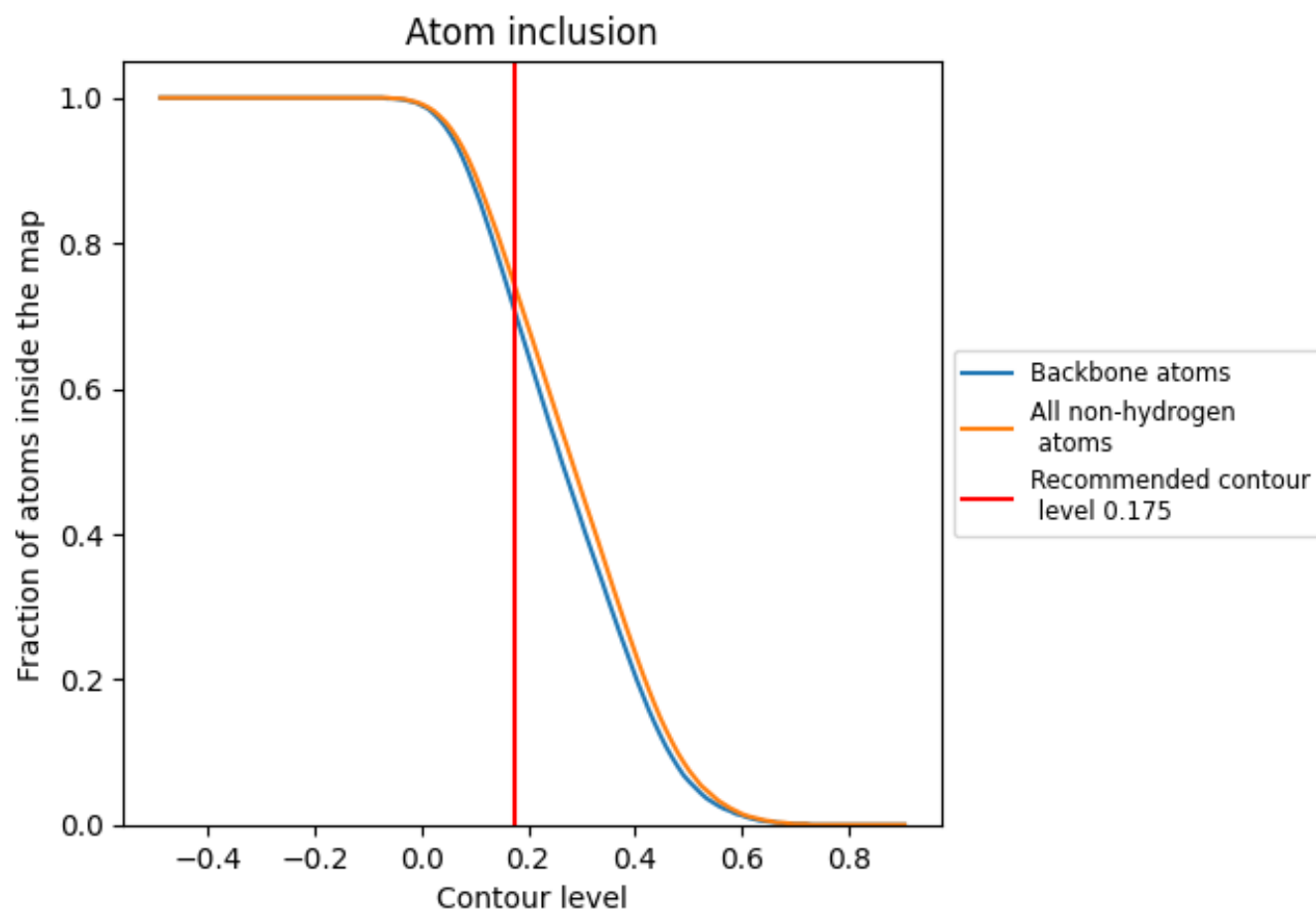
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.175).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.3710
A2	 0.8600	 0.3810
AA	 0.6760	 0.4110
AB	 0.6600	 0.3880
AC	 0.3940	 0.1490
AD	 0.5930	 0.3680
AE	 0.7560	 0.4390
AF	 0.6470	 0.3060
AG	 0.7510	 0.4020
AH	 0.0280	 0.3250
AT	 0.6350	 0.3910
AZ	 0.7240	 0.4020
Aa	 0.6740	 0.3990
Ab	 0.7340	 0.4300
Ac	 0.6500	 0.3710
Ad	 0.7290	 0.4210
Ae	 0.6520	 0.3620
Af	 0.6510	 0.3130
Ag	 0.6710	 0.3600
Ah	 0.7170	 0.4040
Ai	 0.7510	 0.4030
Aj	 0.6900	 0.3310
Ak	 0.6670	 0.4120
Al	 0.3330	 0.1440
Am	 0.7160	 0.4190
An	 0.7180	 0.4140
Ao	 0.6340	 0.3030
Ap	 0.6990	 0.3720
Aq	 0.6880	 0.3610
Ar	 0.6410	 0.3170
As	 0.6820	 0.3330
At	 0.6270	 0.3340
Au	 0.7240	 0.4110
Av	 0.6950	 0.4460
Aw	 0.7440	 0.4470



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Chain	Atom inclusion	Q-score
Ax	 0.7400	 0.3790
Ay	 0.5380	 0.2820
Az	 0.6060	 0.4180
B	 0.7560	 0.3920
B5	 0.8520	 0.3890
B7	 0.9210	 0.4170
B8	 0.8800	 0.4080
BA	 0.7300	 0.4580
BB	 0.7510	 0.4410
BC	 0.7560	 0.4440
BE	 0.6790	 0.3760
BF	 0.7450	 0.4340
BG	 0.7050	 0.3870
BH	 0.7190	 0.4120
BI	 0.7360	 0.4420
BJ	 0.7080	 0.3880
BK	 0.2060	 0.4310
BL	 0.7220	 0.4110
BM	 0.7450	 0.4020
BN	 0.7720	 0.4610
BO	 0.7430	 0.4370
BP	 0.7280	 0.4460
BQ	 0.7530	 0.4590
BR	 0.7160	 0.3890
BS	 0.7550	 0.4500
BT	 0.7140	 0.4400
BU	 0.7220	 0.4260
BV	 0.7000	 0.4500
BW	 0.5760	 0.3170
BX	 0.7130	 0.4280
BY	 0.7160	 0.4270
BZ	 0.7470	 0.3990
Ba	 0.7950	 0.4520
Bb	 0.6600	 0.3700
Bc	 0.6290	 0.3620
Bd	 0.7350	 0.4430
Be	 0.7580	 0.4550
Bf	 0.7740	 0.4620
Bg	 0.7120	 0.4330
Bh	 0.7340	 0.4130
Bi	 0.7240	 0.4000
Bj	 0.8250	 0.4710

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Chain	Atom inclusion	Q-score
Bk	 0.6340	 0.3640
Bl	 0.7260	 0.4500
Bm	 0.7280	 0.4220
Bo	 0.7080	 0.4360
Bp	 0.7130	 0.4270
Br	 0.7430	 0.4560
Bs	 0.0440	 0.0350
Bt	 0.0450	 0.0550
Ct	 0.1950	 0.1080
Cu	 0.3250	 0.2200
DA	 0.0350	 0.0460
DB	 0.1690	 0.0860
DC	 0.1490	 0.0510
EA	 0.1620	 0.0470