



wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 06:17 am BST

PDB ID : 9F1B / pdb_00009f1b
EMDB ID : EMD-50124
Title : Mammalian ternary complex of a translating 80S ribosome, NAC and NatA/E
Authors : Yudin, D.; Scaiola, A.; Ban, N.
Deposited on : 2024-04-18
Resolution : 3.01 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:

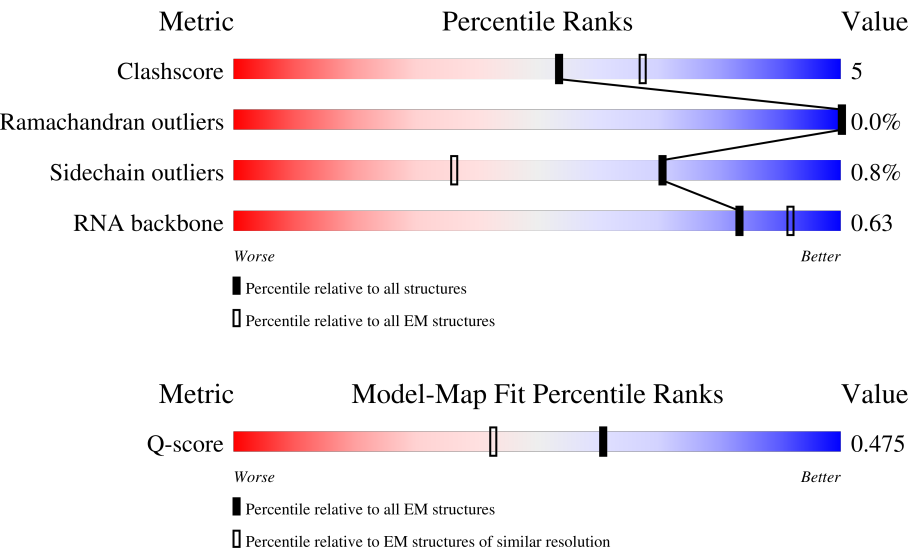
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.01 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	13882 (2.51 - 3.51)

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	BP	184	
2	Aq	135	
3	Bo	106	

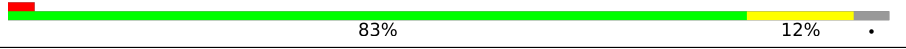
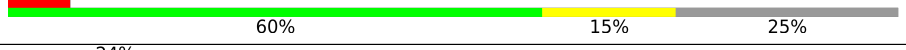
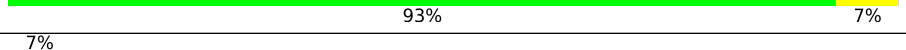
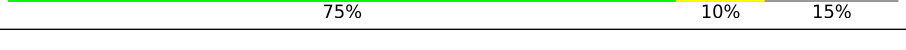
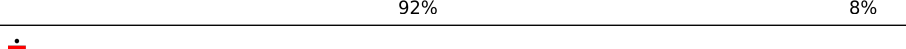
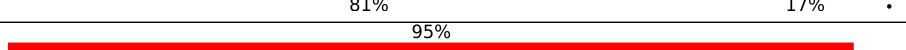
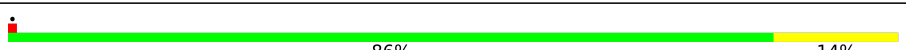
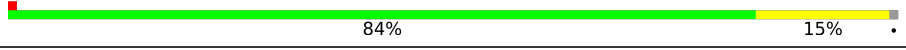
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Mol	Chain	Length	Quality of chain
4	AT	76	
5	Ar	151	
6	Cu	162	
7	BL	211	
8	BX	156	
9	Bp	92	
10	BQ	188	
11	As	145	
12	Br	136	
13	BR	196	
14	At	119	
15	Bs	318	
16	BG	266	
17	BU	128	
18	Av	130	
19	DB	915	
20	Ct	238	
21	BH	192	
22	BV	140	
23	Aw	143	
24	B5	4808	
25	BT	160	
26	BI	214	
27	BW	157	
28	Ax	130	

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Mol	Chain	Length	Quality of chain
29	B7	119	
30	Au	83	
31	BJ	178	
32	AZ	294	
33	Ay	124	
34	B8	158	
35	BK	29	
36	Aa	264	
37	Az	25	
38	BA	257	
39	Bt	165	
40	BM	218	
41	Ab	293	
42	BY	145	
43	BB	403	
44	BS	176	
45	Ac	281	
46	BZ	136	
47	BC	412	
48	BN	204	
49	Ad	263	
50	Ba	148	
51	B	297	
52	BO	203	
53	Ae	204	

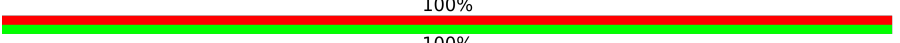
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Mol	Chain	Length	Quality of chain
54	Bb	245	
55	BE	291	
56	DA	403	
57	Af	249	
58	Bc	115	
59	BF	247	
60	DC	235	
61	Ag	432	
62	Bd	125	
63	A2	1870	
64	Ah	208	
65	Be	135	
66	AA	84	
67	Ai	194	
68	Bf	110	
69	AB	69	
70	Aj	165	
71	Bg	115	
72	AC	156	
73	Ak	158	
74	Bh	123	
75	AD	133	
76	Al	132	
77	Bi	105	
78	AE	115	

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Mol	Chain	Length	Quality of chain
79	Am	151	
80	Bj	97	
81	AF	317	
82	An	151	
83	Bk	70	
84	AG	56	
85	Ao	145	
86	Bl	51	
87	AH	3	
88	Ap	172	
89	Bm	128	

2 Entry composition

There are 97 unique types of molecules in this entry. The entry contains 234232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BP	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 2 is a protein called 40S ribosomal protein eS17.

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

- Molecule 3 is a protein called Large ribosomal subunit protein eL42.

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

- 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 protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Cu	105	Total	C	N	O	S	0	0
			813	508	152	150	3		

- Molecule 7 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	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 8 is a protein called Ribosomal_L23eN domain-containing protein.

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

- Molecule 9 is a protein called 60S ribosomal protein L37a.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL18.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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 12 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	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 13 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	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 14 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 15 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 16 is a protein called 60S ribosomal protein L7a.

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

- Molecule 17 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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 18 is a protein called Ribosomal protein S15a.

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

- Molecule 19 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 20 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Ct	115	Total	C	N	O	S	
			895	561	163	167	4	0

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
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 21 is a protein called 60S ribosomal protein L9.

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

- Molecule 22 is a protein called Ribosomal protein L23.

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

- Molecule 23 is a protein called 40S ribosomal protein S23.

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

- Molecule 24 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L10.

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

- Molecule 28 is a protein called 40S ribosomal protein S24.

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

- Molecule 29 is a RNA chain called 5S rRNA.

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

- Molecule 30 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 31 is a protein called 60S ribosomal protein L11.

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 33 is a protein called 40S ribosomal protein S25.

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

- Molecule 34 is a RNA chain called 5.8S rRNA.

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

- Molecule 35 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	BK	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 36 is a protein called 40S ribosomal protein S3a.

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

- Molecule 37 is a protein called 60S ribosomal protein L41.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 39 is a protein called 60S ribosomal protein L12.

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

- Molecule 40 is a protein called 60S ribosomal protein L14.

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

- Molecule 41 is a protein called 40S ribosomal protein S2.

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

- Molecule 42 is a protein called Ribosomal protein L26.

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

- Molecule 43 is a protein called Ribosomal protein L3.

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

- Molecule 44 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 45 is a protein called 40S ribosomal protein S3.

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

- Molecule 46 is a protein called 60S ribosomal protein L27.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 48 is a protein called Ribosomal protein L15.

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

- Molecule 49 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	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 50 is a protein called 60S ribosomal protein L27a.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	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 52 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 53 is a protein called Ribosomal protein S5.

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

- Molecule 54 is a protein called 60S ribosomal protein L29.

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

- Molecule 55 is a protein called 60S ribosomal protein L6.

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

- Molecule 56 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,N-alpha-acetyltransferase 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	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
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 57 is a protein called 40S ribosomal protein S6.

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

- Molecule 58 is a protein called 60S ribosomal protein L30.

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

- Molecule 59 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	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 60 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	DC	165	Total	C	N	O	S	0	0
			1339	844	242	242	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 S7.

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

- Molecule 62 is a protein called 60S ribosomal protein L31.

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

- Molecule 63 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	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 64 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	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 65 is a protein called Ribosomal protein L32.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Be	22	ARG	CYS	variant	UNP G1U6S0
Be	75	ARG	HIS	variant	UNP G1U6S0

- Molecule 66 is a protein called 40S ribosomal protein S27.

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

- Molecule 67 is a protein called 40S ribosomal protein S9.

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

- Molecule 68 is a protein called 60S ribosomal protein L35a.

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

- Molecule 69 is a protein called 40S ribosomal protein S28.

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

- Molecule 70 is a protein called S10_pectin domain-containing protein.

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

- Molecule 71 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 72 is a protein called Ribosomal protein S27a.

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

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

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

- Molecule 74 is a protein called 60S ribosomal protein L35.

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

- Molecule 75 is a protein called 40S ribosomal protein S30.

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

- Molecule 76 is a protein called 40S ribosomal protein S12.

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

- Molecule 77 is a protein called 60S ribosomal protein L36.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 79 is a protein called 40S ribosomal protein S13.

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

- Molecule 80 is a protein called Ribosomal protein L37.

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

- Molecule 81 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 82 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	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 83 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	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 84 is a protein called 40S ribosomal protein S29.

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

- Molecule 85 is a protein called 40S ribosomal protein uS19.

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

- Molecule 86 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 87 is a RNA chain called mRNA.

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

- Molecule 88 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 89 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

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

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	BP	1	Total	Mg	0
			1	1	
90	AT	3	Total	Mg	0
			3	3	
90	BR	1	Total	Mg	0
			1	1	
90	Ct	1	Total	Mg	0
			1	1	
90	BV	1	Total	Mg	0
			1	1	
90	B5	282	Total	Mg	0
			282	282	
90	BI	1	Total	Mg	0
			1	1	
90	B7	9	Total	Mg	0
			9	9	
90	B8	9	Total	Mg	0
			9	9	
90	Ba	1	Total	Mg	0
			1	1	
90	Af	1	Total	Mg	0
			1	1	
90	A2	108	Total	Mg	0
			108	108	
90	Bj	1	Total	Mg	0
			1	1	
90	An	1	Total	Mg	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
91	Bo	1	Total	Zn	0
			1	1	
91	Bp	1	Total	Zn	0
			1	1	

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

- Molecule 92 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

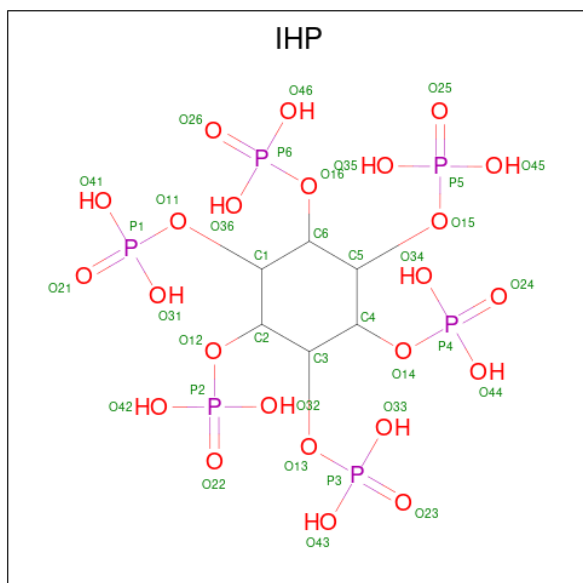
Mol	Chain	Residues	Atoms		AltConf
92	Bo	1	Total 1	X 1	0
92	AT	2	Total 2	X 2	0
92	Ar	1	Total 1	X 1	0
92	BL	1	Total 1	X 1	0
92	BQ	2	Total 2	X 2	0
92	BH	1	Total 1	X 1	0
92	B5	207	Total 207	X 207	0
92	BT	2	Total 2	X 2	0
92	BI	1	Total 1	X 1	0
92	B7	6	Total 6	X 6	0
92	B8	7	Total 7	X 7	0
92	BA	4	Total 4	X 4	0
92	BB	2	Total 2	X 2	0

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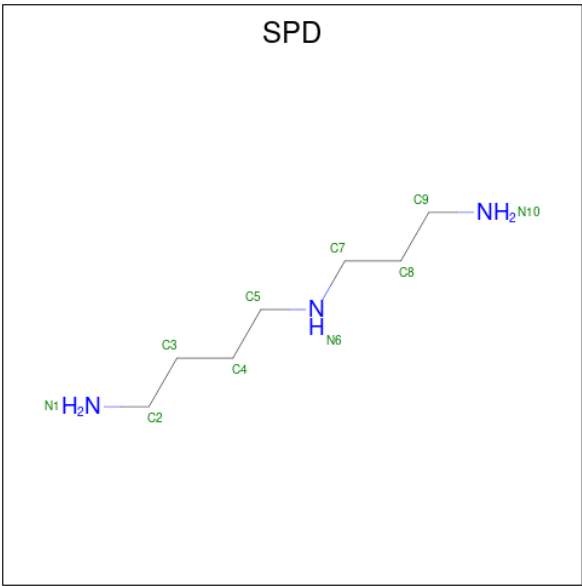
Mol	Chain	Residues	Atoms		AltConf
92	BN	1	Total	X	0
			1	1	
92	Ae	1	Total	X	0
			1	1	
92	Bb	2	Total	X	0
			2	2	
92	A2	57	Total	X	0
			57	57	
92	Be	3	Total	X	0
			3	3	
92	Bf	1	Total	X	0
			1	1	
92	Ak	1	Total	X	0
			1	1	
92	Bj	1	Total	X	0
			1	1	
92	An	1	Total	X	0
			1	1	
92	Bl	1	Total	X	0
			1	1	

- Molecule 93 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- 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	

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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	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 14	C 10	N 4	0
95	B5	1	Total 14	C 10	N 4	0
95	A2	1	Total 14	C 10	N 4	0

- Molecule 96 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

- Molecule 97 is water.

Mol	Chain	Residues	Atoms		AltConf
97	BP	3	Total 3	O 3	0
97	Bo	1	Total 1	O 1	0
97	AT	13	Total 13	O 13	0
97	Ar	1	Total 1	O 1	0
97	BL	2	Total 2	O 2	0
97	BX	1	Total 1	O 1	0
97	As	3	Total 3	O 3	0
97	BR	5	Total 5	O 5	0
97	At	1	Total 1	O 1	0
97	Ct	1	Total 1	O 1	0
97	BH	2	Total 2	O 2	0
97	BV	2	Total 2	O 2	0
97	Aw	5	Total 5	O 5	0
97	B5	1383	Total 1383	O 1383	0
97	BI	3	Total 3	O 3	0
97	B7	43	Total 43	O 43	0
97	BJ	1	Total 1	O 1	0
97	B8	50	Total 50	O 50	0
97	Aa	2	Total 2	O 2	0
97	BA	8	Total 8	O 8	0
97	BM	1	Total 1	O 1	0

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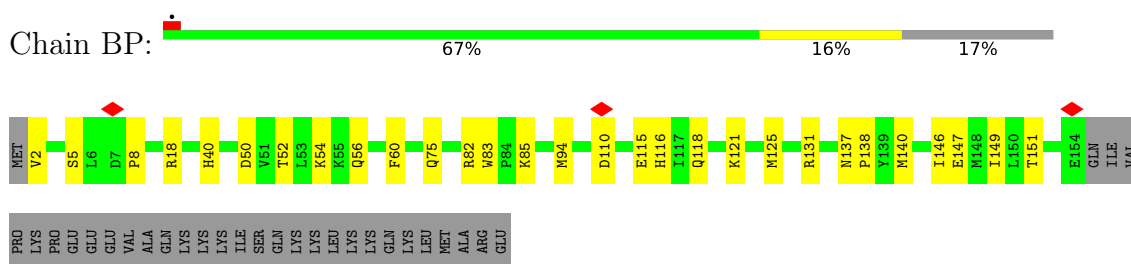
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Mol	Chain	Residues	Atoms		AltConf
97	BB	9	Total 9	O 9	0
97	BC	7	Total 7	O 7	0
97	BN	4	Total 4	O 4	0
97	Ba	8	Total 8	O 8	0
97	B	1	Total 1	O 1	0
97	BO	1	Total 1	O 1	0
97	Af	1	Total 1	O 1	0
97	BF	1	Total 1	O 1	0
97	Bd	1	Total 1	O 1	0
97	A2	526	Total 526	O 526	0
97	Be	5	Total 5	O 5	0
97	Bf	1	Total 1	O 1	0
97	Bg	2	Total 2	O 2	0
97	Ak	2	Total 2	O 2	0
97	AE	1	Total 1	O 1	0
97	Am	1	Total 1	O 1	0
97	Bj	3	Total 3	O 3	0
97	An	3	Total 3	O 3	0
97	Bl	1	Total 1	O 1	0
97	AH	5	Total 5	O 5	0
97	Ap	2	Total 2	O 2	0

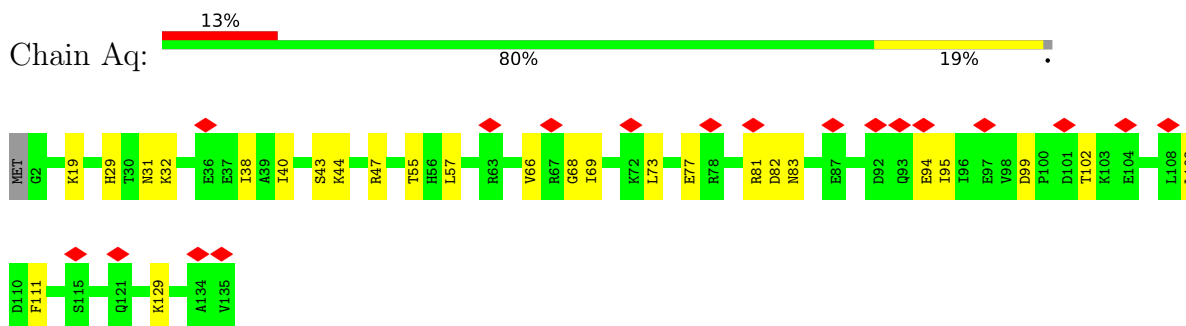
3 Residue-property plots [i](#)

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

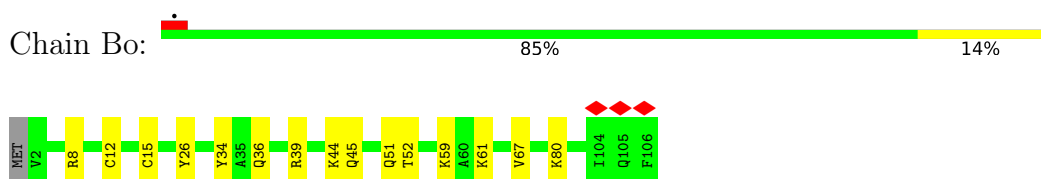
- Molecule 1: Large ribosomal subunit protein uL22



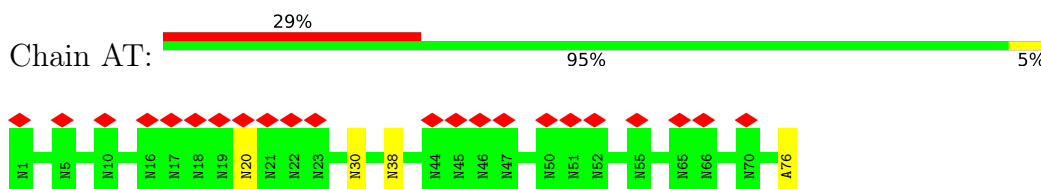
- Molecule 2: 40S ribosomal protein eS17



- Molecule 3: Large ribosomal subunit protein eL42

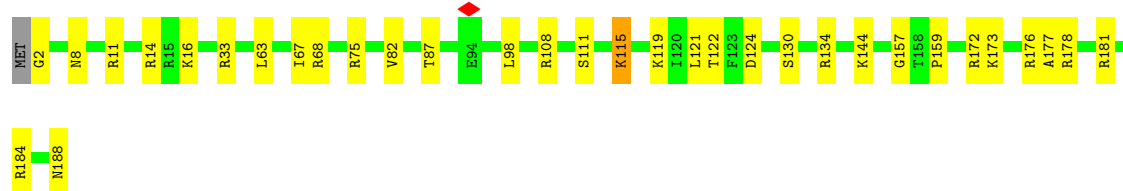


- Molecule 4: P-site tRNA



- Molecule 5: Small ribosomal subunit protein uS13

Chain BQ:  82% 17% ..



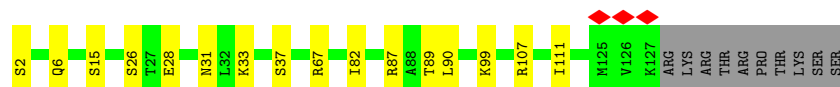
- Molecule 11: 40S ribosomal protein S19

Chain As:  12% 88% 10% .



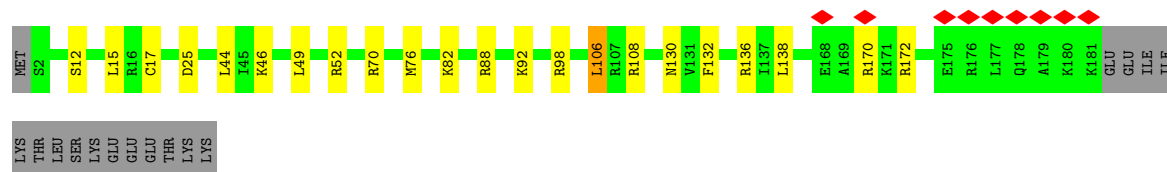
- Molecule 12: Large ribosomal subunit protein eL28

Chain Br:  81% 12% 7%



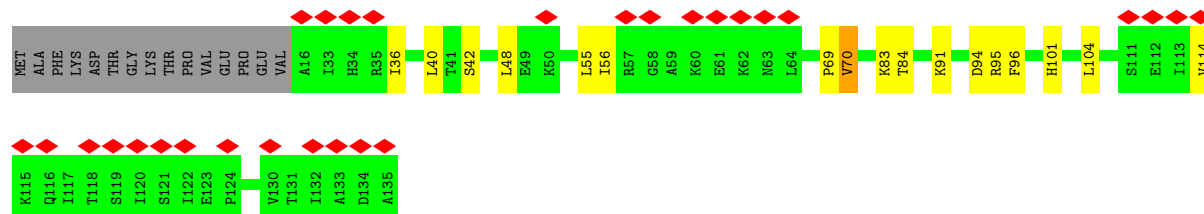
- Molecule 13: Ribosomal protein L19

Chain BR:  5% 81% 11% 8%



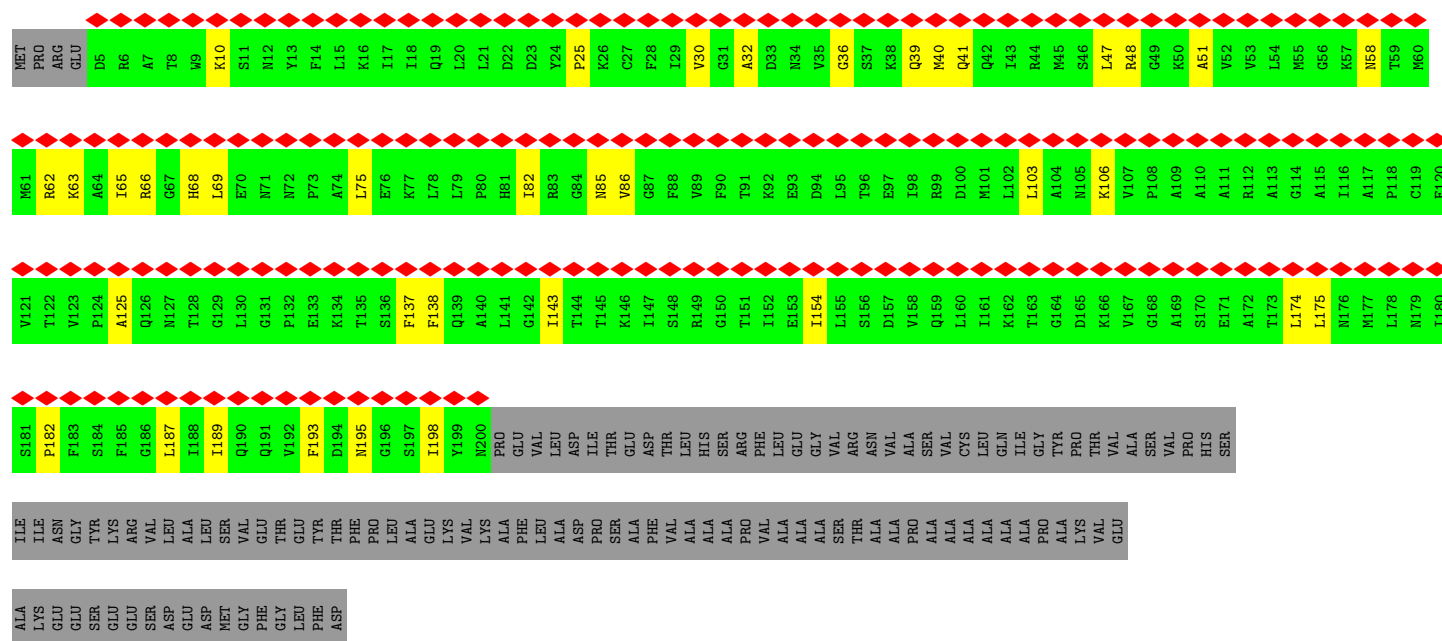
- Molecule 14: Small ribosomal subunit protein uS10

Chain At:  24% 73% 13% 13%

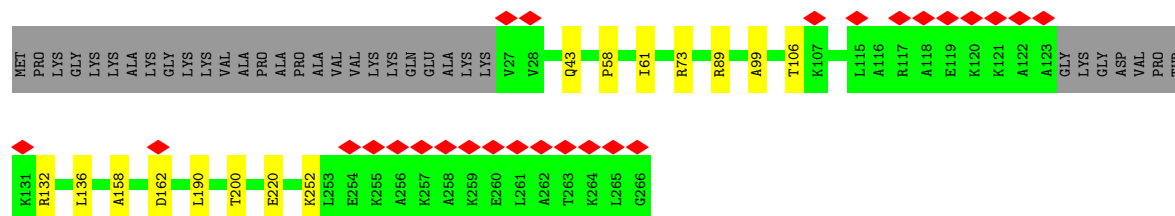
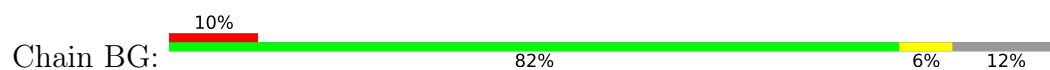


- Molecule 15: 60S acidic ribosomal protein P0

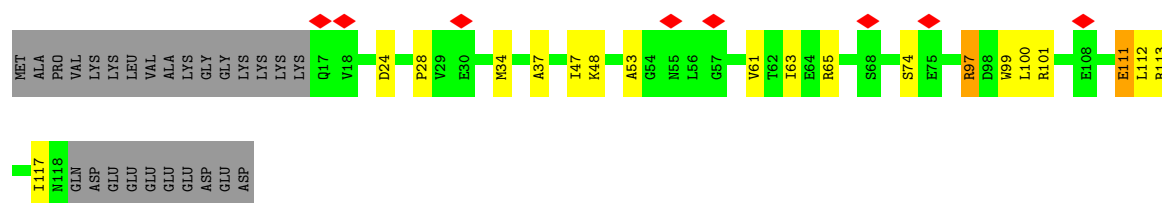
Chain Bs:  62% 50% 12% 38%



• Molecule 16: 60S ribosomal protein L7a



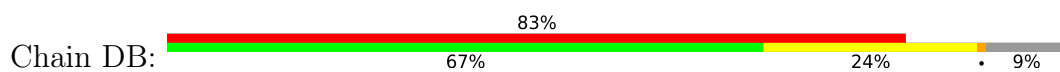
• Molecule 17: 60S ribosomal protein L22



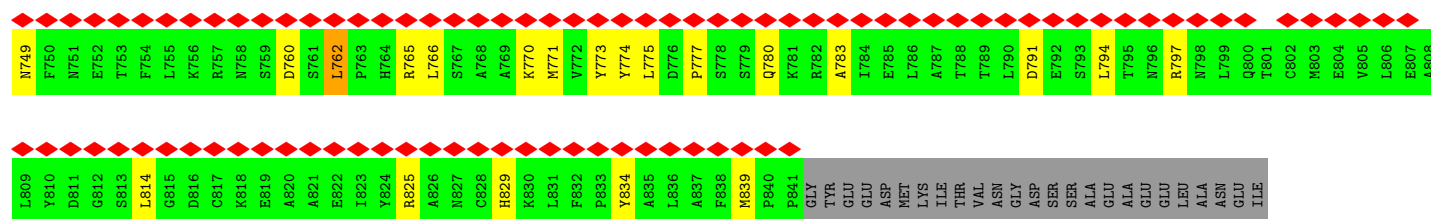
• Molecule 18: Ribosomal protein S15a



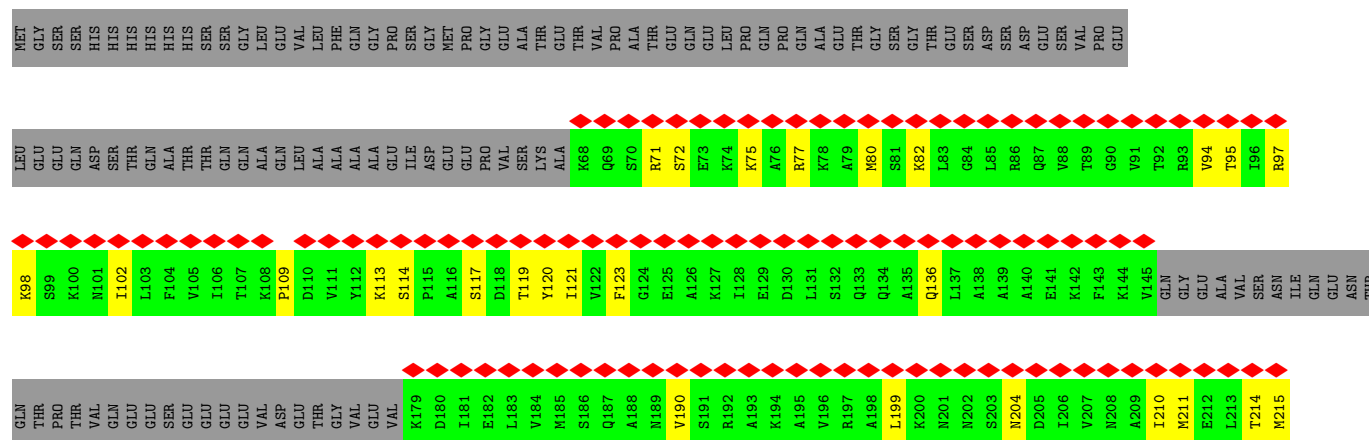
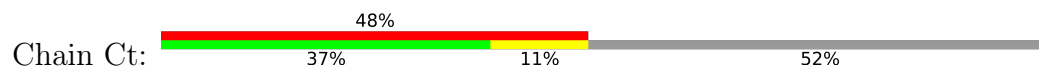
• Molecule 19: N-alpha-acetyltransferase 15, NatA auxiliary subunit



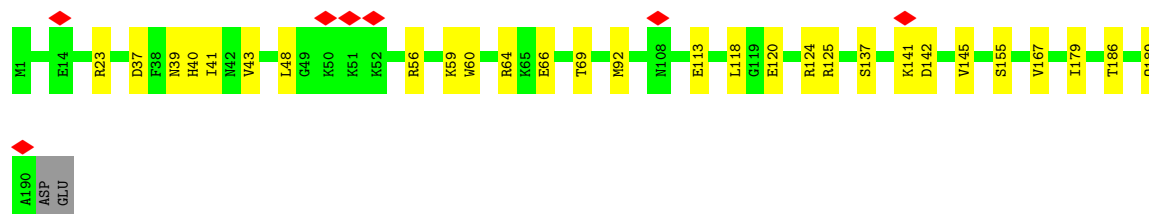
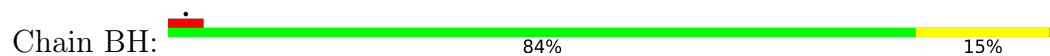
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A12	L13	SER	F14	K15	R16	R19	C20	Y21	K24	Q25	Y26	R27	N28	K31	F32	C33	K34	L37	S38	N39	P40	K41	F42	A43	E44	H45	G46	E47	T48	L49	A50	M51	K52	G53	L54	T55	L56	N57	C58	L59	G60	K61	K62	E63	E64	A65	Y66	E67	L68	V69	R70	R71	G72	L73	R74	N75				
D76	L77	K78	S79	H80	V81	W82	H84	Y85	G86	G87	L88	L89	Q90	R91	S92	D93	K94	K95	Y96	D97	E98	A99	I100	C102	Y103	N105	A106	L107	K108	W109	D110	K111	D112	N113	L114	Q115	I116	L117	R118	D119	L120	S121	L122	L123	Q124	I125	Q126	M127	R128	D129	L130	Y133	R134	E135	T136					
R137	Y138	Q139	L140	L141	Q142	L143	R144	P145	A146	Q147	R148	A149	S150	W151	I152	G153	Y154	A155	I156	A157	Y158	H159	L160	L161	E162	D163	Y164	E165	M166	A167	W169	K169	L170	L171	E172	E173	F174	R175	K176	T177	Q178	Q179	T180	S181	P182	D183	K184	Y185	D186	Y187	E188	Y189	S190	E191	Q192	L193	L194	Y195	Q196	
N197	Q198	Y199	L200	R201	E202	A203	G204	L205	Y206	R207	E208	A209	L210	E211	H212	L213	C214	T215	Y216	E217	K218	Q219	L220	C221	D222	K223	L224	A225	V226	E227	E228	T229	K230	Q231	E232	L233	L234	L235	Q236	L237	C238	R239	L240	E241	D242	A243	A244	D245	V246	Y247	R248	G249	L250	Q251	E252	R253	L254	P255	E256	
W257	W258	A259	Y260	Y261	K262	G263	L264	E265	K266	A267	L268	K269	P270	A271	W272	H273	L274	E275	R276	L277	K278	T279	Y280	E281	E282	A283	W284	T285	K286	Y287	P288	R289	L290	L291	V292	P293	R294	R295	L296	P297	L298	N299	F300	L301	S302	G303	E304	K305	F306	K307	E308	C309	L310	D311	K312	F313	L314	R315	M316	
N317	F318	S319	K320	C321	G322	F323	P324	V325	F326	N327	T328	L329	R330	S331	W332	Y333	K334	D335	K336	E337	Y338	V339	A340	I341	T342	E343	E344	L345	V346	V347	G348	Y349	E350	T351	S352	L353	K354	S355	C356	R357	L358	F359	N360	P361	N362	D363	D364	G365	G366	E367	E368	P369	P370	T371	D372	L373	L374	W375	V376	
Q377	Y378	Y379	L380	A381	Q382	H383	Y384	D385	K386	I387	G388	Q389	S390	S391	Y392	A393	L394	E395	Y396	I397	N398	T399	A400	L401	E402	S403	T404	P405	T406	L407	L408	E409	L410	F411	L412	V413	K414	A415	K416	I417	Y418	K419	H420	A421	Q422	N423	I424	K425	E426	A427	A428	R429	W430	M431	D432	E433	A434	Q435	A436	
L437	D438	T439	A440	D441	R442	F443	I444	N445	S446	K447	C448	A449	K450	Y451	M452	L453	K454	A455	M456	L457	T458	K459	A460	A461	E462	E463	M464	C465	S466	K467	F468	T469	R470	E471	G472	T473	S474	A475	V476	F477	M478	L479	N480	E481	M482	Q483	C484	M485	W486	F487	Q488	R489	Q490	C491	F492	Q493	A494	Y495	K496	
A497	M498	M499	K500	F501	G502	E503	A504	L505	G506	K507	C508	H509	E510	I511	E512	R513	H514	F515	I516	E517	I518	T519	D520	D521	Q522	F523	D524	F525	H526	T527	Y528	C529	M530	R531	K532	I533	T534	L535	R536	S537	Y538	L541	L542	K543	L544	E545	D546	V547	L548	R549	Q620	Q621	R622	M623	Q624	K625	K626	K627	K628	
R559	I560	A561	I562	E563	I564	Y565	L566	K567	L568	H569	D570	N571	P572	L573	T574	D575	E576	N577	K578	E579	H580	E581	A582	D583	T584	A585	M586	M587	S588	D589	K590	E591	R596	N597	K605	I608	E609	E610	E611	K612	K613	M614	A615	E616	K617	E618	K619	Q620	Q621	R622	M623	Q624	K625	K626	K627	K628				
D629	D630	D631	D632	E633	E634	L635	G636	G637	P638	K639	E640	E641	L642	L643	P644	E645	K646	L647	A648	K649	V650	E651	T652	P653	L654	E655	E656	A657	T658	D659	F660	L661	T662	P663	L664	K665	L666	L667	V668	K669	N670	K671	L672	M673	L674	T675	H676	L677	F677	M678	F679	E680	I681	F682	P683	R684	K685	E686	P687	K688
L689	L690	M691	L692	Q693	S694	V695	K696	R697	A698	F699	A700	I701	D702	S703	H705	P706	W707	L708	H709	E710	C711	M712	T713	R714	L715	F716	M717	T718	A719	V720	C721	T722	S723	K724	D725	L726	S727	D728	T729	W730	R731	T732	W733	L734	K735	Q736	F737	M738	N739	R740	L741	F742	G743	T744	T745	N746	P747	K748		



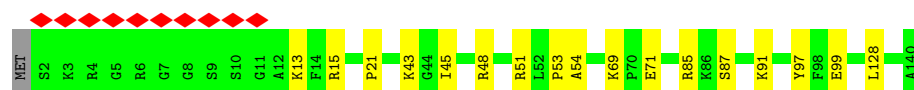
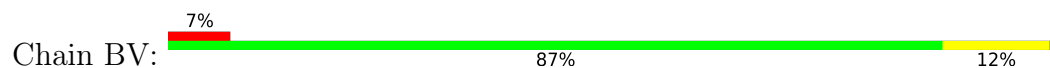
• Molecule 20: Nascent polypeptide-associated complex subunit alpha



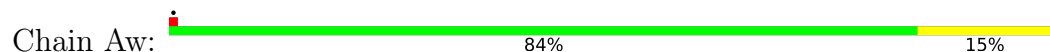
• Molecule 21: 60S ribosomal protein L9



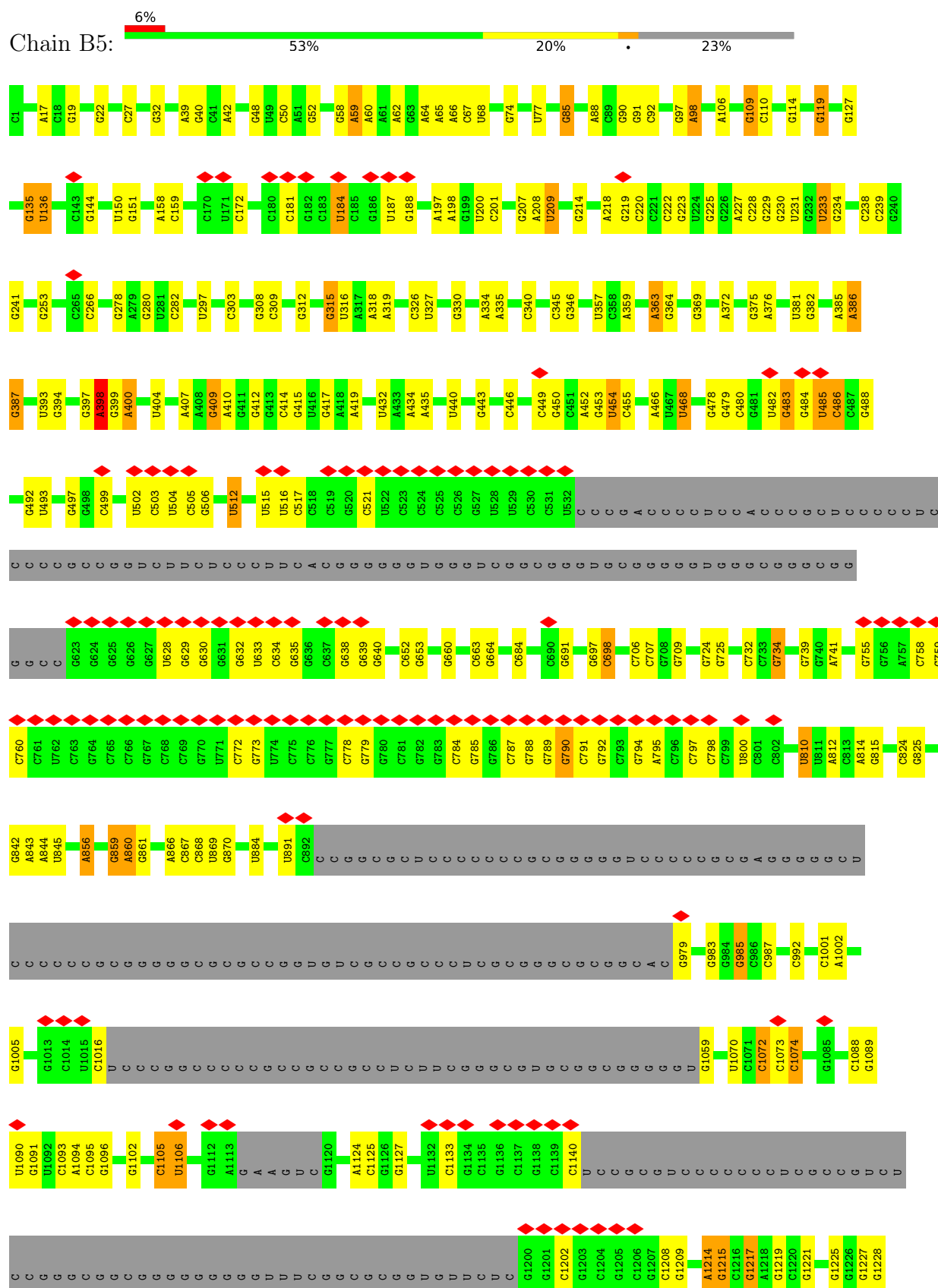
• Molecule 22: Ribosomal protein L23



• Molecule 23: 40S ribosomal protein S23

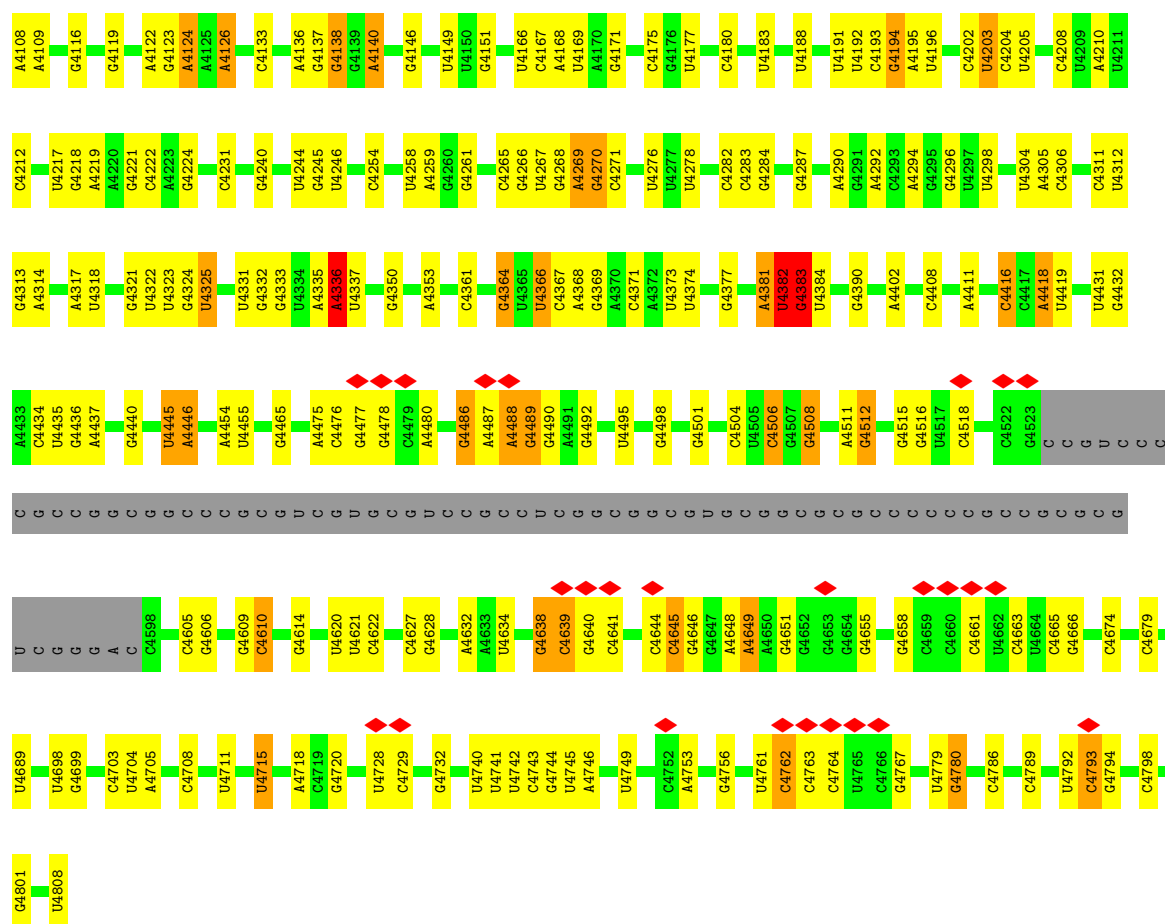


● Molecule 24: 28S rRNA

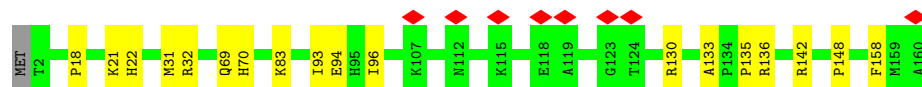
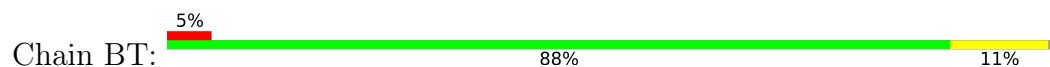




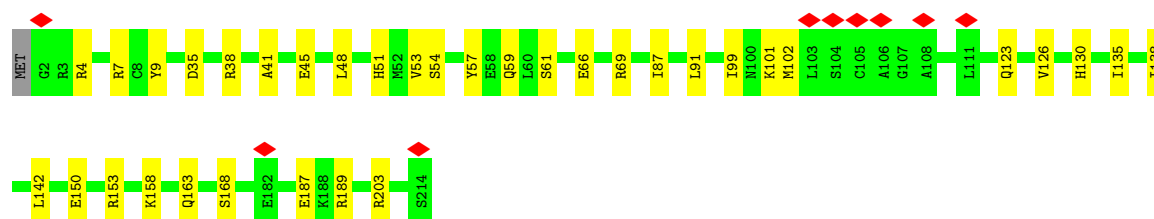
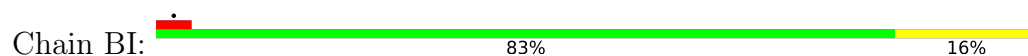




• Molecule 25: 60S ribosomal protein L21



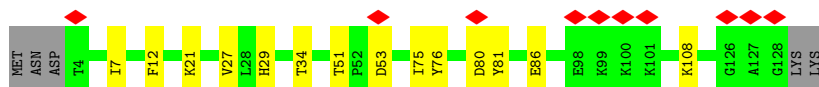
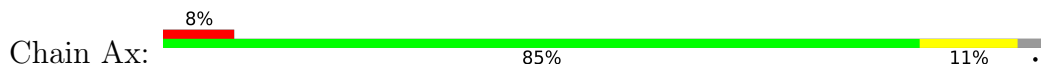
• Molecule 26: 60S ribosomal protein L10



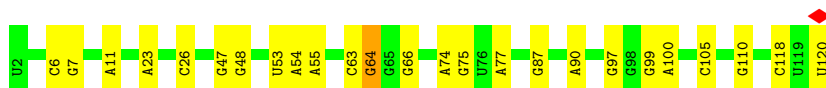
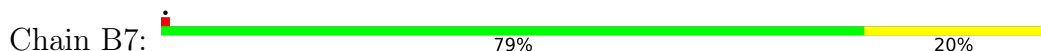
• Molecule 27: Ribosomal protein L24



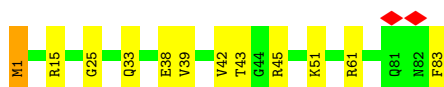
- Molecule 28: 40S ribosomal protein S24



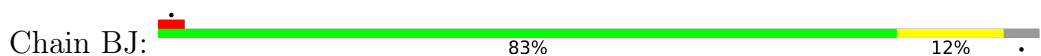
- Molecule 29: 5S rRNA



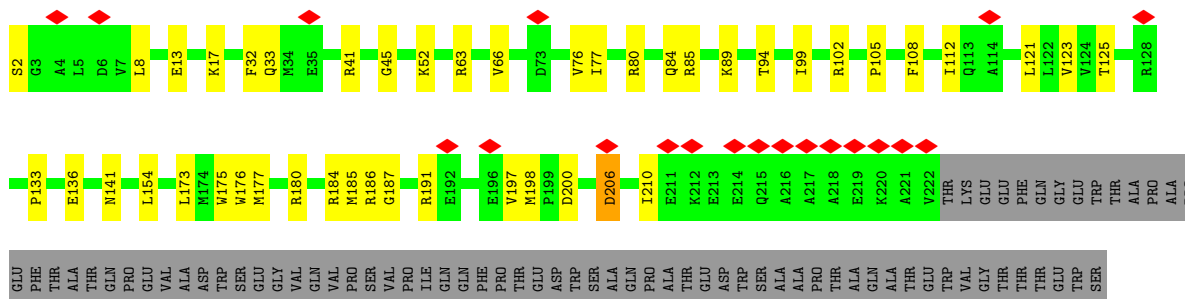
- Molecule 30: Small ribosomal subunit protein eS21

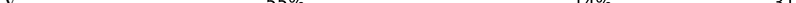


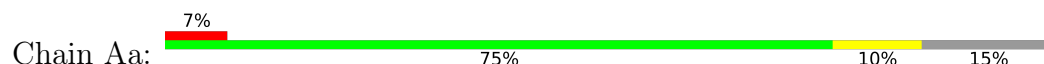
- Molecule 31: 60S ribosomal protein L11



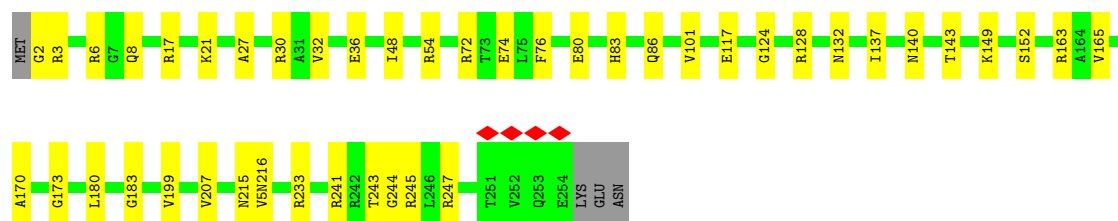
- Molecule 32: Small ribosomal subunit protein uS2



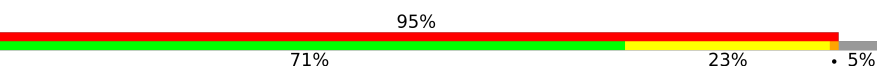
- Chain A_y: 

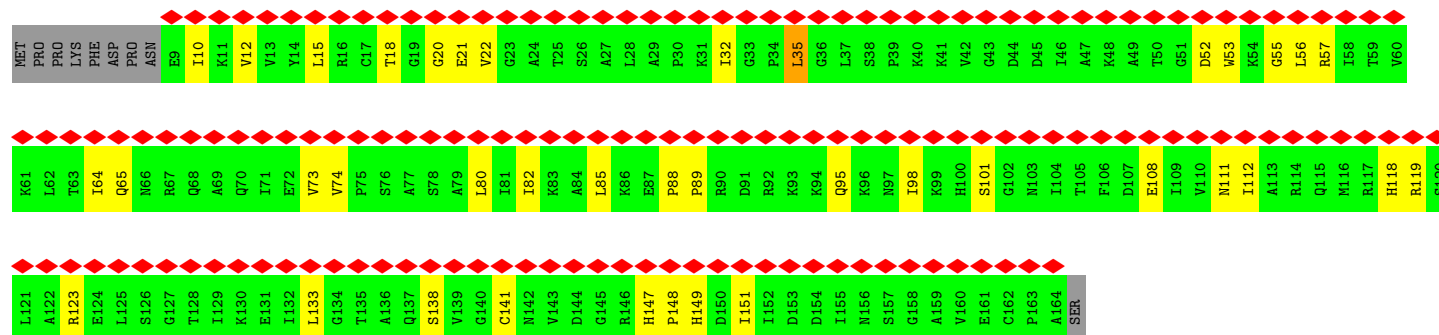


Chain BA: 



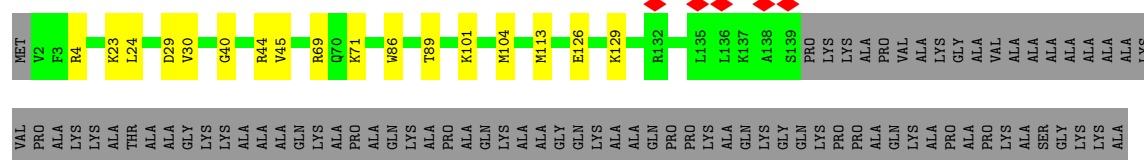
- Molecule 39: 60S ribosomal protein L12

Chain Bt: 



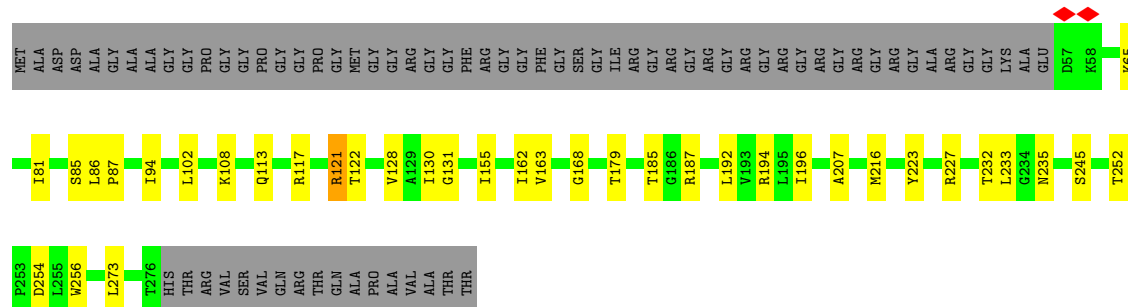
- Molecule 40: 60S ribosomal protein L14

Chain BM: 



- Molecule 41: 40S ribosomal protein S2

Chain Ab: 



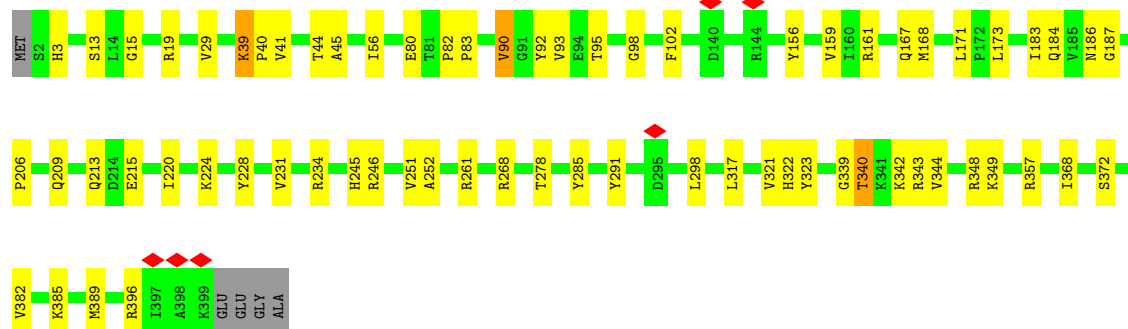
- Molecule 42: Ribosomal protein L26

Chain BY: 



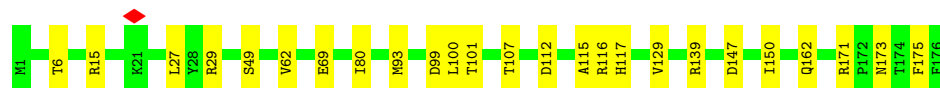
• Molecule 43: Ribosomal protein L3

Chain BB: 



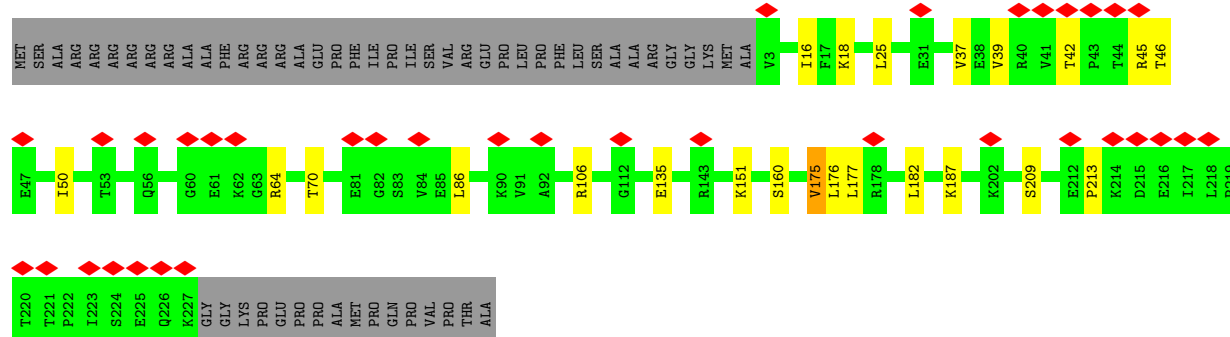
• Molecule 44: Large ribosomal subunit protein eL20

Chain BS: 



• Molecule 45: 40S ribosomal protein S3

Chain Ac: 

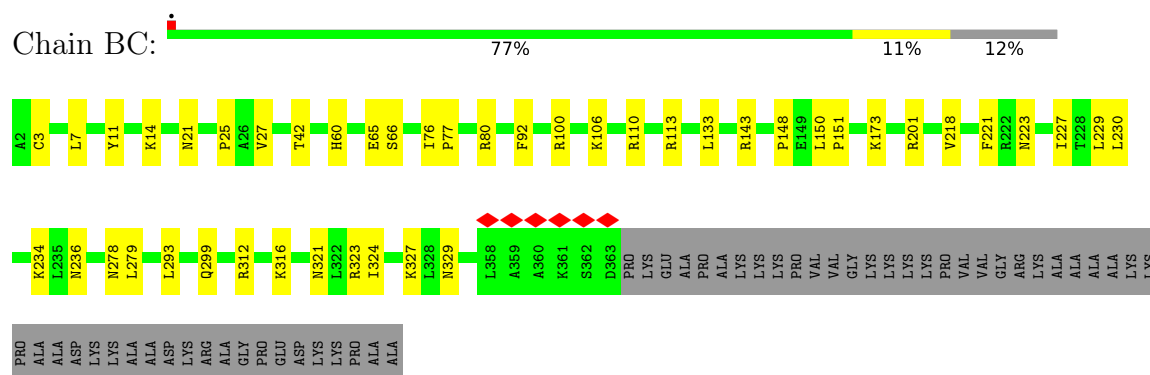


• Molecule 46: 60S ribosomal protein L27

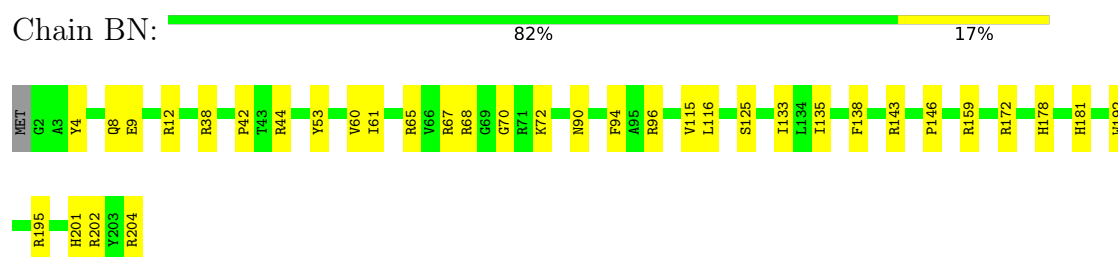
Chain BZ: 



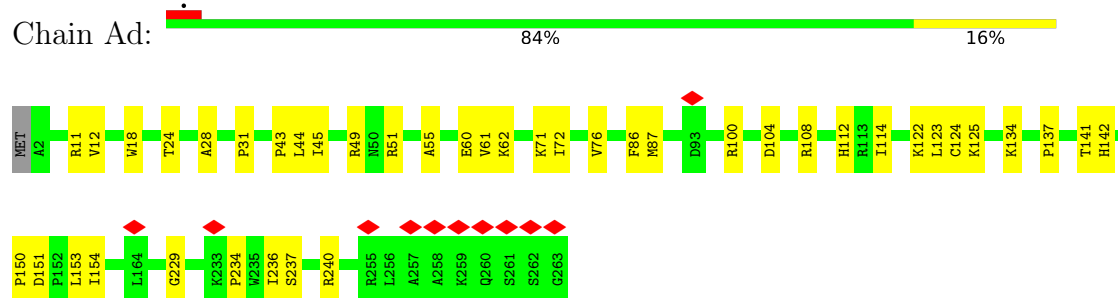
- Molecule 47: Large ribosomal subunit protein uL4



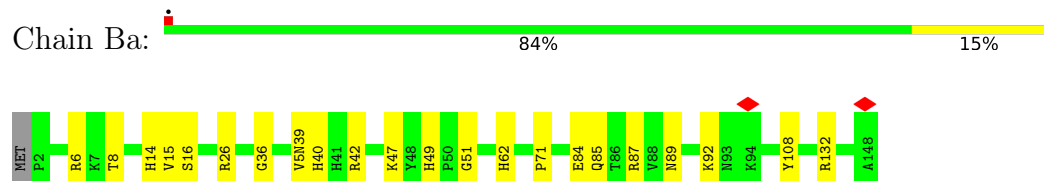
- Molecule 48: Ribosomal protein L15



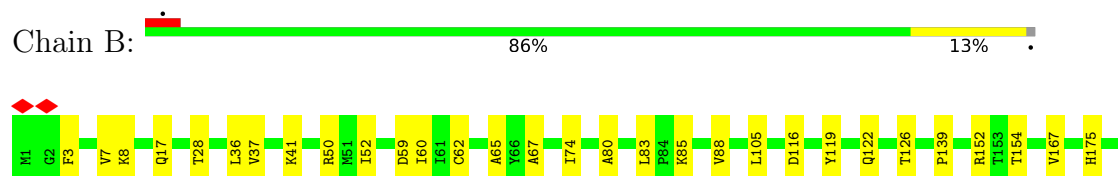
- Molecule 49: 40S ribosomal protein S4



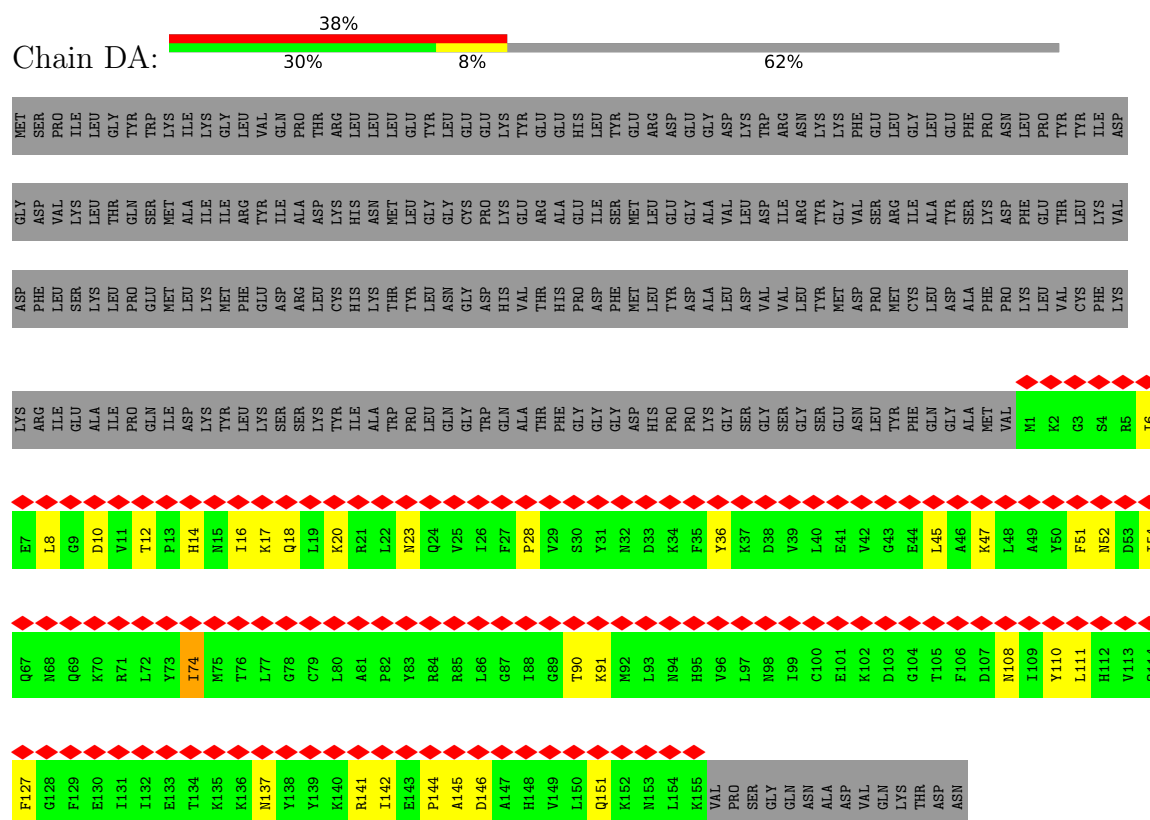
- Molecule 50: 60S ribosomal protein L27a



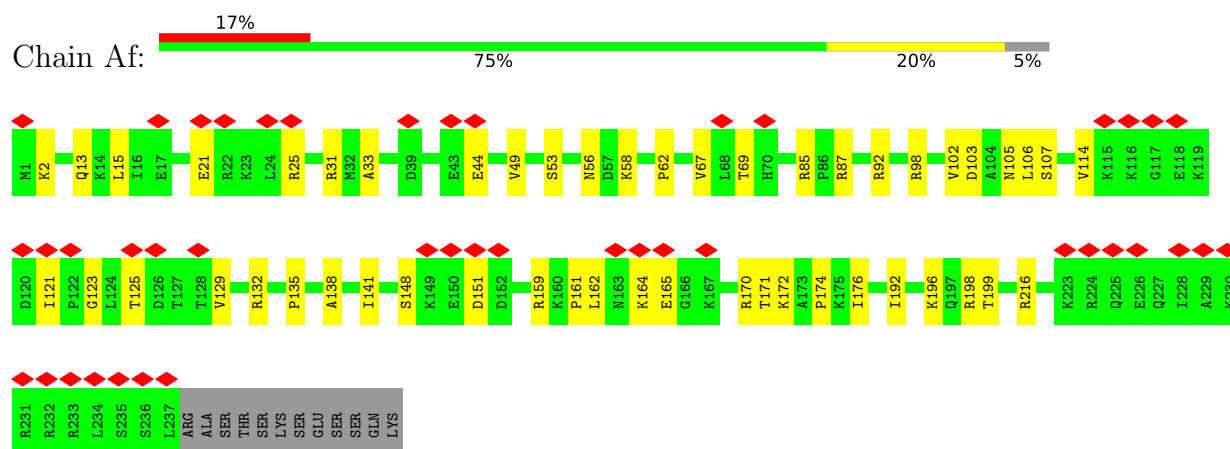
- Molecule 51: Large ribosomal subunit protein uL18



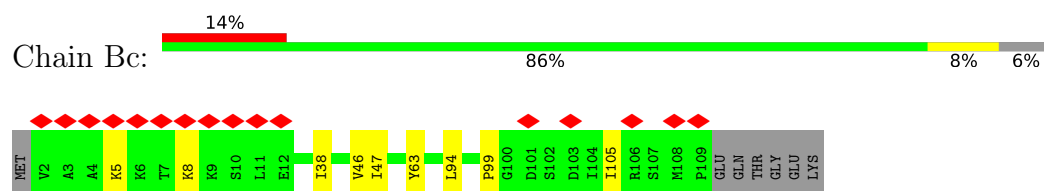
- Molecule 56: Glutathione S-transferase class-mu 26 kDa isozyme,N-alpha-acetyltransferase 50



- Molecule 57: 40S ribosomal protein S6



- Molecule 58: 60S ribosomal protein L30



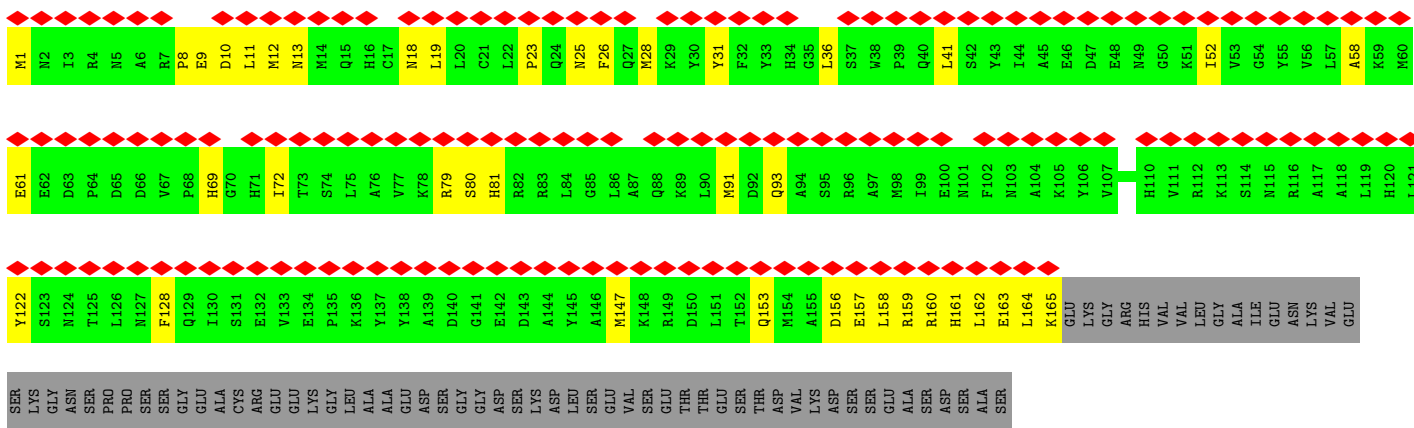
- Molecule 59: Ribosomal Protein uL30

Response	Percentage
Yes, the U.S. is a democracy	78%
No, the U.S. is not a democracy	14%
Don't know	9%



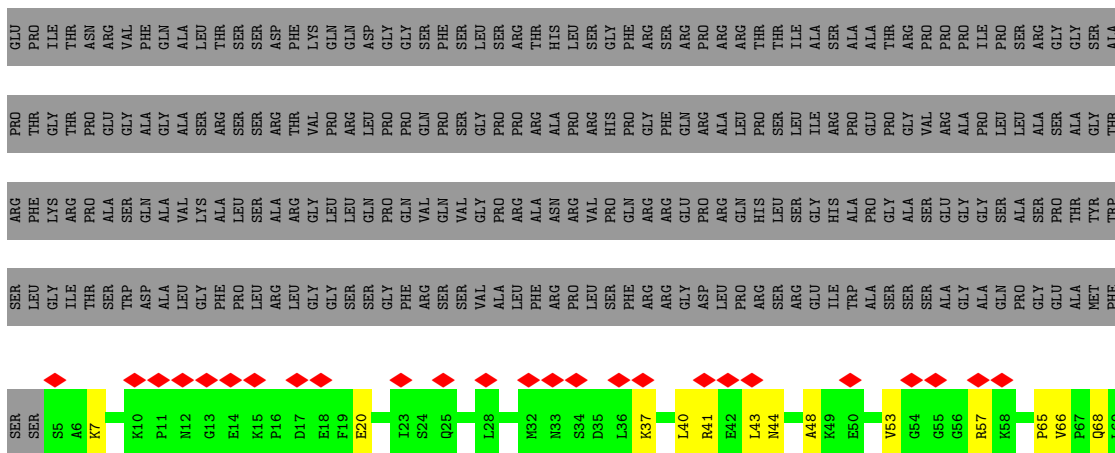
- Molecule 60: N-alpha-acetyltransferase 10

Category	Percentage
Very bad	66%
Bad	53%
Good	17%
Very good	30%



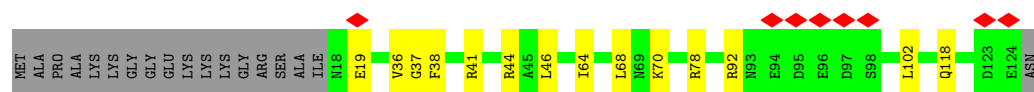
- Molecule 61: 40S ribosomal protein S7

Response	Percentage
Yes	9%
No	37%
Don't know	7%
No answer	56%

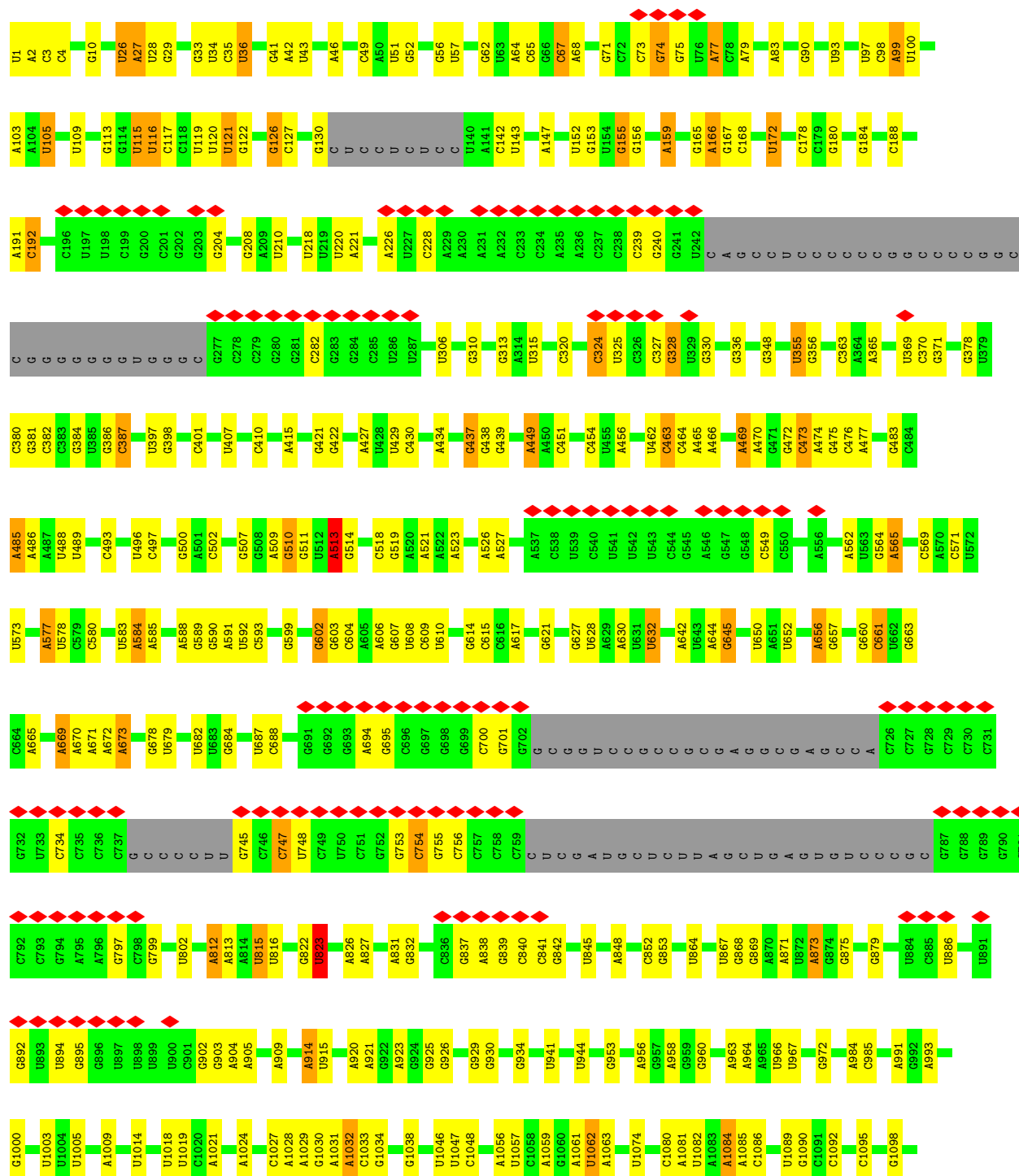


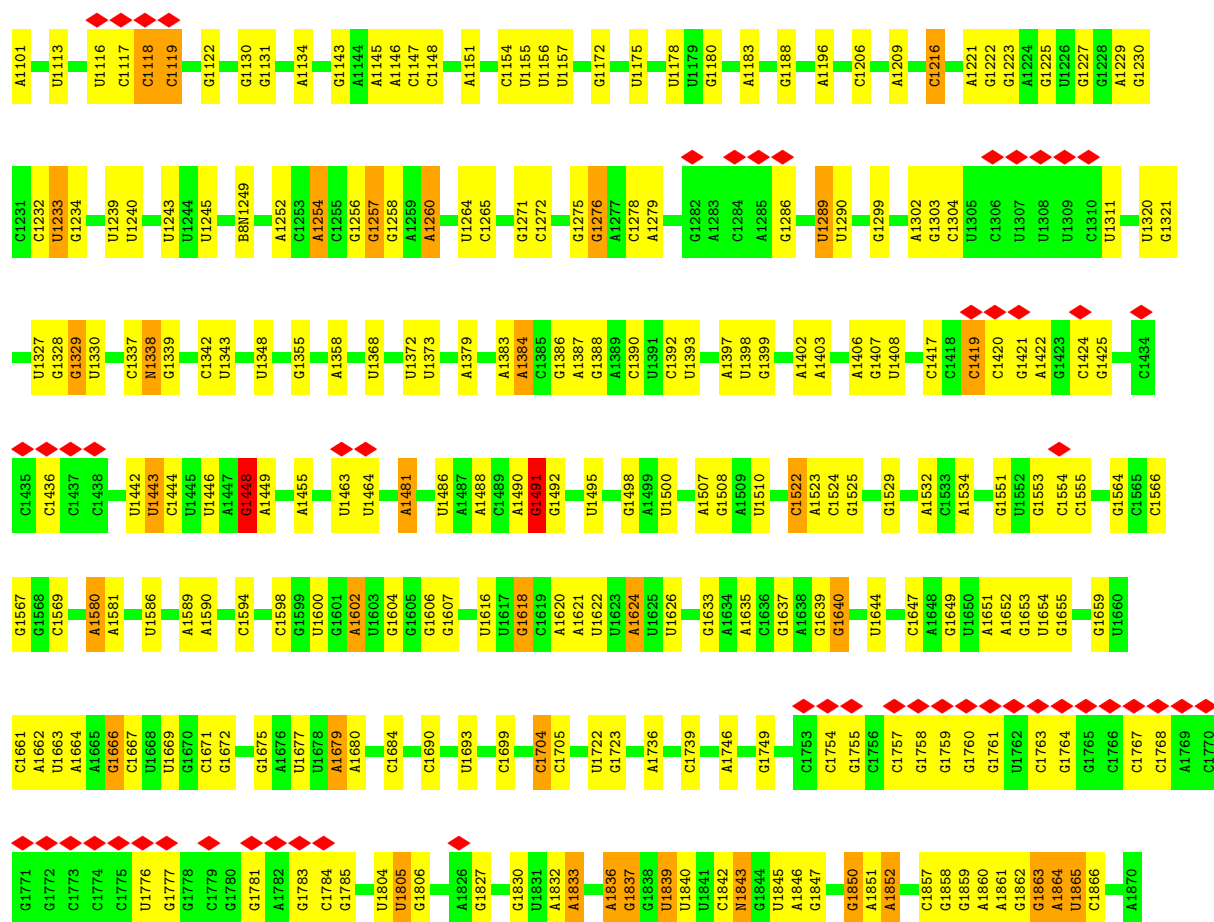
- Molecule 62: 60S ribosomal protein L31

Device Type	Percentage
Smartphone	6%
Tablet	74%
Smart TV	11%
Other	14%

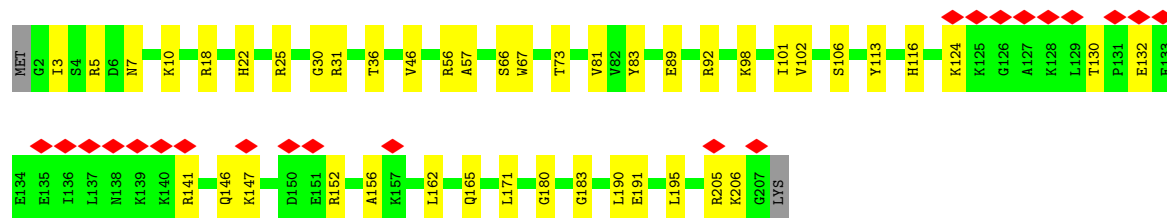
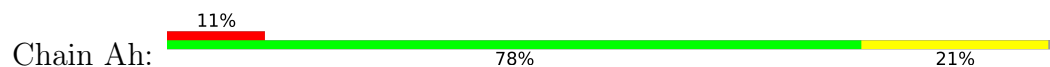


• Molecule 63: 18S rRNA

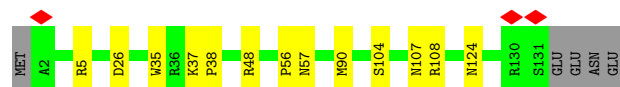
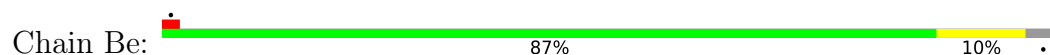




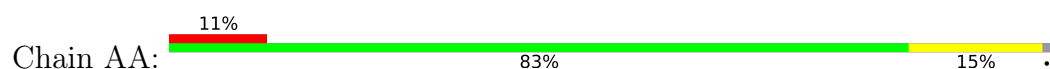
• Molecule 64: 40S ribosomal protein S8

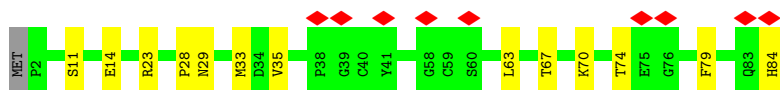


• Molecule 65: Ribosomal protein L32

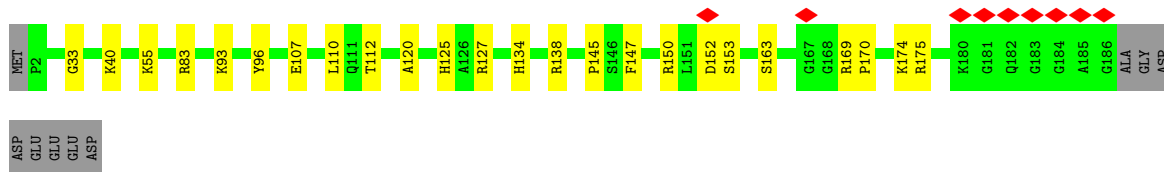
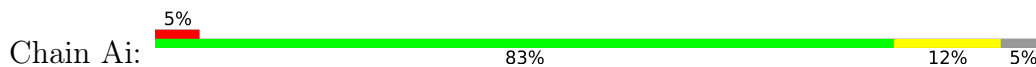


• Molecule 66: 40S ribosomal protein S27





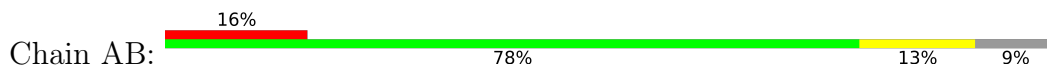
- Molecule 67: 40S ribosomal protein S9



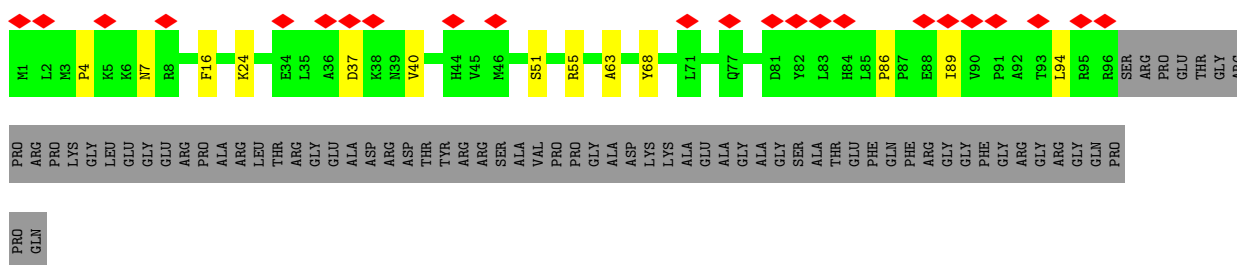
- Molecule 68: 60S ribosomal protein L35a



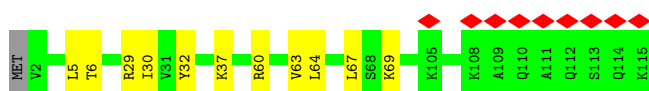
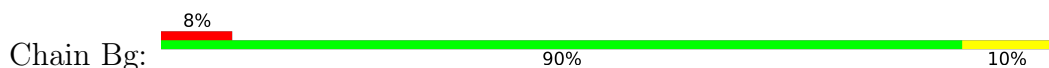
- Molecule 69: 40S ribosomal protein S28



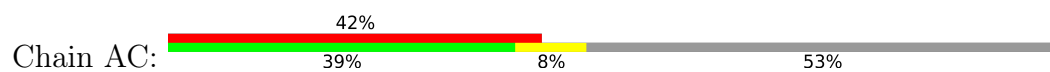
- Molecule 70: S10_pectin domain-containing protein



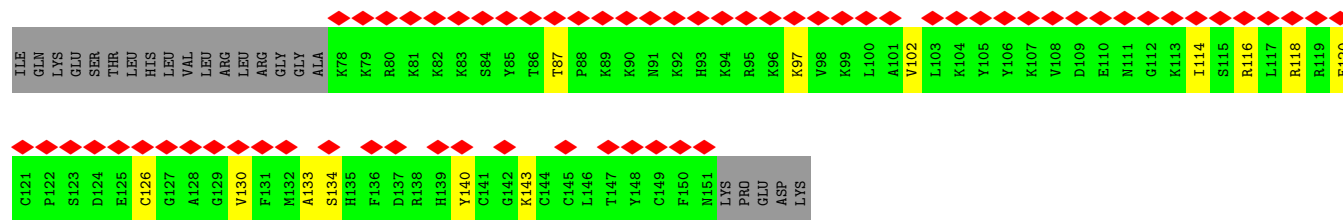
- Molecule 71: Large ribosomal subunit protein eL34



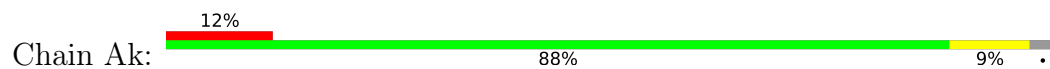
- Molecule 72: Ribosomal protein S27a



MET GLN ILE PHE VAL SER THR LEU THR VAL GLY LYS THR ILE THR LEU GLY VAL GLU PRO SER ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP ASP GLU GLY ILE PRO PRO ASP GLN ASP ARG LEU ILE PHE ALA GLY LYS LEU GLU ASP ARG THR SER ASN

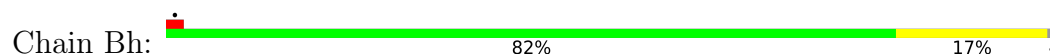


- Molecule 73: 40S ribosomal protein S11



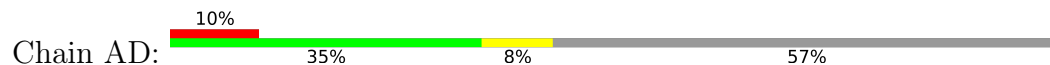
MET ALA D3 Q18 R22 V23 L24 G26 E27 T28 G29 K30 E31 K32 L33 K48 K79 K104 N108 R118 D119 V120 V126 S135 R139 V145 T146 K147 T151 K152 K153 Q154 F155 Q156 LYS PHE

- Molecule 74: 60S ribosomal protein L35

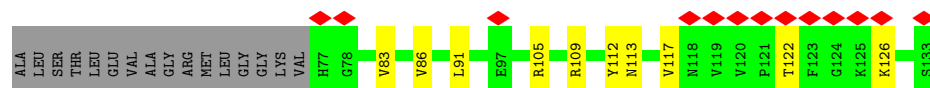


MET A2 K3 I4 K5 A6 R10 K13 E16 S53 N62 K66 L69 K79 P80 L83 R84 P85 K86 R89 R93 R94 L95 T104 R112 A123

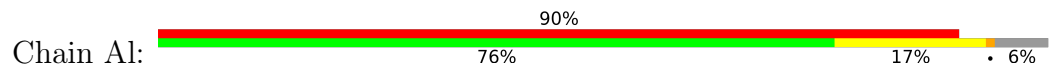
- Molecule 75: 40S ribosomal protein S30



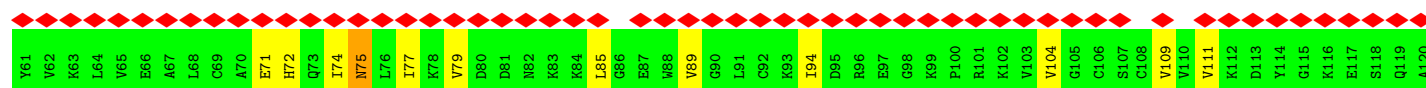
MET GLN LEU PHE THR VAL ARG ALA GLN HIS LEU THR LEU GLY VAL THR ARG GLY THR VAL THR ILE ALA LYS ALA HIS VAL VAL ALA SER LEU GLU GLY ILE PRO GLU ASP GLN VAL VAL LEU LEU ALA GLY THR PRO LEU GLU ASP GLU ALA THR LEU GLY GLN CYS VAL GLU

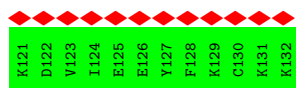


- Molecule 76: 40S ribosomal protein S12

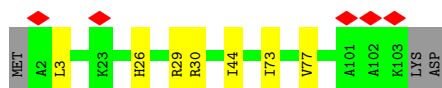
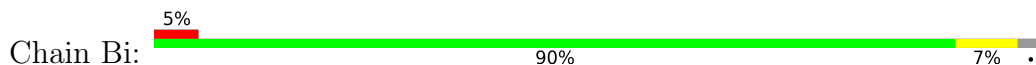


MET ALA GLU THR ILE ALA G9 G10 V11 H12 D13 V14 N15 T16 A17 L18 Q19 E20 V21 L22 K23 T24 A25 L26 I27 H28 D29 G30 L31 A32 R33 G34 I35 R36 E37 A38 A39 K40 A41 L42 D43 K44 R45 Q46 A47 H48 L49 C50 V51 L52 A53 S54 N55 C56 D57 E58 P59 M60

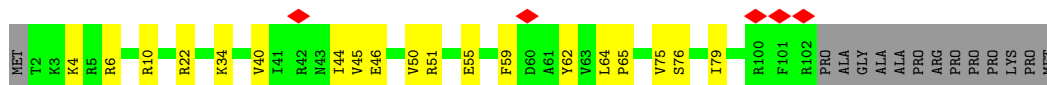




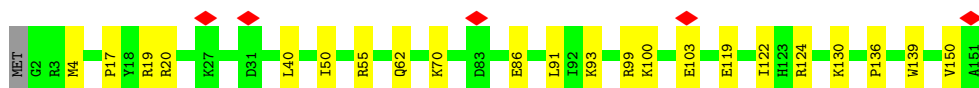
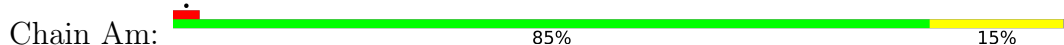
- Molecule 77: 60S ribosomal protein L36



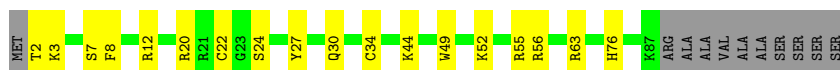
- Molecule 78: Small ribosomal subunit protein eS26



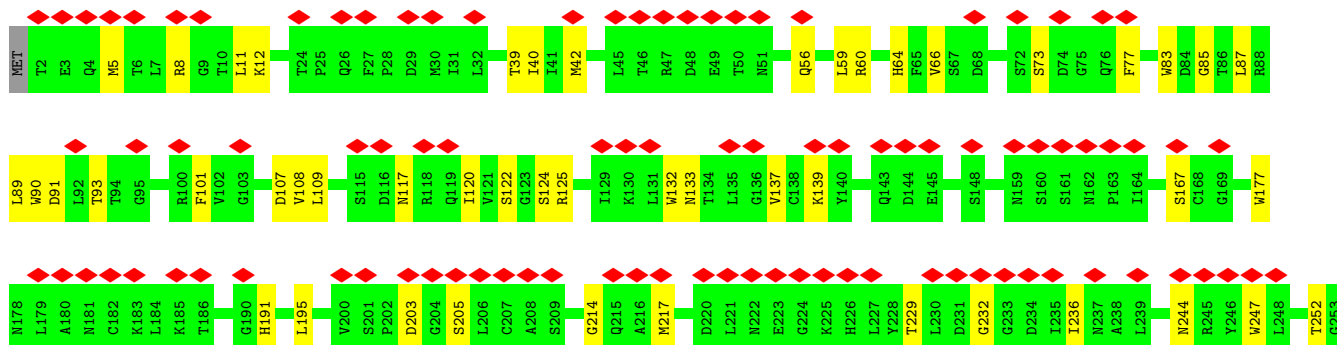
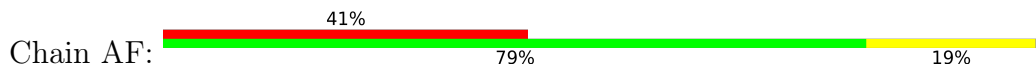
- Molecule 79: 40S ribosomal protein S13

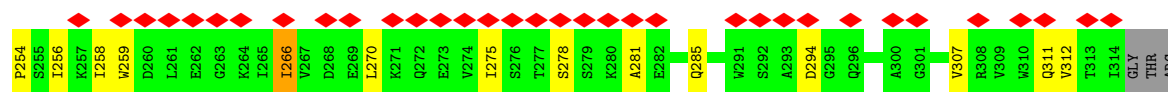


- Molecule 80: Ribosomal protein L37

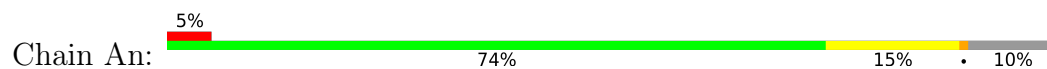


- Molecule 81: Small ribosomal subunit protein RACK1

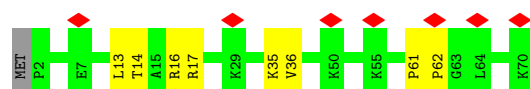




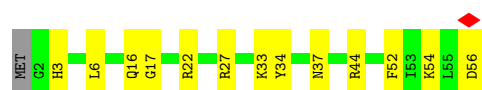
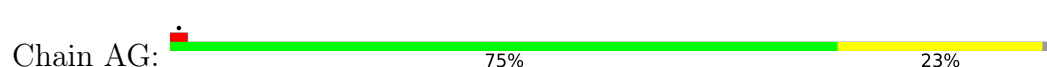
- Molecule 82: Small ribosomal subunit protein uS11



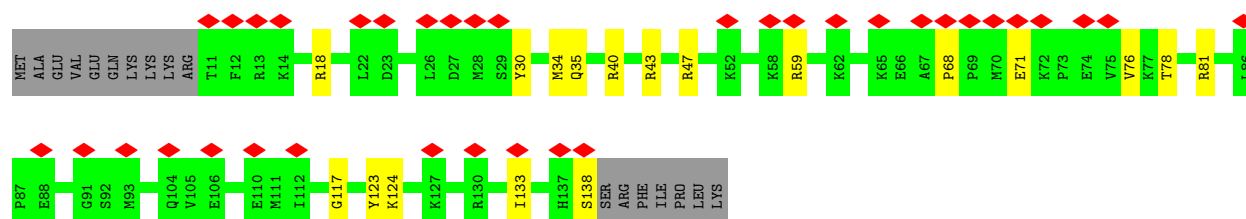
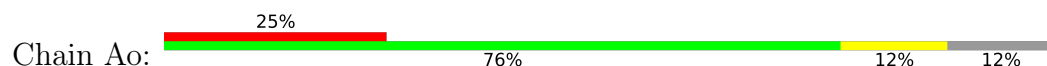
- Molecule 83: 60S ribosomal protein L38



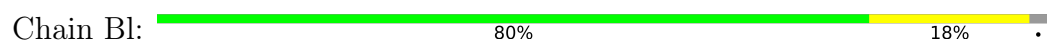
- Molecule 84: 40S ribosomal protein S29



- Molecule 85: 40S ribosomal protein uS19



- Molecule 86: 60S ribosomal protein L39-like

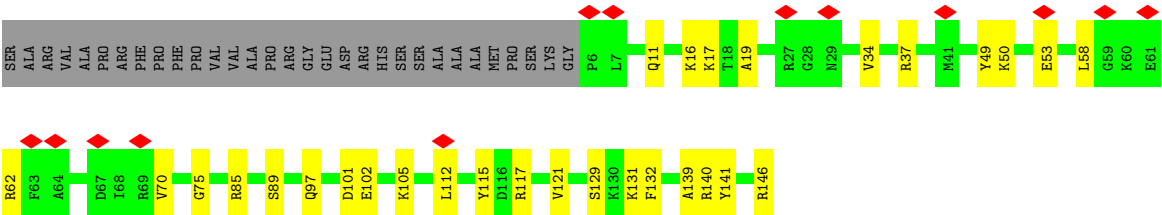


- Molecule 87: mRNA

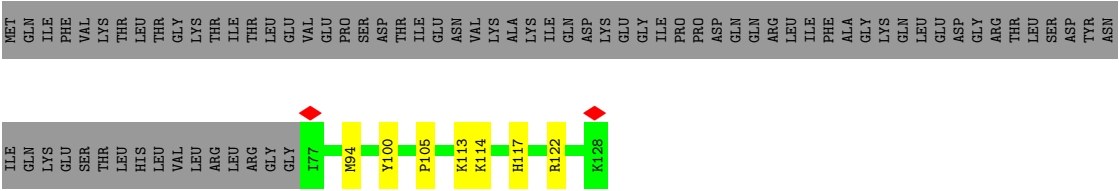
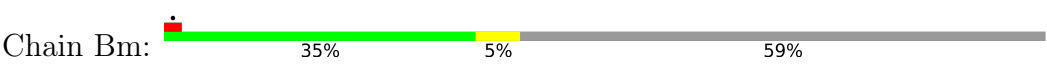




• Molecule 88: Small ribosomal subunit protein uS9



• Molecule 89: Ubiquitin-ribosomal protein eL40 fusion protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.360	Depositor
Minimum map value	-0.419	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.275	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BP	0.07	0/1268	0.21	0/1700
2	Aq	0.07	0/1094	0.19	0/1469
3	Bo	0.13	0/866	0.25	0/1141
4	AT	0.07	0/68	0.15	0/103
5	Ar	0.06	0/1226	0.18	0/1643
6	Cu	0.16	0/821	0.35	0/1101
7	BL	0.07	0/1733	0.19	0/2316
8	BX	0.07	0/984	0.19	0/1323
9	Bp	0.08	0/718	0.21	0/953
10	BQ	0.07	0/1539	0.19	0/2054
11	As	0.06	0/1119	0.17	0/1498
12	Br	0.08	0/1020	0.22	0/1366
13	BR	0.06	0/1524	0.16	0/2013
14	At	0.14	0/832	0.22	0/1117
15	Bs	0.07	0/1530	0.19	0/2064
16	BG	0.07	0/1908	0.19	0/2566
17	BU	0.08	0/845	0.21	0/1134
18	Av	0.08	0/1051	0.18	0/1406
19	DB	0.11	0/7038	0.26	0/9468
20	Ct	0.22	0/900	0.35	0/1202
21	BH	0.07	0/1535	0.19	0/2063
22	BV	0.07	0/1048	0.19	0/1402
23	Aw	0.07	0/1107	0.20	0/1475
24	B5	0.11	2/86006 (0.0%)	0.13	0/134179
25	BT	0.07	0/1326	0.18	0/1770
26	BI	0.07	0/1756	0.20	0/2346
27	BW	0.06	0/1006	0.18	0/1334
28	Ax	0.06	0/1032	0.18	0/1371
29	B7	0.06	0/2835	0.10	0/4418
30	Au	0.07	0/636	0.18	0/852
31	BJ	0.07	0/1385	0.19	0/1852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AZ	0.08	0/1771	0.19	0/2406
33	Ay	0.07	0/691	0.18	0/922
34	B8	0.11	0/3635	0.15	0/5661
36	Aa	0.08	0/1841	0.20	0/2459
37	Az	0.06	0/240	0.13	0/305
38	BA	0.08	0/1965	0.22	0/2633
39	Bt	0.07	0/1193	0.21	0/1609
40	BM	0.07	0/1158	0.18	0/1547
41	Ab	0.07	0/1742	0.21	0/2354
42	BY	0.06	0/1132	0.19	0/1504
43	BB	0.08	0/3261	0.21	0/4364
44	BS	0.08	0/1497	0.20	0/2008
45	Ac	0.07	0/1779	0.19	0/2395
46	BZ	0.06	0/1130	0.17	0/1507
47	BC	0.07	0/2932	0.19	0/3939
48	BN	0.08	0/1746	0.19	0/2338
49	Ad	0.07	0/2118	0.20	0/2849
50	Ba	0.07	0/1179	0.20	0/1572
51	B	0.08	0/2444	0.20	0/3273
52	BO	0.08	0/1662	0.19	0/2222
53	Ae	0.07	0/1531	0.22	0/2059
54	Bb	0.06	0/884	0.18	0/1169
55	BE	0.08	0/1998	0.20	0/2673
56	DA	0.07	0/1284	0.21	0/1728
57	Af	0.06	0/1946	0.17	0/2590
58	Bc	0.07	0/847	0.18	0/1134
59	BF	0.07	0/1922	0.19	0/2563
60	DC	0.21	0/1368	0.37	0/1843
61	Ag	0.07	0/1552	0.19	0/2079
62	Bd	0.08	0/903	0.20	0/1216
63	A2	0.14	0/40342	0.13	0/62877
64	Ah	0.07	0/1715	0.19	0/2287
65	Be	0.07	0/1088	0.19	0/1451
66	AA	0.06	0/665	0.20	0/891
67	Ai	0.06	0/1550	0.18	0/2069
68	Bf	0.08	0/903	0.19	0/1208
69	AB	0.06	0/497	0.19	0/666
70	Aj	0.07	0/834	0.21	0/1125
71	Bg	0.07	0/916	0.19	0/1220
72	AC	0.06	0/622	0.18	0/822
73	Ak	0.07	0/1284	0.19	0/1717
74	Bh	0.06	0/1021	0.16	0/1348
75	AD	0.06	0/462	0.18	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Al	0.07	0/968	0.20	0/1296
77	Bi	0.06	0/841	0.18	0/1112
78	AE	0.07	0/828	0.20	0/1109
79	Am	0.06	0/1232	0.18	0/1656
80	Bj	0.07	0/720	0.20	0/952
81	AF	0.08	0/2493	0.20	0/3394
82	An	0.07	0/1020	0.20	0/1366
83	Bk	0.07	0/575	0.17	0/761
84	AG	0.07	0/470	0.19	0/623
85	Ao	0.07	0/1069	0.19	0/1429
86	Bl	0.07	0/459	0.18	0/608
88	Ap	0.08	0/1142	0.25	0/1528
89	Bm	0.08	0/426	0.21	0/564
All	All	0.10	2/241249 (0.0%)	0.16	0/352306

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B5	4269	A2M	O3'-P	5.03	1.61	1.56
24	B5	3517	A2M	O3'-P	5.00	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	BP	1242	0	1274	19	0
2	Aq	1080	0	1135	18	0
3	Bo	863	0	929	9	0
4	AT	939	0	617	3	0
5	Ar	1217	0	1279	20	0
6	Cu	813	0	856	23	0
7	BL	1702	0	1820	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BX	967	0	1040	10	0
9	Bp	708	0	756	9	0
10	BQ	1515	0	1634	24	0
11	As	1113	0	1145	15	0
12	Br	1014	0	1083	12	0
13	BR	1508	0	1664	16	0
14	At	822	0	887	12	0
15	Bs	1507	0	1564	28	0
16	BG	1877	0	2023	11	0
17	BU	831	0	852	12	0
18	Av	1034	0	1080	12	0
19	DB	6900	0	6944	176	0
20	Ct	895	0	960	29	0
21	BH	1516	0	1597	17	0
22	BV	1034	0	1097	16	0
23	Aw	1099	0	1162	12	0
24	B5	79525	0	40251	628	0
25	BT	1298	0	1366	18	0
26	BI	1717	0	1764	21	0
27	BW	991	0	1048	12	0
28	Ax	1015	0	1086	9	0
29	B7	2538	0	1283	16	0
30	Au	640	0	633	9	0
31	BJ	1362	0	1399	15	0
32	AZ	1743	0	1748	28	0
33	Ay	683	0	761	11	0
34	B8	3319	0	1684	30	0
35	BK	145	0	32	1	0
36	Aa	1815	0	1908	20	0
37	Az	239	0	289	2	0
38	BA	1940	0	2028	33	0
39	Bt	1178	0	1235	24	0
40	BM	1137	0	1211	12	0
41	Ab	1706	0	1796	25	0
42	BY	1115	0	1205	12	0
43	BB	3206	0	3352	50	0
44	BS	1457	0	1492	16	0
45	Ac	1751	0	1846	15	0
46	BZ	1107	0	1182	13	0
47	BC	2886	0	3057	32	0
48	BN	1701	0	1749	29	0
49	Ad	2076	0	2177	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	Ba	1163	0	1202	19	0
51	B	2398	0	2428	30	0
52	BO	1630	0	1778	19	0
53	Ae	1509	0	1563	24	0
54	Bb	881	0	957	10	0
55	BE	1960	0	2153	29	0
56	DA	1260	0	1282	21	0
57	Af	1923	0	2089	41	0
58	Bc	836	0	888	6	0
59	BF	1886	0	2008	25	0
60	DC	1339	0	1315	31	0
61	Ag	1529	0	1627	19	0
62	Bd	888	0	930	10	0
63	A2	37833	0	19167	310	0
64	Ah	1686	0	1772	30	0
65	Be	1070	0	1164	10	0
66	AA	651	0	672	9	0
67	Ai	1525	0	1640	16	0
68	Bf	884	0	923	6	0
69	AB	495	0	523	5	0
70	Aj	810	0	836	8	0
71	Bg	906	0	998	7	0
72	AC	610	0	634	10	0
73	Ak	1262	0	1335	11	0
74	Bh	1013	0	1147	21	0
75	AD	457	0	502	11	0
76	Al	958	0	993	15	0
77	Bi	830	0	916	6	0
78	AE	814	0	863	12	0
79	Am	1208	0	1293	16	0
80	Bj	705	0	737	16	0
81	AF	2436	0	2393	36	0
82	An	1016	0	1038	17	0
83	Bk	569	0	637	5	0
84	AG	459	0	448	11	0
85	Ao	1048	0	1093	14	0
86	Bl	447	0	478	7	0
87	AH	36	0	25	0	0
88	Ap	1124	0	1193	23	0
89	Bm	432	0	470	6	0
90	A2	108	0	0	0	0
90	AT	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	Af	1	0	0	0	0
90	An	1	0	0	0	0
90	B5	282	0	0	0	0
90	B7	9	0	0	0	0
90	B8	9	0	0	0	0
90	BI	1	0	0	0	0
90	BP	1	0	0	0	0
90	BR	1	0	0	0	0
90	BV	1	0	0	0	0
90	Ba	1	0	0	0	0
90	Bj	1	0	0	0	0
90	Ct	1	0	0	0	0
91	AC	1	0	0	0	0
91	AE	1	0	0	0	0
91	AG	1	0	0	0	0
91	Bg	1	0	0	0	0
91	Bj	1	0	0	0	0
91	Bm	1	0	0	0	0
91	Bo	1	0	0	0	0
91	Bp	1	0	0	0	0
92	A2	57	0	0	1	0
92	AT	2	0	0	0	0
92	Ae	1	0	0	0	0
92	Ak	1	0	0	0	0
92	An	1	0	0	0	0
92	Ar	1	0	0	0	0
92	B5	207	0	0	4	0
92	B7	6	0	0	1	0
92	B8	7	0	0	0	0
92	BA	4	0	0	0	0
92	BB	2	0	0	0	0
92	BH	1	0	0	0	0
92	BI	1	0	0	0	0
92	BL	1	0	0	0	0
92	BN	1	0	0	0	0
92	BQ	2	0	0	0	0
92	BT	2	0	0	0	0
92	Bb	2	0	0	0	0
92	Be	3	0	0	0	0
92	Bf	1	0	0	0	0
92	Bj	1	0	0	0	0
92	Bl	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	Bo	1	0	0	0	0
93	DB	36	0	6	0	0
94	A2	80	0	152	9	0
94	B5	220	0	418	17	0
95	A2	14	0	26	3	0
95	B5	28	0	52	3	0
96	B7	32	0	11	0	0
97	A2	526	0	0	11	0
97	AE	1	0	0	0	0
97	AH	5	0	0	0	0
97	AT	13	0	0	0	0
97	Aa	2	0	0	0	0
97	Af	1	0	0	0	0
97	Ak	2	0	0	0	0
97	Am	1	0	0	0	0
97	An	3	0	0	0	0
97	Ap	2	0	0	0	0
97	Ar	1	0	0	0	0
97	As	3	0	0	0	0
97	At	1	0	0	1	0
97	Aw	5	0	0	0	0
97	B	1	0	0	0	0
97	B5	1383	0	0	36	0
97	B7	43	0	0	0	0
97	B8	50	0	0	0	0
97	BA	8	0	0	0	0
97	BB	9	0	0	0	0
97	BC	7	0	0	1	0
97	BF	1	0	0	0	0
97	BH	2	0	0	0	0
97	BI	3	0	0	0	0
97	BJ	1	0	0	0	0
97	BL	2	0	0	0	0
97	BM	1	0	0	0	0
97	BN	4	0	0	0	0
97	BO	1	0	0	0	0
97	BP	3	0	0	0	0
97	BR	5	0	0	0	0
97	BV	2	0	0	0	0
97	BX	1	0	0	0	0
97	Ba	8	0	0	1	0
97	Bd	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	Be	5	0	0	0	0
97	Bf	1	0	0	0	0
97	Bg	2	0	0	0	0
97	Bj	3	0	0	0	0
97	Bl	1	0	0	0	0
97	Bo	1	0	0	0	0
97	Ct	1	0	0	0	0
All	All	234232	0	175755	2016	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 2016 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)
92:B5:4968:UNX:UNK	97:B5:6243:HOH:O	1.45	0.96
34:B8:81:C:HO2'	74:Bh:2:ALA:N	1.66	0.93
18:Av:2:VAL:N	63:A2:1092:C:HO2'	1.66	0.92
82:An:34:PHE:HB3	82:An:41:PHE:HB2	1.66	0.77
49:Ad:125:LYS:H	49:Ad:142:HIS:HD2	1.34	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
2	Aq	132/135 (98%)	132 (100%)	0	0	100	100
3	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
5	Ar	146/151 (97%)	143 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Cu	103/162 (64%)	95 (92%)	8 (8%)	0	100	100
7	BL	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
8	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
9	Bp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
10	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
11	As	140/145 (97%)	140 (100%)	0	0	100	100
12	Br	124/136 (91%)	122 (98%)	2 (2%)	0	100	100
13	BR	178/196 (91%)	178 (100%)	0	0	100	100
14	At	102/119 (86%)	98 (96%)	4 (4%)	0	100	100
15	Bs	194/318 (61%)	189 (97%)	5 (3%)	0	100	100
16	BG	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
17	BU	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
18	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
19	DB	835/915 (91%)	822 (98%)	13 (2%)	0	100	100
20	Ct	111/238 (47%)	110 (99%)	1 (1%)	0	100	100
21	BH	188/192 (98%)	188 (100%)	0	0	100	100
22	BV	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
23	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
25	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
26	BI	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
27	BW	119/157 (76%)	118 (99%)	1 (1%)	0	100	100
28	Ax	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
30	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
31	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
32	AZ	219/294 (74%)	214 (98%)	5 (2%)	0	100	100
33	Ay	83/124 (67%)	81 (98%)	2 (2%)	0	100	100
36	Aa	220/264 (83%)	217 (99%)	3 (1%)	0	100	100
37	Az	23/25 (92%)	23 (100%)	0	0	100	100
38	BA	250/257 (97%)	240 (96%)	10 (4%)	0	100	100
39	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
40	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	Ab	218/293 (74%)	218 (100%)	0	0	100	100
42	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
43	BB	395/403 (98%)	392 (99%)	3 (1%)	0	100	100
44	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
45	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
46	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
47	BC	360/412 (87%)	357 (99%)	3 (1%)	0	100	100
48	BN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
49	Ad	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
50	Ba	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	18	51
51	B	293/297 (99%)	289 (99%)	4 (1%)	0	100	100
52	BO	197/203 (97%)	197 (100%)	0	0	100	100
53	Ae	189/204 (93%)	185 (98%)	4 (2%)	0	100	100
54	Bb	103/245 (42%)	97 (94%)	6 (6%)	0	100	100
55	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
56	DA	153/403 (38%)	152 (99%)	1 (1%)	0	100	100
57	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
58	Bc	106/115 (92%)	106 (100%)	0	0	100	100
59	BF	224/247 (91%)	218 (97%)	5 (2%)	1 (0%)	30	63
60	DC	163/235 (69%)	162 (99%)	1 (1%)	0	100	100
61	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
62	Bd	105/125 (84%)	105 (100%)	0	0	100	100
64	Ah	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
65	Be	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
66	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
67	Ai	183/194 (94%)	179 (98%)	4 (2%)	0	100	100
68	Bf	108/110 (98%)	108 (100%)	0	0	100	100
69	AB	61/69 (88%)	61 (100%)	0	0	100	100
70	Aj	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
71	Bg	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
72	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	Ak	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
74	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
75	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
76	Al	122/132 (92%)	118 (97%)	4 (3%)	0	100	100
77	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
78	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
79	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
80	Bj	84/97 (87%)	84 (100%)	0	0	100	100
81	AF	311/317 (98%)	305 (98%)	6 (2%)	0	100	100
82	An	132/151 (87%)	128 (97%)	4 (3%)	0	100	100
83	Bk	67/70 (96%)	67 (100%)	0	0	100	100
84	AG	53/56 (95%)	53 (100%)	0	0	100	100
85	Ao	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
86	Bl	48/51 (94%)	48 (100%)	0	0	100	100
88	Ap	139/172 (81%)	133 (96%)	6 (4%)	0	100	100
89	Bm	49/128 (38%)	49 (100%)	0	0	100	100
All	All	13062/15567 (84%)	12867 (98%)	193 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
50	Ba	15	VAL
59	BF	196	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BP	134/163 (82%)	134 (100%)	0	100	100
2	Aq	120/121 (99%)	119 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Bo	92/93 (99%)	92 (100%)	0	100	100
5	Ar	127/130 (98%)	123 (97%)	4 (3%)	35	67
6	Cu	89/136 (65%)	89 (100%)	0	100	100
7	BL	175/176 (99%)	173 (99%)	2 (1%)	65	82
8	BX	106/134 (79%)	106 (100%)	0	100	100
9	Bp	74/75 (99%)	73 (99%)	1 (1%)	59	79
10	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	81
11	As	112/114 (98%)	112 (100%)	0	100	100
12	Br	109/119 (92%)	109 (100%)	0	100	100
13	BR	159/175 (91%)	158 (99%)	1 (1%)	78	87
14	At	94/107 (88%)	92 (98%)	2 (2%)	47	74
15	Bs	164/258 (64%)	164 (100%)	0	100	100
16	BG	199/223 (89%)	197 (99%)	2 (1%)	68	83
17	BU	91/113 (80%)	88 (97%)	3 (3%)	33	65
18	Av	112/113 (99%)	111 (99%)	1 (1%)	70	84
19	DB	746/806 (93%)	729 (98%)	17 (2%)	44	72
20	Ct	99/202 (49%)	97 (98%)	2 (2%)	48	75
21	BH	169/171 (99%)	169 (100%)	0	100	100
22	BV	106/107 (99%)	106 (100%)	0	100	100
23	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	76
25	BT	139/140 (99%)	139 (100%)	0	100	100
26	BI	180/181 (99%)	179 (99%)	1 (1%)	78	87
27	BW	100/126 (79%)	99 (99%)	1 (1%)	68	83
28	Ax	107/112 (96%)	107 (100%)	0	100	100
30	Au	67/67 (100%)	65 (97%)	2 (3%)	36	68
31	BJ	143/149 (96%)	143 (100%)	0	100	100
32	AZ	182/242 (75%)	179 (98%)	3 (2%)	55	78
33	Ay	75/102 (74%)	74 (99%)	1 (1%)	61	80
36	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	83
37	Az	24/24 (100%)	24 (100%)	0	100	100
38	BA	194/198 (98%)	193 (100%)	1 (0%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	56
40	BM	117/161 (73%)	117 (100%)	0	100	100
41	Ab	185/223 (83%)	183 (99%)	2 (1%)	65	82
42	BY	124/135 (92%)	124 (100%)	0	100	100
43	BB	344/347 (99%)	340 (99%)	4 (1%)	63	81
44	BS	154/154 (100%)	154 (100%)	0	100	100
45	Ac	189/232 (82%)	187 (99%)	2 (1%)	65	82
46	BZ	117/118 (99%)	117 (100%)	0	100	100
47	BC	302/336 (90%)	302 (100%)	0	100	100
48	BN	171/172 (99%)	171 (100%)	0	100	100
49	Ad	224/225 (100%)	224 (100%)	0	100	100
50	Ba	118/119 (99%)	118 (100%)	0	100	100
51	B	247/250 (99%)	247 (100%)	0	100	100
52	BO	171/173 (99%)	169 (99%)	2 (1%)	63	81
53	Ae	161/170 (95%)	161 (100%)	0	100	100
54	Bb	87/183 (48%)	87 (100%)	0	100	100
55	BE	216/251 (86%)	215 (100%)	1 (0%)	81	88
56	DA	137/355 (39%)	136 (99%)	1 (1%)	76	85
57	Af	207/218 (95%)	206 (100%)	1 (0%)	81	88
58	Bc	92/98 (94%)	92 (100%)	0	100	100
59	BF	197/215 (92%)	197 (100%)	0	100	100
60	DC	141/202 (70%)	140 (99%)	1 (1%)	76	85
61	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	87
62	Bd	98/110 (89%)	98 (100%)	0	100	100
64	Ah	178/180 (99%)	177 (99%)	1 (1%)	78	87
65	Be	116/121 (96%)	116 (100%)	0	100	100
66	AA	75/76 (99%)	74 (99%)	1 (1%)	61	80
67	Ai	161/168 (96%)	160 (99%)	1 (1%)	78	87
68	Bf	89/89 (100%)	89 (100%)	0	100	100
69	AB	56/62 (90%)	55 (98%)	1 (2%)	51	76
70	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	Bg	98/99 (99%)	97 (99%)	1 (1%)	68	83
72	AC	67/140 (48%)	67 (100%)	0	100	100
73	Ak	139/142 (98%)	139 (100%)	0	100	100
74	Bh	109/110 (99%)	109 (100%)	0	100	100
75	AD	47/106 (44%)	47 (100%)	0	100	100
76	Al	104/108 (96%)	101 (97%)	3 (3%)	37	68
77	Bi	86/89 (97%)	86 (100%)	0	100	100
78	AE	88/98 (90%)	86 (98%)	2 (2%)	44	72
79	Am	130/131 (99%)	130 (100%)	0	100	100
80	Bj	73/80 (91%)	73 (100%)	0	100	100
81	AF	272/275 (99%)	269 (99%)	3 (1%)	65	82
82	An	105/118 (89%)	102 (97%)	3 (3%)	37	68
83	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	78
84	AG	48/49 (98%)	48 (100%)	0	100	100
85	Ao	114/130 (88%)	113 (99%)	1 (1%)	70	84
86	Bl	47/48 (98%)	47 (100%)	0	100	100
88	Ap	117/140 (84%)	117 (100%)	0	100	100
89	Bm	47/115 (41%)	47 (100%)	0	100	100
All	All	11381/13206 (86%)	11290 (99%)	91 (1%)	70	85

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	Ab	121	ARG
61	Ag	53	VAL
43	BB	39	LYS
52	BO	126	VAL
69	AB	14	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
64	Ah	7	ASN
88	Ap	97	GLN
66	AA	29	ASN

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Mol	Chain	Res	Type
77	Bi	15	HIS
27	BW	120	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	B5	3694/4808 (76%)	434 (11%)	2 (0%)
29	B7	118/119 (99%)	6 (5%)	0
34	B8	155/158 (98%)	15 (9%)	0
4	AT	2/76 (2%)	1 (50%)	0
63	A2	1765/1870 (94%)	208 (11%)	1 (0%)
87	AH	0/3	-	-
All	All	5734/7034 (81%)	664 (11%)	3 (0%)

5 of 664 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	AT	76	A
24	B5	39	A
24	B5	42	A
24	B5	59	A
24	B5	64	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	B5	1588	G
24	B5	4445	U
63	A2	1	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
63	PSU	A2	1239	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
89	M3L	Bm	98	89	10,11,12	0.83	0	9,14,16	0.53	0
63	OMU	A2	429	63	19,22,23	1.20	2 (10%)	26,31,34	1.69	4 (15%)
47	AYA	BC	2	47	6,7,8	0.71	0	5,8,10	0.36	0
63	PSU	A2	36	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	1718	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	4298	24	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
24	A2M	B5	3557	24	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
24	PSU	B5	4169	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
24	OMG	B5	1477	24	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
63	PSU	A2	109	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	1057	63	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	1491	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	4267	90,24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	967	63	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	OMG	B5	4240	24	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
24	PSU	B5	3462	24	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	573	63	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
63	A2M	A2	577	63	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
63	OMG	A2	645	63	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
63	PSU	A2	1046	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
63	PSU	A2	1175	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
24	A2M	B5	400	24	22,25,26	1.47	4 (18%)	31,36,39	2.09	10 (32%)
24	PSU	B5	3585	90,24	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
63	PSU	A2	610	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
38	V5N	BA	216	38	9,11,12	2.09	2 (22%)	9,14,16	1.72	2 (22%)
63	OMG	A2	1448	63	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
24	A2M	B5	4269	90,24	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
30	AME	Au	1	30	9,10,11	0.48	0	9,11,13	0.86	1 (11%)
24	OMG	B5	1260	24	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
24	UY1	B5	3550	24	19,22,23	1.39	3 (15%)	22,31,34	1.89	5 (22%)
63	4AC	A2	1843	63	21,24,25	1.11	2 (9%)	29,34,37	1.27	3 (10%)
63	PSU	A2	1693	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	OMU	A2	1443	90,63	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)
24	OMG	B5	3524	24	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PSU	A2	867	63	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	6MZ	B5	3966	24	22,25,26	1.44	4 (18%)	30,36,39	2.18	9 (30%)
34	OMG	B8	75	34	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
24	OMC	B5	2647	24	19,22,23	0.81	0	26,31,34	0.82	0
63	OMG	A2	868	63	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
24	PSU	B5	3554	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	2208	90,24	19,22,23	0.81	0	26,31,34	0.83	0
24	PSU	B5	4374	24	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
63	PSU	A2	119	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
63	PSU	A2	1626	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
63	OMC	A2	174	90,63	19,22,23	0.81	0	26,31,34	0.82	0
63	PSU	A2	650	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	1082	63	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
63	PSU	A2	407	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	4202	24	19,22,23	0.81	0	26,31,34	0.77	0
24	OMC	B5	2704	24	19,22,23	0.81	0	26,31,34	0.83	0
24	PSU	B5	4749	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
43	HIC	BB	245	43	10,11,12	0.61	0	8,14,16	0.39	0
63	A2M	A2	1679	63	22,25,26	1.45	4 (18%)	31,36,39	2.24	10 (32%)
63	MA6	A2	1851	63	23,26,27	2.28	5 (21%)	34,38,41	3.71	13 (38%)
24	PSU	B5	4099	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
63	6MZ	A2	1833	90,63	22,25,26	1.45	4 (18%)	30,36,39	2.16	9 (30%)
63	A2M	A2	669	90,63	22,25,26	1.45	4 (18%)	31,36,39	2.12	10 (32%)
24	OMG	B5	2207	24	23,26,27	1.18	3 (13%)	33,38,41	1.93	6 (18%)
24	PSU	B5	4435	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	34	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
24	UR3	B5	4276	24	19,22,23	0.99	0	26,32,35	1.41	1 (3%)
63	A2M	A2	513	63	22,25,26	1.48	4 (18%)	31,36,39	2.13	10 (32%)
24	PSU	B5	2351	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	OMG	B5	4369	24	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
24	A2M	B5	2206	90,24	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
24	OMG	B5	4138	24	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
24	PSU	B5	3427	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	4177	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	A2M	B5	2658	90,24	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
24	OMG	B5	3676	24	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	A2M	B5	2244	90,24	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
63	PSU	A2	218	63	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	3500	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
63	A2M	A2	99	90,63	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
63	PSU	A2	1233	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	4042	24	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
24	A2M	B5	3450	24	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
24	A2M	B5	4317	24	22,25,26	1.47	4 (18%)	31,36,39	2.14	9 (29%)
63	PSU	A2	93	63	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	OMU	B5	4244	24	19,22,23	1.21	2 (10%)	26,31,34	1.70	5 (19%)
63	OMU	A2	355	63	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
24	PSU	B5	3466	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	1799	24	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	3494	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	4149	24	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
24	PSU	B5	4217	24	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
63	OMU	A2	1805	63	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
63	B8N	A2	1249	63	24,29,30	1.31	3 (12%)	29,42,45	1.30	3 (10%)
63	4AC	A2	1338	63	21,24,25	1.07	2 (9%)	29,34,37	1.21	3 (10%)
63	PSU	A2	802	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
63	OMU	A2	121	63	19,22,23	1.21	3 (15%)	26,31,34	1.66	4 (15%)
24	OMG	B5	4245	24	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
24	A2M	B5	3517	24	22,25,26	1.44	4 (18%)	31,36,39	2.22	11 (35%)
24	PSU	B5	3652	90,24	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	105	63	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	682	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
63	OMC	A2	463	63	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
24	OMG	B5	2267	24	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
24	OMC	B5	3573	24	19,22,23	0.81	0	26,31,34	0.91	1 (3%)
24	OMC	B5	3601	24	19,22,23	0.81	0	26,31,34	0.80	0
50	V5N	Ba	39	50	9,11,12	2.09	2 (22%)	9,14,16	1.71	2 (22%)
24	PSU	B5	4058	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
63	A2M	A2	591	63	22,25,26	1.49	4 (18%)	31,36,39	2.20	7 (22%)
63	A2M	A2	1032	63	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
24	A2M	B5	1270	24	22,25,26	1.46	4 (18%)	31,36,39	2.10	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	OMC	B5	3433	24	19,22,23	0.79	0	26,31,34	0.75	0
24	PSU	B5	3583	24	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
24	OMC	B5	4282	90,24	19,22,23	0.82	0	26,31,34	0.85	0
24	A2M	B5	1479	24	22,25,26	1.46	4 (18%)	31,36,39	2.11	8 (25%)
63	PSU	A2	1047	63	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
24	OMG	B5	4116	24	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
63	A2M	A2	485	63	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
24	PSU	B5	2475	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4278	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
24	PSU	B5	4382	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	A2M	B5	1489	90,24	22,25,26	1.46	4 (18%)	31,36,39	2.09	9 (29%)
24	OMG	B5	3359	24	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
63	PSU	A2	864	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4166	24	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
63	OMG	A2	684	63	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
24	PSU	B5	1720	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	1638	24	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	PSU	A2	210	63	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
24	OMC	B5	3540	24	19,22,23	0.82	0	26,31,34	0.81	0
24	PSU	B5	3447	24	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
24	A2M	B5	4336	24	22,25,26	1.45	4 (18%)	31,36,39	2.15	10 (32%)
63	OMG	A2	510	90,63	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
63	PSU	A2	1368	63	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
63	OMG	A2	437	63	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
63	A2M	A2	469	63	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
24	PSU	B5	4107	24	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
34	PSU	B8	55	34	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
63	PSU	A2	816	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	1348	63	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	3496	24	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
24	OMG	B5	3974	24	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
63	OMC	A2	518	63	19,22,23	0.82	0	26,31,34	0.81	0
24	A2M	B5	2630	90,24	22,25,26	1.45	4 (18%)	31,36,39	2.15	9 (29%)
24	1MA	B5	1266	90,24	21,25,26	1.38	4 (19%)	31,37,40	1.71	5 (16%)
63	MA6	A2	1852	63	23,26,27	2.25	5 (21%)	34,38,41	3.68	13 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	OMU	B5	3657	24	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
24	PSU	B5	3576	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4740	24	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
24	PSU	B5	1537	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	2265	90,24	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
63	OMU	A2	172	63	19,22,23	1.20	2 (10%)	26,31,34	1.68	5 (19%)
63	OMU	A2	116	63	19,22,23	1.18	2 (10%)	26,31,34	1.69	5 (19%)
63	A2M	A2	1384	63	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
24	OMC	B5	1820	90,24	19,22,23	0.80	0	26,31,34	0.79	0
82	IAS	An	138	82	6,7,8	0.97	0	6,8,10	1.38	1 (16%)
63	PSU	A2	1178	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	PSU	A2	1005	63	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
23	HY3	Aw	62	23	6,8,9	2.06	1 (16%)	5,10,12	1.12	1 (20%)
24	PSU	B5	3502	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
63	A2M	A2	27	90,63	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
24	PSU	B5	4039	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	5MC	B5	4193	24	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
3	MLZ	Bo	53	3	8,9,10	0.40	0	4,9,11	0.15	0
63	OMG	A2	1329	63	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
63	PSU	A2	687	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	1284	24	19,22,23	0.81	0	26,31,34	0.79	0
11	NMM	As	67	11	9,11,12	0.60	0	6,12,14	0.43	0
24	PSU	B5	1801	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
63	PSU	A2	1245	63	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
63	OMC	A2	1392	63	19,22,23	0.82	0	26,31,34	0.83	0
24	PSU	B5	4045	24	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
24	OMU	B5	4052	24	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
24	PSU	B5	1632	24	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
24	PSU	B5	1721	24	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	4203	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
63	PSU	A2	1446	63	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
24	OMG	B5	4383	24	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
5	SAC	Ar	2	5	7,8,9	0.54	0	8,9,11	0.90	1 (12%)
24	OMU	B5	2680	24	19,22,23	1.21	2 (10%)	26,31,34	1.72	4 (15%)
63	OMU	A2	1289	63	19,22,23	1.23	3 (15%)	26,31,34	1.68	5 (19%)
12	SAC	Br	2	12	7,8,9	0.52	0	8,9,11	0.83	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	B5	4419	24	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
63	OMC	A2	1704	63	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
63	G7M	A2	1640	63	23,26,27	3.14	9 (39%)	35,39,42	3.33	13 (37%)
63	OMG	A2	602	63	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
54	MLZ	Bb	5	54	8,9,10	0.49	0	4,9,11	0.18	0
24	5MC	B5	3514	90,24	18,22,23	0.95	2 (11%)	26,32,35	1.14	3 (11%)
24	OMC	B5	2194	90,24	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
63	A2M	A2	159	63	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
63	PSU	A2	823	63	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
24	PSU	B5	1731	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMU	B5	2258	24	19,22,23	1.22	3 (15%)	26,31,34	1.67	4 (15%)
24	OMG	B5	3631	24	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
63	OMU	A2	1327	90,63	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
24	PSU	B5	1683	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	PSU	B5	3490	24	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	4325	24	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	A2M	B5	3456	24	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
34	PSU	B8	69	34	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
24	OMG	B5	3942	4,24	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
24	PSU	B5	4188	24	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
24	A2M	B5	398	24	22,25,26	1.47	4 (18%)	31,36,39	2.16	10 (32%)
24	PSU	B5	4322	24	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
24	A2M	B5	3492	24,63	22,25,26	1.47	4 (18%)	31,36,39	2.17	10 (32%)
24	OMU	B5	4366	24	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
24	OMU	B5	3973	24	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)
24	OMG	B5	1580	24	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
24	PSU	B5	3369	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
24	PSU	B5	3371	24	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
63	OMU	A2	628	63	19,22,23	1.17	2 (10%)	26,31,34	1.69	5 (19%)
24	OMG	B5	3476	24	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
24	OMG	B5	2719	24	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)
24	PSU	B5	4246	24	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
63	PSU	A2	815	63	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
24	OMC	B5	2667	24	19,22,23	0.81	0	26,31,34	0.80	0
24	OMG	B5	4364	24	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	A2M	B5	3599	24	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
63	OMG	A2	1491	90,63	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
63	PSU	A2	652	63	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
24	PSU	B5	3616	24	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
63	PSU	A2	1644	90,63	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
24	OMC	B5	3619	24	19,22,23	0.81	0	26,31,34	0.84	0
24	A2M	B5	1810	90,24	22,25,26	1.47	4 (18%)	31,36,39	2.18	10 (32%)
24	A2M	B5	3562	24	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
32	SAC	AZ	2	32	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
24	PSU	B5	4711	24	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
63	A2M	A2	166	63	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)

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
63	PSU	A2	1239	63	-	0/7/25/26	0/2/2/2
89	M3L	Bm	98	89	-	0/9/10/12	-
63	OMU	A2	429	63	-	6/9/27/28	0/2/2/2
47	AYA	BC	2	47	-	3/4/6/8	-
63	PSU	A2	36	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	1718	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4298	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3557	24	-	1/9/27/28	0/3/3/3
24	PSU	B5	4169	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	1477	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	109	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1057	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	1491	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4267	90,24	-	0/7/25/26	0/2/2/2
63	PSU	A2	967	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4240	24	-	0/9/27/28	0/3/3/3
24	PSU	B5	3462	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	573	63	-	0/7/25/26	0/2/2/2
63	A2M	A2	577	63	-	2/9/27/28	0/3/3/3
63	OMG	A2	645	63	-	3/9/27/28	0/3/3/3
63	PSU	A2	1046	63	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PSU	A2	1175	63	-	0/7/25/26	0/2/2/2
24	A2M	B5	400	24	-	0/9/27/28	0/3/3/3
24	PSU	B5	3585	90,24	-	0/7/25/26	0/2/2/2
63	PSU	A2	610	63	-	0/7/25/26	0/2/2/2
38	V5N	BA	216	38	-	3/9/10/12	0/1/1/1
63	OMG	A2	1448	63	-	3/9/27/28	0/3/3/3
24	A2M	B5	4269	90,24	-	0/9/27/28	0/3/3/3
30	AME	Au	1	30	-	2/9/10/12	-
24	OMG	B5	1260	24	-	1/9/27/28	0/3/3/3
24	UY1	B5	3550	24	-	1/9/27/28	0/2/2/2
63	4AC	A2	1843	63	-	4/11/29/30	0/2/2/2
63	PSU	A2	1693	63	-	0/7/25/26	0/2/2/2
63	OMU	A2	1443	90,63	-	0/9/27/28	0/2/2/2
24	OMG	B5	3524	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	867	63	-	0/7/25/26	0/2/2/2
24	6MZ	B5	3966	24	-	0/9/27/28	0/3/3/3
34	OMG	B8	75	34	-	0/9/27/28	0/3/3/3
24	OMC	B5	2647	24	-	0/9/27/28	0/2/2/2
63	OMG	A2	868	63	-	2/9/27/28	0/3/3/3
24	PSU	B5	3554	24	-	0/7/25/26	0/2/2/2
24	OMC	B5	2208	90,24	-	0/9/27/28	0/2/2/2
24	PSU	B5	4374	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	119	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1626	63	-	0/7/25/26	0/2/2/2
63	OMC	A2	174	90,63	-	0/9/27/28	0/2/2/2
63	PSU	A2	650	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1082	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	407	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	4202	24	-	0/9/27/28	0/2/2/2
24	OMC	B5	2704	24	-	1/9/27/28	0/2/2/2
24	PSU	B5	4749	24	-	0/7/25/26	0/2/2/2
43	HIC	BB	245	43	-	2/5/6/8	0/1/1/1
63	A2M	A2	1679	63	-	0/9/27/28	0/3/3/3
63	MA6	A2	1851	63	-	0/11/29/30	0/3/3/3
24	PSU	B5	4099	24	-	0/7/25/26	0/2/2/2
63	6MZ	A2	1833	90,63	-	0/9/27/28	0/3/3/3
63	A2M	A2	669	90,63	-	3/9/27/28	0/3/3/3
24	OMG	B5	2207	24	-	3/9/27/28	0/3/3/3
24	PSU	B5	4435	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	34	63	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	UR3	B5	4276	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	513	63	-	2/9/27/28	0/3/3/3
24	PSU	B5	2351	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	4369	24	-	0/9/27/28	0/3/3/3
24	A2M	B5	2206	90,24	-	0/9/27/28	0/3/3/3
24	OMG	B5	4138	24	-	1/9/27/28	0/3/3/3
24	PSU	B5	3427	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4177	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	2658	90,24	-	0/9/27/28	0/3/3/3
24	OMG	B5	3676	24	-	2/9/27/28	0/3/3/3
24	A2M	B5	2244	90,24	-	0/9/27/28	0/3/3/3
63	PSU	A2	218	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3500	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	99	90,63	-	2/9/27/28	0/3/3/3
63	PSU	A2	1233	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4042	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3450	24	-	0/9/27/28	0/3/3/3
24	A2M	B5	4317	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	93	63	-	0/7/25/26	0/2/2/2
24	OMU	B5	4244	24	-	0/9/27/28	0/2/2/2
63	OMU	A2	355	63	-	1/9/27/28	0/2/2/2
24	PSU	B5	3466	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1799	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	3494	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4149	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4217	24	-	0/7/25/26	0/2/2/2
63	OMU	A2	1805	63	-	0/9/27/28	0/2/2/2
63	B8N	A2	1249	63	-	4/16/34/35	0/2/2/2
63	4AC	A2	1338	63	-	3/11/29/30	0/2/2/2
63	PSU	A2	802	63	-	0/7/25/26	0/2/2/2
63	OMU	A2	121	63	-	0/9/27/28	0/2/2/2
24	OMG	B5	4245	24	-	0/9/27/28	0/3/3/3
24	A2M	B5	3517	24	-	2/9/27/28	0/3/3/3
24	PSU	B5	3652	90,24	-	0/7/25/26	0/2/2/2
63	PSU	A2	105	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	682	63	-	0/7/25/26	0/2/2/2
63	OMC	A2	463	63	-	0/9/27/28	0/2/2/2
24	OMG	B5	2267	24	-	0/9/27/28	0/3/3/3
24	OMC	B5	3573	24	-	0/9/27/28	0/2/2/2
24	OMC	B5	3601	24	-	0/9/27/28	0/2/2/2
50	V5N	Ba	39	50	-	1/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	B5	4058	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	591	63	-	4/9/27/28	0/3/3/3
63	A2M	A2	1032	63	-	0/9/27/28	0/3/3/3
24	A2M	B5	1270	24	-	0/9/27/28	0/3/3/3
24	OMC	B5	3433	24	-	4/9/27/28	0/2/2/2
24	PSU	B5	3583	24	-	0/7/25/26	0/2/2/2
24	OMC	B5	4282	90,24	-	1/9/27/28	0/2/2/2
24	A2M	B5	1479	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	1047	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4116	24	-	0/9/27/28	0/3/3/3
63	A2M	A2	485	63	-	0/9/27/28	0/3/3/3
24	PSU	B5	2475	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4278	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4382	24	-	4/7/25/26	0/2/2/2
24	A2M	B5	1489	90,24	-	2/9/27/28	0/3/3/3
24	OMG	B5	3359	24	-	0/9/27/28	0/3/3/3
63	PSU	A2	864	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	4166	24	-	2/7/25/26	0/2/2/2
63	OMG	A2	684	63	-	1/9/27/28	0/3/3/3
24	PSU	B5	1720	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1638	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	210	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	3540	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	3447	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	4336	24	-	1/9/27/28	0/3/3/3
63	OMG	A2	510	90,63	-	2/9/27/28	0/3/3/3
63	PSU	A2	1368	63	-	0/7/25/26	0/2/2/2
63	OMG	A2	437	63	-	0/9/27/28	0/3/3/3
63	A2M	A2	469	63	-	0/9/27/28	0/3/3/3
24	PSU	B5	4107	24	-	0/7/25/26	0/2/2/2
34	PSU	B8	55	34	-	0/7/25/26	0/2/2/2
63	PSU	A2	816	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1348	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3496	24	-	0/7/25/26	0/2/2/2
24	OMG	B5	3974	24	-	0/9/27/28	0/3/3/3
63	OMC	A2	518	63	-	0/9/27/28	0/2/2/2
24	A2M	B5	2630	90,24	-	2/9/27/28	0/3/3/3
24	1MA	B5	1266	90,24	-	0/7/25/26	0/3/3/3
63	MA6	A2	1852	63	-	2/11/29/30	0/3/3/3
24	OMU	B5	3657	24	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	B5	3576	24	-	1/7/25/26	0/2/2/2
24	PSU	B5	4740	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1537	24	-	0/7/25/26	0/2/2/2
24	OMC	B5	2265	90,24	-	1/9/27/28	0/2/2/2
63	OMU	A2	172	63	-	0/9/27/28	0/2/2/2
63	OMU	A2	116	63	-	0/9/27/28	0/2/2/2
63	A2M	A2	1384	63	-	0/9/27/28	0/3/3/3
24	OMC	B5	1820	90,24	-	1/9/27/28	0/2/2/2
82	IAS	An	138	82	-	2/7/7/8	-
63	PSU	A2	1178	63	-	0/7/25/26	0/2/2/2
63	PSU	A2	1005	63	-	0/7/25/26	0/2/2/2
23	HY3	Aw	62	23	-	1/1/12/14	0/1/1/1
24	PSU	B5	3502	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	27	90,63	-	1/9/27/28	0/3/3/3
24	PSU	B5	4039	24	-	0/7/25/26	0/2/2/2
24	5MC	B5	4193	24	-	4/7/25/26	0/2/2/2
3	MLZ	Bo	53	3	-	1/7/8/10	-
63	OMG	A2	1329	63	-	0/9/27/28	0/3/3/3
63	PSU	A2	687	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	1284	24	-	1/9/27/28	0/2/2/2
11	NMM	As	67	11	-	0/9/11/13	-
24	PSU	B5	1801	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	1245	63	-	0/7/25/26	0/2/2/2
63	OMC	A2	1392	63	-	0/9/27/28	0/2/2/2
24	PSU	B5	4045	24	-	0/7/25/26	0/2/2/2
24	OMU	B5	4052	24	-	0/9/27/28	0/2/2/2
24	PSU	B5	1632	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	1721	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4203	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	1446	63	-	0/7/25/26	0/2/2/2
24	OMG	B5	4383	24	-	1/9/27/28	0/3/3/3
5	SAC	Ar	2	5	-	0/7/8/10	-
24	OMU	B5	2680	24	-	1/9/27/28	0/2/2/2
63	OMU	A2	1289	63	-	0/9/27/28	0/2/2/2
12	SAC	Br	2	12	-	0/7/8/10	-
24	PSU	B5	4419	24	-	0/7/25/26	0/2/2/2
63	OMC	A2	1704	63	-	1/9/27/28	0/2/2/2
63	G7M	A2	1640	63	-	2/7/25/26	0/3/3/3
63	OMG	A2	602	63	-	0/9/27/28	0/3/3/3
54	MLZ	Bb	5	54	-	2/7/8/10	-
24	5MC	B5	3514	90,24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OMC	B5	2194	90,24	-	2/9/27/28	0/2/2/2
63	A2M	A2	159	63	-	0/9/27/28	0/3/3/3
63	PSU	A2	823	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	1731	24	-	0/7/25/26	0/2/2/2
24	OMU	B5	2258	24	-	0/9/27/28	0/2/2/2
24	OMG	B5	3631	24	-	1/9/27/28	0/3/3/3
63	OMU	A2	1327	90,63	-	0/9/27/28	0/2/2/2
24	PSU	B5	1683	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	3490	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	4325	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3456	24	-	0/9/27/28	0/3/3/3
34	PSU	B8	69	34	-	0/7/25/26	0/2/2/2
24	OMG	B5	3942	4,24	-	0/9/27/28	0/3/3/3
24	PSU	B5	4188	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	398	24	-	4/9/27/28	0/3/3/3
24	PSU	B5	4322	24	-	0/7/25/26	0/2/2/2
24	A2M	B5	3492	24,63	-	2/9/27/28	0/3/3/3
24	OMU	B5	4366	24	-	0/9/27/28	0/2/2/2
24	OMU	B5	3973	24	-	0/9/27/28	0/2/2/2
24	OMG	B5	1580	24	-	0/9/27/28	0/3/3/3
24	PSU	B5	3369	24	-	0/7/25/26	0/2/2/2
24	PSU	B5	3371	24	-	0/7/25/26	0/2/2/2
63	OMU	A2	628	63	-	4/9/27/28	0/2/2/2
24	OMG	B5	3476	24	-	1/9/27/28	0/3/3/3
24	OMG	B5	2719	24	-	0/9/27/28	0/3/3/3
24	PSU	B5	4246	24	-	1/7/25/26	0/2/2/2
63	PSU	A2	815	63	-	0/7/25/26	0/2/2/2
24	OMC	B5	2667	24	-	1/9/27/28	0/2/2/2
24	OMG	B5	4364	24	-	0/9/27/28	0/3/3/3
24	A2M	B5	3599	24	-	0/9/27/28	0/3/3/3
63	OMG	A2	1491	90,63	-	0/9/27/28	0/3/3/3
63	PSU	A2	652	63	-	0/7/25/26	0/2/2/2
24	PSU	B5	3616	24	-	0/7/25/26	0/2/2/2
63	PSU	A2	1644	90,63	-	0/7/25/26	0/2/2/2
24	OMC	B5	3619	24	-	3/9/27/28	0/2/2/2
24	A2M	B5	1810	90,24	-	1/9/27/28	0/3/3/3
24	A2M	B5	3562	24	-	0/9/27/28	0/3/3/3
32	SAC	AZ	2	32	-	2/7/8/10	-
24	PSU	B5	4711	24	-	0/7/25/26	0/2/2/2
63	A2M	A2	166	63	-	0/9/27/28	0/3/3/3

The worst 5 of 505 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	A2	1640	G7M	C4-N9	7.86	1.58	1.38
63	A2	1640	G7M	O6-C6	7.68	1.38	1.23
63	A2	1851	MA6	C5-N7	6.88	1.52	1.39
63	A2	1852	MA6	C5-N7	6.78	1.51	1.39
63	A2	1640	G7M	C5-C4	6.21	1.54	1.38

The worst 5 of 956 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	A2	1851	MA6	C4-N9-C8	14.73	121.69	105.73
63	A2	1852	MA6	C4-N9-C8	14.45	121.39	105.73
63	A2	1640	G7M	C8-N7-C5	11.45	122.10	107.78
63	A2	591	A2M	C5-C4-N3	-6.94	117.69	126.75
63	A2	1852	MA6	N3-C4-N9	6.89	138.43	127.08

There are no chirality outliers.

5 of 125 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Bo	53	MLZ	O-C-CA-CB
24	B5	3433	OMC	C2'-C1'-N1-C2
24	B5	3433	OMC	C2'-C1'-N1-C6
24	B5	3517	A2M	O4'-C4'-C5'-O5'
24	B5	4166	PSU	C2'-C1'-C5-C4

There are no ring outliers.

87 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	A2	36	PSU	1	0
24	B5	1718	PSU	1	0
24	B5	3557	A2M	1	0
63	A2	577	A2M	1	0
24	B5	400	A2M	1	0
63	A2	1448	OMG	2	0
24	B5	4269	A2M	2	0
30	Au	1	AME	1	0
24	B5	1260	OMG	1	0
24	B5	3550	UY1	2	0
63	A2	1843	4AC	2	0
63	A2	1443	OMU	1	0
24	B5	3524	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B8	75	OMG	1	0
24	B5	2647	OMC	1	0
24	B5	4202	OMC	1	0
24	B5	2704	OMC	1	0
43	BB	245	HIC	1	0
63	A2	1679	A2M	1	0
24	B5	4099	PSU	1	0
63	A2	1833	6MZ	1	0
24	B5	2207	OMG	2	0
63	A2	513	A2M	1	0
24	B5	2206	A2M	2	0
24	B5	4138	OMG	1	0
24	B5	2658	A2M	2	0
24	B5	3676	OMG	1	0
63	A2	99	A2M	2	0
63	A2	1233	PSU	2	0
24	B5	3450	A2M	2	0
63	A2	355	OMU	1	0
63	A2	1805	OMU	2	0
63	A2	1338	4AC	4	0
63	A2	121	OMU	2	0
24	B5	3517	A2M	2	0
63	A2	105	PSU	1	0
63	A2	463	OMC	2	0
24	B5	3573	OMC	1	0
24	B5	4058	PSU	1	0
63	A2	1032	A2M	2	0
24	B5	1270	A2M	2	0
24	B5	4282	OMC	1	0
63	A2	485	A2M	1	0
24	B5	4382	PSU	2	0
24	B5	3540	OMC	1	0
24	B5	4336	A2M	1	0
63	A2	510	OMG	1	0
63	A2	437	OMG	1	0
63	A2	469	A2M	1	0
24	B5	3974	OMG	1	0
63	A2	518	OMC	1	0
63	A2	172	OMU	2	0
63	A2	116	OMU	1	0
63	A2	1384	A2M	1	0
82	An	138	IAS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	A2	27	A2M	1	0
24	B5	4039	PSU	1	0
63	A2	1329	OMG	1	0
24	B5	1284	OMC	3	0
63	A2	1392	OMC	1	0
24	B5	4052	OMU	2	0
24	B5	1632	PSU	1	0
24	B5	4203	PSU	1	0
24	B5	4383	OMG	1	0
63	A2	1289	OMU	2	0
63	A2	1704	OMC	1	0
63	A2	1640	G7M	1	0
63	A2	602	OMG	1	0
24	B5	2194	OMC	1	0
63	A2	159	A2M	1	0
63	A2	823	PSU	1	0
24	B5	2258	OMU	2	0
24	B5	3631	OMG	1	0
24	B5	4325	PSU	1	0
24	B5	3456	A2M	2	0
24	B5	3942	OMG	2	0
24	B5	398	A2M	1	0
24	B5	4366	OMU	3	0
24	B5	3476	OMG	1	0
63	A2	815	PSU	1	0
24	B5	4364	OMG	1	0
63	A2	1491	OMG	1	0
24	B5	3616	PSU	1	0
24	B5	3619	OMC	1	0
24	B5	1810	A2M	2	0
24	B5	3562	A2M	2	0
63	A2	166	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 769 ligands modelled in this entry, 428 are monoatomic and 306 are unknown - 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	A2	1978	-	9,9,9	0.15	0	8,8,8	0.20	0
94	SPD	A2	1971	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	A2	1950	-	9,9,9	0.15	0	8,8,8	0.19	0
94	SPD	B5	5041	-	9,9,9	0.14	0	8,8,8	0.20	0
94	SPD	A2	1985	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	5082	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5343	-	9,9,9	0.15	0	8,8,8	0.17	0
95	SPM	B5	5018	-	13,13,13	0.15	0	12,12,12	0.22	0
94	SPD	A2	1957	-	9,9,9	0.15	0	8,8,8	0.19	0
95	SPM	A2	1994	-	13,13,13	0.15	0	12,12,12	0.16	0
96	GTP	B7	216	29	30,34,34	0.50	0	46,54,54	0.55	0
94	SPD	A2	1964	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	4933	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5244	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5205	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	A2	1943	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	B5	5322	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	4975	-	9,9,9	0.16	0	8,8,8	0.19	0
95	SPM	B5	5061	-	13,13,13	0.15	0	12,12,12	0.14	0
94	SPD	B5	4945	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5144	-	9,9,9	0.15	0	8,8,8	0.22	0
94	SPD	B5	4997	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5103	-	9,9,9	0.15	0	8,8,8	0.17	0
94	SPD	A2	1986	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	4912	-	9,9,9	0.16	0	8,8,8	0.17	0
94	SPD	B5	5165	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5405	-	9,9,9	0.16	0	8,8,8	0.18	0
94	SPD	B5	5363	-	9,9,9	0.16	0	8,8,8	0.19	0
94	SPD	B5	5123	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	4954	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5385	-	9,9,9	0.15	0	8,8,8	0.18	0
94	SPD	B5	5263	-	9,9,9	0.16	0	8,8,8	0.15	0
94	SPD	B5	5302	-	9,9,9	0.15	0	8,8,8	0.15	0
93	IHP	DB	901	-	36,36,36	1.55	6 (16%)	54,60,60	1.09	3 (5%)
94	SPD	B5	5224	-	9,9,9	0.16	0	8,8,8	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	SPD	A2	1978	-	-	1/7/7/7	-
94	SPD	A2	1971	-	-	0/7/7/7	-
94	SPD	A2	1950	-	-	0/7/7/7	-
94	SPD	B5	5041	-	-	0/7/7/7	-
94	SPD	A2	1985	-	-	1/7/7/7	-
94	SPD	B5	5082	-	-	0/7/7/7	-
94	SPD	B5	5343	-	-	1/7/7/7	-
95	SPM	B5	5018	-	-	1/11/11/11	-
94	SPD	A2	1957	-	-	0/7/7/7	-
95	SPM	A2	1994	-	-	2/11/11/11	-
96	GTP	B7	216	29	-	0/22/38/38	0/3/3/3
94	SPD	A2	1964	-	-	0/7/7/7	-
94	SPD	B5	4933	-	-	0/7/7/7	-
94	SPD	B5	5244	-	-	0/7/7/7	-
94	SPD	B5	5205	-	-	0/7/7/7	-
94	SPD	A2	1943	-	-	0/7/7/7	-
94	SPD	B5	5322	-	-	1/7/7/7	-
94	SPD	B5	4975	-	-	2/7/7/7	-
95	SPM	B5	5061	-	-	0/11/11/11	-
94	SPD	B5	4945	-	-	0/7/7/7	-
94	SPD	B5	5144	-	-	0/7/7/7	-
94	SPD	B5	4997	-	-	0/7/7/7	-
94	SPD	B5	5103	-	-	0/7/7/7	-
94	SPD	A2	1986	-	-	0/7/7/7	-
94	SPD	B5	4912	-	-	0/7/7/7	-
94	SPD	B5	5165	-	-	1/7/7/7	-
94	SPD	B5	5405	-	-	1/7/7/7	-
94	SPD	B5	5363	-	-	0/7/7/7	-
94	SPD	B5	5123	-	-	0/7/7/7	-
94	SPD	B5	4954	-	-	0/7/7/7	-
94	SPD	B5	5385	-	-	1/7/7/7	-
94	SPD	B5	5263	-	-	1/7/7/7	-
94	SPD	B5	5302	-	-	1/7/7/7	-
93	IHP	DB	901	-	-	8/30/54/54	0/1/1/1
94	SPD	B5	5224	-	-	1/7/7/7	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	DB	901	IHP	P2-O12	3.53	1.66	1.59
93	DB	901	IHP	P5-O15	3.43	1.65	1.59
93	DB	901	IHP	P1-O11	3.25	1.65	1.59
93	DB	901	IHP	P6-O16	3.24	1.65	1.59
93	DB	901	IHP	P4-O14	3.18	1.65	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	DB	901	IHP	C6-C5-C4	4.26	119.74	110.41
93	DB	901	IHP	C5-C4-C3	3.49	118.05	110.41
93	DB	901	IHP	C5-C6-C1	3.40	117.86	110.41

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
93	DB	901	IHP	C1-C2-O12-P2
93	DB	901	IHP	C4-C5-O15-P5
93	DB	901	IHP	C4-O14-P4-O24
95	A2	1994	SPM	C8-C9-N10-C11
93	DB	901	IHP	C2-O12-P2-O32

There are no ring outliers.

20 monomers are involved in 32 short contacts:

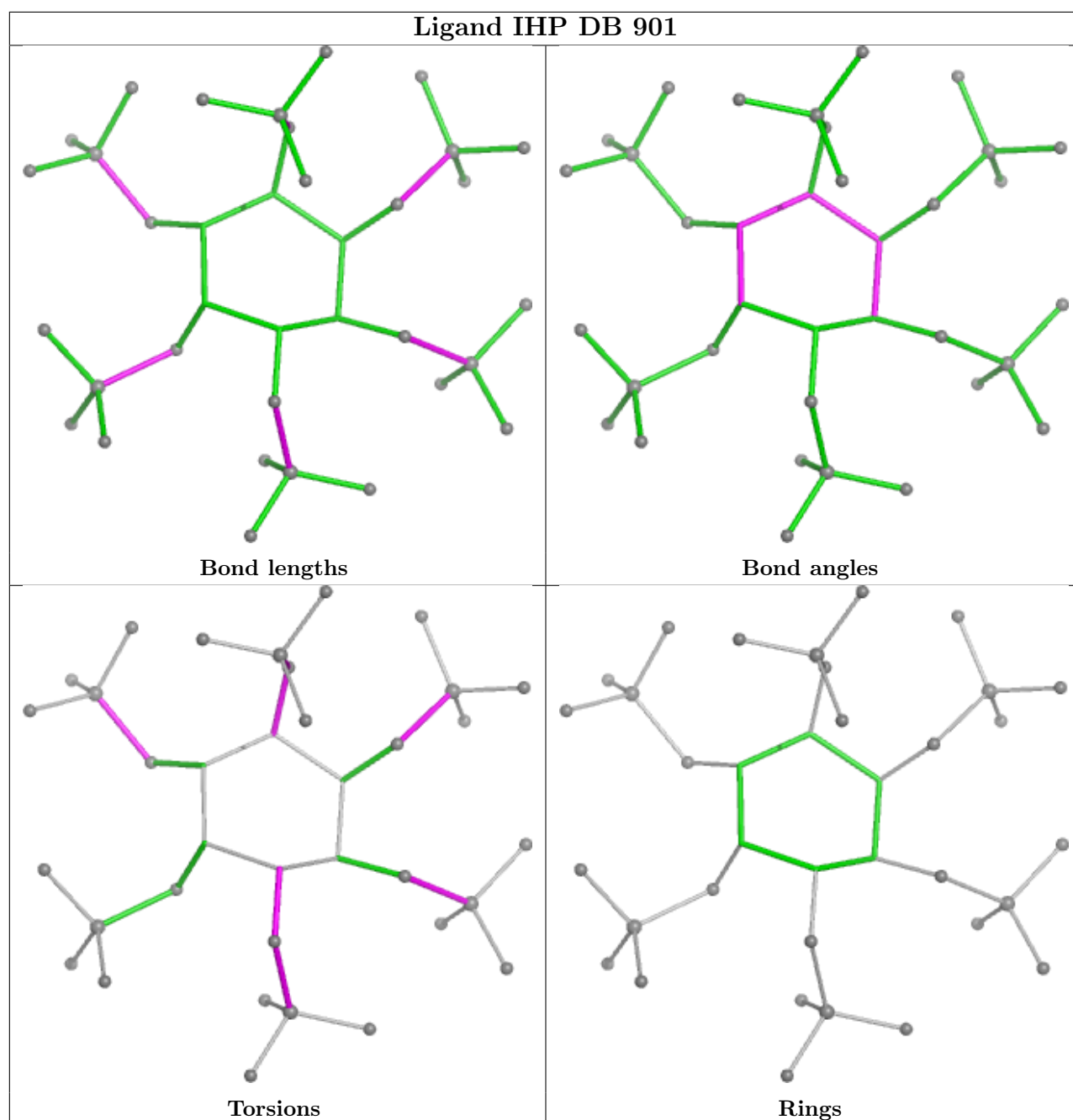
Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	A2	1978	SPD	1	0
94	A2	1971	SPD	1	0
94	A2	1950	SPD	2	0
94	A2	1985	SPD	2	0
94	B5	5082	SPD	2	0
94	B5	5343	SPD	1	0
95	B5	5018	SPM	3	0
94	A2	1957	SPD	1	0
95	A2	1994	SPM	3	0
94	A2	1964	SPD	1	0
94	B5	4933	SPD	2	0
94	B5	5244	SPD	1	0
94	B5	4975	SPD	1	0
94	B5	5144	SPD	2	0
94	A2	1986	SPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	B5	4912	SPD	1	0
94	B5	5165	SPD	1	0
94	B5	5405	SPD	1	0
94	B5	4954	SPD	2	0
94	B5	5263	SPD	3	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.

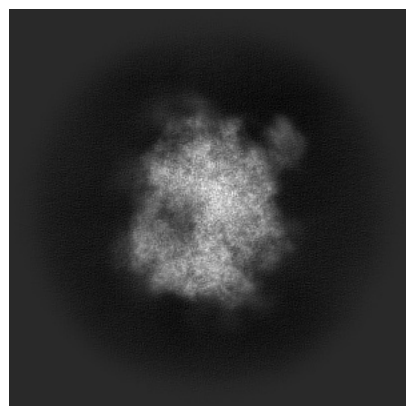
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50124. These allow visual inspection of the internal detail of the map and identification of artifacts.

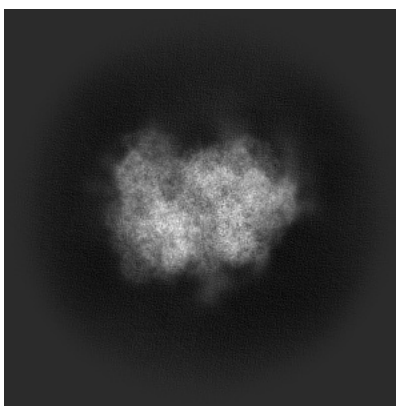
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

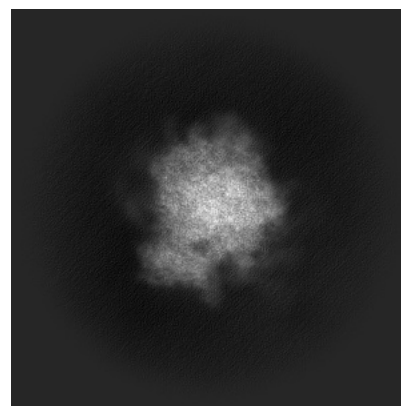
6.1.1 Primary map



X

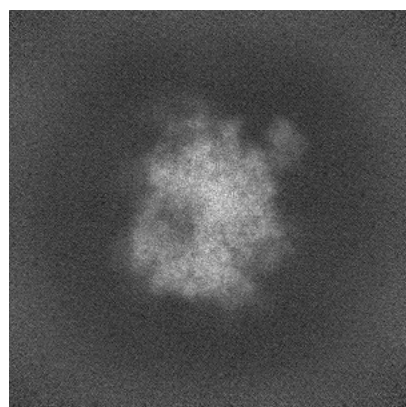


Y

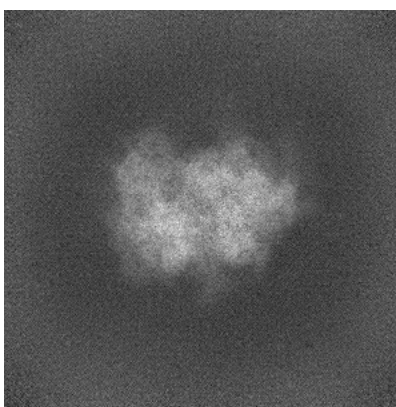


Z

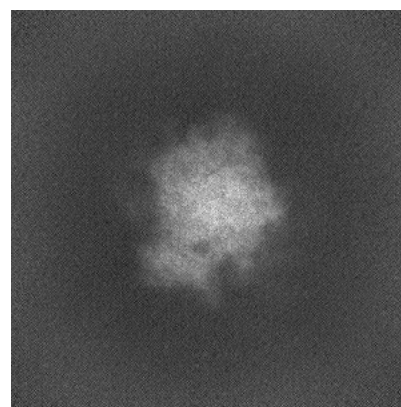
6.1.2 Raw map



X



Y

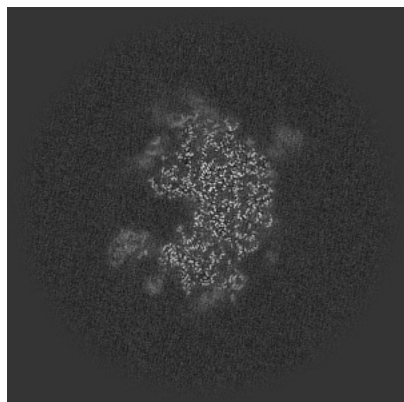


Z

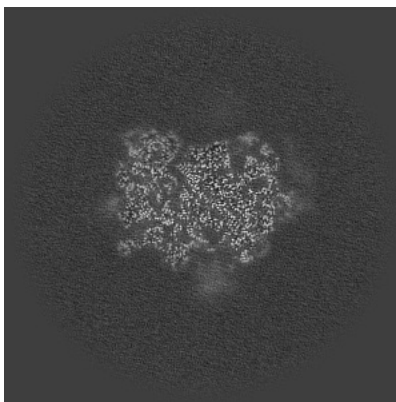
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

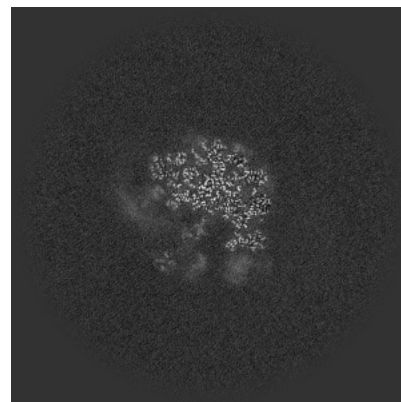
6.2.1 Primary map



X Index: 280

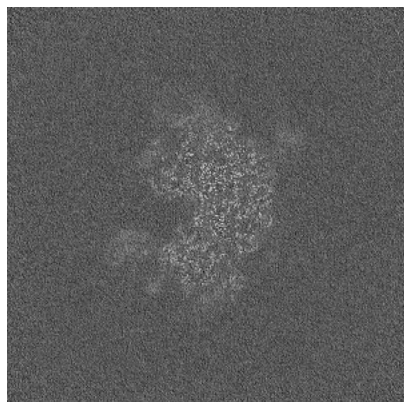


Y Index: 280

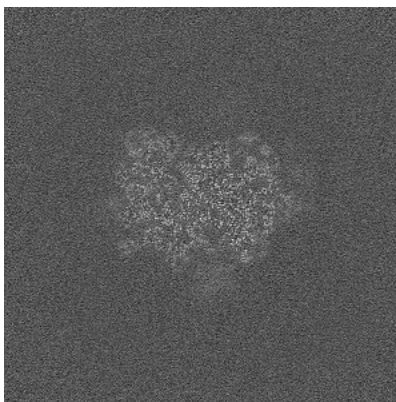


Z Index: 280

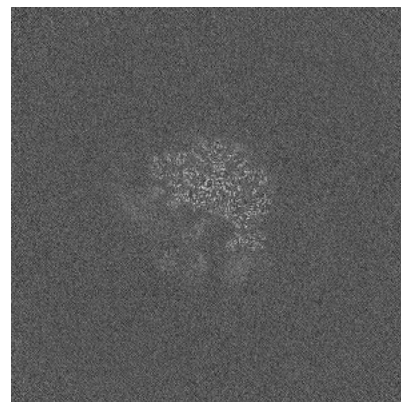
6.2.2 Raw map



X Index: 280



Y Index: 280

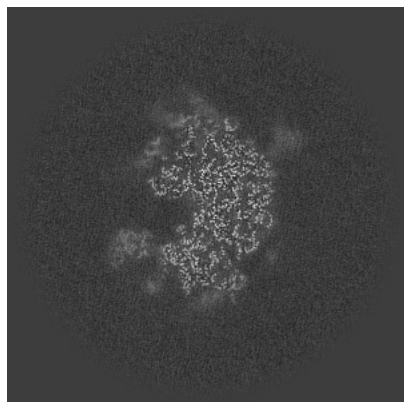


Z Index: 280

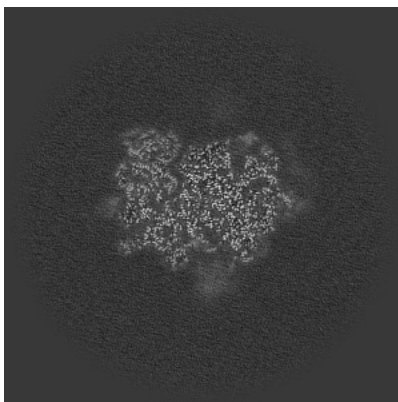
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

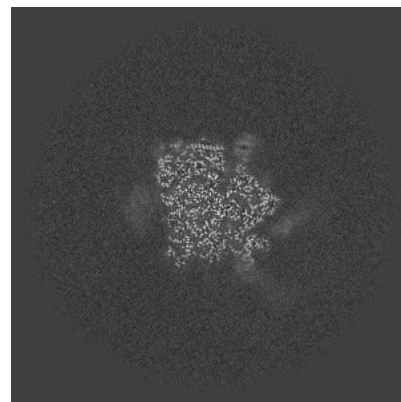
6.3.1 Primary map



X Index: 279

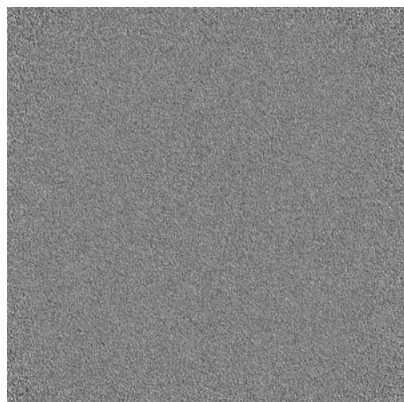


Y Index: 281

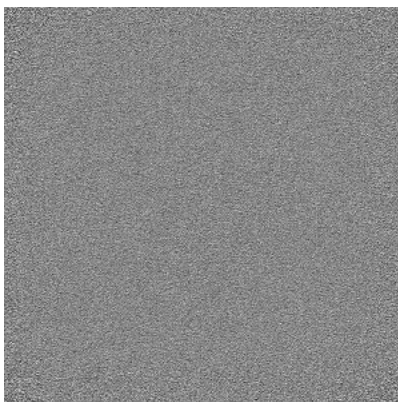


Z Index: 309

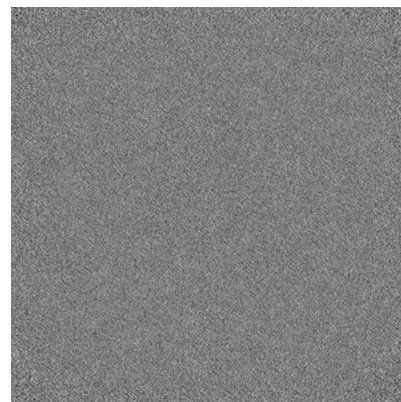
6.3.2 Raw map



X Index: 0



Y Index: 0

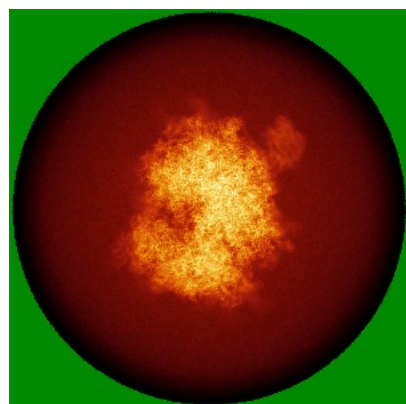


Z Index: 0

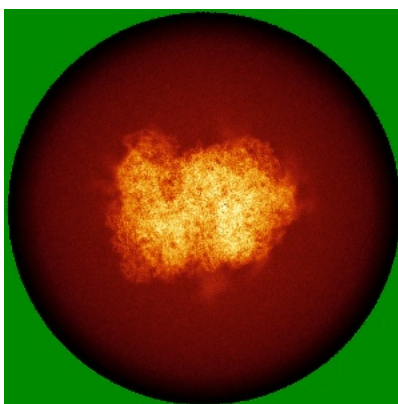
The images above show the largest variance slices of the map in three orthogonal directions.

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

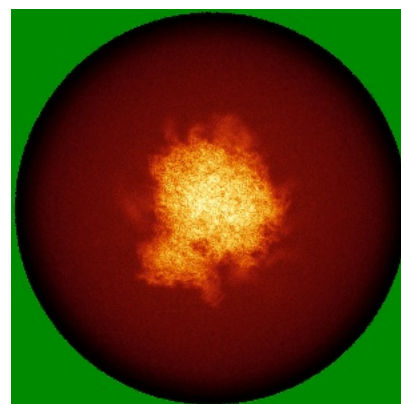
6.4.1 Primary map



X

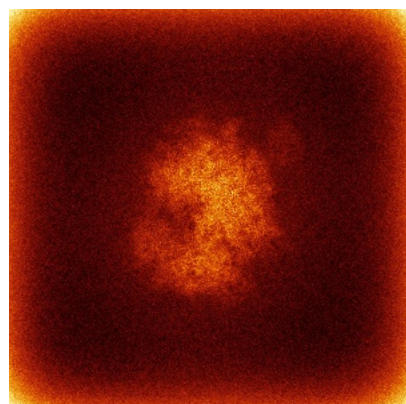


Y

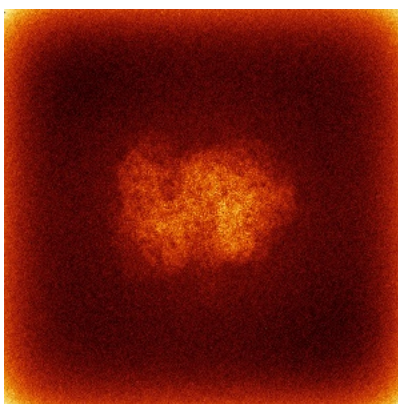


Z

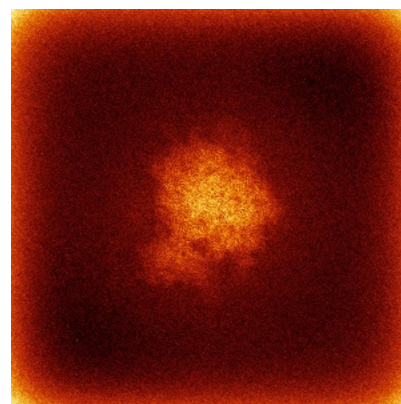
6.4.2 Raw map



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



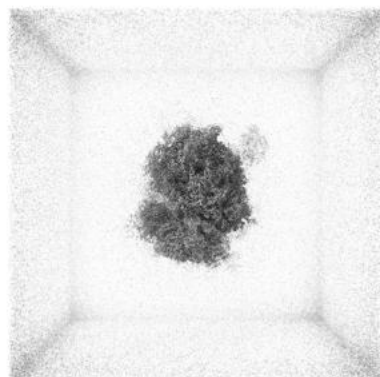
Y



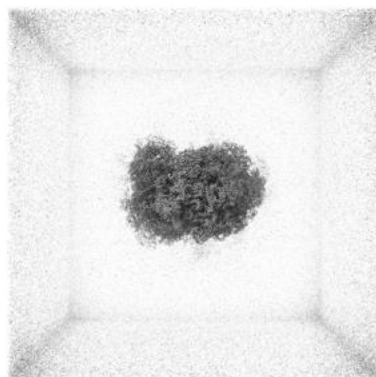
Z

The images above show the 3D surface view of the map at the recommended contour level 0.275. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

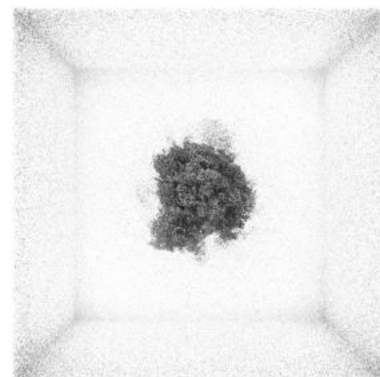
6.5.2 Raw map



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.

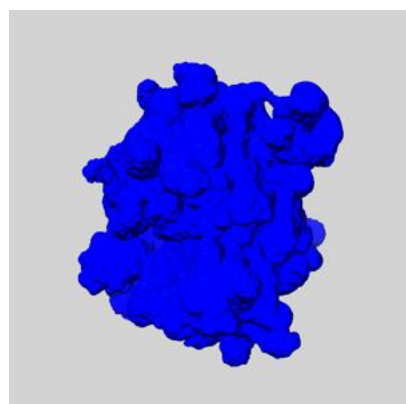
6.6 Mask visualisation [i](#)

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

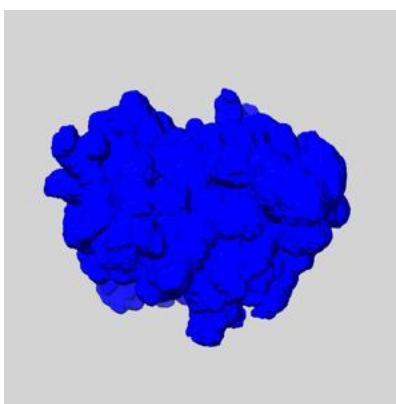
A mask typically either:

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

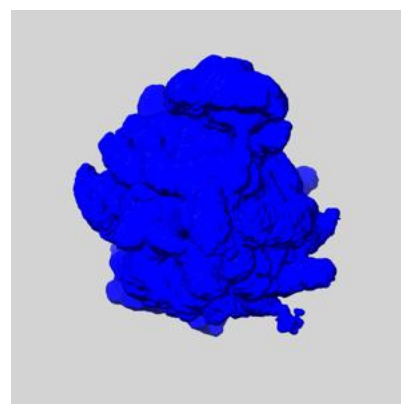
6.6.1 emd_50124_msk_1.map [i](#)



X

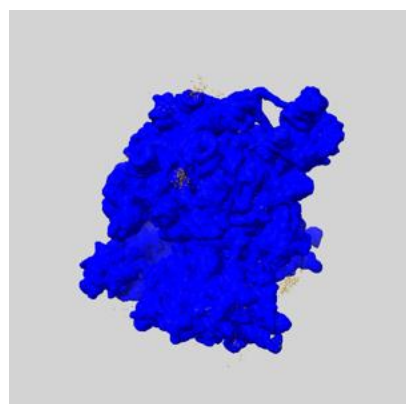


Y

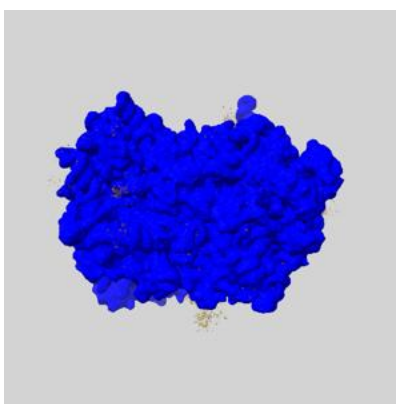


Z

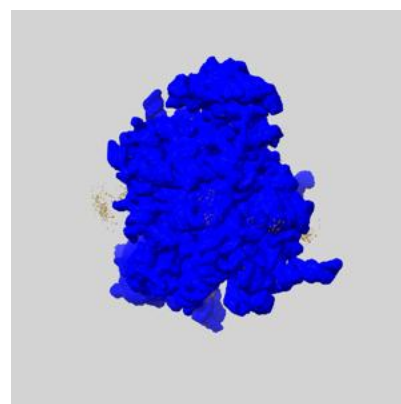
6.6.2 emd_50124_msk_2.map [i](#)



X



Y

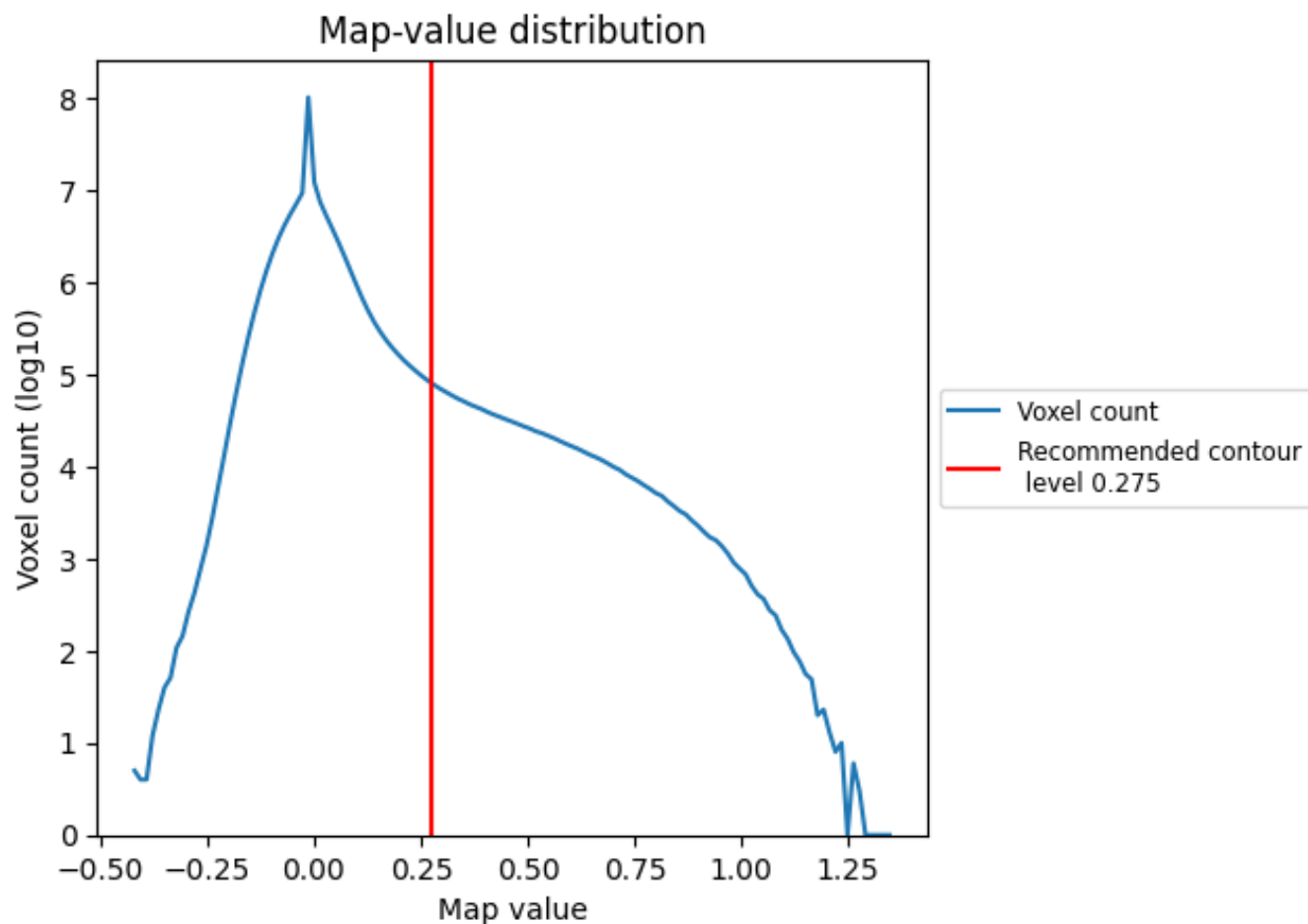


Z

7 Map analysis [i](#)

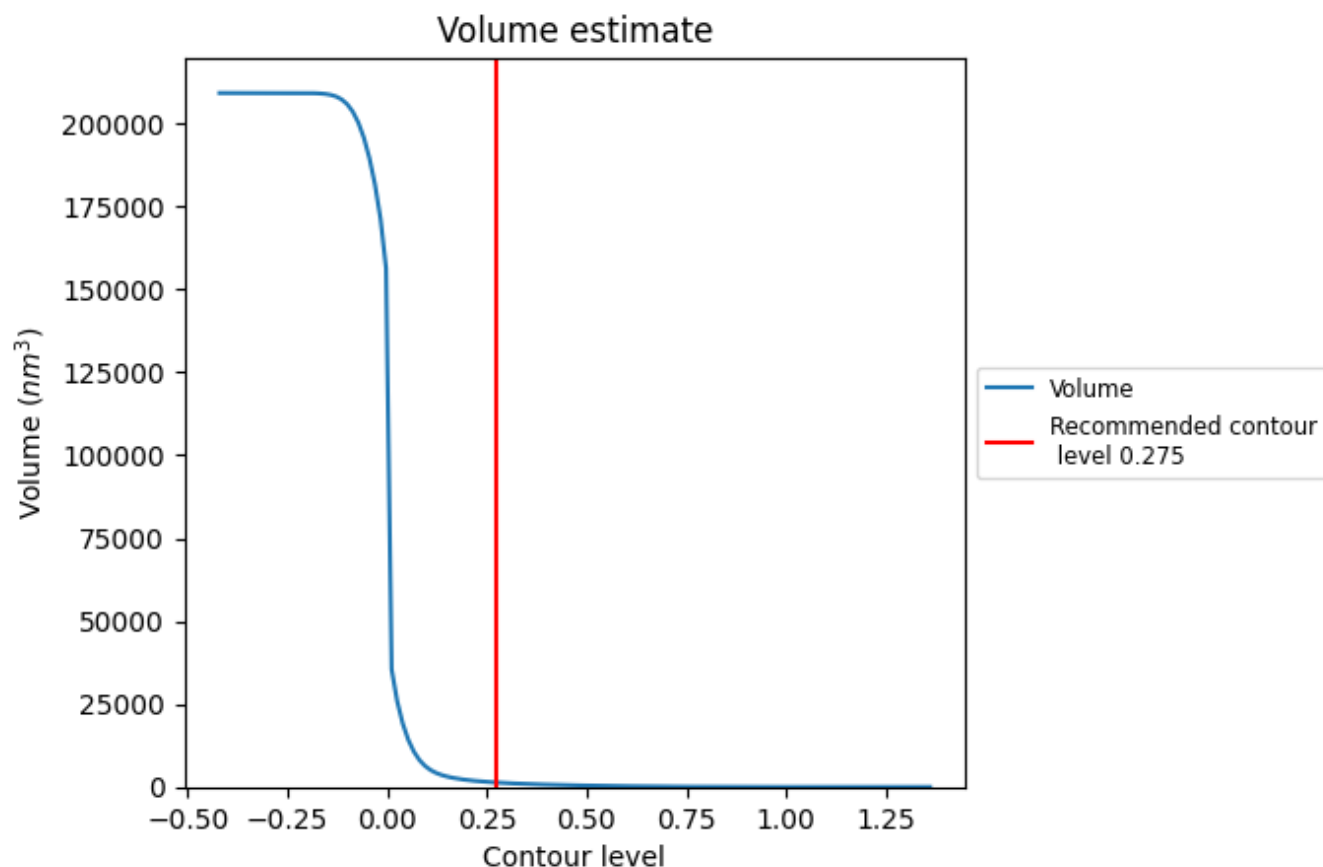
This section contains the results of statistical analysis of the map.

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.

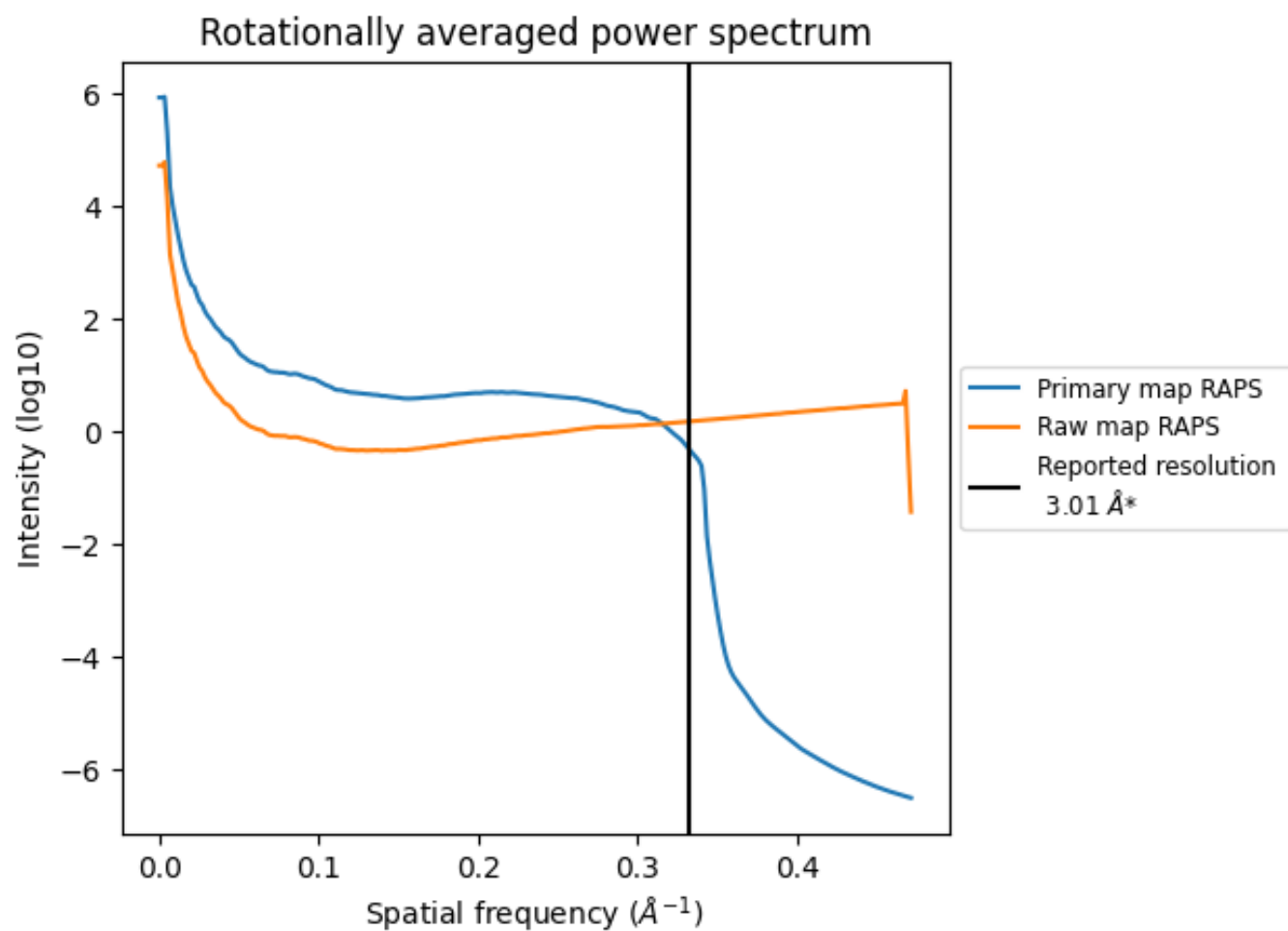
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1330 nm^3 ; this corresponds to an approximate mass of 1201 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 ⓘ

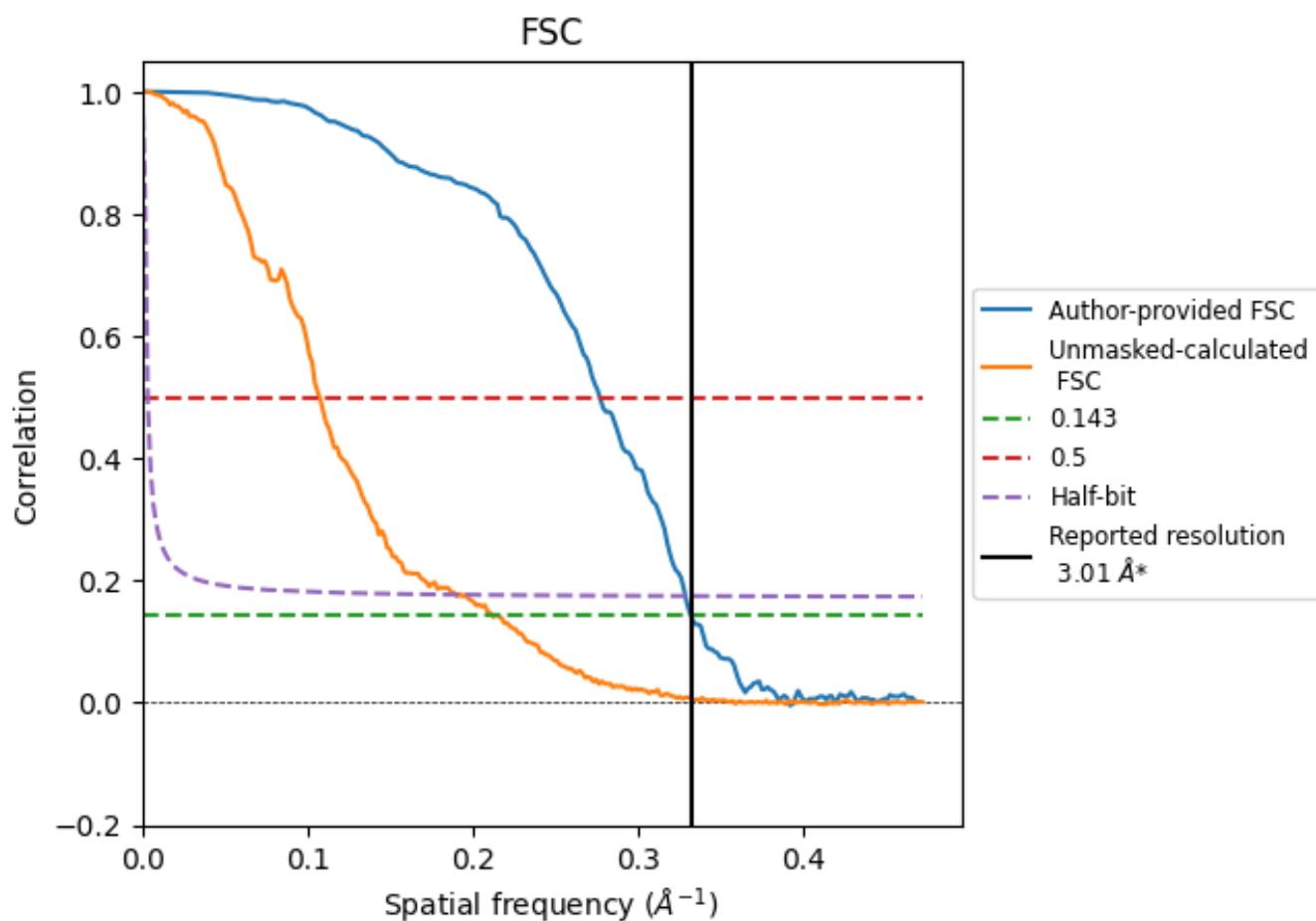


*Reported resolution corresponds to spatial frequency of 0.332 $\text{\AA}^{-1}$

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 $0.332 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

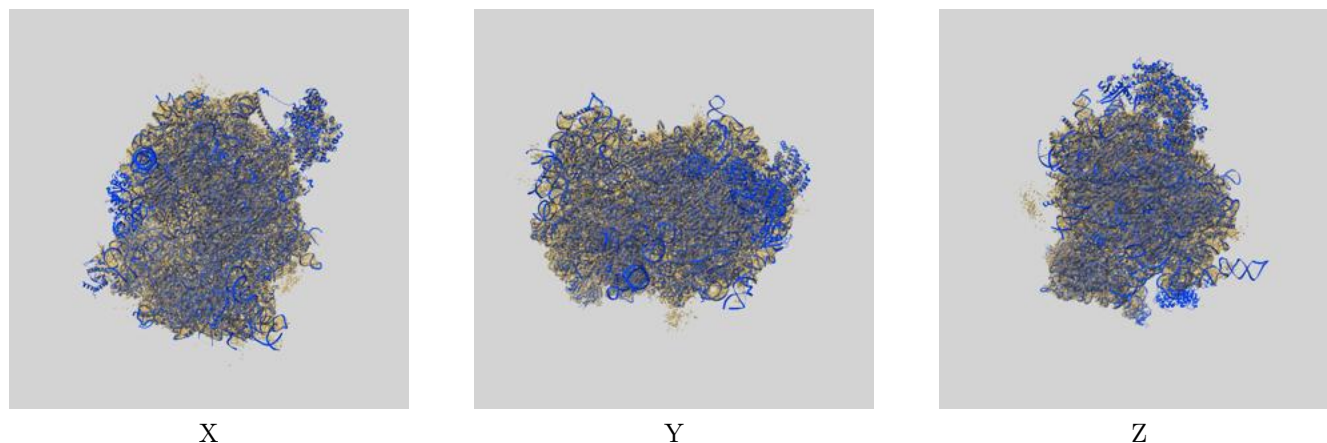
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.61	3.04
Unmasked-calculated*	4.73	9.33	5.27

*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 4.73 differs from the reported value 3.01 by more than 10 %

9 Map-model fit [i](#)

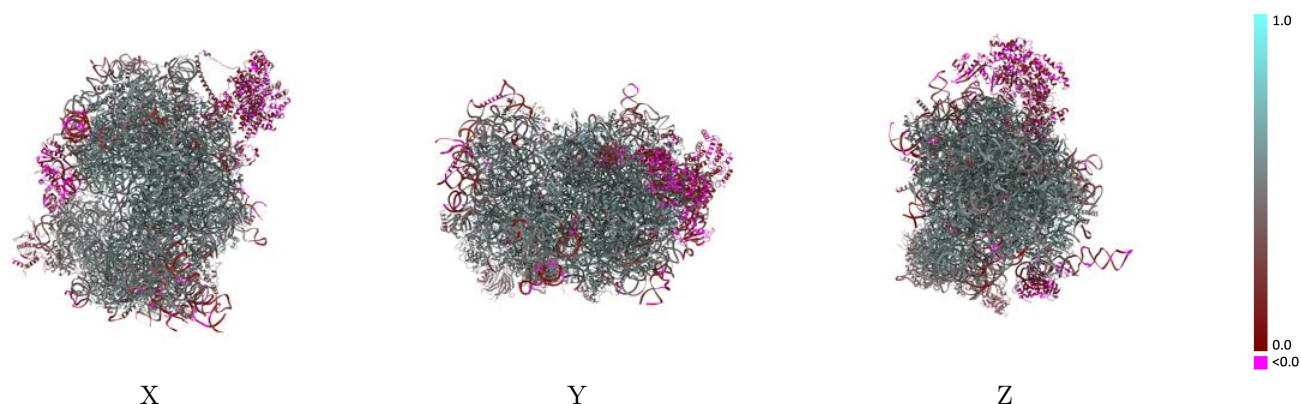
This section contains information regarding the fit between EMDB map EMD-50124 and PDB model 9F1B. Per-residue inclusion information can be found in [section 3](#) on [page 32](#).

9.1 Map-model overlay [i](#)



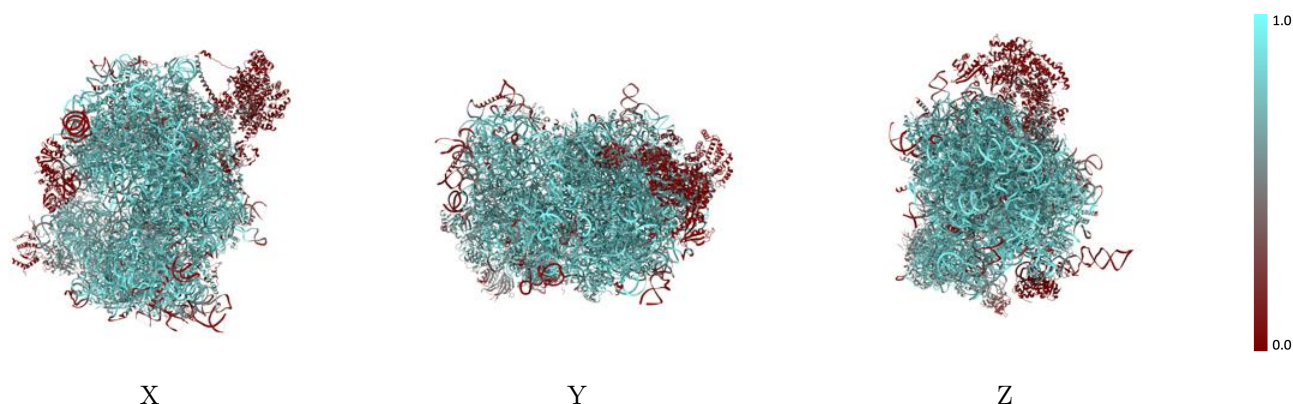
The images above show the 3D surface view of the map at the recommended contour level 0.275 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



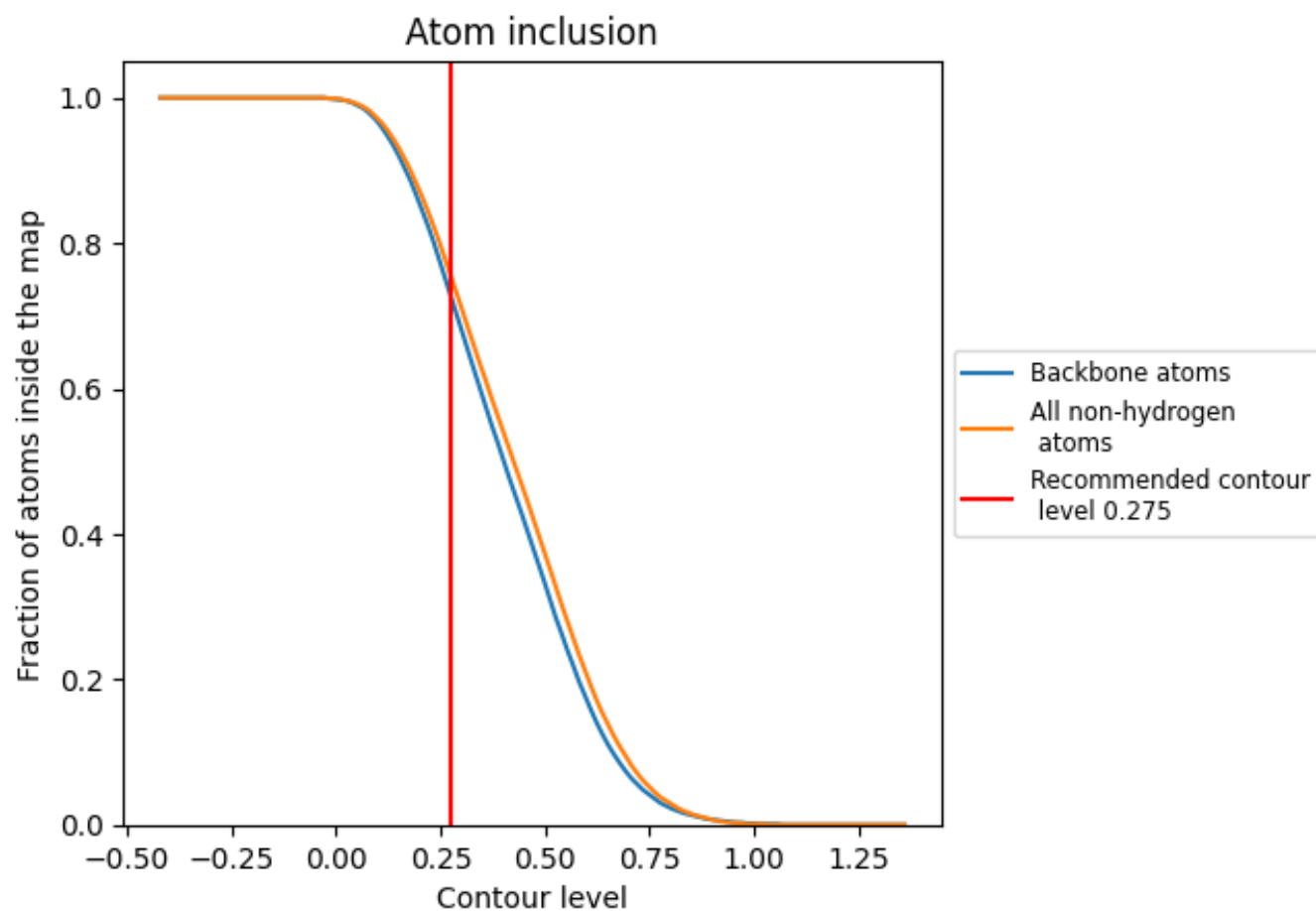
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.275).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 76% 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 (0.275) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.4750
A2	 0.8340	 0.4770
AA	 0.6760	 0.4940
AB	 0.6040	 0.4780
AC	 0.1580	 0.2200
AD	 0.5770	 0.4370
AE	 0.7980	 0.5180
AF	 0.4480	 0.3760
AG	 0.8120	 0.4960
AH	 0.1110	 0.3930
AT	 0.5350	 0.4300
AZ	 0.7000	 0.5000
Aa	 0.6880	 0.5030
Ab	 0.7800	 0.5250
Ac	 0.6100	 0.4320
Ad	 0.7770	 0.5190
Ae	 0.6640	 0.4740
Af	 0.6150	 0.4160
Ag	 0.5810	 0.4320
Ah	 0.7380	 0.5060
Ai	 0.7500	 0.4960
Aj	 0.5520	 0.3920
Ak	 0.7490	 0.5000
Al	 0.0760	 0.1840
Am	 0.7700	 0.5270
An	 0.7710	 0.5310
Ao	 0.5590	 0.4140
Ap	 0.7010	 0.4760
Aq	 0.6430	 0.4560
Ar	 0.6120	 0.4400
As	 0.6700	 0.4420
At	 0.6020	 0.4150
Au	 0.7330	 0.5060
Av	 0.8070	 0.5460
Aw	 0.8050	 0.5450



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Chain	Atom inclusion	Q-score
Ax	 0.7070	 0.4830
Ay	 0.5010	 0.3960
Az	 0.7390	 0.5400
B	 0.7510	 0.5210
B5	 0.8560	 0.5010
B7	 0.9420	 0.5520
B8	 0.9030	 0.5280
BA	 0.8510	 0.5690
BB	 0.8300	 0.5580
BC	 0.8460	 0.5570
BE	 0.7190	 0.4990
BF	 0.8490	 0.5600
BG	 0.7080	 0.4880
BH	 0.7620	 0.5330
BI	 0.7880	 0.5470
BJ	 0.6930	 0.5030
BK	 0.3310	 0.3920
BL	 0.7930	 0.5170
BM	 0.7900	 0.5200
BN	 0.9040	 0.5760
BO	 0.8470	 0.5610
BP	 0.8530	 0.5640
BQ	 0.8600	 0.5680
BR	 0.7950	 0.5200
BS	 0.8660	 0.5670
BT	 0.7900	 0.5340
BU	 0.6780	 0.4800
BV	 0.7760	 0.5450
BW	 0.5410	 0.3730
BX	 0.8060	 0.5380
BY	 0.7740	 0.5400
BZ	 0.7880	 0.5270
Ba	 0.8760	 0.5730
Bb	 0.6860	 0.4710
Bc	 0.6760	 0.4860
Bd	 0.8030	 0.5370
Be	 0.8540	 0.5620
Bf	 0.8500	 0.5750
Bg	 0.7930	 0.5360
Bh	 0.7850	 0.5290
Bi	 0.7700	 0.5150
Bj	 0.9140	 0.5780

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Chain	Atom inclusion	Q-score
Bk	 0.6550	 0.4820
Bl	 0.8760	 0.5530
Bm	 0.8190	 0.5500
Bo	 0.7960	 0.5480
Bp	 0.7920	 0.5460
Br	 0.8380	 0.5520
Bs	 0.0050	 0.0570
Bt	 0.0020	 0.0470
Ct	 0.1020	 0.1340
Cu	 0.2310	 0.2170
DA	 0.0050	 0.0410
DB	 0.1280	 0.1010
DC	 0.1200	 0.0860