



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 05:54 am BST

PDB ID : 8P2K / pdb_00008p2k
EMDB ID : EMD-17367
Title : Ternary complex of translating ribosome, NAC and METAP1
Authors : Jia, M.; Jaskolowski, M.; Scaiola, A.; Jomaa, A.; Ban, N.
Deposited on : 2023-05-16
Resolution : 2.90 Å (reported)
Based on initial models : 2B3K, 7QWR, 7O7Y

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

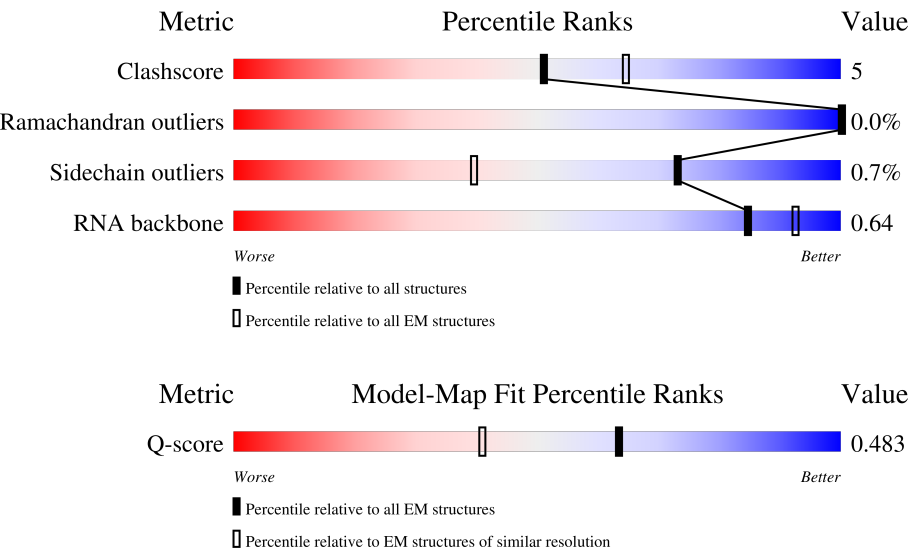
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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.



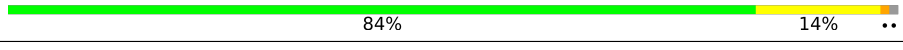
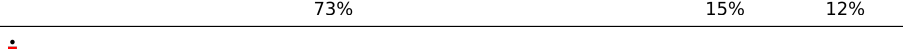
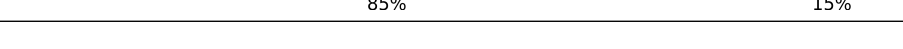
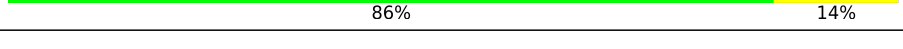
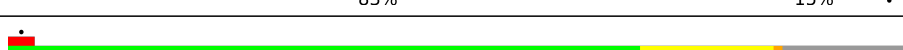
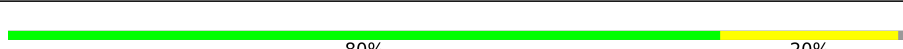
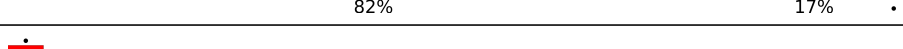
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	B5	4808	53%22%22%
2	B7	120	78%21%..
3	B8	158	70%25%..

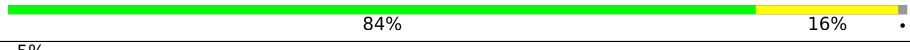
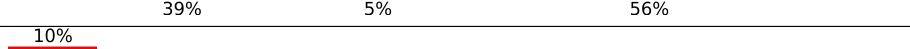
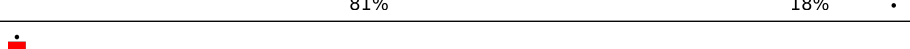
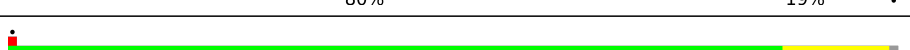
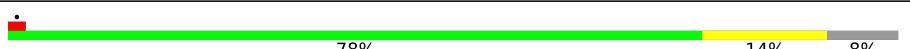
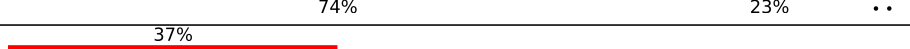
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Mol	Chain	Length	Quality of chain
4	BA	257	
5	BB	403	
6	BC	413	
7	BD	297	
8	BE	291	
9	BF	247	
10	BG	266	
11	BH	192	
12	BI	214	
13	BJ	178	
14	BK	65	
15	BL	211	
16	BM	218	
17	BN	204	
18	BO	203	
19	BP	184	
20	BQ	188	
21	BR	196	
22	BS	176	
23	BT	160	
24	BU	128	
25	BV	140	
26	BW	157	
27	BX	156	
28	BY	145	

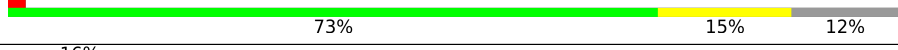
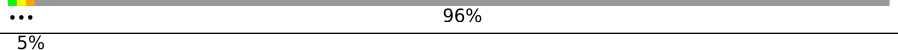
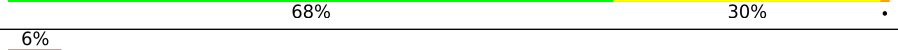
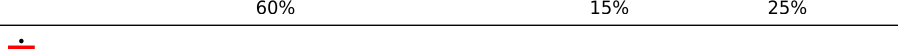
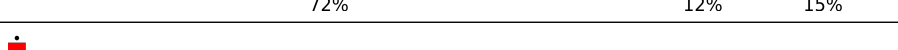
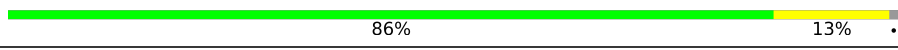
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Mol	Chain	Length	Quality of chain
29	BZ	136	
30	Ba	148	
31	Bb	245	
32	Bc	115	
33	Bd	125	
34	Be	135	
35	Bf	110	
36	Bg	117	
37	Bh	123	
38	Bi	105	
39	Bj	97	
40	Bk	70	
41	Bl	51	
42	Bm	128	
43	Bo	106	
44	Bp	92	
45	Br	137	
46	Bs	318	
47	Bt	165	
48	Bv	217	
49	MA	386	
50	Na	215	
51	Nb	132	
52	A2	1870	
53	AA	84	

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Mol	Chain	Length	Quality of chain
54	AB	69	
55	AC	156	
56	AD	133	
57	AE	115	
58	AF	317	
59	AG	56	
60	AI	76	
61	AT	76	
62	AZ	295	
63	Aa	264	
64	Ab	293	
65	Ac	281	
66	Ad	263	
67	Ae	204	
68	Af	249	
69	Ag	432	
70	Ah	208	
71	Ai	194	
72	Aj	165	
73	Ak	158	
74	Al	132	
75	Am	151	
76	An	151	
77	Ao	145	
78	Ap	172	

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Mol	Chain	Length	Quality of chain
79	Aq	135	
80	Ar	152	
81	As	145	
82	At	119	
83	Au	83	
84	Av	130	
85	Aw	143	
86	Ax	130	
87	Ay	124	
88	Az	25	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	UNX	B5	5277	-	-	X	-
93	UNX	B1	102	-	-	X	-

2 Entry composition [i](#)

There are 97 unique types of molecules in this entry. The entry contains 231486 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA.

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

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

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

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called Ribosomal protein L3.

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

- Molecule 6 is a protein called 60S ribosomal protein L4.

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

- Molecule 7 is a protein called Ribosomal protein L5 eukaryotic C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BD	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called 60S ribosomal protein L6.

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

- Molecule 9 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	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	conflict	UNP G1TUB1
BF	93	ARG	GLY	conflict	UNP G1TUB1
BF	131	MET	VAL	conflict	UNP G1TUB1
BF	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 10 is a protein called 60S ribosomal protein L7a.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	184	LEU	ILE	conflict	UNP P62424

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L10.

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

- Molecule 13 is a protein called 60S ribosomal protein L11.

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

- Molecule 14 is a protein called Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BK	29	Total	C	N	O	S	0	0
			237	152	40	40	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	60	MET	VAL	conflict	UNP P06744
BK	61	MET	-	expression tag	UNP P06744
BK	62	MET	-	expression tag	UNP P06744
BK	63	MET	-	expression tag	UNP P06744
BK	64	MET	-	expression tag	UNP P06744
BK	65	VAL	-	expression tag	UNP P06744

- Molecule 15 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	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	conflict	UNP G1TKB3
BL	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 16 is a protein called 60S ribosomal protein L14.

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

- Molecule 17 is a protein called Ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	174	LEU	ILE	conflict	UNP A0A0N8ETI8
BO	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 19 is a protein called uL22.

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

- Molecule 20 is a protein called eL18.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 21 is a protein called Ribosomal protein L19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	38	ARG	HIS	conflict	UNP G1TYL6
BR	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	36	ASN	ILE	conflict	UNP A0A1Z5LHJ5

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called 60S ribosomal protein L22.

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

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	GLY	ARG	conflict	UNP G1TSG1
BU	36	ALA	GLU	conflict	UNP G1TSG1

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Chain	Residue	Modelled	Actual	Comment	Reference
BU	39	PHE	SER	conflict	UNP G1TSG1
BU	54	GLY	ARG	conflict	UNP G1TSG1
BU	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 25 is a protein called Ribosomal protein L23.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called Ribosomal_L23eN domain-containing protein.

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

- Molecule 28 is a protein called Ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

- Molecule 31 is a protein called 60S ribosomal protein L29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31.

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

- Molecule 34 is a protein called Ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called Ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 41 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 43 is a protein called eL42.

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

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	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 46 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 47 is a protein called 60S ribosomal protein L12.

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

- Molecule 48 is a protein called Ribosomal protein uL1.

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

- Molecule 49 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	MA	315	Total	C	N	O	S	0	0
			2485	1562	444	461	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MA	220	ASN	ASP	conflict	UNP P53582

- Molecule 50 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Na	67	Total	C	N	O	S	0	0
			531	335	97	98	1		

- Molecule 51 is a protein called Transcription factor BTF3.

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

- Molecule 52 is a RNA chain called 18s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	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 53 is a protein called 40S ribosomal protein S27.

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

- Molecule 54 is a protein called 40S ribosomal protein S28.

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

- Molecule 55 is a protein called Ribosomal protein S27a.

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

- Molecule 56 is a protein called 40S ribosomal protein S30.

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

- Molecule 57 is a protein called eS26.

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

- Molecule 58 is a protein called RACK1.

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

- Molecule 59 is a protein called 40S ribosomal protein S29.

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

- Molecule 60 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AI	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 61 is a RNA chain called P-site Val-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AT	76	Total	C	N	O	P	0	0
			1621	724	290	531	76		

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

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

- Molecule 63 is a protein called 40S ribosomal protein S3a.

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

- Molecule 64 is a protein called 40S ribosomal protein S2.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	33	ILE	VAL	conflict	UNP O18789
Ab	101	ALA	SER	conflict	UNP O18789

- Molecule 65 is a protein called 40S ribosomal protein S3.

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

- Molecule 66 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	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	conflict	UNP G1TK17
Ad	51	ARG	LYS	conflict	UNP G1TK17
Ad	78	THR	ALA	conflict	UNP G1TK17
Ad	156	VAL	MET	conflict	UNP G1TK17

- Molecule 67 is a protein called Ribosomal protein S5.

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

- Molecule 68 is a protein called 40S ribosomal protein S6.

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

- Molecule 69 is a protein called 40S ribosomal protein S7.

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

- Molecule 70 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 71 is a protein called 40S ribosomal protein S9.

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

- Molecule 72 is a protein called S10_ plectin domain-containing protein.

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

- 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 40S ribosomal protein S12.

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

- Molecule 75 is a protein called 40S ribosomal protein S13.

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

- Molecule 76 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	136	Total	C	N	O	S	0	0
			1017	622	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	5F0	ASP	conflict	UNP G1U472

- Molecule 77 is a protein called 40S ribosomal protein uS19.

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

- Molecule 78 is a protein called uS9.

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

- Molecule 79 is a protein called 40S ribosomal protein eS17.

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

- Molecule 80 is a protein called 40S ribosomal protein S18.

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

- Molecule 81 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	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	conflict	UNP G1TN62
As	142	ASN	LYS	conflict	UNP G1TN62

- Molecule 82 is a protein called 40S ribosomal protein uS10.

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

- Molecule 83 is a protein called 40S ribosomal protein S21.

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

- Molecule 84 is a protein called Ribosomal protein S15a.

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

- Molecule 85 is a protein called 40S ribosomal protein S23.

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

- Molecule 86 is a protein called 40S ribosomal protein S24.

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

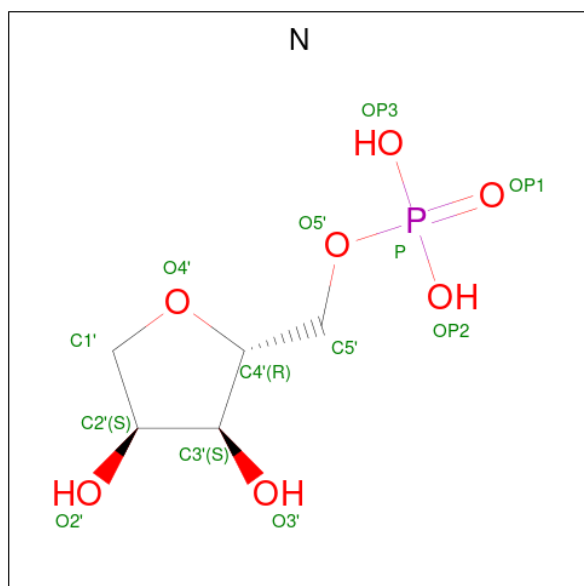
- Molecule 87 is a protein called 40S ribosomal protein S25.

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

- Molecule 88 is a protein called 60S ribosomal protein L41.

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

- Molecule 89 is ANY 5'-MONOPHOSPHATE NUCLEOTIDE (CCD ID: N) (formula: $C_5H_{11}O_7P$).



Mol	Chain	Residues	Atoms				AltConf
89	B5	1	Total	C	O	P	0
			12	5	6	1	
89	B5	1	Total	C	O	P	0
			12	5	6	1	
89	B5	1	Total	C	O	P	0
			12	5	6	1	
89	B5	1	Total	C	O	P	0
			12	5	6	1	

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Mol	Chain	Residues	Atoms				AltConf
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	B5	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 13	C 5	O 7	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bo	1	Total 12	C 5	O 6	P 1	0
89	Bv	1	Total 12	C 5	O 6	P 1	0
89	Bv	1	Total 12	C 5	O 6	P 1	0
89	Bv	1	Total 12	C 5	O 6	P 1	0
89	Bv	1	Total 12	C 5	O 6	P 1	0
89	Bv	1	Total 12	C 5	O 6	P 1	0
89	Bv	1	Total 12	C 5	O 6	P 1	0
89	Bv	1	Total 12	C 5	O 6	P 1	0
89	Bv	1	Total 12	C 5	O 6	P 1	0
89	A2	1	Total 12	C 5	O 6	P 1	0
89	A2	1	Total 12	C 5	O 6	P 1	0
89	A2	1	Total 12	C 5	O 6	P 1	0
89	AI	1	Total 12	C 5	O 6	P 1	0
89	AT	1	Total 12	C 5	O 6	P 1	0
89	AT	1	Total 12	C 5	O 6	P 1	0
89	AT	1	Total 12	C 5	O 6	P 1	0
89	AT	1	Total 12	C 5	O 6	P 1	0

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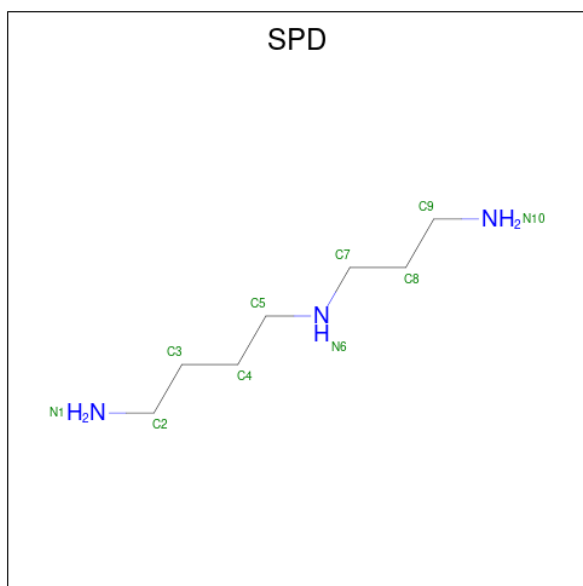
Mol	Chain	Residues	Atoms				AltConf
89	AT	1	Total 12	C 5	O 6	P 1	0
89	AT	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Aa	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0
89	Ae	1	Total 12	C 5	O 6	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
89	Ae	1	Total	C	O	P	0
			12	5	6	1	
89	Ay	1	Total	C	O	P	0
			12	5	6	1	
89	Ay	1	Total	C	O	P	0
			12	5	6	1	
89	Ay	1	Total	C	O	P	0
			12	5	6	1	
89	Ay	1	Total	C	O	P	0
			12	5	6	1	
89	Ay	1	Total	C	O	P	0
			12	5	6	1	

- Molecule 90 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

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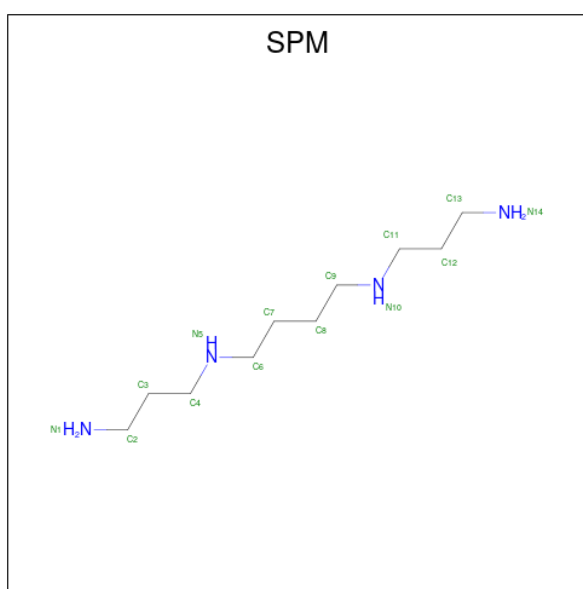
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3	0
90	B5	1	10	7	3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

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

- Molecule 91 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



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

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

Mol	Chain	Residues	Atoms		AltConf
92	B5	282	Total	Mg	0
			282	282	
92	B7	9	Total	Mg	0
			9	9	

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Mol	Chain	Residues	Atoms		AltConf
92	B8	9	Total 9	Mg 9	0
92	BI	1	Total 1	Mg 1	0
92	BP	1	Total 1	Mg 1	0
92	BR	1	Total 1	Mg 1	0
92	BV	1	Total 1	Mg 1	0
92	Ba	1	Total 1	Mg 1	0
92	Bj	1	Total 1	Mg 1	0
92	Na	1	Total 1	Mg 1	0
92	A2	108	Total 108	Mg 108	0
92	AT	3	Total 3	Mg 3	0
92	Af	1	Total 1	Mg 1	0
92	An	1	Total 1	Mg 1	0

- Molecule 93 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

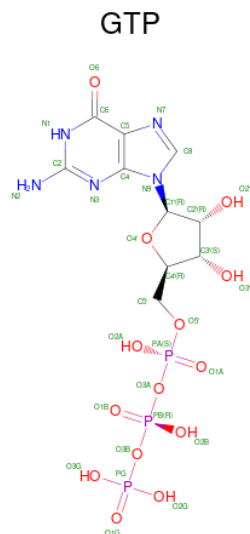
Mol	Chain	Residues	Atoms		AltConf
93	B5	214	Total 214	X 214	0
93	B7	6	Total 6	X 6	0
93	B8	6	Total 6	X 6	0
93	BA	3	Total 3	X 3	0
93	BB	2	Total 2	X 2	0
93	BH	1	Total 1	X 1	0
93	BI	1	Total 1	X 1	0

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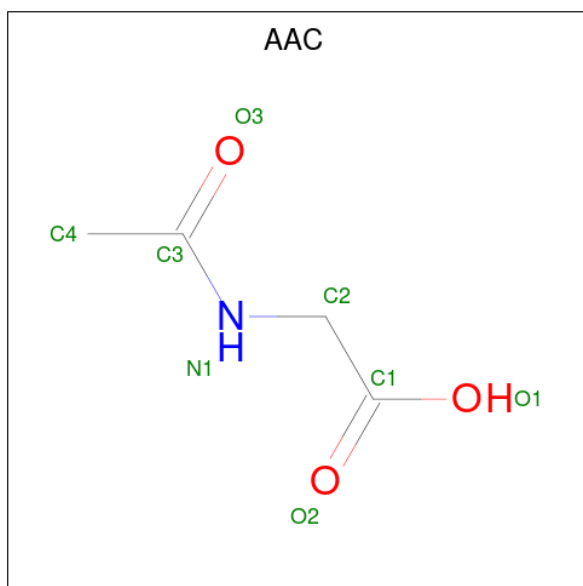
Mol	Chain	Residues	Atoms		AltConf
93	BL	1	Total 1	X 1	0
93	BN	1	Total 1	X 1	0
93	BP	1	Total 1	X 1	0
93	BQ	2	Total 2	X 2	0
93	BT	1	Total 1	X 1	0
93	Bb	2	Total 2	X 2	0
93	Be	3	Total 3	X 3	0
93	Bf	1	Total 1	X 1	0
93	Bl	2	Total 2	X 2	0
93	Bo	1	Total 1	X 1	0
93	A2	56	Total 56	X 56	0
93	AE	1	Total 1	X 1	0
93	AT	2	Total 2	X 2	0
93	Ae	1	Total 1	X 1	0
93	Ak	1	Total 1	X 1	0
93	An	1	Total 1	X 1	0
93	Ar	1	Total 1	X 1	0
93	Az	1	Total 1	X 1	0

- Molecule 94 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 95 is ACETYLAMINO-ACETIC ACID (CCD ID: AAC) (formula: $\text{C}_4\text{H}_7\text{NO}_3$).



Mol	Chain	Residues	Atoms				AltConf
95	BD	1	Total	C	N	O	0
			7	4	1	2	

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

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

- Molecule 97 is water.

Mol	Chain	Residues	Atoms		AltConf
97	B5	1388	Total 1388	O 1388	0
97	B7	44	Total 44	O 44	0
97	B8	49	Total 49	O 49	0
97	BA	9	Total 9	O 9	0
97	BB	6	Total 6	O 6	0
97	BC	7	Total 7	O 7	0
97	BD	1	Total 1	O 1	0
97	BF	1	Total 1	O 1	0
97	BH	2	Total 2	O 2	0
97	BI	1	Total 1	O 1	0
97	BL	3	Total 3	O 3	0
97	BN	5	Total 5	O 5	0

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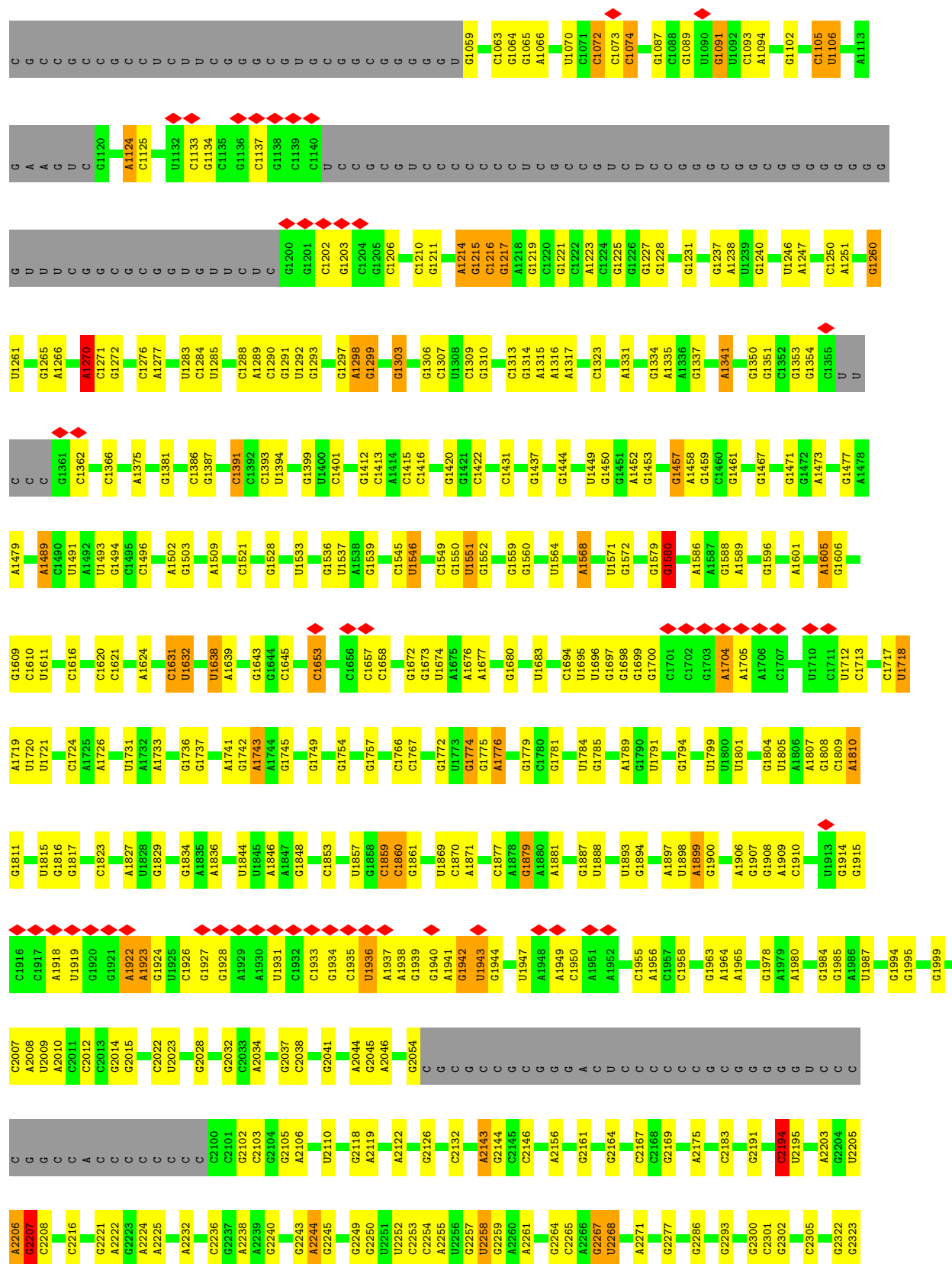
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Mol	Chain	Residues	Atoms		AltConf
97	BP	2	Total 2	O 2	0
97	BR	5	Total 5	O 5	0
97	BT	1	Total 1	O 1	0
97	BV	3	Total 3	O 3	0
97	BX	1	Total 1	O 1	0
97	Ba	7	Total 7	O 7	0
97	Bb	1	Total 1	O 1	0
97	Bd	1	Total 1	O 1	0
97	Be	5	Total 5	O 5	0
97	Bg	2	Total 2	O 2	0
97	Bj	2	Total 2	O 2	0
97	Bl	1	Total 1	O 1	0
97	Bo	1	Total 1	O 1	0
97	Na	3	Total 3	O 3	0
97	A2	530	Total 530	O 530	0
97	AI	1	Total 1	O 1	0
97	AT	13	Total 13	O 13	0
97	Aa	2	Total 2	O 2	0
97	Ad	1	Total 1	O 1	0
97	Af	1	Total 1	O 1	0
97	Ak	2	Total 2	O 2	0

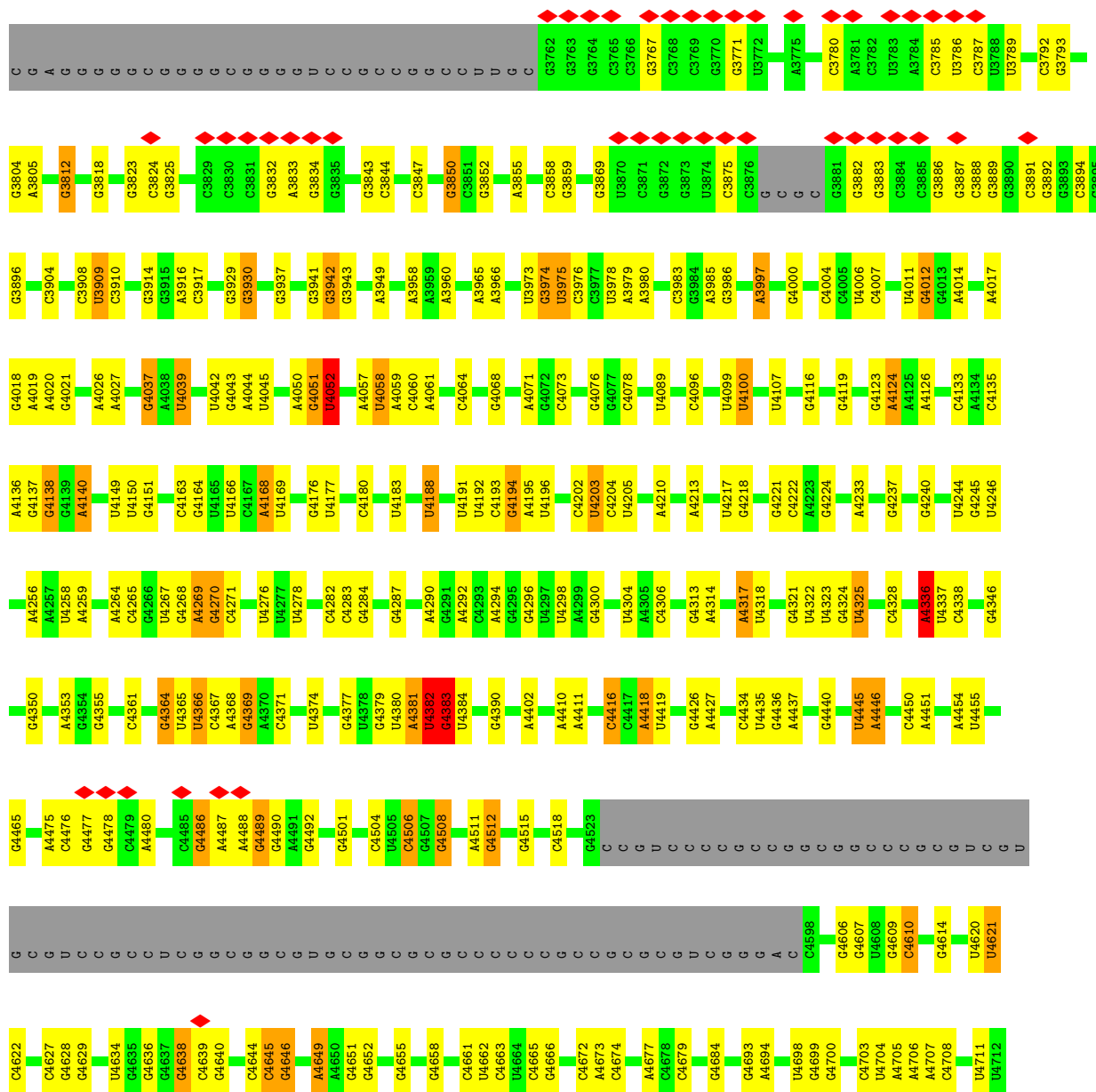
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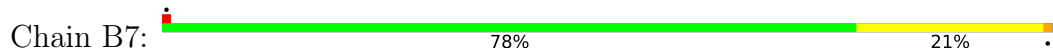
Mol	Chain	Residues	Atoms		AltConf
97	Am	1	Total 1	O 1	0
97	An	3	Total 3	O 3	0
97	Ap	2	Total 2	O 2	0
97	Ar	2	Total 2	O 2	0
97	As	2	Total 2	O 2	0
97	At	1	Total 1	O 1	0
97	Aw	5	Total 5	O 5	0







• Molecule 2: 5S rRNA

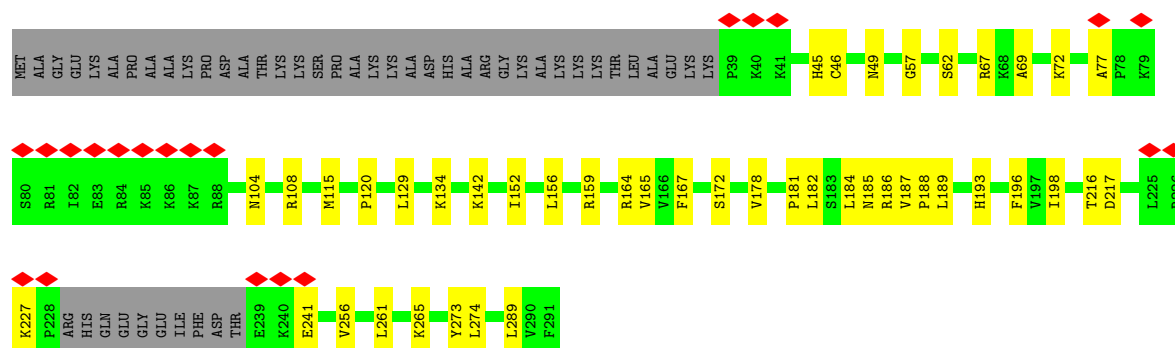


• Molecule 3: 5.8S rRNA

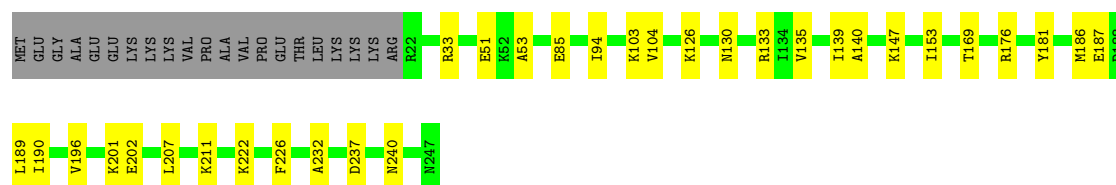
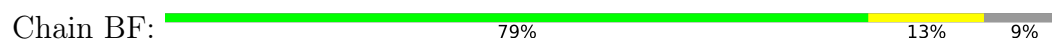




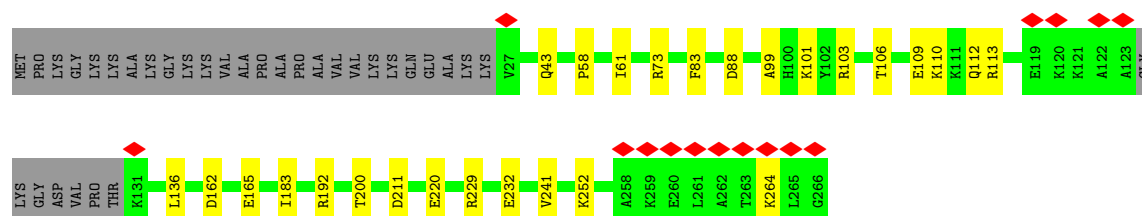
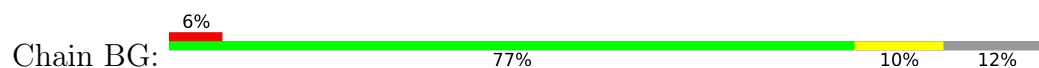
• Molecule 8: 60S ribosomal protein L6



• Molecule 9: Ribosomal Protein uL30



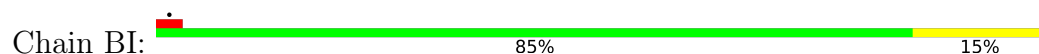
• Molecule 10: 60S ribosomal protein L7a



• Molecule 11: 60S ribosomal protein L9

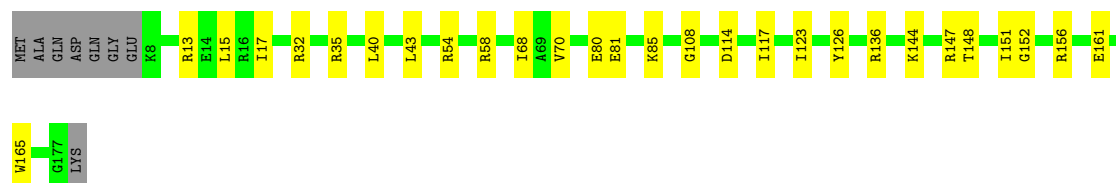


• Molecule 12: 60S ribosomal protein L10

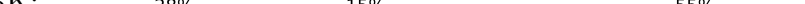


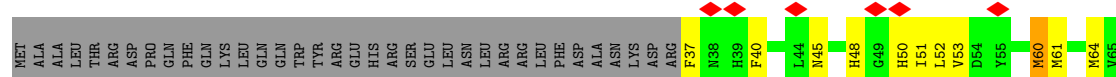
- Molecule 13: 60S ribosomal protein L11

Chain BJ:  80% 16% .

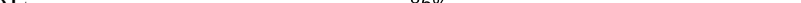


- Molecule 14: Glucose-6-phosphate isomerase

Chain BK: 

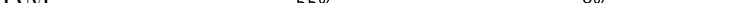


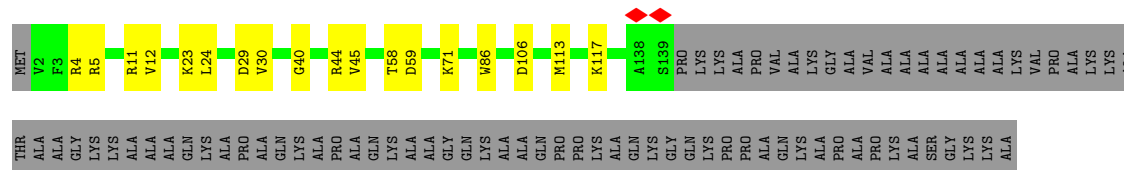
- Molecule 15: 60S ribosomal protein L13

Chain BL: 

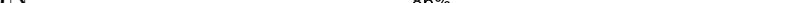


- Molecule 16: 60S ribosomal protein L14

Chain BM: 



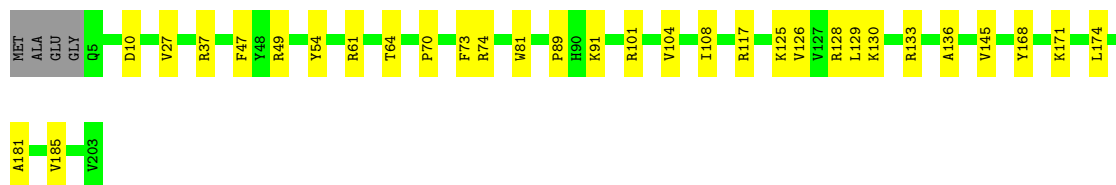
- Molecule 17: Ribosomal protein L15

Chain BN:  86% 14%



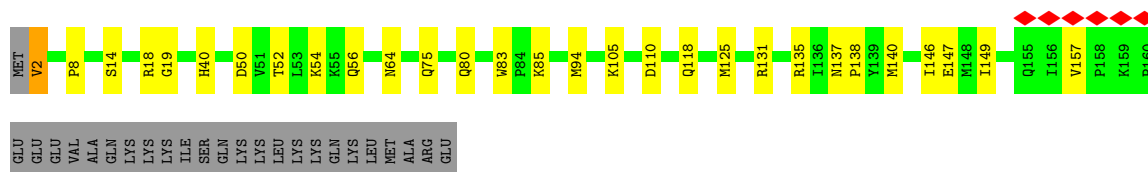
- Molecule 18: 60S ribosomal protein L13a

Chain BO:  83% 15% .



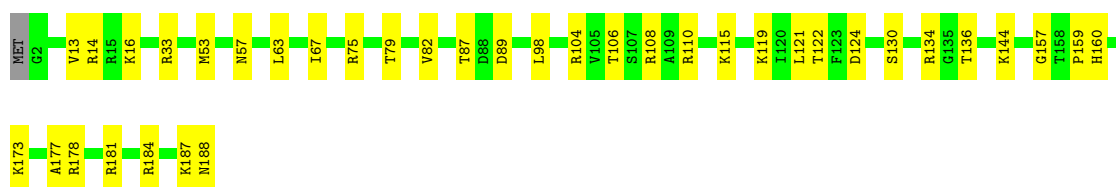
• Molecule 19: uL22

Chain BP:  71% 15% 14% .



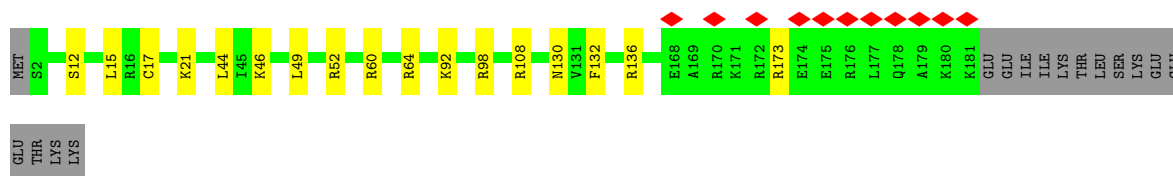
• Molecule 20: eL18

Chain BQ:  80% 20% .



• Molecule 21: Ribosomal protein L19

Chain BR:  6% 83% 9% 8% .



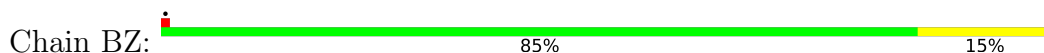
• Molecule 22: 60S ribosomal protein L18a

Chain BS:  87% 13% .



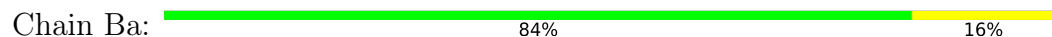
• Molecule 23: 60S ribosomal protein L21

Chain BT:  82% 17% .

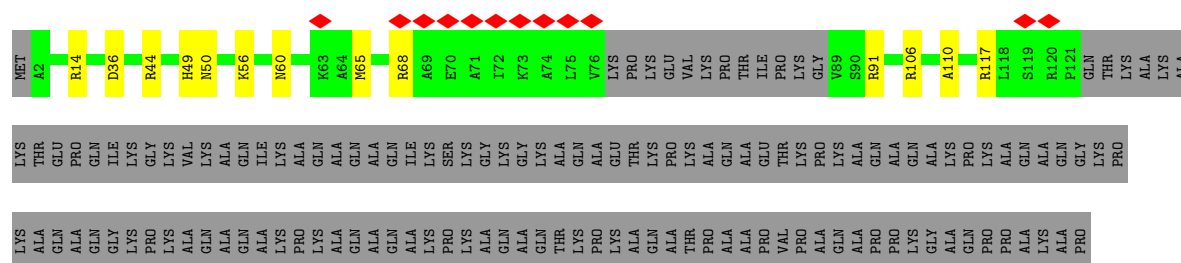
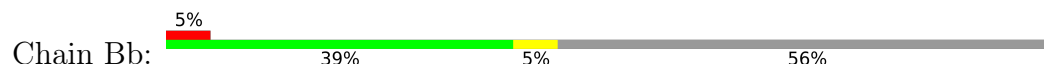




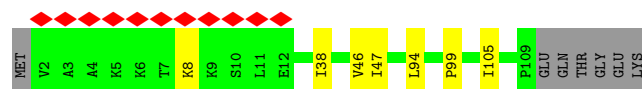
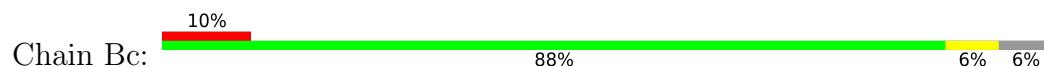
- Molecule 30: 60S ribosomal protein L27a



- Molecule 31: 60S ribosomal protein L29



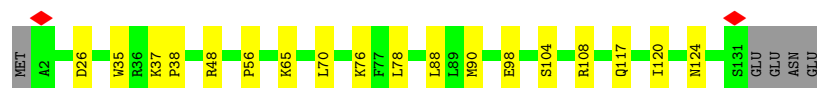
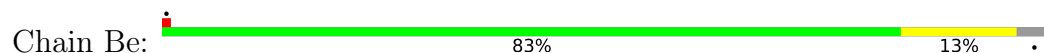
- Molecule 32: 60S ribosomal protein L30



- Molecule 33: 60S ribosomal protein L31

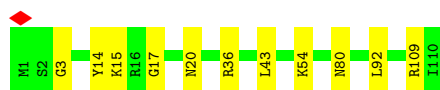


- Molecule 34: Ribosomal protein L32

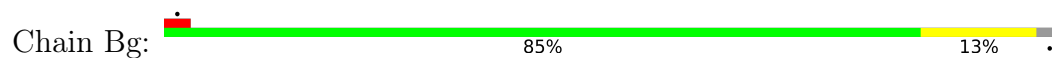


- Molecule 35: 60S ribosomal protein L35a

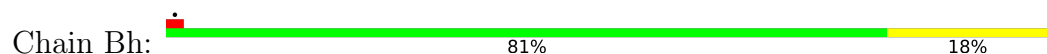




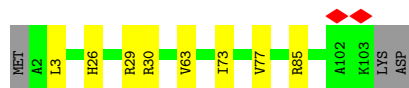
- Molecule 36: 60S ribosomal protein L34



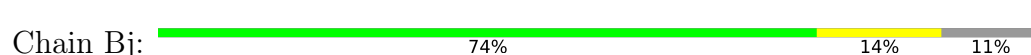
- Molecule 37: 60S ribosomal protein L35



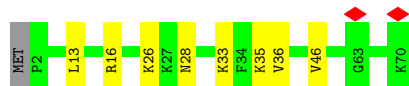
- Molecule 38: 60S ribosomal protein L36



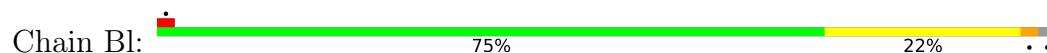
- Molecule 39: Ribosomal protein L37



- Molecule 40: 60S ribosomal protein L38



- Molecule 41: 60S ribosomal protein L39-like



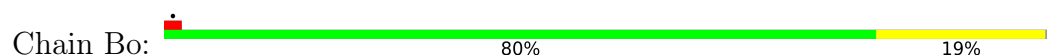
- Molecule 42: Ubiquitin-60S ribosomal protein L40



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

ILE GLN LYS SER THR LEU HIS VAL LEU ARG LEU ARG GLY I77 M94 Y100 P105 K112 K113 K114 K128

- Molecule 43: eL42



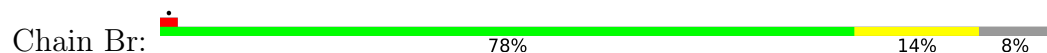
MET V2 R8 H18 Y26 K27 K28 D31 Y34 A35 Q36 R39 K44 Q45 Q51 T52 K53 P54 K59 A60 K61 T62 T63 V67 E74 C77 Q105 F106

- Molecule 44: 60S ribosomal protein L37a



MET A2 T5 V8 V11 L22 L23 T33 T45 V52 Q53 K62 A65 W69 D91 Q92

- Molecule 45: 60S ribosomal protein L28



MET S2 D6 R20 S26 T27 E28 N31 L32 K33 S37 R67 T82 A88 T89 L90 R98 R99 R107 I111 R112 R119 M125 V126 K127 ARG LYS THR ARG ARG PRO LYS SER

- Molecule 46: 60S acidic ribosomal protein P0

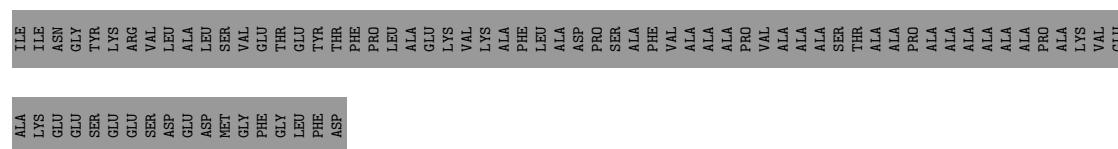


MET PRO ARG GLU D5 R6 A7 T8 W9 K10 S11 N12 N13 F14 L15 K16 I17 I18 Q19 L20 L21 L22 D23 Y24 P25 K26 C27 F28 I29 V30 G31 A32 D33 N34 V35 G36 S37 K38 Q39 M40 Q41 Q42 Q43 R44 M45 S46 L47 R48 G49 K50 A51 V52 V53 L54 M55 G56 K57 N58 T59 M60

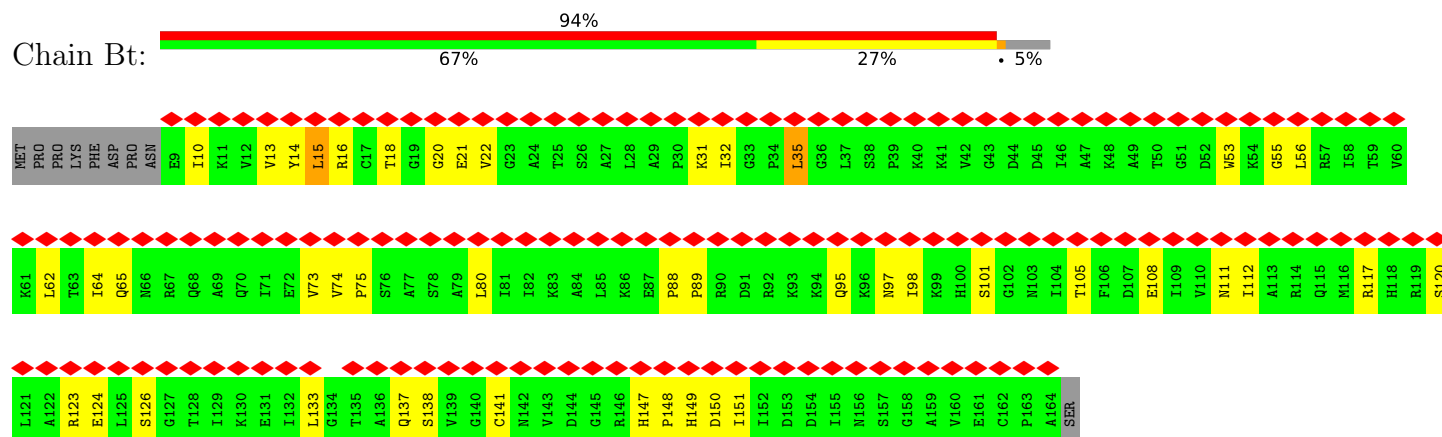
M61 R62 K63 A64 T65 R66 G67 H68 L69 E70 N71 N72 P73 A74 L75 E76 K77 L78 L79 P80 H81 I82 R83 G84 N85 V86 G87 F88 V89 F90 T91 K92 E93 D94 L95 T96 E97 I98 A99 D100 M101 L102 L103 A104 M105 K106 V107 P108 A109 A110 A111 R112 A113 G114 A115 I116 A117 C119 E120

V121 T122 V123 P124 A125 Q126 N127 T128 L129 L130 G131 P132 E133 K134 T135 S136 F137 Q138 Q139 A140 A141 G142 I143 T144 T145 K146 I147 S148 L149 H150 G151 T151 I152 E153 L154 L155 S156 D157 V158 A159 Q159 D160 L161 L162 K163 T163 G164 D165 K166 V167 P168 A169 S170 E171 A172 T173 L174 L175 N176 M177 L178 N179 I180

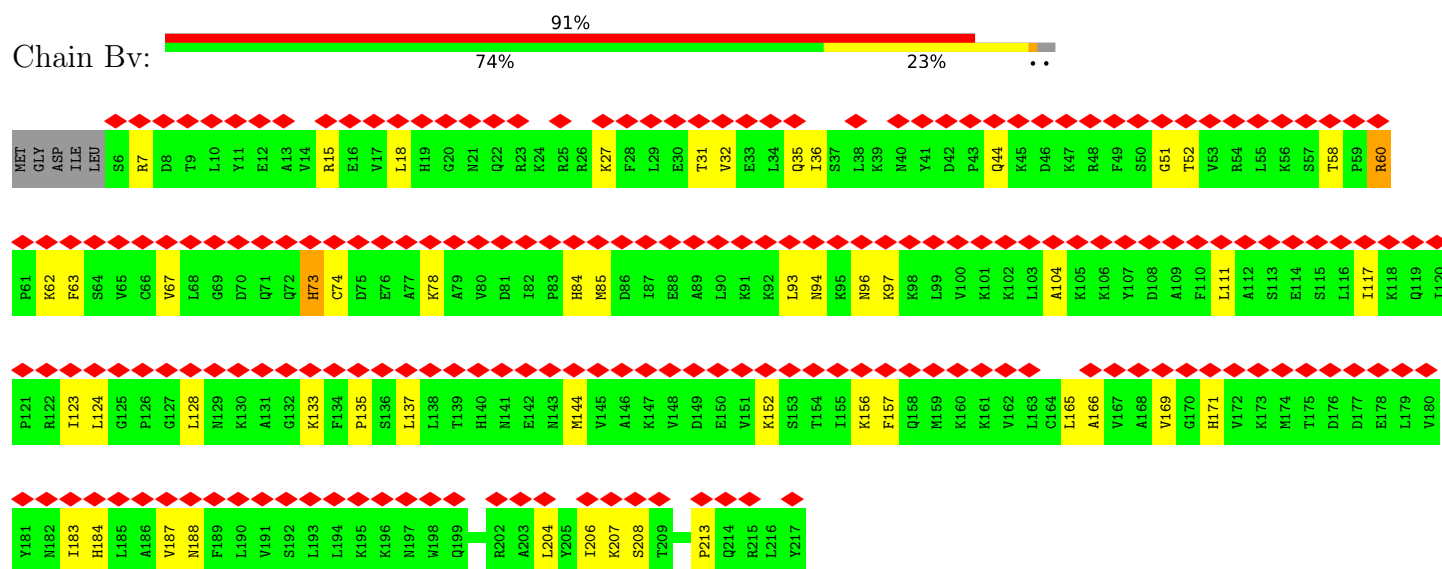
S181 P182 F183 S184 F185 G186 L187 I188 I189 Q190 Q191 V192 F193 D194 N195 G196 S197 I198 Y199 N200 PRO GLU VAL LEU ASP ILE THR GLU ASP THR LEU HIS SER ARG PHE LEU GLY VAL ARG ASN VAL SER ALA VAL CYS LEU GLN ILE GLY TYR PRO THR VAL ALA SER VAL PRO HIS SER



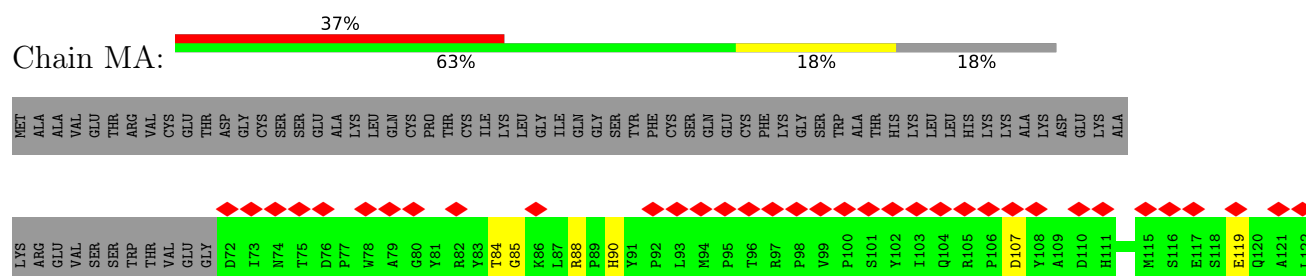
• Molecule 47: 60S ribosomal protein L12

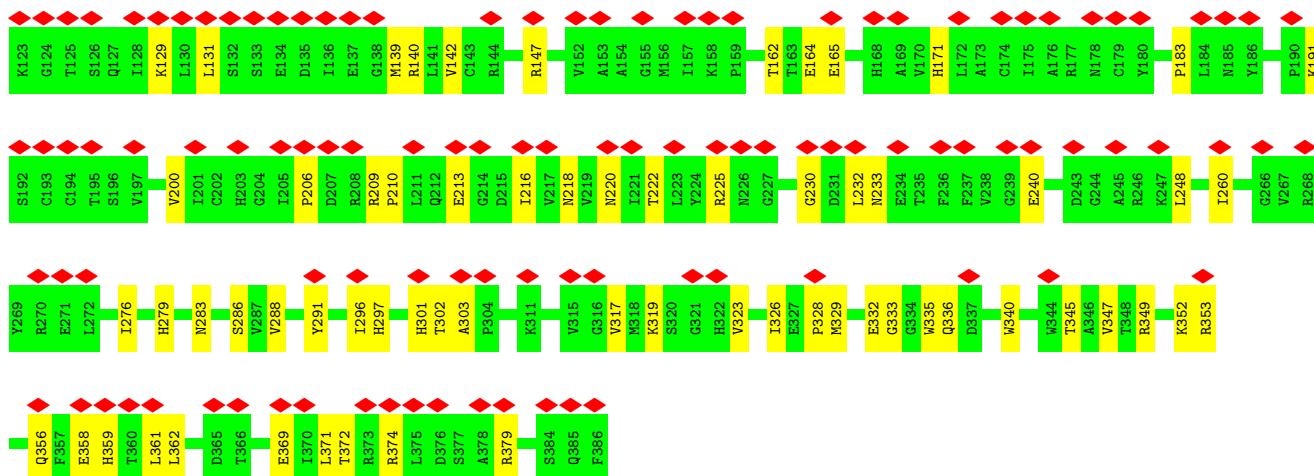


• Molecule 48: Ribosomal protein uL1

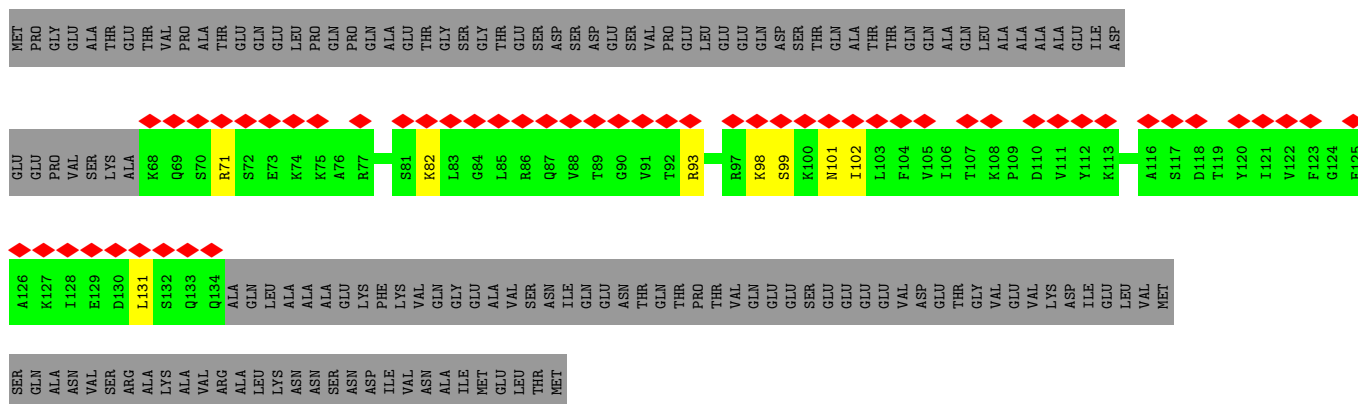


• Molecule 49: Methionine aminopeptidase 1

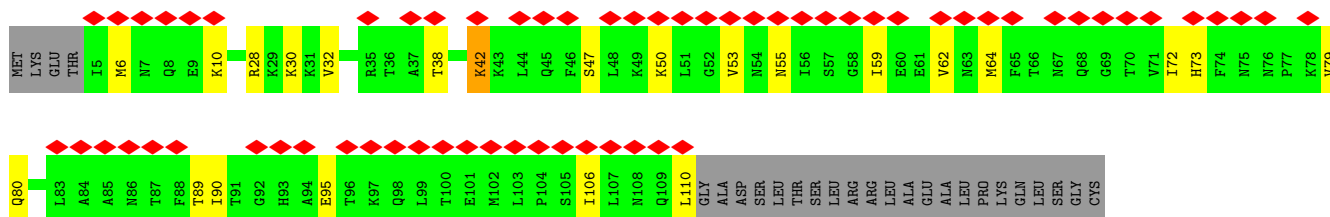




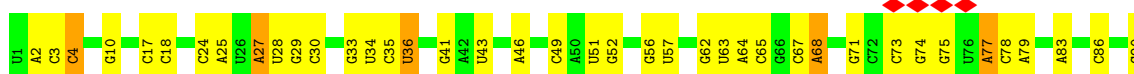
- Molecule 50: Nascent polypeptide-associated complex subunit alpha



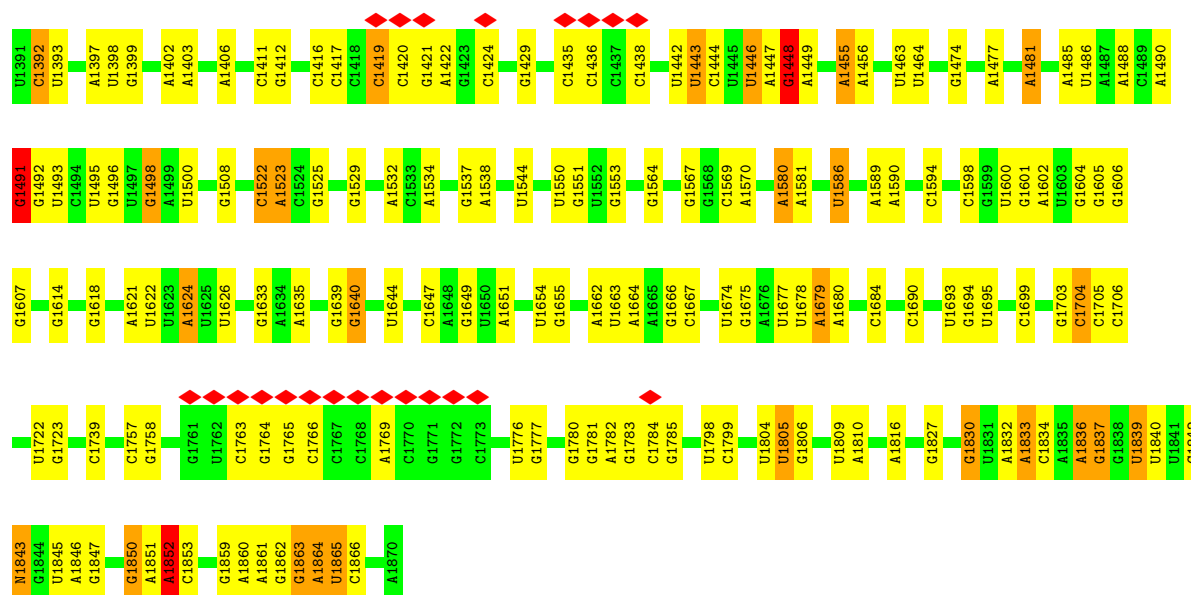
- Molecule 51: Transcription factor BTF3



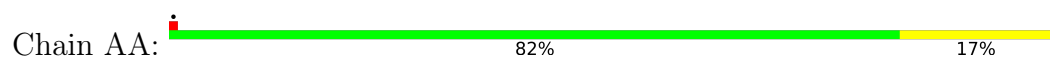
- Molecule 52: 18s rRNA



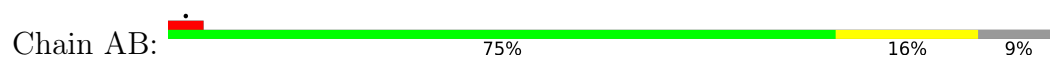




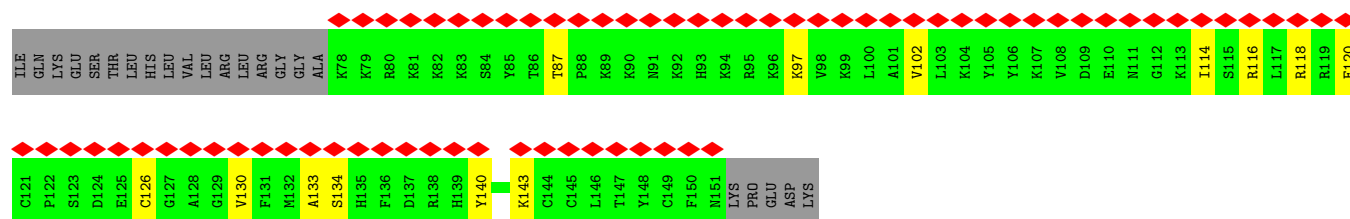
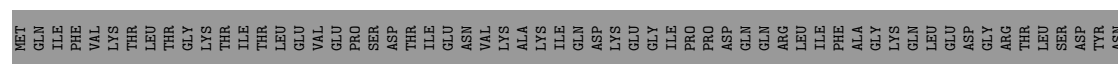
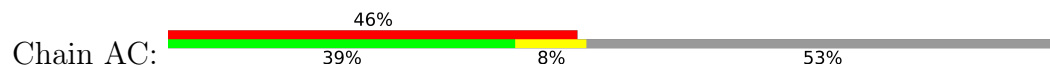
• Molecule 53: 40S ribosomal protein S27



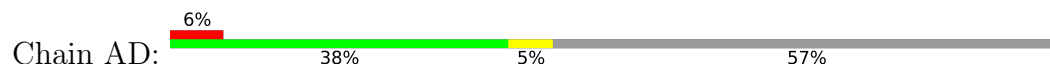
• Molecule 54: 40S ribosomal protein S28



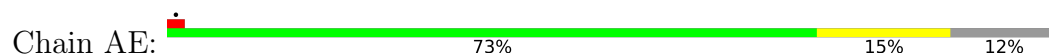
• Molecule 55: Ribosomal protein S27a



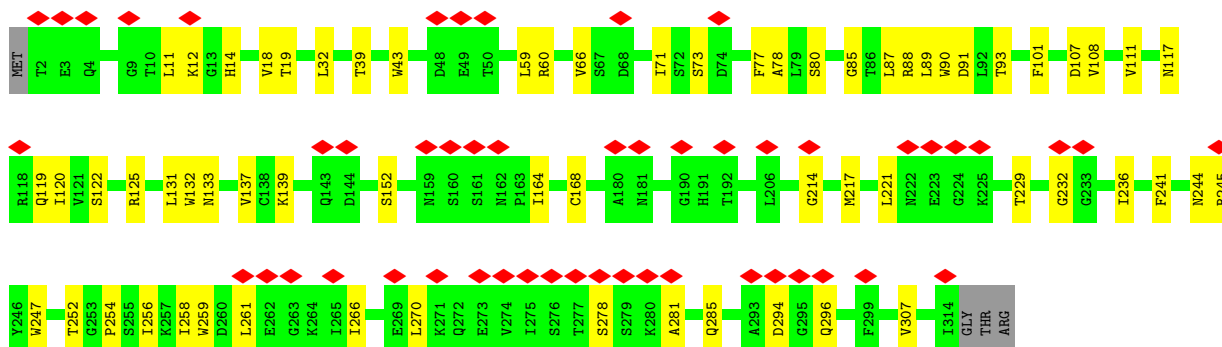
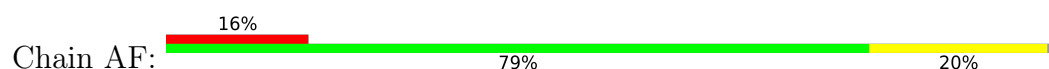
• Molecule 56: 40S ribosomal protein S30



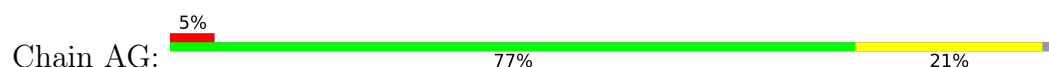
- Molecule 57: eS26



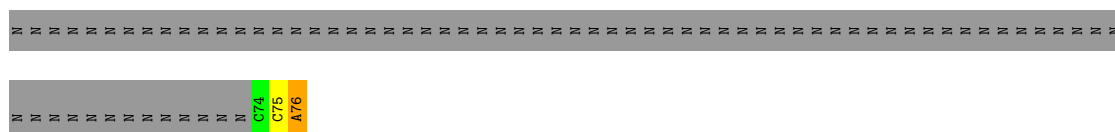
- Molecule 58: RACK1



- Molecule 59: 40S ribosomal protein S29



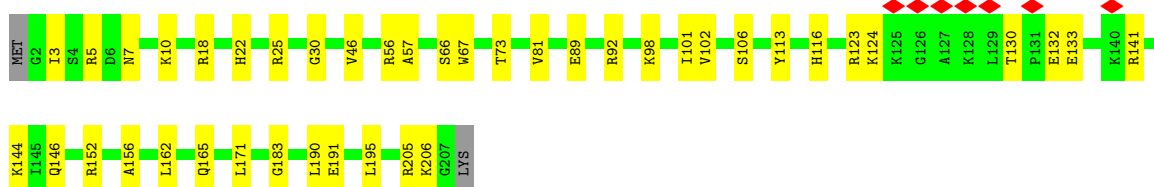
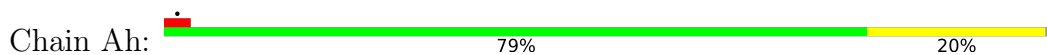
- Molecule 60: E-site tRNA



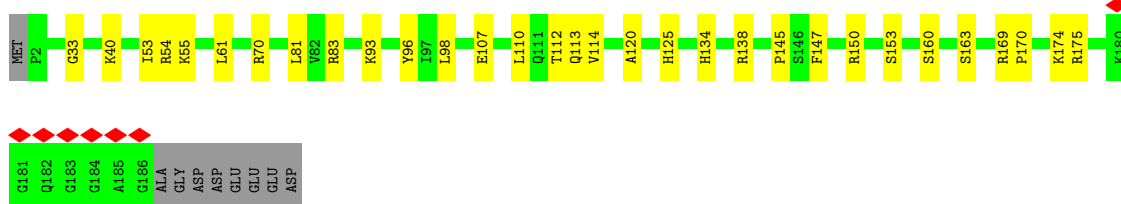
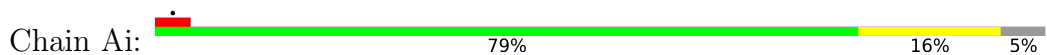
- Molecule 61: P-site Val-tRNA



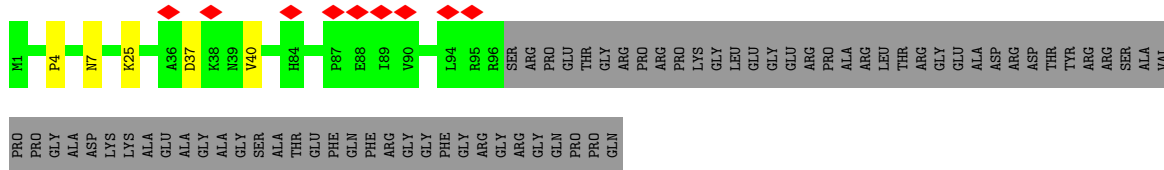
- Molecule 70: 40S ribosomal protein S8



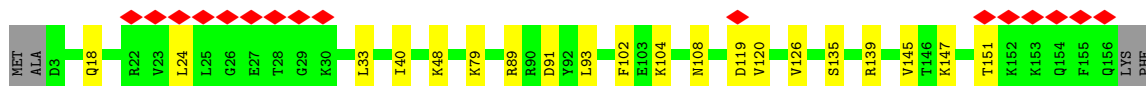
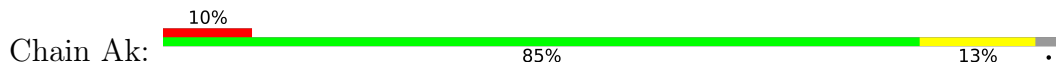
- Molecule 71: 40S ribosomal protein S9



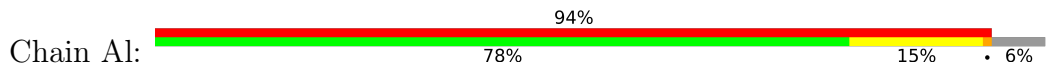
- Molecule 72: S10 plectin domain-containing protein

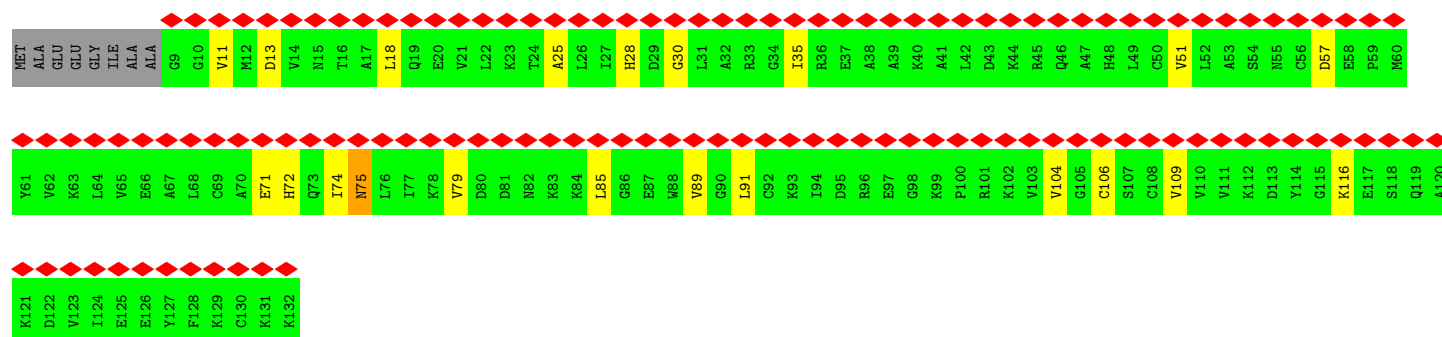


- Molecule 73: 40S ribosomal protein S11



- Molecule 74: 40S ribosomal protein S12





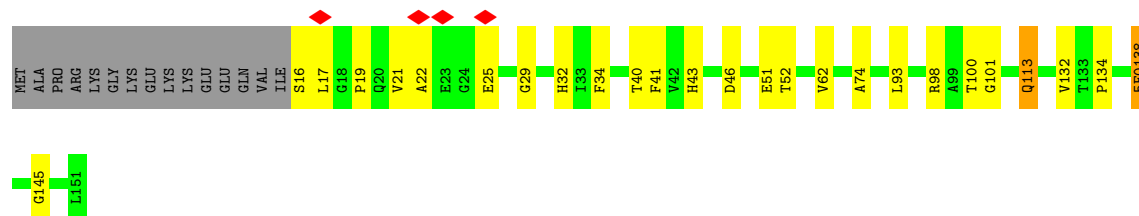
- Molecule 75: 40S ribosomal protein S13

Chain Am: 86% 13% .



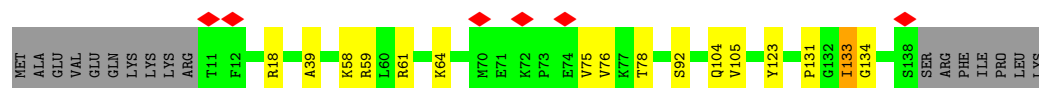
- Molecule 76: 40S ribosomal protein S14

Chain An: 73% 16% 10% .



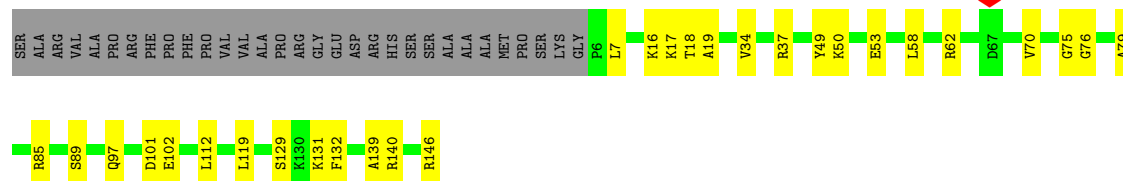
- Molecule 77: 40S ribosomal protein uS19

Chain Ao: 77% 10% 12% .



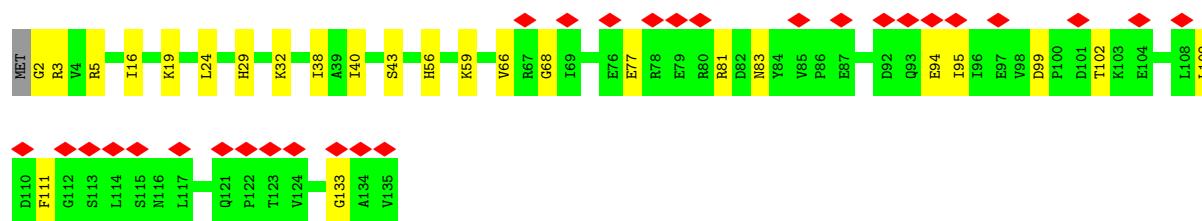
- Molecule 78: uS9

Chain Ap: 65% 17% 18% .

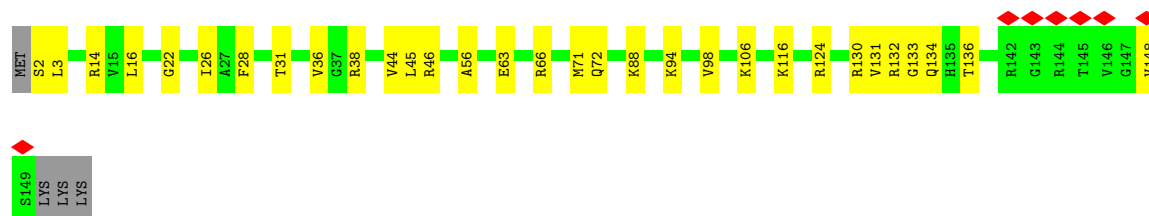
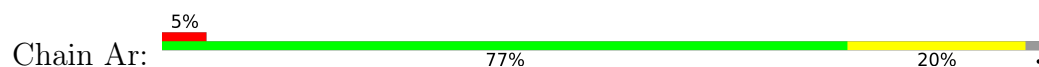


- Molecule 79: 40S ribosomal protein eS17

Chain Aq: 21% 81% 19% .



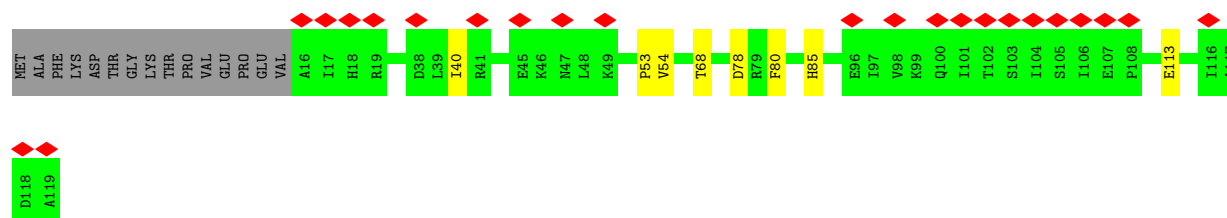
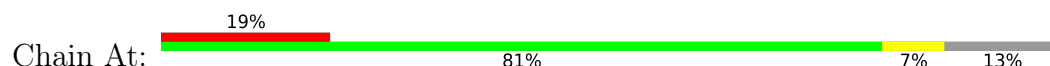
- Molecule 80: 40S ribosomal protein S18



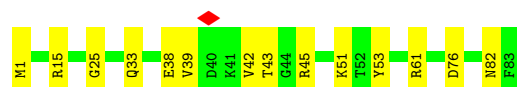
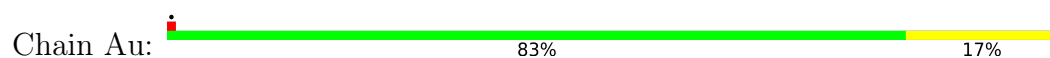
- Molecule 81: 40S ribosomal protein S19



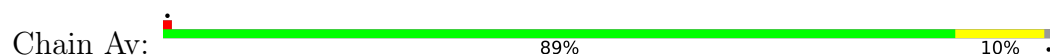
- Molecule 82: 40S ribosomal protein uS10



- Molecule 83: 40S ribosomal protein S21

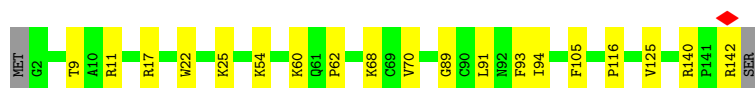
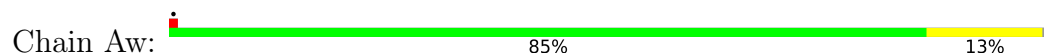


- Molecule 84: Ribosomal protein S15a

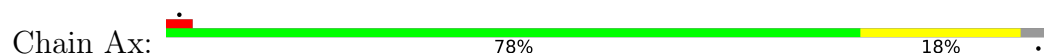




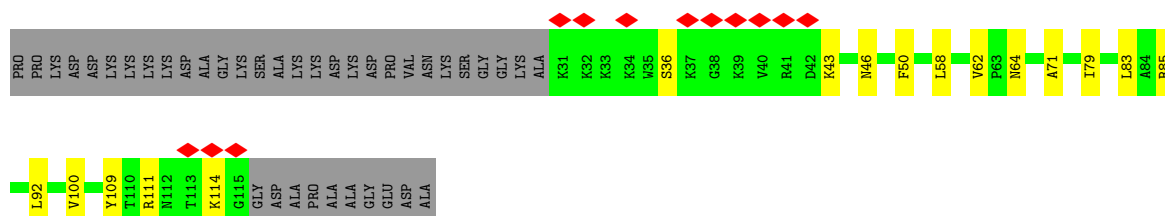
- Molecule 85: 40S ribosomal protein S23



- Molecule 86: 40S ribosomal protein S24



- Molecule 87: 40S ribosomal protein S25



- Molecule 88: 60S ribosomal protein L41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21221	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	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.350	Depositor
Minimum map value	-1.922	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.221	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	542.717, 542.717, 542.717	wwPDB
Map dimensions	434, 434, 434	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2505, 1.2505, 1.2505	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SAC, AYA, M3L, AME, ZN, 1MA, SPD, MA6, A2M, G7M, B8N, 5MC, OMU, OMG, GTP, HIC, UR3, UY1, PSU, UNX, AAC, SPM, 5F0, 5MU, NMM, 4AC, V5N, MLZ, HY3, OMC, 6MZ

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	B5	0.11	0/87403	0.13	0/136359
2	B7	0.07	0/2835	0.10	0/4418
3	B8	0.07	0/3635	0.12	0/5661
4	BA	0.08	0/1965	0.22	0/2633
5	BB	0.08	0/3261	0.20	0/4364
6	BC	0.07	0/2932	0.18	0/3939
7	BD	0.07	0/2437	0.18	0/3264
8	BE	0.08	0/1998	0.20	0/2673
9	BF	0.08	0/1922	0.19	0/2563
10	BG	0.07	0/1908	0.19	0/2566
11	BH	0.07	0/1535	0.18	0/2063
12	BI	0.07	0/1756	0.19	0/2346
13	BJ	0.06	0/1385	0.18	0/1852
14	BK	0.13	0/242	0.31	0/324
15	BL	0.07	0/1733	0.19	0/2316
16	BM	0.07	0/1158	0.18	0/1547
17	BN	0.08	0/1746	0.19	0/2338
18	BO	0.07	0/1662	0.18	0/2222
19	BP	0.07	0/1317	0.20	0/1768
20	BQ	0.08	0/1539	0.20	0/2054
21	BR	0.06	0/1524	0.16	0/2013
22	BS	0.08	0/1497	0.19	0/2008
23	BT	0.07	0/1326	0.17	0/1770
24	BU	0.07	0/820	0.19	0/1100
25	BV	0.08	0/1048	0.20	0/1402
26	BW	0.07	0/1006	0.18	0/1334
27	BX	0.07	0/984	0.19	0/1323
28	BY	0.07	0/1132	0.19	0/1504
29	BZ	0.07	0/1130	0.16	0/1507
30	Ba	0.08	0/1179	0.21	0/1572
31	Bb	0.07	0/884	0.18	0/1169

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Bc	0.07	0/847	0.16	0/1134
33	Bd	0.07	0/903	0.18	0/1216
34	Be	0.07	0/1088	0.20	0/1451
35	Bf	0.08	0/903	0.19	0/1208
36	Bg	0.07	0/916	0.21	0/1220
37	Bh	0.06	0/1021	0.16	0/1348
38	Bi	0.07	0/841	0.20	0/1112
39	Bj	0.08	0/720	0.21	0/952
40	Bk	0.06	0/575	0.17	0/761
41	Bl	0.07	0/459	0.17	0/608
42	Bm	0.07	0/426	0.20	0/564
43	Bo	0.07	0/866	0.20	0/1141
44	Bp	0.07	0/718	0.19	0/953
45	Br	0.07	0/1020	0.20	0/1366
46	Bs	0.06	0/1530	0.18	0/2064
47	Bt	0.07	0/1193	0.21	0/1609
48	Bv	0.07	0/1735	0.23	0/2328
49	MA	0.06	0/2549	0.20	0/3462
50	Na	0.10	0/536	0.23	0/715
51	Nb	0.10	0/829	0.31	0/1112
52	A2	0.14	0/40342	0.13	0/62877
53	AA	0.06	0/665	0.20	0/891
54	AB	0.06	0/497	0.17	0/666
55	AC	0.07	0/622	0.21	0/822
56	AD	0.05	0/462	0.17	0/607
57	AE	0.07	0/828	0.20	0/1109
58	AF	0.06	0/2493	0.20	0/3394
59	AG	0.08	0/470	0.18	0/623
60	AI	0.07	0/68	0.12	0/103
61	AT	0.05	0/1766	0.09	0/2749
62	AZ	0.07	0/1771	0.19	0/2406
63	Aa	0.07	0/1841	0.19	0/2459
64	Ab	0.07	0/1742	0.19	0/2354
65	Ac	0.07	0/1779	0.19	0/2395
66	Ad	0.07	0/2118	0.20	0/2849
67	Ae	0.07	0/1531	0.26	0/2059
68	Af	0.06	0/1946	0.17	0/2590
69	Ag	0.06	0/1552	0.20	0/2079
70	Ah	0.07	0/1715	0.19	0/2287
71	Ai	0.07	0/1550	0.18	0/2069
72	Aj	0.06	0/834	0.18	0/1125
73	Ak	0.07	0/1284	0.19	0/1717
74	Al	0.06	0/968	0.20	0/1296

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Am	0.06	0/1232	0.18	0/1656
76	An	0.08	0/1020	0.20	0/1366
77	Ao	0.07	0/1069	0.18	0/1429
78	Ap	0.08	0/1142	0.24	0/1528
79	Aq	0.06	0/1094	0.18	0/1469
80	Ar	0.06	0/1226	0.17	0/1643
81	As	0.06	0/1119	0.17	0/1498
82	At	0.06	0/831	0.19	0/1115
83	Au	0.06	0/636	0.18	0/852
84	Av	0.08	0/1051	0.19	0/1406
85	Aw	0.07	0/1107	0.19	0/1475
86	Ax	0.06	0/1032	0.17	0/1371
87	Ay	0.06	0/691	0.17	0/922
88	Az	0.07	0/240	0.16	0/305
All	All	0.10	0/238908	0.16	0/349857

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

Mol	Chain	#Chirality outliers	#Planarity outliers
43	Bo	0	1
76	An	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
76	An	138	5F0	Peptide
43	Bo	53	MLZ	Mainchain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B5	80772	0	40877	688	0
2	B7	2538	0	1283	17	0
3	B8	3319	0	1684	32	0
4	BA	1940	0	2029	32	0
5	BB	3206	0	3352	38	0
6	BC	2886	0	3057	41	0
7	BD	2391	0	2424	29	0
8	BE	1960	0	2153	28	0
9	BF	1886	0	2008	25	0
10	BG	1877	0	2023	17	0
11	BH	1516	0	1596	15	0
12	BI	1717	0	1764	20	0
13	BJ	1362	0	1399	19	0
14	BK	237	0	233	9	0
15	BL	1702	0	1820	22	0
16	BM	1137	0	1211	13	0
17	BN	1701	0	1749	23	0
18	BO	1630	0	1778	20	0
19	BP	1289	0	1329	20	0
20	BQ	1515	0	1634	27	0
21	BR	1508	0	1664	14	0
22	BS	1457	0	1492	14	0
23	BT	1298	0	1366	25	0
24	BU	806	0	827	7	0
25	BV	1034	0	1097	12	0
26	BW	991	0	1048	13	0
27	BX	967	0	1040	6	0
28	BY	1115	0	1205	12	0
29	BZ	1107	0	1182	13	0
30	Ba	1163	0	1202	18	0
31	Bb	881	0	957	12	0
32	Bc	836	0	888	5	0
33	Bd	888	0	930	12	0
34	Be	1070	0	1165	14	0
35	Bf	884	0	922	7	0
36	Bg	906	0	998	13	0
37	Bh	1013	0	1147	21	0
38	Bi	830	0	916	6	0
39	Bj	705	0	737	13	0
40	Bk	569	0	637	5	0
41	Bl	447	0	479	11	0
42	Bm	432	0	470	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	Bo	863	0	929	14	0
44	Bp	708	0	756	8	0
45	Br	1014	0	1083	15	0
46	Bs	1507	0	1564	30	0
47	Bt	1178	0	1235	30	0
48	Bv	1707	0	1815	33	0
49	MA	2485	0	2418	42	0
50	Na	531	0	573	6	0
51	Nb	821	0	867	13	0
52	A2	37833	0	19167	328	0
53	AA	651	0	672	9	0
54	AB	495	0	523	6	0
55	AC	610	0	634	10	0
56	AD	457	0	502	6	0
57	AE	814	0	863	14	0
58	AF	2436	0	2393	40	0
59	AG	459	0	448	11	0
60	AI	62	0	34	2	0
61	AT	1621	0	823	12	0
62	AZ	1743	0	1748	31	0
63	Aa	1815	0	1908	25	0
64	Ab	1706	0	1796	28	0
65	Ac	1751	0	1846	21	0
66	Ad	2076	0	2177	25	0
67	Ae	1509	0	1563	21	0
68	Af	1923	0	2089	35	0
69	Ag	1529	0	1627	19	0
70	Ah	1686	0	1772	27	0
71	Ai	1525	0	1640	19	0
72	Aj	810	0	836	3	0
73	Ak	1262	0	1335	14	0
74	Al	958	0	993	13	0
75	Am	1208	0	1294	15	0
76	An	1017	0	1035	17	0
77	Ao	1048	0	1093	11	0
78	Ap	1124	0	1193	21	0
79	Aq	1080	0	1135	20	0
80	Ar	1217	0	1279	22	0
81	As	1113	0	1145	14	0
82	At	821	0	883	6	0
83	Au	640	0	633	9	0
84	Av	1034	0	1080	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	Aw	1099	0	1162	12	0
86	Ax	1015	0	1086	16	0
87	Ay	683	0	761	12	0
88	Az	239	0	289	2	0
89	A2	36	0	24	1	0
89	AI	12	0	8	0	0
89	AT	72	0	48	0	0
89	Aa	120	0	80	1	0
89	Ae	120	0	80	2	0
89	Ay	60	0	40	0	0
89	B5	240	0	160	1	0
89	Bo	133	0	88	1	0
89	Bv	84	0	56	1	0
90	A2	80	0	152	12	0
90	B5	220	0	418	18	0
91	A2	14	0	26	3	0
91	B5	28	0	52	1	0
92	A2	108	0	0	0	0
92	AT	3	0	0	0	0
92	Af	1	0	0	0	0
92	An	1	0	0	0	0
92	B5	282	0	0	0	0
92	B7	9	0	0	0	0
92	B8	9	0	0	0	0
92	BI	1	0	0	0	0
92	BP	1	0	0	0	0
92	BR	1	0	0	0	0
92	BV	1	0	0	0	0
92	Ba	1	0	0	0	0
92	Bj	1	0	0	0	0
92	Na	1	0	0	0	0
93	A2	56	0	0	0	0
93	AE	1	0	0	0	0
93	AT	2	0	0	0	0
93	Ae	1	0	0	0	0
93	Ak	1	0	0	0	0
93	An	1	0	0	0	0
93	Ar	1	0	0	0	0
93	Az	1	0	0	0	0
93	B5	214	0	0	8	0
93	B7	6	0	0	0	0
93	B8	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	BA	3	0	0	0	0
93	BB	2	0	0	0	0
93	BH	1	0	0	0	0
93	BI	1	0	0	0	0
93	BL	1	0	0	0	0
93	BN	1	0	0	0	0
93	BP	1	0	0	0	0
93	BQ	2	0	0	0	0
93	BT	1	0	0	0	0
93	Bb	2	0	0	0	0
93	Be	3	0	0	0	0
93	Bf	1	0	0	0	0
93	Bl	2	0	0	3	0
93	Bo	1	0	0	0	0
94	B7	32	0	11	1	0
95	BD	7	0	6	0	0
96	AC	1	0	0	0	0
96	AE	1	0	0	0	0
96	AG	1	0	0	0	0
96	Bg	1	0	0	0	0
96	Bj	1	0	0	0	0
96	Bm	1	0	0	0	0
96	Bo	1	0	0	0	0
96	Bp	1	0	0	0	0
97	A2	530	0	0	16	0
97	AI	1	0	0	1	0
97	AT	13	0	0	3	0
97	Aa	2	0	0	0	0
97	Ad	1	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	2	0	0	1	0
97	As	2	0	0	0	0
97	At	1	0	0	0	0
97	Aw	5	0	0	0	0
97	B5	1388	0	0	49	0
97	B7	44	0	0	1	0
97	B8	49	0	0	0	0
97	BA	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	BB	6	0	0	0	0
97	BC	7	0	0	1	0
97	BD	1	0	0	0	0
97	BF	1	0	0	0	0
97	BH	2	0	0	0	0
97	BI	1	0	0	0	0
97	BL	3	0	0	0	0
97	BN	5	0	0	0	0
97	BP	2	0	0	0	0
97	BR	5	0	0	0	0
97	BT	1	0	0	0	0
97	BV	3	0	0	0	0
97	BX	1	0	0	0	0
97	Ba	7	0	0	2	0
97	Bb	1	0	0	0	0
97	Bd	1	0	0	0	0
97	Be	5	0	0	0	0
97	Bg	2	0	0	1	0
97	Bj	2	0	0	0	0
97	Bl	1	0	0	0	0
97	Bo	1	0	0	0	0
97	Na	3	0	0	0	0
All	All	231486	0	171718	1980	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 1980 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)
41:Bl:8:ARG:NH1	93:Bl:102:UNX:UNK	1.53	1.02
3:B8:81:C:HO2'	37:Bh:2:ALA:N	1.63	0.97
52:A2:1092:C:HO2'	84:Av:2:VAL:N	1.66	0.92
93:B5:5318:UNX:UNK	97:B5:6024:HOH:O	1.53	0.88
93:B5:5254:UNX:UNK	97:B5:6137:HOH:O	1.61	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BA	250/257 (97%)	242 (97%)	8 (3%)	0	100	100
5	BB	395/403 (98%)	390 (99%)	5 (1%)	0	100	100
6	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
7	BD	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
8	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
9	BF	224/247 (91%)	219 (98%)	4 (2%)	1 (0%)	30	59
10	BG	229/266 (86%)	227 (99%)	2 (1%)	0	100	100
11	BH	188/192 (98%)	188 (100%)	0	0	100	100
12	BI	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
13	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
14	BK	27/65 (42%)	25 (93%)	2 (7%)	0	100	100
15	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
16	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
17	BN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
18	BO	197/203 (97%)	197 (100%)	0	0	100	100
19	BP	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
20	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
21	BR	178/196 (91%)	178 (100%)	0	0	100	100
22	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
23	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
25	BV	137/140 (98%)	134 (98%)	3 (2%)	0	100	100
26	BW	119/157 (76%)	118 (99%)	1 (1%)	0	100	100
27	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
28	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
30	Ba	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	18	48
31	Bb	103/245 (42%)	100 (97%)	3 (3%)	0	100	100
32	Bc	106/115 (92%)	106 (100%)	0	0	100	100
33	Bd	105/125 (84%)	105 (100%)	0	0	100	100
34	Be	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
35	Bf	108/110 (98%)	108 (100%)	0	0	100	100
36	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
37	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
38	Bi	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
39	Bj	84/97 (87%)	84 (100%)	0	0	100	100
40	Bk	67/70 (96%)	67 (100%)	0	0	100	100
41	Bl	48/51 (94%)	48 (100%)	0	0	100	100
42	Bm	49/128 (38%)	49 (100%)	0	0	100	100
43	Bo	102/106 (96%)	102 (100%)	0	0	100	100
44	Bp	89/92 (97%)	89 (100%)	0	0	100	100
45	Br	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
46	Bs	194/318 (61%)	190 (98%)	4 (2%)	0	100	100
47	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
48	Bv	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
49	MA	313/386 (81%)	309 (99%)	4 (1%)	0	100	100
50	Na	65/215 (30%)	63 (97%)	2 (3%)	0	100	100
51	Nb	104/132 (79%)	100 (96%)	4 (4%)	0	100	100
53	AA	81/84 (96%)	81 (100%)	0	0	100	100
54	AB	61/69 (88%)	61 (100%)	0	0	100	100
55	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
56	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
57	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
58	AF	311/317 (98%)	305 (98%)	6 (2%)	0	100	100
59	AG	53/56 (95%)	53 (100%)	0	0	100	100
62	AZ	219/295 (74%)	218 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	Aa	220/264 (83%)	217 (99%)	3 (1%)	0	100	100
64	Ab	218/293 (74%)	218 (100%)	0	0	100	100
65	Ac	223/281 (79%)	222 (100%)	1 (0%)	0	100	100
66	Ad	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
67	Ae	189/204 (93%)	188 (100%)	1 (0%)	0	100	100
68	Af	235/249 (94%)	235 (100%)	0	0	100	100
69	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100
70	Ah	204/208 (98%)	202 (99%)	2 (1%)	0	100	100
71	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
72	Aj	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
73	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
74	Al	122/132 (92%)	121 (99%)	1 (1%)	0	100	100
75	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
76	An	133/151 (88%)	129 (97%)	4 (3%)	0	100	100
77	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
78	Ap	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
79	Aq	132/135 (98%)	132 (100%)	0	0	100	100
80	Ar	146/152 (96%)	144 (99%)	2 (1%)	0	100	100
81	As	140/145 (97%)	140 (100%)	0	0	100	100
82	At	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
83	Au	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
84	Av	127/130 (98%)	127 (100%)	0	0	100	100
85	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
86	Ax	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
87	Ay	83/124 (67%)	82 (99%)	1 (1%)	0	100	100
88	Az	23/25 (92%)	23 (100%)	0	0	100	100
All	All	12418/14635 (85%)	12262 (99%)	154 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	BF	196	VAL
30	Ba	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BA	194/198 (98%)	193 (100%)	1 (0%)	81	93
5	BB	344/347 (99%)	340 (99%)	4 (1%)	63	86
6	BC	302/337 (90%)	302 (100%)	0	100	100
7	BD	247/250 (99%)	247 (100%)	0	100	100
8	BE	216/251 (86%)	215 (100%)	1 (0%)	81	93
9	BF	197/215 (92%)	197 (100%)	0	100	100
10	BG	199/223 (89%)	196 (98%)	3 (2%)	57	84
11	BH	169/171 (99%)	169 (100%)	0	100	100
12	BI	180/181 (99%)	180 (100%)	0	100	100
13	BJ	143/149 (96%)	143 (100%)	0	100	100
14	BK	28/61 (46%)	26 (93%)	2 (7%)	13	40
15	BL	175/176 (99%)	174 (99%)	1 (1%)	78	93
16	BM	117/161 (73%)	117 (100%)	0	100	100
17	BN	171/172 (99%)	171 (100%)	0	100	100
18	BO	171/173 (99%)	169 (99%)	2 (1%)	63	86
19	BP	140/163 (86%)	139 (99%)	1 (1%)	76	92
20	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	86
21	BR	159/175 (91%)	159 (100%)	0	100	100
22	BS	154/154 (100%)	153 (99%)	1 (1%)	78	93
23	BT	139/140 (99%)	138 (99%)	1 (1%)	76	92
24	BU	88/113 (78%)	88 (100%)	0	100	100
25	BV	106/107 (99%)	106 (100%)	0	100	100
26	BW	100/126 (79%)	100 (100%)	0	100	100
27	BX	106/134 (79%)	106 (100%)	0	100	100
28	BY	124/135 (92%)	124 (100%)	0	100	100
29	BZ	117/118 (99%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Ba	118/119 (99%)	118 (100%)	0	100	100
31	Bb	87/183 (48%)	87 (100%)	0	100	100
32	Bc	92/98 (94%)	92 (100%)	0	100	100
33	Bd	98/110 (89%)	98 (100%)	0	100	100
34	Be	116/121 (96%)	116 (100%)	0	100	100
35	Bf	89/89 (100%)	89 (100%)	0	100	100
36	Bg	98/100 (98%)	97 (99%)	1 (1%)	68	89
37	Bh	109/110 (99%)	109 (100%)	0	100	100
38	Bi	86/89 (97%)	86 (100%)	0	100	100
39	Bj	73/80 (91%)	73 (100%)	0	100	100
40	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	83
41	Bl	47/48 (98%)	46 (98%)	1 (2%)	47	77
42	Bm	47/115 (41%)	47 (100%)	0	100	100
43	Bo	92/93 (99%)	92 (100%)	0	100	100
44	Bp	74/75 (99%)	73 (99%)	1 (1%)	59	85
45	Br	109/120 (91%)	109 (100%)	0	100	100
46	Bs	164/258 (64%)	163 (99%)	1 (1%)	78	93
47	Bt	128/137 (93%)	123 (96%)	5 (4%)	28	63
48	Bv	191/195 (98%)	187 (98%)	4 (2%)	47	77
49	MA	270/330 (82%)	267 (99%)	3 (1%)	65	88
50	Na	60/183 (33%)	59 (98%)	1 (2%)	53	82
51	Nb	90/111 (81%)	85 (94%)	5 (6%)	19	50
53	AA	75/76 (99%)	74 (99%)	1 (1%)	61	86
54	AB	56/62 (90%)	55 (98%)	1 (2%)	51	80
55	AC	67/140 (48%)	67 (100%)	0	100	100
56	AD	47/106 (44%)	47 (100%)	0	100	100
57	AE	88/98 (90%)	87 (99%)	1 (1%)	65	88
58	AF	272/275 (99%)	271 (100%)	1 (0%)	84	94
59	AG	48/49 (98%)	48 (100%)	0	100	100
62	AZ	182/243 (75%)	180 (99%)	2 (1%)	65	88
63	Aa	203/231 (88%)	201 (99%)	2 (1%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	Ab	185/223 (83%)	184 (100%)	1 (0%)	81	93
65	Ac	189/232 (82%)	188 (100%)	1 (0%)	81	93
66	Ad	224/225 (100%)	224 (100%)	0	100	100
67	Ae	161/170 (95%)	161 (100%)	0	100	100
68	Af	207/218 (95%)	206 (100%)	1 (0%)	81	93
69	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	93
70	Ah	178/180 (99%)	177 (99%)	1 (1%)	78	93
71	Ai	161/168 (96%)	160 (99%)	1 (1%)	78	93
72	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	88
73	Ak	139/142 (98%)	139 (100%)	0	100	100
74	Al	104/108 (96%)	102 (98%)	2 (2%)	50	79
75	Am	130/131 (99%)	130 (100%)	0	100	100
76	An	105/118 (89%)	101 (96%)	4 (4%)	29	64
77	Ao	114/130 (88%)	112 (98%)	2 (2%)	51	80
78	Ap	117/140 (84%)	116 (99%)	1 (1%)	70	90
79	Aq	120/121 (99%)	120 (100%)	0	100	100
80	Ar	127/131 (97%)	126 (99%)	1 (1%)	73	90
81	As	112/114 (98%)	111 (99%)	1 (1%)	70	90
82	At	94/107 (88%)	92 (98%)	2 (2%)	47	77
83	Au	67/67 (100%)	65 (97%)	2 (3%)	36	70
84	Av	112/113 (99%)	111 (99%)	1 (1%)	70	90
85	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	80
86	Ax	107/112 (96%)	107 (100%)	0	100	100
87	Ay	75/102 (74%)	75 (100%)	0	100	100
88	Az	24/24 (100%)	24 (100%)	0	100	100
All	All	10811/12390 (87%)	10736 (99%)	75 (1%)	73	92

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
74	Al	75	ASN
83	Au	61	ARG
76	An	21	VAL

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Mol	Chain	Res	Type
78	Ap	18	THR
47	Bt	15	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
70	Ah	146	GLN
72	Aj	77	GLN
78	Ap	114	GLN
19	BP	75	GLN
18	BO	180	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3752/4808 (78%)	423 (11%)	2 (0%)
2	B7	118/120 (98%)	6 (5%)	0
3	B8	155/158 (98%)	14 (9%)	0
52	A2	1764/1870 (94%)	206 (11%)	0
60	AI	2/76 (2%)	1 (50%)	0
61	AT	75/76 (98%)	10 (13%)	0
All	All	5866/7108 (82%)	660 (11%)	2 (0%)

5 of 660 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	39	A
1	B5	42	A
1	B5	58	G
1	B5	59	A
1	B5	64	A

All (2) RNA pucker outliers are listed below:

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

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

225 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
52	PSU	A2	1348	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4435	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	1718	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	1626	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
30	V5N	Ba	39	30	9,11,12	2.07	2 (22%)	9,14,16	1.70	2 (22%)
1	PSU	B5	3427	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	B5	4244	1	19,22,23	1.21	2 (10%)	26,31,34	1.70	5 (19%)
52	PSU	A2	1175	52	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	B5	2244	92,1	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
1	OMG	B5	4116	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	1801	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	398	1	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
52	OMU	A2	355	52	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
1	1MA	B5	1266	92,1	21,25,26	1.38	4 (19%)	31,37,40	1.69	5 (16%)
1	A2M	B5	2630	92,1	22,25,26	1.45	4 (18%)	31,36,39	2.16	9 (29%)
3	OMG	B8	75	3	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	A2M	B5	3557	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
1	OMC	B5	3573	1	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
61	5MU	AT	54	61	19,22,23	1.41	5 (26%)	28,32,35	2.03	6 (21%)
1	OMC	B5	2704	1	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
1	PSU	B5	4042	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	A2M	B5	3517	1	22,25,26	1.43	4 (18%)	31,36,39	2.21	11 (35%)
1	PSU	B5	3585	92,1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4099	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	OMG	A2	602	52	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	B5	4245	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	B5	3562	1	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
52	PSU	A2	109	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	OMC	A2	463	52	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
52	OMG	A2	868	52	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
52	PSU	A2	1057	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
3	PSU	B8	69	3	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	A2M	A2	669	52,92	22,25,26	1.45	4 (18%)	31,36,39	2.10	9 (29%)
1	OMG	B5	3359	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
52	OMU	A2	116	52	19,22,23	1.20	3 (15%)	26,31,34	1.67	4 (15%)
1	OMG	B5	1477	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4419	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	3619	1	19,22,23	0.80	0	26,31,34	0.84	0
1	OMG	B5	3524	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	A2M	A2	577	52	22,25,26	1.47	4 (18%)	31,36,39	2.10	10 (32%)
1	PSU	B5	4169	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	B8N	A2	1249	52	24,29,30	1.29	3 (12%)	29,42,45	1.28	3 (10%)
52	A2M	A2	485	52	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
52	OMC	A2	518	52	19,22,23	0.81	0	26,31,34	0.81	0
1	PSU	B5	4749	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	5MC	B5	4193	1	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
52	A2M	A2	1032	52	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
52	OMG	A2	645	52	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
52	OMU	A2	1327	52,92	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)
1	OMG	B5	4138	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4267	92,1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
52	PSU	A2	1046	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	3942	61,1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	B5	1284	1	19,22,23	0.81	0	26,31,34	0.81	0
1	OMC	B5	2647	1	19,22,23	0.81	0	26,31,34	0.82	0
83	AME	Au	1	83	9,10,11	0.48	0	9,11,13	0.85	1 (11%)
6	AYA	BC	2	6	6,7,8	0.72	0	5,8,10	0.30	0
1	PSU	B5	4322	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	3631	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
52	PSU	A2	682	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4203	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	OMG	A2	684	52	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
1	A2M	B5	4336	1	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	B5	1638	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4711	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
4	V5N	BA	216	4	9,11,12	2.09	2 (22%)	9,14,16	1.72	2 (22%)
1	OMG	B5	4369	1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
43	MLZ	Bo	53	43	8,9,10	0.48	0	4,9,11	0.09	0
52	OMU	A2	429	52	19,22,23	1.20	3 (15%)	26,31,34	1.68	4 (15%)
1	OMU	B5	3657	1	19,22,23	1.23	2 (10%)	26,31,34	1.75	5 (19%)
1	PSU	B5	4217	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	1731	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
76	5F0	An	138	76	8,8,9	1.47	2 (25%)	7,9,11	1.74	1 (14%)
1	A2M	B5	1479	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
52	OMU	A2	121	52	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
52	4AC	A2	1843	52	21,24,25	1.12	2 (9%)	29,34,37	1.32	3 (10%)
61	PSU	AT	55	61	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4149	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
52	PSU	A2	218	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1178	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	4240	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	3502	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	B5	3492	52,1	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
52	PSU	A2	407	52	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	3490	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	6MZ	B5	3966	1	22,25,26	1.43	4 (18%)	30,36,39	2.18	9 (30%)
52	PSU	A2	1233	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	1489	92,1	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
1	OMG	B5	2719	1	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)
52	OMC	A2	1392	52	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
52	PSU	A2	687	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4298	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	OMC	B5	1820	92,1	19,22,23	0.80	0	26,31,34	0.80	0
1	PSU	B5	4325	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	119	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	OMG	A2	510	52,92	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	B5	2265	92,1	19,22,23	0.82	0	26,31,34	0.86	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	3371	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
52	MA6	A2	1851	52	23,26,27	2.27	5 (21%)	34,38,41	3.69	13 (38%)
52	PSU	A2	210	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	A2M	A2	27	52,92	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
1	A2M	B5	400	1	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
1	PSU	B5	3494	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4278	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	B5	4374	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	864	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	4269	92,1	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)
1	PSU	B5	2475	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	1644	52,92	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	3974	1	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
1	OMU	B5	4052	1	19,22,23	1.22	2 (10%)	26,31,34	1.67	4 (15%)
52	PSU	A2	1368	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1632	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
1	OMU	B5	3973	1	19,22,23	1.23	3 (15%)	26,31,34	1.70	4 (15%)
1	OMG	B5	2267	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	OMC	B5	3601	1	19,22,23	0.82	0	26,31,34	0.85	0
52	PSU	A2	650	52	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	B5	1721	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	815	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	3462	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	5MC	B5	3514	92,1	18,22,23	0.94	2 (11%)	26,32,35	1.13	3 (11%)
52	4AC	A2	1338	52	21,24,25	1.07	1 (4%)	29,34,37	1.21	3 (10%)
1	OMC	B5	2208	92,1	19,22,23	0.81	0	26,31,34	0.80	0
52	PSU	A2	1082	52	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	4058	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	A2M	A2	99	52,92	22,25,26	1.47	4 (18%)	31,36,39	2.12	10 (32%)
1	OMG	B5	1260	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	UR3	B5	4276	1	19,22,23	0.99	0	26,32,35	1.41	1 (3%)
52	PSU	A2	34	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	802	52	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	3450	1	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
52	A2M	A2	1384	52	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	M3L	Bm	98	42	10,11,12	0.83	0	9,14,16	0.55	0
52	OMG	A2	1448	52	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	4740	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1005	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	816	52	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
3	PSU	B8	55	3	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	573	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	1799	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	4282	92,1	19,22,23	0.82	0	26,31,34	0.84	0
1	OMG	B5	3476	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	3369	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
1	OMC	B5	2194	92,1	19,22,23	0.82	0	26,31,34	0.93	1 (3%)
1	OMC	B5	3540	1	19,22,23	0.82	0	26,31,34	0.82	0
1	PSU	B5	4177	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	A2M	A2	1679	52	22,25,26	1.46	4 (18%)	31,36,39	2.19	10 (32%)
1	PSU	B5	3447	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3500	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	OMG	A2	1491	52,92	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	B5	4364	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	B5	3466	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	1270	1	22,25,26	1.45	4 (18%)	31,36,39	2.08	9 (29%)
52	A2M	A2	166	52	22,25,26	1.47	4 (18%)	31,36,39	2.14	10 (32%)
52	OMU	A2	1289	52	19,22,23	1.21	3 (15%)	26,31,34	1.67	4 (15%)
52	OMU	A2	1805	52	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
52	OMU	A2	172	52	19,22,23	1.19	2 (10%)	26,31,34	1.70	4 (15%)
52	PSU	A2	93	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
31	MLZ	Bb	5	31	8,9,10	0.49	0	4,9,11	0.13	0
1	PSU	B5	3576	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1047	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1693	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	B5	2258	1	19,22,23	1.21	2 (10%)	26,31,34	1.68	4 (15%)
1	OMG	B5	4383	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	6MZ	A2	1833	52,92	22,25,26	1.44	4 (18%)	30,36,39	2.15	9 (30%)
1	PSU	B5	3583	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	OMU	B5	2680	1	19,22,23	1.21	2 (10%)	26,31,34	1.72	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	4246	1	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	B5	3676	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	1683	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	3433	1	19,22,23	0.79	0	26,31,34	0.75	0
1	OMG	B5	1580	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	1537	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	1491	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
1	A2M	B5	4317	1	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
52	PSU	A2	652	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	B5	2658	92,1	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
1	PSU	B5	1720	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3554	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
52	OMC	A2	174	52,92	19,22,23	0.82	0	26,31,34	0.81	0
1	A2M	B5	2206	92,1	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
52	MA6	A2	1852	52	23,26,27	2.26	5 (21%)	34,38,41	3.67	13 (38%)
80	SAC	Ar	2	80	7,8,9	0.53	0	8,9,11	0.91	1 (12%)
52	OMG	A2	1329	52	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	A2M	A2	159	52	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
62	SAC	AZ	2	62	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
1	UY1	B5	3550	1	19,22,23	1.37	3 (15%)	22,31,34	1.90	5 (22%)
1	PSU	B5	4188	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	OMU	B5	4366	1	19,22,23	1.21	2 (10%)	26,31,34	1.72	4 (15%)
52	PSU	A2	105	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
81	NMM	As	67	81	9,11,12	0.59	0	6,12,14	0.44	0
52	PSU	A2	36	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1446	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	628	52	19,22,23	1.17	2 (10%)	26,31,34	1.69	5 (19%)
1	PSU	B5	4382	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	967	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
85	HY3	Aw	62	85	6,8,9	2.01	1 (16%)	5,10,12	1.14	1 (20%)
1	PSU	B5	2351	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
5	HIC	BB	245	5	10,11,12	0.61	0	8,14,16	0.40	0
1	A2M	B5	1810	92,1	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
1	PSU	B5	4045	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
52	OMU	A2	1443	52,92	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	A2	867	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	A2M	A2	591	52	22,25,26	1.47	4 (18%)	31,36,39	2.21	7 (22%)
1	PSU	B5	3616	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	B5	4107	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	2207	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
52	A2M	A2	513	52	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
52	A2M	A2	469	52	22,25,26	1.47	4 (18%)	31,36,39	2.09	10 (32%)
1	PSU	B5	3652	92,1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4039	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	3456	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
1	OMC	B5	2667	1	19,22,23	0.82	0	26,31,34	0.82	0
52	OMC	A2	1704	52	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	A2M	B5	3599	1	22,25,26	1.46	4 (18%)	31,36,39	2.10	10 (32%)
52	PSU	A2	823	52	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
52	PSU	A2	1239	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3496	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
52	PSU	A2	610	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
45	SAC	Br	2	45	7,8,9	0.52	0	8,9,11	0.85	1 (12%)
52	OMG	A2	437	52	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	B5	4166	1	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
52	G7M	A2	1640	61,52	23,26,27	3.12	9 (39%)	35,39,42	3.31	13 (37%)
1	OMC	B5	4202	1	19,22,23	0.81	0	26,31,34	0.79	0
52	PSU	A2	1245	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	A2	1348	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4435	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1718	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1626	52	-	0/7/25/26	0/2/2/2
30	V5N	Ba	39	30	-	1/9/10/12	0/1/1/1
1	PSU	B5	3427	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	4244	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	1175	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	2244	92,1	-	0/9/27/28	0/3/3/3
1	OMG	B5	4116	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	1801	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	398	1	-	3/9/27/28	0/3/3/3
52	OMU	A2	355	52	-	1/9/27/28	0/2/2/2
1	1MA	B5	1266	92,1	-	0/7/25/26	0/3/3/3
1	A2M	B5	2630	92,1	-	2/9/27/28	0/3/3/3
3	OMG	B8	75	3	-	0/9/27/28	0/3/3/3
1	A2M	B5	3557	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	3573	1	-	0/9/27/28	0/2/2/2
61	5MU	AT	54	61	-	0/7/25/26	0/2/2/2
1	OMC	B5	2704	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4042	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3517	1	-	2/9/27/28	0/3/3/3
1	PSU	B5	3585	92,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4099	1	-	0/7/25/26	0/2/2/2
52	OMG	A2	602	52	-	0/9/27/28	0/3/3/3
1	OMG	B5	4245	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	3562	1	-	0/9/27/28	0/3/3/3
52	PSU	A2	109	52	-	0/7/25/26	0/2/2/2
52	OMC	A2	463	52	-	0/9/27/28	0/2/2/2
52	OMG	A2	868	52	-	0/9/27/28	0/3/3/3
52	PSU	A2	1057	52	-	0/7/25/26	0/2/2/2
3	PSU	B8	69	3	-	0/7/25/26	0/2/2/2
52	A2M	A2	669	52,92	-	3/9/27/28	0/3/3/3
1	OMG	B5	3359	1	-	0/9/27/28	0/3/3/3
52	OMU	A2	116	52	-	1/9/27/28	0/2/2/2
1	OMG	B5	1477	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4419	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3619	1	-	2/9/27/28	0/2/2/2
1	OMG	B5	3524	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	577	52	-	2/9/27/28	0/3/3/3
1	PSU	B5	4169	1	-	0/7/25/26	0/2/2/2
52	B8N	A2	1249	52	-	4/16/34/35	0/2/2/2
52	A2M	A2	485	52	-	0/9/27/28	0/3/3/3
52	OMC	A2	518	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	4749	1	-	0/7/25/26	0/2/2/2
1	5MC	B5	4193	1	-	4/7/25/26	0/2/2/2
52	A2M	A2	1032	52	-	0/9/27/28	0/3/3/3
52	OMG	A2	645	52	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	OMU	A2	1327	52,92	-	0/9/27/28	0/2/2/2
1	OMG	B5	4138	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	4267	92,1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1046	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	3942	61,1	-	0/9/27/28	0/3/3/3
1	OMC	B5	1284	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	2647	1	-	0/9/27/28	0/2/2/2
83	AME	Au	1	83	-	2/9/10/12	-
6	AYA	BC	2	6	-	3/4/6/8	-
1	PSU	B5	4322	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3631	1	-	1/9/27/28	0/3/3/3
52	PSU	A2	682	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4203	1	-	0/7/25/26	0/2/2/2
52	OMG	A2	684	52	-	2/9/27/28	0/3/3/3
1	A2M	B5	4336	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	1638	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4711	1	-	0/7/25/26	0/2/2/2
4	V5N	BA	216	4	-	3/9/10/12	0/1/1/1
1	OMG	B5	4369	1	-	1/9/27/28	0/3/3/3
43	MLZ	Bo	53	43	-	0/7/8/10	-
52	OMU	A2	429	52	-	4/9/27/28	0/2/2/2
1	OMU	B5	3657	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4217	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1731	1	-	0/7/25/26	0/2/2/2
76	5F0	An	138	76	-	1/9/9/10	-
1	A2M	B5	1479	1	-	0/9/27/28	0/3/3/3
52	OMU	A2	121	52	-	0/9/27/28	0/2/2/2
52	4AC	A2	1843	52	-	4/11/29/30	0/2/2/2
61	PSU	AT	55	61	-	0/7/25/26	0/2/2/2
1	PSU	B5	4149	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	218	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1178	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	4240	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3502	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3492	52,1	-	3/9/27/28	0/3/3/3
52	PSU	A2	407	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3490	1	-	0/7/25/26	0/2/2/2
1	6MZ	B5	3966	1	-	0/9/27/28	0/3/3/3
52	PSU	A2	1233	52	-	0/7/25/26	0/2/2/2
1	A2M	B5	1489	92,1	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	B5	2719	1	-	0/9/27/28	0/3/3/3
52	OMC	A2	1392	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	687	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4298	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	1820	92,1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4325	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	119	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	510	52,92	-	1/9/27/28	0/3/3/3
1	OMC	B5	2265	92,1	-	2/9/27/28	0/2/2/2
1	PSU	B5	3371	1	-	0/7/25/26	0/2/2/2
52	MA6	A2	1851	52	-	0/11/29/30	0/3/3/3
52	PSU	A2	210	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	27	52,92	-	1/9/27/28	0/3/3/3
1	A2M	B5	400	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3494	1	-	1/7/25/26	0/2/2/2
1	PSU	B5	4278	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4374	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	864	52	-	0/7/25/26	0/2/2/2
1	A2M	B5	4269	92,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	2475	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1644	52,92	-	0/7/25/26	0/2/2/2
1	OMG	B5	3974	1	-	0/9/27/28	0/3/3/3
1	OMU	B5	4052	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	1368	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1632	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3973	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	2267	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	3601	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	650	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1721	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	815	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3462	1	-	0/7/25/26	0/2/2/2
1	5MC	B5	3514	92,1	-	0/7/25/26	0/2/2/2
52	4AC	A2	1338	52	-	4/11/29/30	0/2/2/2
1	OMC	B5	2208	92,1	-	0/9/27/28	0/2/2/2
52	PSU	A2	1082	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4058	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	99	52,92	-	2/9/27/28	0/3/3/3
1	OMG	B5	1260	1	-	1/9/27/28	0/3/3/3
1	UR3	B5	4276	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	34	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	802	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	3450	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	1384	52	-	0/9/27/28	0/3/3/3
42	M3L	Bm	98	42	-	0/9/10/12	-
52	OMG	A2	1448	52	-	3/9/27/28	0/3/3/3
1	PSU	B5	4740	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1005	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	816	52	-	0/7/25/26	0/2/2/2
3	PSU	B8	55	3	-	0/7/25/26	0/2/2/2
52	PSU	A2	573	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1799	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	4282	92,1	-	0/9/27/28	0/2/2/2
1	OMG	B5	3476	1	-	2/9/27/28	0/3/3/3
1	PSU	B5	3369	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2194	92,1	-	2/9/27/28	0/2/2/2
1	OMC	B5	3540	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4177	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	1679	52	-	0/9/27/28	0/3/3/3
1	PSU	B5	3447	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3500	1	-	0/7/25/26	0/2/2/2
52	OMG	A2	1491	52,92	-	0/9/27/28	0/3/3/3
1	OMG	B5	4364	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3466	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1270	1	-	0/9/27/28	0/3/3/3
52	A2M	A2	166	52	-	0/9/27/28	0/3/3/3
52	OMU	A2	1289	52	-	0/9/27/28	0/2/2/2
52	OMU	A2	1805	52	-	0/9/27/28	0/2/2/2
52	OMU	A2	172	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	93	52	-	0/7/25/26	0/2/2/2
31	MLZ	Bb	5	31	-	2/7/8/10	-
1	PSU	B5	3576	1	-	1/7/25/26	0/2/2/2
52	PSU	A2	1047	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1693	52	-	0/7/25/26	0/2/2/2
1	OMU	B5	2258	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	4383	1	-	1/9/27/28	0/3/3/3
52	6MZ	A2	1833	52,92	-	0/9/27/28	0/3/3/3
1	PSU	B5	3583	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	2680	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4246	1	-	1/7/25/26	0/2/2/2
1	OMG	B5	3676	1	-	2/9/27/28	0/3/3/3
1	PSU	B5	1683	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3433	1	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	B5	1580	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	1537	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1491	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	4317	1	-	0/9/27/28	0/3/3/3
52	PSU	A2	652	52	-	0/7/25/26	0/2/2/2
1	A2M	B5	2658	92,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	1720	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3554	1	-	0/7/25/26	0/2/2/2
52	OMC	A2	174	52,92	-	0/9/27/28	0/2/2/2
1	A2M	B5	2206	92,1	-	0/9/27/28	0/3/3/3
52	MA6	A2	1852	52	-	2/11/29/30	0/3/3/3
80	SAC	Ar	2	80	-	0/7/8/10	-
52	OMG	A2	1329	52	-	0/9/27/28	0/3/3/3
52	A2M	A2	159	52	-	1/9/27/28	0/3/3/3
62	SAC	AZ	2	62	-	2/7/8/10	-
1	UY1	B5	3550	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4188	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	4366	1	-	1/9/27/28	0/2/2/2
52	PSU	A2	105	52	-	0/7/25/26	0/2/2/2
81	NMM	As	67	81	-	1/9/11/13	-
52	PSU	A2	36	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1446	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	628	52	-	4/9/27/28	0/2/2/2
1	PSU	B5	4382	1	-	4/7/25/26	0/2/2/2
52	PSU	A2	967	52	-	0/7/25/26	0/2/2/2
85	HY3	Aw	62	85	-	1/1/12/14	0/1/1/1
1	PSU	B5	2351	1	-	0/7/25/26	0/2/2/2
5	HIC	BB	245	5	-	2/5/6/8	0/1/1/1
1	A2M	B5	1810	92,1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4045	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	1443	52,92	-	1/9/27/28	0/2/2/2
52	PSU	A2	867	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	591	52	-	3/9/27/28	0/3/3/3
1	PSU	B5	3616	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4107	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	2207	1	-	3/9/27/28	0/3/3/3
52	A2M	A2	513	52	-	2/9/27/28	0/3/3/3
52	A2M	A2	469	52	-	1/9/27/28	0/3/3/3
1	PSU	B5	3652	92,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4039	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	3456	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	2667	1	-	1/9/27/28	0/2/2/2
52	OMC	A2	1704	52	-	1/9/27/28	0/2/2/2
1	A2M	B5	3599	1	-	1/9/27/28	0/3/3/3
52	PSU	A2	823	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1239	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3496	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	610	52	-	0/7/25/26	0/2/2/2
45	SAC	Br	2	45	-	0/7/8/10	-
52	OMG	A2	437	52	-	0/9/27/28	0/3/3/3
1	PSU	B5	4166	1	-	0/7/25/26	0/2/2/2
52	G7M	A2	1640	61,52	-	2/7/25/26	0/3/3/3
1	OMC	B5	4202	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	1245	52	-	0/7/25/26	0/2/2/2

The worst 5 of 513 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1640	G7M	C4-N9	7.81	1.58	1.38
52	A2	1640	G7M	O6-C6	7.64	1.38	1.23
52	A2	1851	MA6	C5-N7	6.82	1.51	1.39
52	A2	1852	MA6	C5-N7	6.78	1.51	1.39
52	A2	1640	G7M	C5-C4	6.18	1.53	1.38

The worst 5 of 969 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1851	MA6	C4-N9-C8	14.63	121.58	105.73
52	A2	1852	MA6	C4-N9-C8	14.47	121.41	105.73
52	A2	1640	G7M	C8-N7-C5	11.39	122.02	107.78
52	A2	591	A2M	C5-C4-N3	-6.87	117.79	126.75
52	A2	1852	MA6	N3-C4-N9	6.76	138.22	127.08

There are no chirality outliers.

5 of 123 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BA	216	V5N	O-C-CA-CB
6	BC	2	AYA	OT-CT-N-CA
6	BC	2	AYA	CM-CT-N-CA
31	Bb	5	MLZ	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
52	A2	429	OMU	C2'-C1'-N1-C2

There are no ring outliers.

96 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	1718	PSU	2	0
1	B5	2244	A2M	1	0
52	A2	355	OMU	1	0
3	B8	75	OMG	1	0
1	B5	3557	A2M	1	0
1	B5	3573	OMC	1	0
1	B5	2704	OMC	1	0
1	B5	3517	A2M	1	0
52	A2	602	OMG	1	0
1	B5	3562	A2M	2	0
52	A2	463	OMC	1	0
52	A2	116	OMU	1	0
1	B5	3619	OMC	1	0
1	B5	3524	OMG	1	0
52	A2	577	A2M	2	0
52	A2	485	A2M	1	0
52	A2	518	OMC	1	0
52	A2	1032	A2M	2	0
52	A2	645	OMG	1	0
1	B5	4138	OMG	1	0
1	B5	3942	OMG	2	0
1	B5	1284	OMC	2	0
1	B5	2647	OMC	1	0
1	B5	3631	OMG	1	0
52	A2	682	PSU	2	0
1	B5	4203	PSU	1	0
1	B5	4336	A2M	1	0
1	B5	1638	PSU	1	0
1	B5	4369	OMG	1	0
52	A2	121	OMU	1	0
52	A2	1843	4AC	2	0
1	B5	3502	PSU	1	0
1	B5	3492	A2M	1	0
52	A2	1233	PSU	2	0
52	A2	1392	OMC	1	0
1	B5	4325	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A2	510	OMG	1	0
1	B5	3371	PSU	1	0
52	A2	27	A2M	1	0
1	B5	400	A2M	1	0
52	A2	864	PSU	1	0
1	B5	4269	A2M	1	0
1	B5	3974	OMG	1	0
1	B5	4052	OMU	1	0
1	B5	2267	OMG	1	0
52	A2	1338	4AC	2	0
1	B5	2208	OMC	1	0
1	B5	4058	PSU	1	0
52	A2	99	A2M	2	0
1	B5	1260	OMG	1	0
1	B5	3450	A2M	2	0
52	A2	1384	A2M	1	0
52	A2	1448	OMG	2	0
1	B5	4282	OMC	1	0
1	B5	3476	OMG	1	0
1	B5	2194	OMC	1	0
1	B5	3540	OMC	1	0
52	A2	1679	A2M	2	0
52	A2	1491	OMG	1	0
1	B5	4364	OMG	1	0
1	B5	1270	A2M	2	0
52	A2	166	A2M	2	0
52	A2	1289	OMU	2	0
52	A2	1805	OMU	2	0
52	A2	172	OMU	2	0
1	B5	2258	OMU	2	0
1	B5	4383	OMG	1	0
52	A2	1833	6MZ	1	0
1	B5	3676	OMG	1	0
1	B5	3433	OMC	1	0
1	B5	1580	OMG	1	0
1	B5	4317	A2M	1	0
1	B5	2658	A2M	2	0
1	B5	2206	A2M	2	0
52	A2	1852	MA6	1	0
52	A2	1329	OMG	1	0
1	B5	3550	UY1	2	0
1	B5	4188	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	4366	OMU	4	0
52	A2	105	PSU	1	0
52	A2	36	PSU	2	0
52	A2	1446	PSU	1	0
1	B5	4382	PSU	2	0
1	B5	1810	A2M	2	0
52	A2	1443	OMU	1	0
1	B5	2207	OMG	2	0
52	A2	513	A2M	1	0
52	A2	469	A2M	1	0
1	B5	4039	PSU	1	0
1	B5	3456	A2M	2	0
1	B5	2667	OMC	1	0
52	A2	1704	OMC	2	0
1	B5	3599	A2M	2	0
52	A2	437	OMG	1	0
52	A2	1640	G7M	1	0
1	B5	4202	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 848 ligands modelled in this entry, 428 are monoatomic and 312 are unknown - leaving 108 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	$\# Z > 2$
89	N	Bo	206	89	9,12,13	0.65	0	10,16,19	0.69	0
89	N	Ay	203	89	9,12,13	0.66	0	10,16,19	0.67	0
89	N	Bv	301	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	AT	104	89	9,12,13	0.65	0	10,16,19	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	N	Aa	301	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	B5	4904	89	9,12,13	0.65	0	10,16,19	0.68	0
90	SPD	A2	1911	-	9,9,9	0.15	0	8,8,8	0.17	0
90	SPD	B5	4938	-	9,9,9	0.15	0	8,8,8	0.18	0
89	N	B5	4910	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	Bo	203	89	9,12,13	0.65	0	10,16,19	0.63	0
89	N	AT	102	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	B5	4907	89	9,12,13	0.66	0	10,16,19	0.65	0
89	N	Ae	308	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	B5	4916	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Ae	302	89	9,12,13	0.66	0	10,16,19	0.68	0
89	N	Ae	304	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	Bv	302	89	9,12,13	0.66	0	10,16,19	0.68	0
89	N	Ae	307	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	B5	4915	89	9,12,13	0.65	0	10,16,19	0.64	0
89	N	Aa	310	89	9,12,13	0.65	0	10,16,19	0.68	0
91	SPM	B5	4935	-	13,13,13	0.15	0	12,12,12	0.14	0
89	N	Ae	309	89	9,12,13	0.65	0	10,16,19	0.69	0
89	N	AT	101	89	9,12,13	0.66	0	10,16,19	0.65	0
89	N	Bo	211	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	B5	4911	89	9,12,13	0.65	0	10,16,19	0.65	0
90	SPD	B5	4928	-	9,9,9	0.15	0	8,8,8	0.16	0
89	N	AT	105	89	9,12,13	0.66	0	10,16,19	0.65	0
89	N	Aa	309	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	B5	4914	89	9,12,13	0.64	0	10,16,19	0.70	0
89	N	B5	4917	89	9,12,13	0.66	0	10,16,19	0.69	0
89	N	Bv	307	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Ae	306	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	B5	4923	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	A2	1905	-	9,9,9	0.16	0	8,8,8	0.16	0
89	N	Ae	303	89	9,12,13	0.64	0	10,16,19	0.68	0
90	SPD	B5	4926	-	9,9,9	0.16	0	8,8,8	0.18	0
90	SPD	A2	1910	-	9,9,9	0.15	0	8,8,8	0.19	0
90	SPD	B5	4931	-	9,9,9	0.15	0	8,8,8	0.19	0
89	N	Aa	304	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	Aa	306	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	Bo	208	89	9,12,13	0.64	0	10,16,19	0.68	0
89	N	Ay	201	89	9,12,13	0.66	0	10,16,19	0.68	0
90	SPD	B5	4929	-	9,9,9	0.16	0	8,8,8	0.17	0
90	SPD	B5	4937	-	9,9,9	0.15	0	8,8,8	0.17	0
89	N	AI	101	60,89	9,12,13	0.65	0	10,16,19	0.68	0
90	SPD	B5	4934	-	9,9,9	0.15	0	8,8,8	0.19	0
89	N	Bo	202	89	13,13,13	0.80	0	17,19,19	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
90	SPD	B5	4921	-	9,9,9	0.15	0	8,8,8	0.14	0
89	N	B5	4903	89	9,12,13	0.66	0	10,16,19	0.69	0
89	N	Ay	202	89	9,12,13	0.65	0	10,16,19	0.68	0
90	SPD	B5	4922	-	9,9,9	0.15	0	8,8,8	0.18	0
91	SPM	A2	1912	-	13,13,13	0.15	0	12,12,12	0.16	0
89	N	Bo	204	89	9,12,13	0.65	0	10,16,19	0.65	0
89	N	B5	4902	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	Ae	310	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	B5	4913	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Ay	204	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	B5	4944	-	9,9,9	0.15	0	8,8,8	0.15	0
89	N	A2	1901	89	9,12,13	0.65	0	10,16,19	0.69	0
90	SPD	A2	1904	-	9,9,9	0.15	0	8,8,8	0.18	0
89	N	B5	4909	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	Ae	305	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	Aa	305	89	9,12,13	0.65	0	10,16,19	0.65	0
89	N	Bv	304	89	9,12,13	0.65	0	10,16,19	0.65	0
89	N	Ay	205	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	Bv	305	89	9,12,13	0.66	0	10,16,19	0.68	0
90	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.20	0
94	GTP	B7	201	2	30,34,34	0.50	0	46,54,54	0.56	0
89	N	AT	106	89	9,12,13	0.66	0	10,16,19	0.65	0
89	N	Aa	308	89	9,12,13	0.65	0	10,16,19	0.68	0
90	SPD	B5	4933	-	9,9,9	0.15	0	8,8,8	0.20	0
89	N	Bo	209	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	B5	4936	-	9,9,9	0.15	0	8,8,8	0.17	0
89	N	B5	4912	89	9,12,13	0.66	0	10,16,19	0.67	0
90	SPD	A2	1909	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	B5	4941	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	A2	1908	-	9,9,9	0.16	0	8,8,8	0.16	0
90	SPD	B5	4939	-	9,9,9	0.15	0	8,8,8	0.17	0
90	SPD	B5	4924	-	9,9,9	0.15	0	8,8,8	0.21	0
90	SPD	B5	4927	-	9,9,9	0.16	0	8,8,8	0.19	0
89	N	B5	4919	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	Bv	303	89	9,12,13	0.66	0	10,16,19	0.67	0
89	N	Bo	212	89	9,12,13	0.66	0	10,16,19	0.68	0
89	N	Aa	303	89	9,12,13	0.64	0	10,16,19	0.66	0
89	N	B5	4908	89	9,12,13	0.66	0	10,16,19	0.64	0
89	N	B5	4905	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	B5	4943	-	9,9,9	0.15	0	8,8,8	0.21	0
89	N	A2	1903	89	9,12,13	0.65	0	10,16,19	0.64	0
89	N	AT	103	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	Aa	307	89	9,12,13	0.65	0	10,16,19	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	N	B5	4906	89	9,12,13	0.64	0	10,16,19	0.64	0
89	N	Bv	306	89	9,12,13	0.65	0	10,16,19	0.68	0
91	SPM	B5	4932	-	13,13,13	0.15	0	12,12,12	0.22	0
90	SPD	B5	4930	-	9,9,9	0.15	0	8,8,8	0.20	0
90	SPD	B5	4942	-	9,9,9	0.15	0	8,8,8	0.18	0
89	N	Aa	302	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	Bo	207	89	9,12,13	0.64	0	10,16,19	0.66	0
89	N	Bo	205	89	9,12,13	0.66	0	10,16,19	0.67	0
90	SPD	A2	1906	-	9,9,9	0.15	0	8,8,8	0.19	0
89	N	Bo	210	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	B5	4940	-	9,9,9	0.15	0	8,8,8	0.20	0
89	N	A2	1902	89	9,12,13	0.66	0	10,16,19	0.66	0
90	SPD	B5	4925	-	9,9,9	0.15	0	8,8,8	0.19	0
89	N	B5	4901	89	9,12,13	0.65	0	10,16,19	0.69	0
95	AAC	BD	301	7	6,6,7	0.88	0	6,6,8	1.13	1 (16%)
89	N	B5	4918	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	B5	4920	89	9,12,13	0.64	0	10,16,19	0.68	0
89	N	Ae	301	89	9,12,13	0.65	0	10,16,19	0.68	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
89	N	Bo	206	89	-	3/3/18/19	0/1/1/1
89	N	Ay	203	89	-	2/3/18/19	0/1/1/1
89	N	Bv	301	89	-	0/3/18/19	0/1/1/1
89	N	AT	104	89	-	0/3/18/19	0/1/1/1
89	N	Aa	301	89	-	0/3/18/19	0/1/1/1
89	N	B5	4904	89	-	0/3/18/19	0/1/1/1
90	SPD	A2	1911	-	-	0/7/7/7	-
90	SPD	B5	4938	-	-	0/7/7/7	-
89	N	B5	4910	89	-	2/3/18/19	0/1/1/1
89	N	Bo	203	89	-	2/3/18/19	0/1/1/1
89	N	AT	102	89	-	0/3/18/19	0/1/1/1
89	N	B5	4907	89	-	0/3/18/19	0/1/1/1
89	N	Ae	308	89	-	0/3/18/19	0/1/1/1
89	N	B5	4916	89	-	3/3/18/19	0/1/1/1
89	N	Ae	302	89	-	2/3/18/19	0/1/1/1
89	N	Ae	304	89	-	3/3/18/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	N	Bv	302	89	-	3/3/18/19	0/1/1/1
89	N	Ae	307	89	-	0/3/18/19	0/1/1/1
89	N	B5	4915	89	-	1/3/18/19	0/1/1/1
89	N	Aa	310	89	-	2/3/18/19	0/1/1/1
91	SPM	B5	4935	-	-	0/11/11/11	-
89	N	Ae	309	89	-	3/3/18/19	0/1/1/1
89	N	AT	101	89	-	3/3/18/19	0/1/1/1
89	N	Bo	211	89	-	2/3/18/19	0/1/1/1
89	N	B5	4911	89	-	2/3/18/19	0/1/1/1
90	SPD	B5	4928	-	-	0/7/7/7	-
89	N	AT	105	89	-	1/3/18/19	0/1/1/1
89	N	Aa	309	89	-	2/3/18/19	0/1/1/1
89	N	B5	4914	89	-	1/3/18/19	0/1/1/1
89	N	B5	4917	89	-	3/3/18/19	0/1/1/1
89	N	Bv	307	89	-	3/3/18/19	0/1/1/1
89	N	Ae	306	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4923	-	-	1/7/7/7	-
90	SPD	A2	1905	-	-	0/7/7/7	-
89	N	Ae	303	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4926	-	-	1/7/7/7	-
90	SPD	A2	1910	-	-	1/7/7/7	-
90	SPD	B5	4931	-	-	0/7/7/7	-
89	N	Aa	304	89	-	2/3/18/19	0/1/1/1
89	N	Aa	306	89	-	1/3/18/19	0/1/1/1
89	N	Bo	208	89	-	3/3/18/19	0/1/1/1
89	N	Ay	201	89	-	2/3/18/19	0/1/1/1
90	SPD	B5	4929	-	-	0/7/7/7	-
90	SPD	B5	4937	-	-	0/7/7/7	-
89	N	AI	101	60,89	-	1/3/18/19	0/1/1/1
90	SPD	B5	4934	-	-	0/7/7/7	-
89	N	Bo	202	89	-	0/6/19/19	0/1/1/1
90	SPD	B5	4921	-	-	1/7/7/7	-
89	N	B5	4903	89	-	0/3/18/19	0/1/1/1
89	N	Ay	202	89	-	2/3/18/19	0/1/1/1
90	SPD	B5	4922	-	-	1/7/7/7	-
91	SPM	A2	1912	-	-	2/11/11/11	-
89	N	Bo	204	89	-	0/3/18/19	0/1/1/1
89	N	B5	4902	89	-	2/3/18/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	N	Ae	310	89	-	0/3/18/19	0/1/1/1
89	N	B5	4913	89	-	3/3/18/19	0/1/1/1
89	N	Ay	204	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4944	-	-	1/7/7/7	-
89	N	A2	1901	89	-	3/3/18/19	0/1/1/1
90	SPD	A2	1904	-	-	1/7/7/7	-
89	N	B5	4909	89	-	1/3/18/19	0/1/1/1
89	N	Ae	305	89	-	2/3/18/19	0/1/1/1
89	N	Aa	305	89	-	1/3/18/19	0/1/1/1
89	N	Bv	304	89	-	1/3/18/19	0/1/1/1
89	N	Ay	205	89	-	2/3/18/19	0/1/1/1
89	N	Bv	305	89	-	2/3/18/19	0/1/1/1
90	SPD	A2	1907	-	-	0/7/7/7	-
94	GTP	B7	201	2	-	0/22/38/38	0/3/3/3
89	N	AT	106	89	-	2/3/18/19	0/1/1/1
89	N	Aa	308	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4933	-	-	0/7/7/7	-
89	N	Bo	209	89	-	0/3/18/19	0/1/1/1
90	SPD	B5	4936	-	-	1/7/7/7	-
89	N	B5	4912	89	-	0/3/18/19	0/1/1/1
90	SPD	A2	1909	-	-	0/7/7/7	-
90	SPD	B5	4941	-	-	0/7/7/7	-
90	SPD	A2	1908	-	-	0/7/7/7	-
90	SPD	B5	4939	-	-	0/7/7/7	-
90	SPD	B5	4924	-	-	0/7/7/7	-
90	SPD	B5	4927	-	-	0/7/7/7	-
89	N	B5	4919	89	-	0/3/18/19	0/1/1/1
89	N	Bv	303	89	-	0/3/18/19	0/1/1/1
89	N	Bo	212	89	-	2/3/18/19	0/1/1/1
89	N	Aa	303	89	-	0/3/18/19	0/1/1/1
89	N	B5	4908	89	-	2/3/18/19	0/1/1/1
89	N	B5	4905	89	-	1/3/18/19	0/1/1/1
90	SPD	B5	4943	-	-	0/7/7/7	-
89	N	A2	1903	89	-	2/3/18/19	0/1/1/1
89	N	AT	103	89	-	3/3/18/19	0/1/1/1
89	N	Aa	307	89	-	0/3/18/19	0/1/1/1
89	N	B5	4906	89	-	1/3/18/19	0/1/1/1
89	N	Bv	306	89	-	3/3/18/19	0/1/1/1
91	SPM	B5	4932	-	-	0/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SPD	B5	4930	-	-	1/7/7/7	-
90	SPD	B5	4942	-	-	1/7/7/7	-
89	N	Aa	302	89	-	0/3/18/19	0/1/1/1
89	N	Bo	207	89	-	3/3/18/19	0/1/1/1
89	N	Bo	205	89	-	0/3/18/19	0/1/1/1
90	SPD	A2	1906	-	-	0/7/7/7	-
89	N	Bo	210	89	-	0/3/18/19	0/1/1/1
90	SPD	B5	4940	-	-	1/7/7/7	-
89	N	A2	1902	89	-	2/3/18/19	0/1/1/1
90	SPD	B5	4925	-	-	1/7/7/7	-
89	N	B5	4901	89	-	3/3/18/19	0/1/1/1
95	AAC	BD	301	7	-	0/3/4/5	-
89	N	B5	4918	89	-	2/3/18/19	0/1/1/1
89	N	B5	4920	89	-	3/3/18/19	0/1/1/1
89	N	Ae	301	89	-	3/3/18/19	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	Bo	202	N	OP2-P-OP1	2.27	119.58	110.68
95	BD	301	AAC	O2-C1-C2	-2.25	118.92	125.42

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	B5	4911	N	O4'-C4'-C5'-O5'
89	A2	1902	N	C3'-C4'-C5'-O5'
89	Aa	304	N	C3'-C4'-C5'-O5'
89	B5	4908	N	O4'-C4'-C5'-O5'
89	B5	4910	N	O4'-C4'-C5'-O5'

There are no ring outliers.

29 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	A2	1911	SPD	1	0
89	B5	4915	N	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	B5	4928	SPD	1	0
90	B5	4923	SPD	1	0
90	A2	1905	SPD	1	0
89	Ae	303	N	2	0
90	A2	1910	SPD	3	0
90	B5	4931	SPD	1	0
90	B5	4929	SPD	2	0
90	B5	4937	SPD	1	0
91	A2	1912	SPM	3	0
89	Bo	204	N	1	0
90	B5	4944	SPD	3	0
90	A2	1904	SPD	2	0
90	A2	1907	SPD	1	0
94	B7	201	GTP	1	0
90	B5	4936	SPD	3	0
90	A2	1909	SPD	1	0
90	A2	1908	SPD	1	0
90	B5	4939	SPD	1	0
89	Aa	303	N	1	0
89	Bv	306	N	1	0
91	B5	4932	SPM	1	0
90	B5	4930	SPD	2	0
90	B5	4942	SPD	1	0
89	Aa	302	N	1	0
90	A2	1906	SPD	2	0
90	B5	4940	SPD	2	0
89	A2	1902	N	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

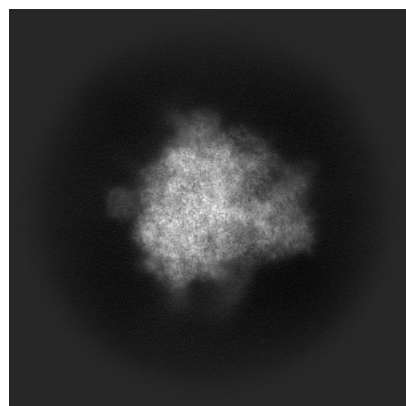
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17367. These allow visual inspection of the internal detail of the map and identification of artifacts.

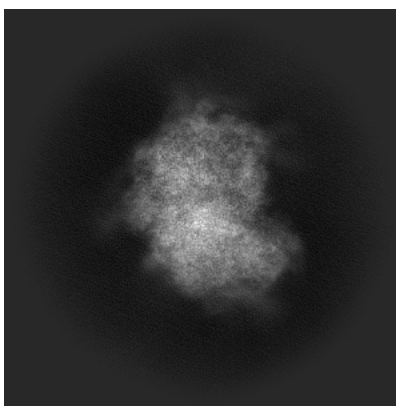
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

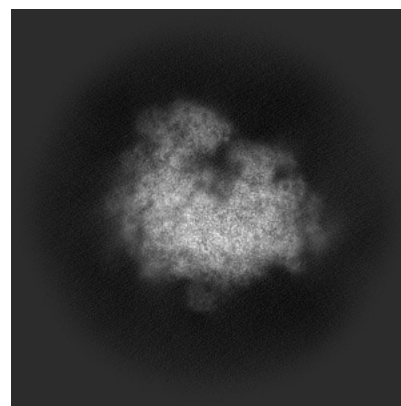
6.1.1 Primary map



X

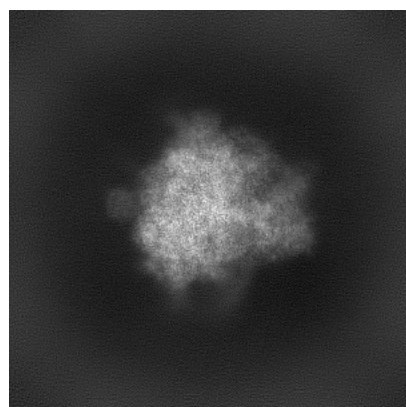


Y

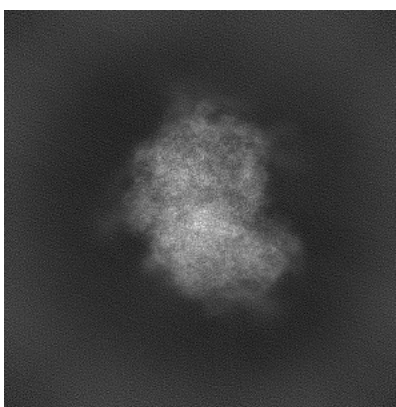


Z

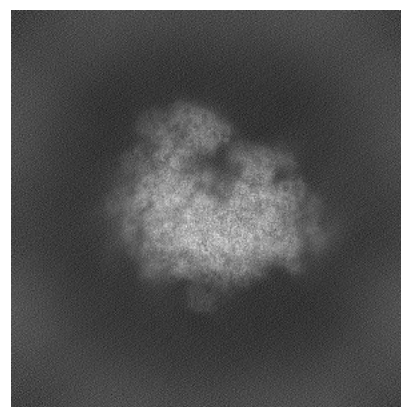
6.1.2 Raw map



X



Y

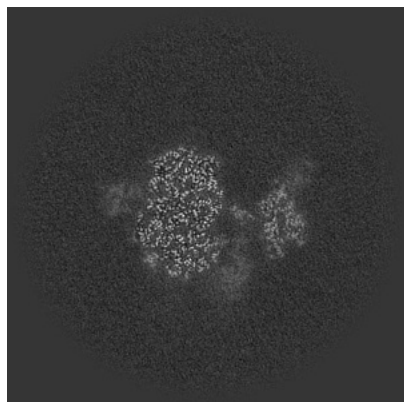


Z

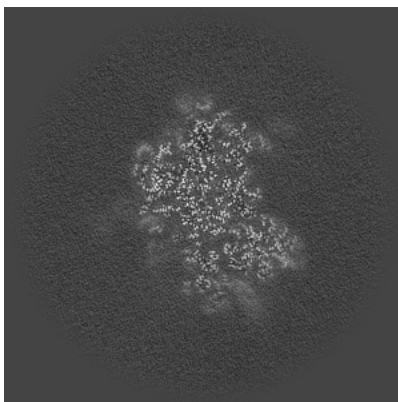
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

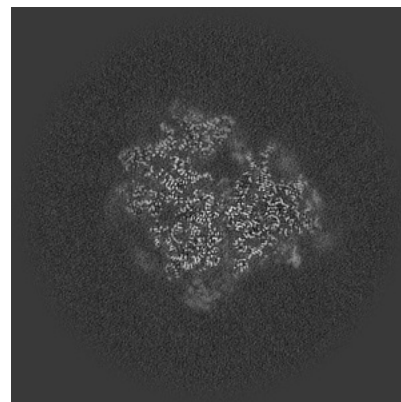
6.2.1 Primary map



X Index: 217

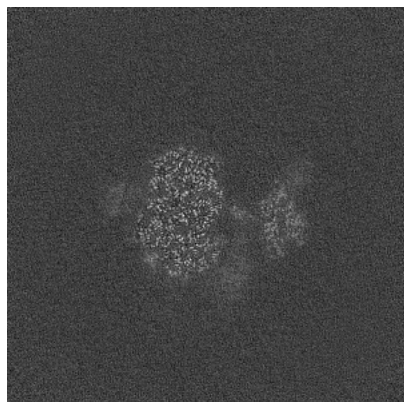


Y Index: 217

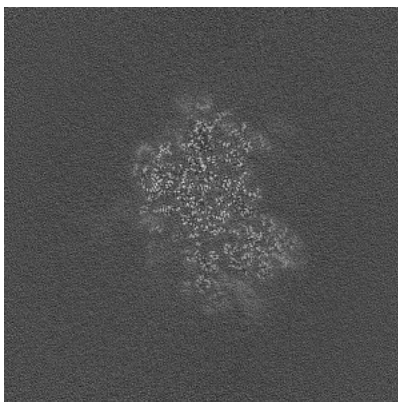


Z Index: 217

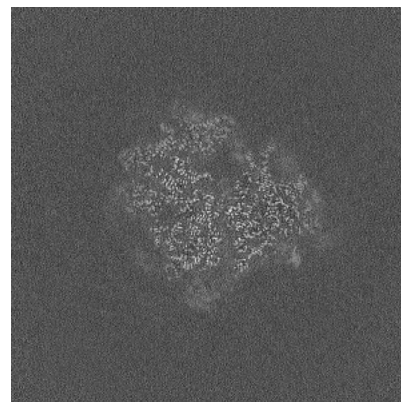
6.2.2 Raw map



X Index: 217



Y Index: 217

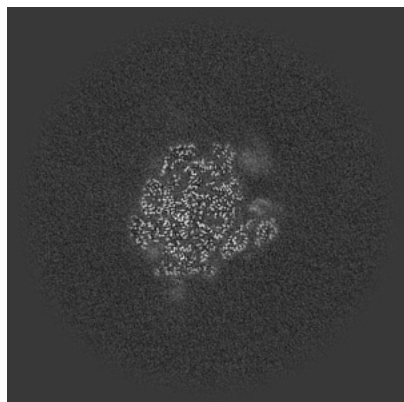


Z Index: 217

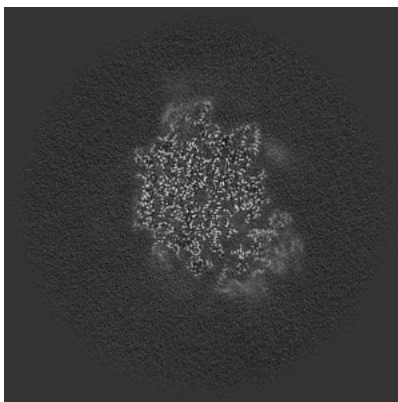
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

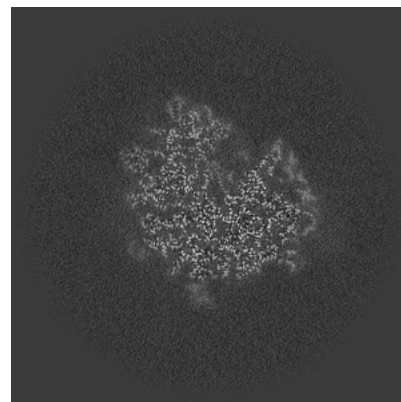
6.3.1 Primary map



X Index: 250

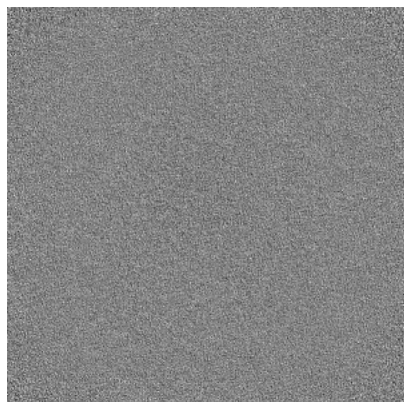


Y Index: 199

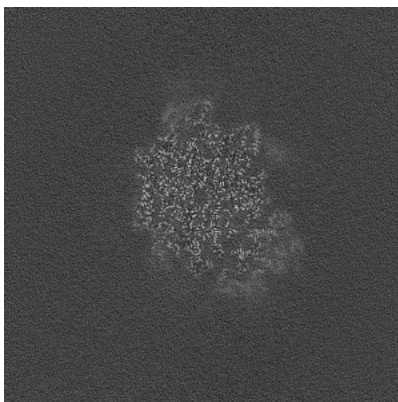


Z Index: 208

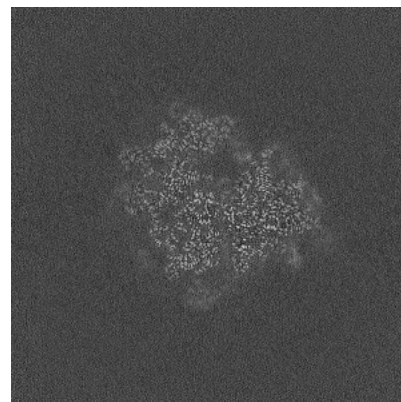
6.3.2 Raw map



X Index: 0



Y Index: 199

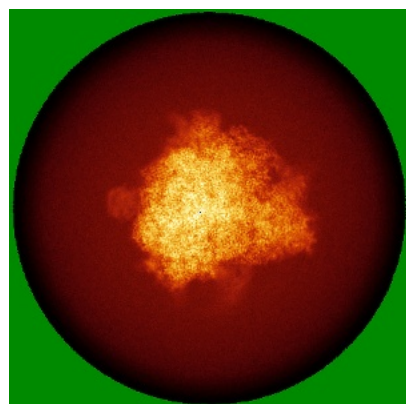


Z Index: 216

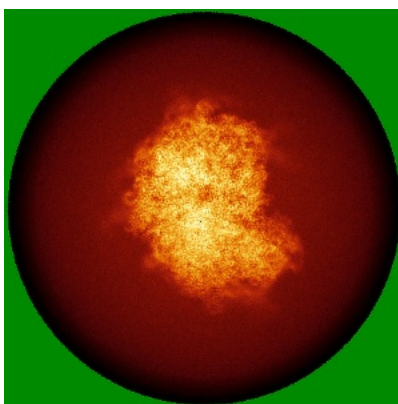
The images above show the largest variance slices of the map in three orthogonal directions.

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

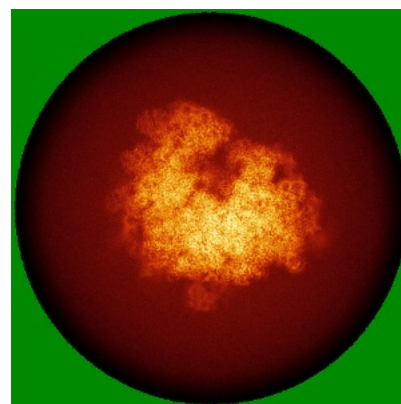
6.4.1 Primary map



X

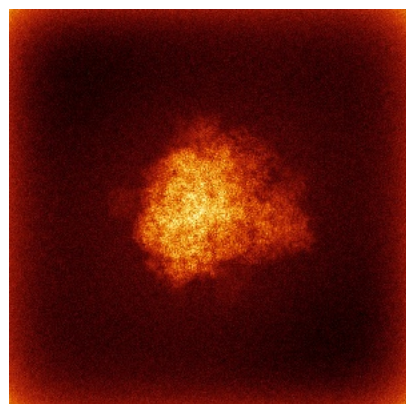


Y

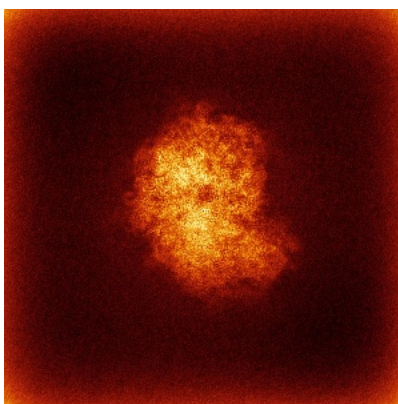


Z

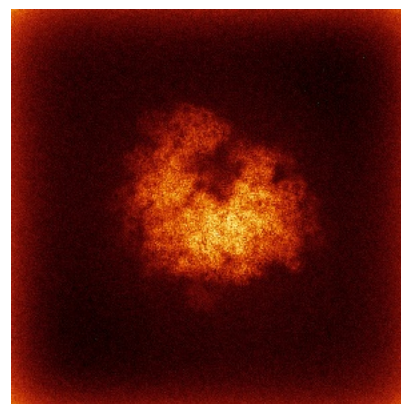
6.4.2 Raw map



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](#)

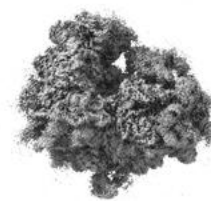
6.5.1 Primary map



X



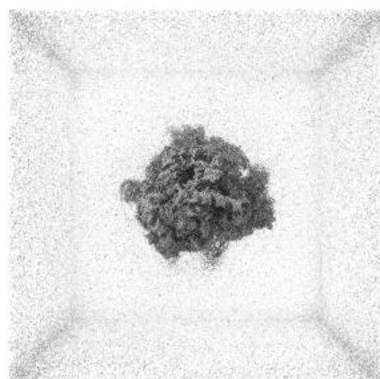
Y



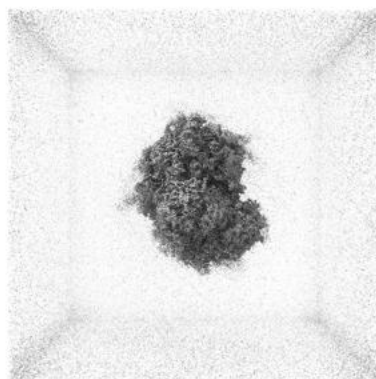
Z

The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

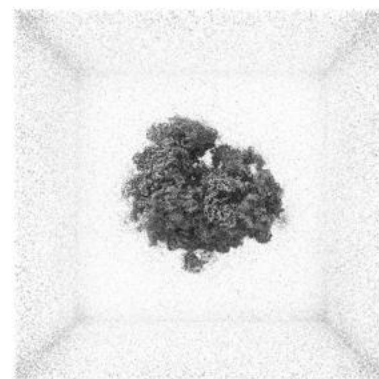
6.5.2 Raw map



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.

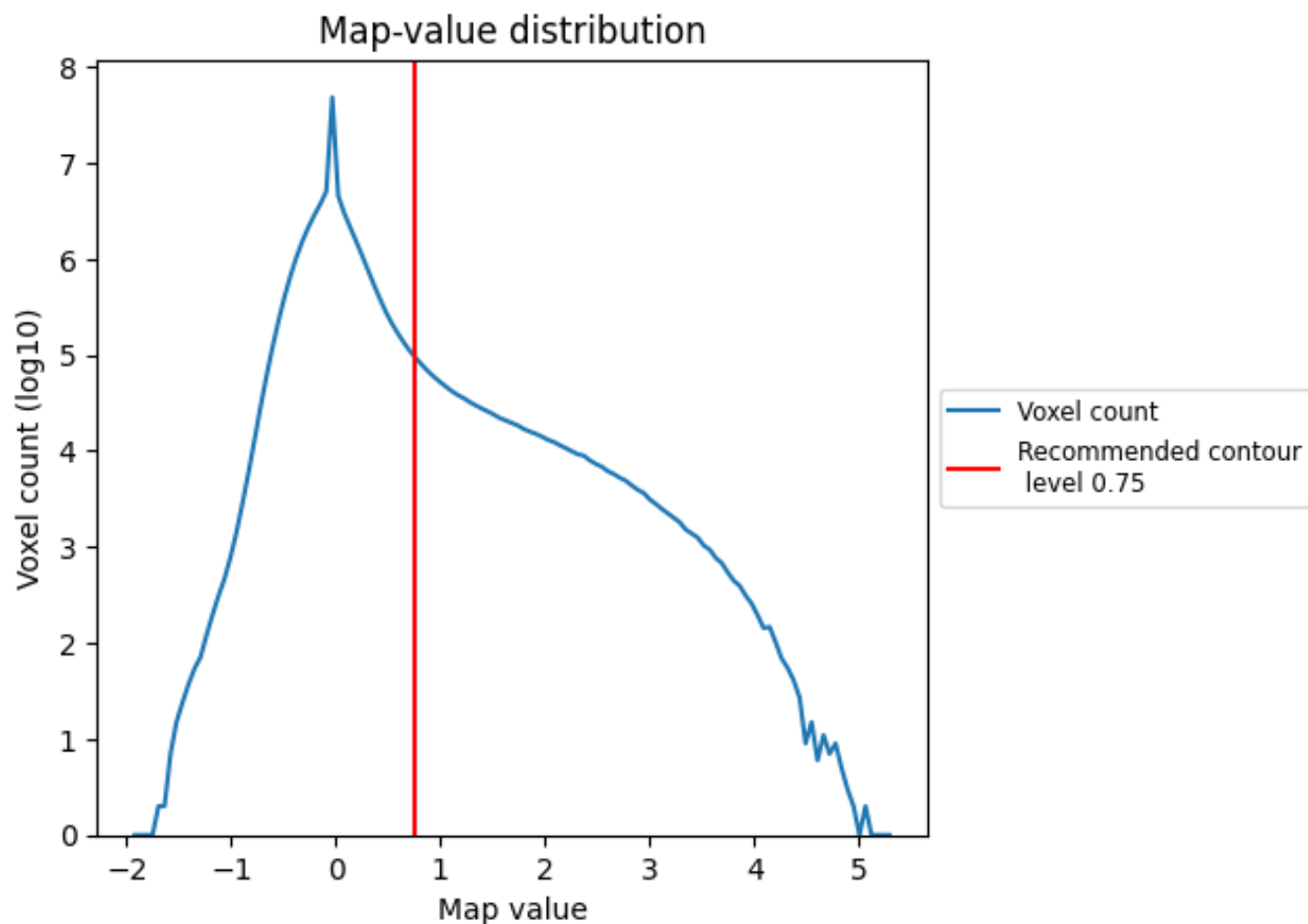
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

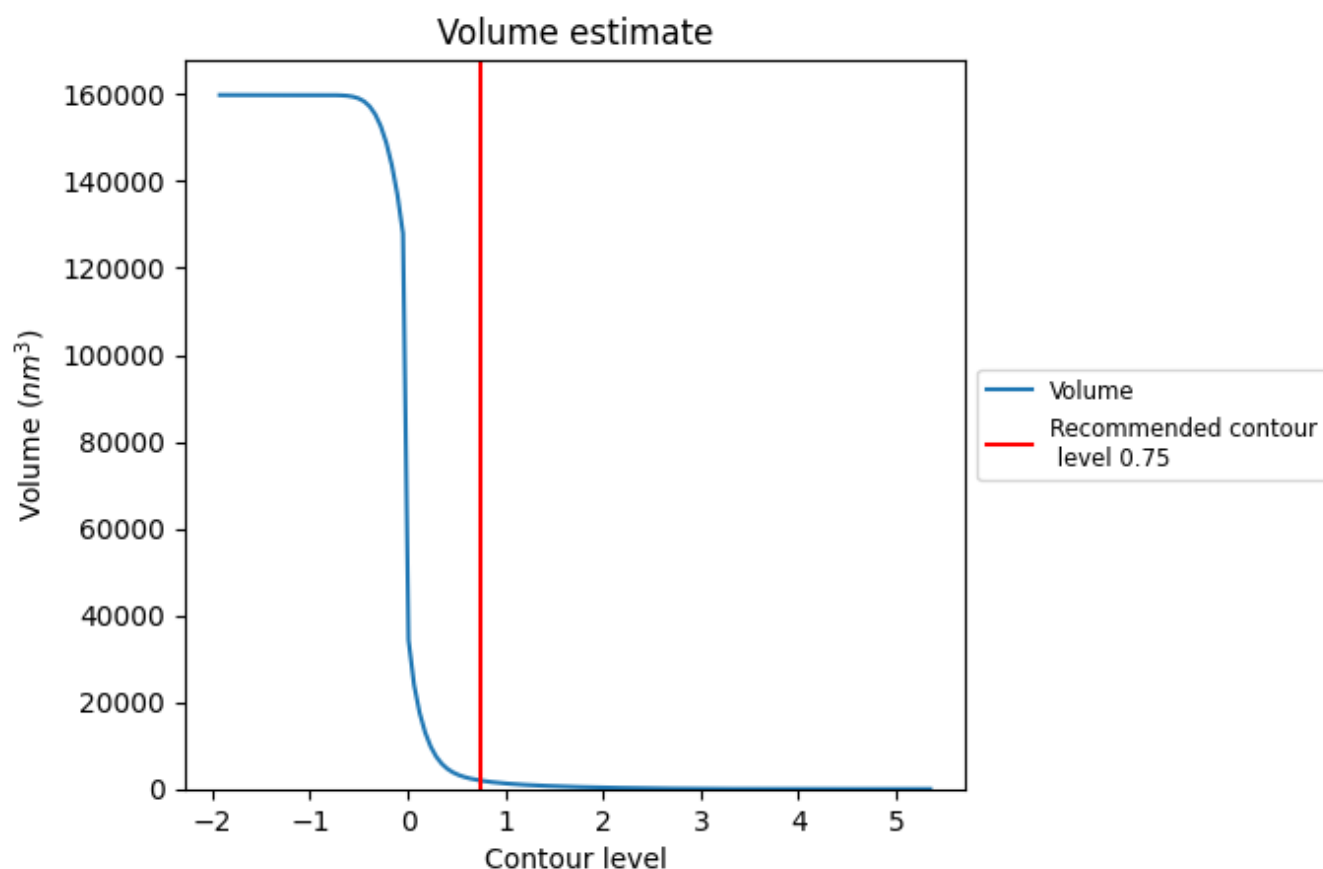
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

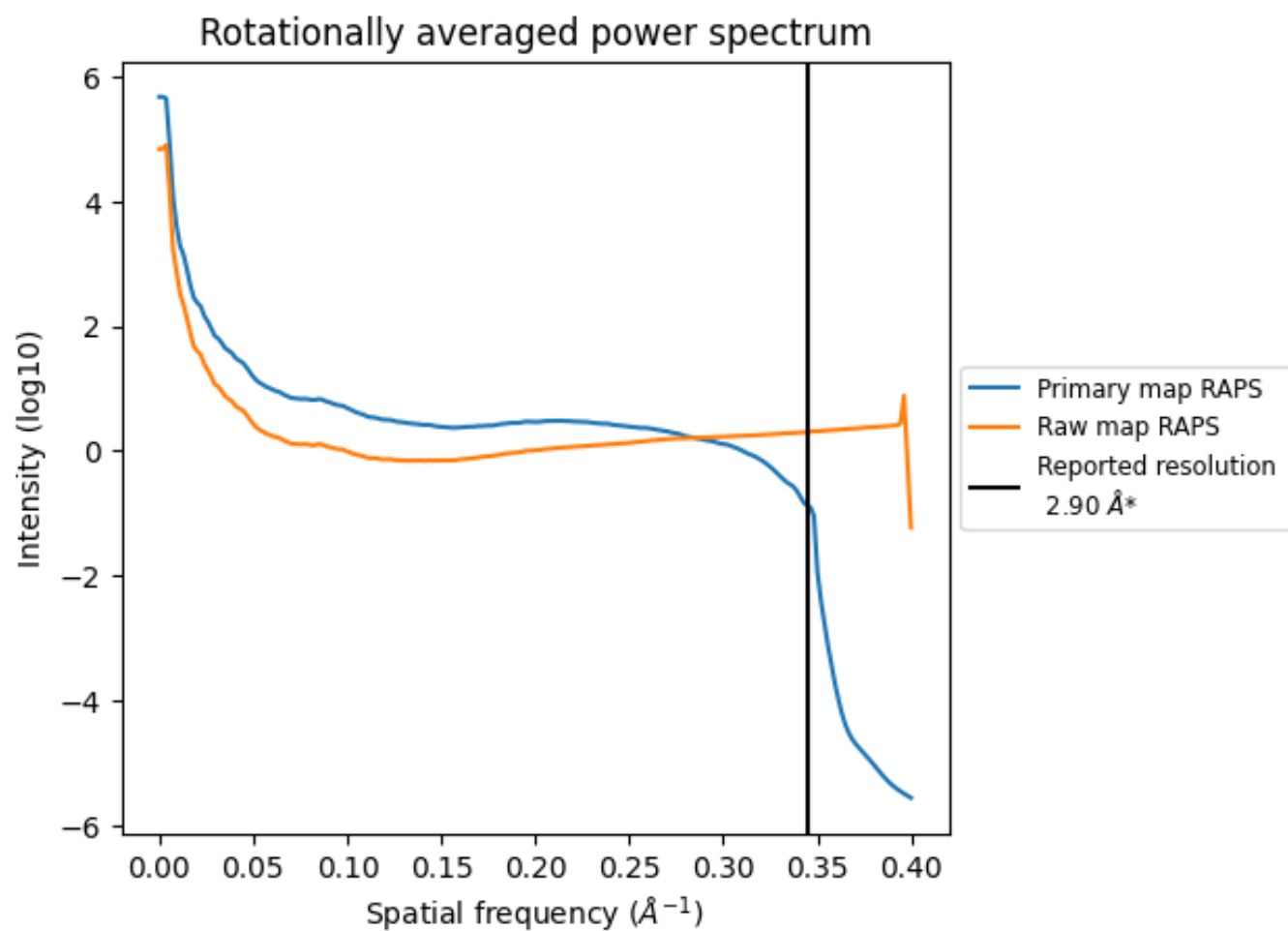
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1923 nm^3 ; this corresponds to an approximate mass of 1737 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 ⓘ

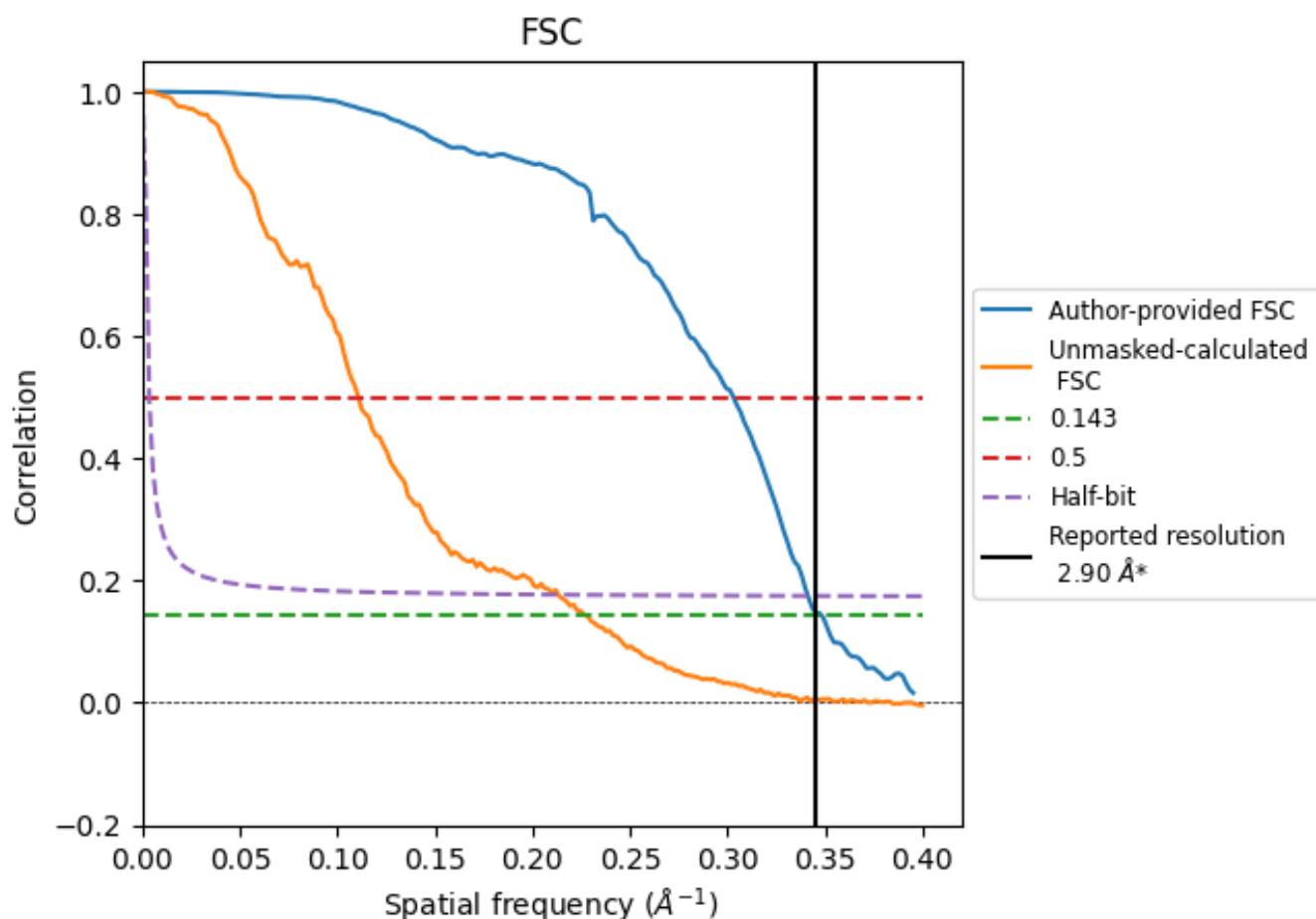


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

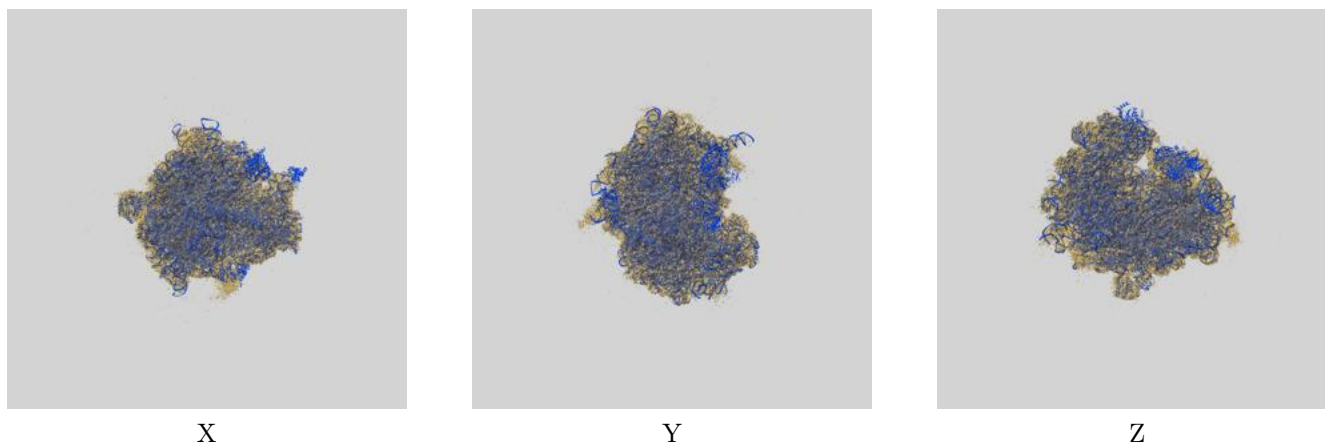
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.30	2.93
Unmasked-calculated*	4.40	9.03	4.69

*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 4.40 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

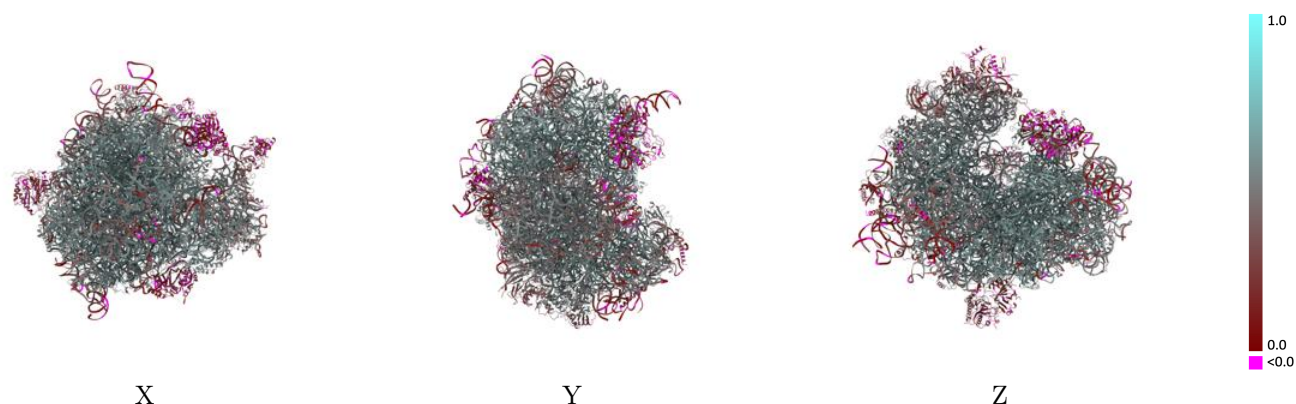
This section contains information regarding the fit between EMDB map EMD-17367 and PDB model 8P2K. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



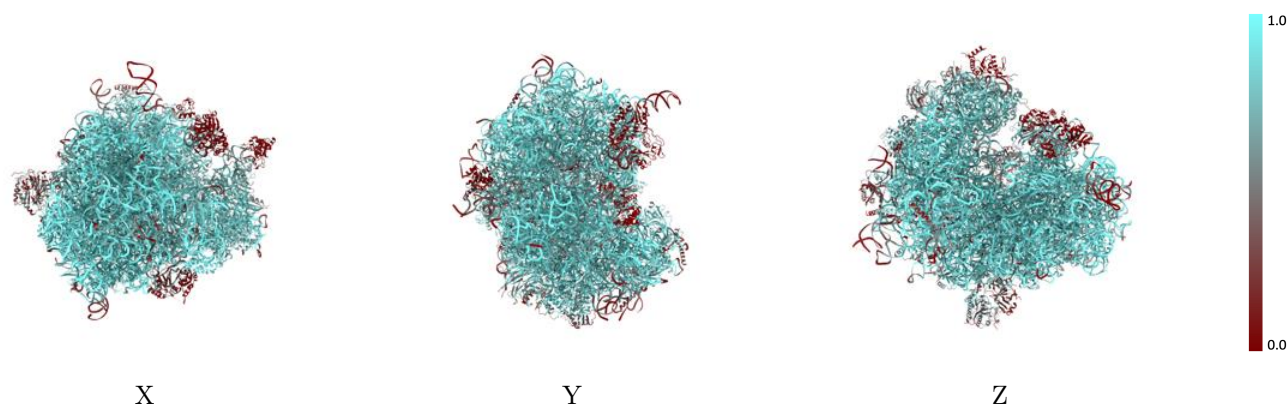
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



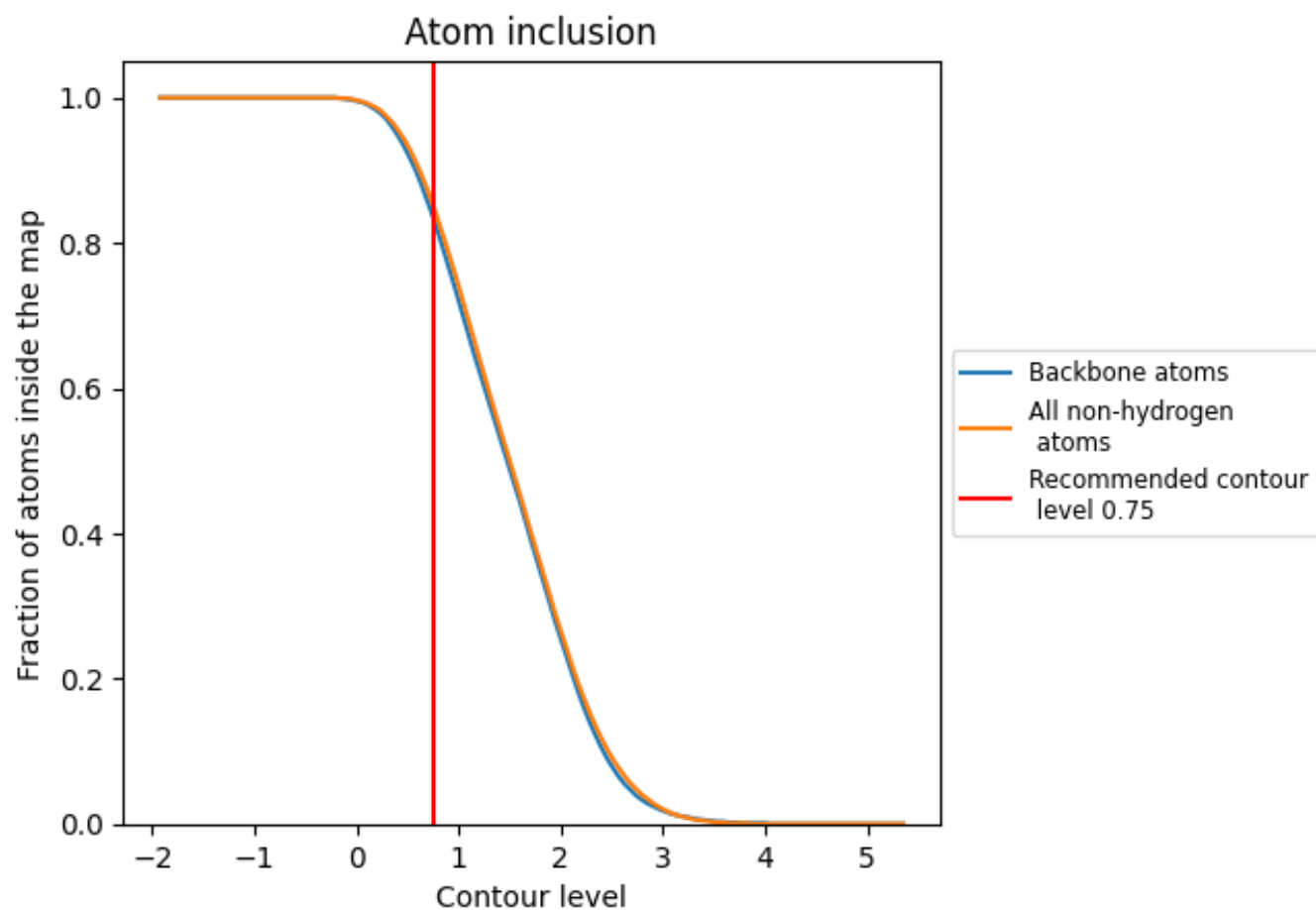
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 85% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.4830
A2	 0.8920	 0.4740
AA	 0.8010	 0.4780
AB	 0.7860	 0.4830
AC	 0.0470	 0.1220
AD	 0.7250	 0.4230
AE	 0.8790	 0.5200
AF	 0.6310	 0.3680
AG	 0.8620	 0.4800
AI	 0.7840	 0.4710
AT	 0.7900	 0.4410
AZ	 0.7640	 0.4670
Aa	 0.8090	 0.4860
Ab	 0.8520	 0.5200
Ac	 0.7370	 0.4370
Ad	 0.8850	 0.5090
Ae	 0.7630	 0.4660
Af	 0.7590	 0.4030
Ag	 0.5680	 0.3850
Ah	 0.8530	 0.4960
Ai	 0.8540	 0.4920
Aj	 0.7280	 0.3800
Ak	 0.8270	 0.4980
Al	 0.0090	 0.1370
Am	 0.8810	 0.5250
An	 0.8760	 0.5240
Ao	 0.7610	 0.4290
Ap	 0.8370	 0.4760
Aq	 0.6590	 0.4260
Ar	 0.7960	 0.4620
As	 0.8330	 0.4620
At	 0.6550	 0.3890
Au	 0.7940	 0.4790
Av	 0.8920	 0.5440
Aw	 0.8910	 0.5410



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Chain	Atom inclusion	Q-score
Ax	 0.8200	 0.4770
Ay	 0.6560	 0.4100
Az	 0.9450	 0.5650
B5	 0.9130	 0.5000
B7	 0.9870	 0.5590
B8	 0.9570	 0.5330
BA	 0.9360	 0.5690
BB	 0.9190	 0.5560
BC	 0.9350	 0.5540
BD	 0.8950	 0.5230
BE	 0.8190	 0.4910
BF	 0.9180	 0.5500
BG	 0.8410	 0.4870
BH	 0.8900	 0.5400
BI	 0.8970	 0.5470
BJ	 0.8600	 0.5040
BK	 0.5890	 0.3770
BL	 0.8960	 0.5310
BM	 0.8930	 0.5240
BN	 0.9680	 0.5820
BO	 0.9380	 0.5590
BP	 0.9010	 0.5560
BQ	 0.9370	 0.5670
BR	 0.8560	 0.5160
BS	 0.9410	 0.5600
BT	 0.9030	 0.5390
BU	 0.8170	 0.4400
BV	 0.8960	 0.5470
BW	 0.6500	 0.3800
BX	 0.8940	 0.5400
BY	 0.9020	 0.5420
BZ	 0.9050	 0.5290
Ba	 0.9510	 0.5770
Bb	 0.7830	 0.4580
Bc	 0.8070	 0.4920
Bd	 0.8980	 0.5430
Be	 0.9270	 0.5640
Bf	 0.9380	 0.5650
Bg	 0.8970	 0.5380
Bh	 0.9010	 0.5330
Bi	 0.9120	 0.5230
Bj	 0.9660	 0.5750

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Chain	Atom inclusion	Q-score
Bk	 0.8040	 0.4830
Bl	 0.9280	 0.5470
Bm	 0.9120	 0.5390
Bo	 0.8170	 0.5170
Bp	 0.9100	 0.5540
Br	 0.9240	 0.5440
Bs	 0.0090	 0.0580
Bt	 0.0190	 0.0570
Bv	 0.1200	 0.1370
MA	 0.4630	 0.1940
Na	 0.2130	 0.1450
Nb	 0.3510	 0.2510