



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:01 PM UTC

PDB ID : 8FKP / pdb_00008fkp
EMDB ID : EMD-29252
Title : Human nucleolar pre-60S ribosomal subunit (State A1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.85 Å(reported)

This is a Full wwPDB EM Validation 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 : 2022.3.0, CSD as543be (2022)
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

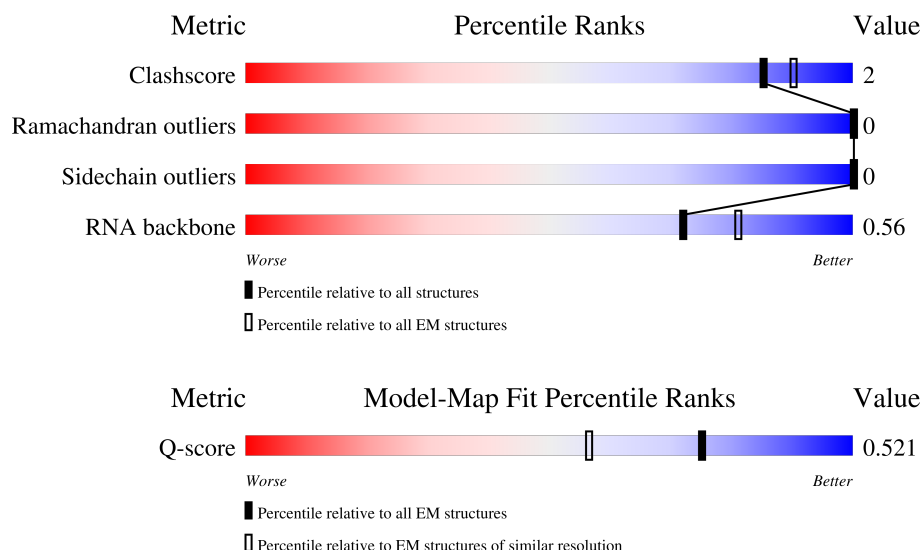
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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	11965 (2.35 - 3.35)

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	L1	157	26% 82% 13% • •
2	L2	1167	94% • •
3	L3	5070	24% 5% 70% •

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Mol	Chain	Length	Quality of chain
4	L6	211	
5	L7	203	
6	L8	215	
7	L9	204	
8	LA	184	
9	LB	188	
10	LC	176	
11	LE	160	
12	LG	140	
13	LH	156	
14	LI	145	
15	LK	148	
16	LN	403	
17	LQ	135	
18	LS	123	
19	LT	110	
20	LU	105	
21	LW	97	
22	NB	549	
23	NE	361	
24	NG	282	
25	NM	300	
26	NN	473	
27	NO	461	
28	NQ	385	

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Mol	Chain	Length	Quality of chain
29	NS	349	
30	SA	427	
31	SC	288	
32	SD	248	
33	SE	266	
34	SH	293	
35	SI	255	
36	SJ	847	
37	SK	245	
38	SL	490	
39	SM	588	
40	SN	306	
41	SO	353	
42	SR	634	
43	SS	746	
44	ST	365	
45	SV	163	
46	SW	670	
47	SZ	178	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 101451 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 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	152	Total	C	N	O	P	0	0
			3234	1443	571	1068	152		

- Molecule 2 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	69	Total	C	N	O	P	0	0
			1468	653	263	483	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	1507	Total	C	N	O	P	0	0
			32319	14383	5932	10497	1507		

- Molecule 4 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L6	114	Total	C	N	O	S	0	0
			936	583	206	146	1		

- Molecule 5 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L7	184	Total	C	N	O	S	0	0
			1507	976	290	237	4		

- Molecule 6 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L8	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 7 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L9	183	Total	C	N	O	S	0	0
			1546	974	325	243	4		

- Molecule 8 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LA	143	Total	C	N	O	S	0	0
			1161	732	214	208	7		

- Molecule 9 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LB	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 10 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LC	174	Total	C	N	O	S	0	0
			1438	912	282	233	11		

- Molecule 11 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	LE	108	Total	C	N	O	0	0
			702	430	138	134		

- Molecule 12 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	114	Total	C	N	O	S	0	0
			844	532	155	152	5		

- Molecule 13 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	LH	20	Total	C	N	O	0	0
			146	95	29	22		

- Molecule 14 is a protein called 60S ribosomal protein L26.

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

- Molecule 15 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LK	108	Total	C	N	O	S	0	0
			642	388	137	115	2		

- Molecule 16 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	377	Total	C	N	O	S	0	0
			3044	1937	566	527	14		

- Molecule 17 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LQ	133	Total	C	N	O	S	0	0
			1096	690	225	176	5		

- Molecule 18 is a protein called 60S ribosomal protein L35.

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

- Molecule 19 is a protein called 60S ribosomal protein L35a.

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

- Molecule 20 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LU	102	Total	C	N	O	S	1	0
			840	526	180	129	5		

- Molecule 21 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LW	69	Total	C	N	O	S	0	0
			563	346	126	86	5		

- Molecule 22 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	NB	31	Total	C	N	O	S	0	0
			257	164	49	43	1		

- Molecule 23 is a protein called Surfeit locus protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	NE	156	Total	C	N	O	S	0	0
			1331	810	293	226	2		

- Molecule 24 is a protein called RRP15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NG	89	Total	C	N	O	S	0	0
			738	456	145	133	4		

- Molecule 25 is a protein called Protein MAK16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	NM	182	Total	C	N	O	S	0	0
			1550	983	286	273	8		

- Molecule 26 is a protein called Suppressor of SWI4 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	NN	244	Total	C	N	O	S	0	0
			1950	1230	371	338	11		

- Molecule 27 is a protein called Ribosomal RNA processing protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	NO	305	Total	C	N	O	S	0	0
			2487	1577	437	461	12		

- Molecule 28 is a protein called WD repeat-containing protein 74.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	NQ	324	Total	C	N	O	S	0	0
			2502	1559	471	457	15		

- Molecule 29 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	NS	305	Total	C	N	O	S	0	0
			2529	1607	472	444	6		

- Molecule 30 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SA	331	Total	C	N	O	S	0	0
			2656	1681	524	437	14		

- Molecule 31 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SC	199	Total	C	N	O	S	0	0
			1627	1046	305	274	2		

- Molecule 32 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SD	239	Total	C	N	O	S	0	0
			1985	1275	381	320	9		

- Molecule 33 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SE	186	Total	C	N	O	S	0	0
			1498	951	290	253	4		

- Molecule 34 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SH	150	Total	C	N	O	S	0	0
			1267	819	224	220	4		

- Molecule 35 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SI	199	Total	C	N	O	S	1	0
			1661	1076	311	270	4		

- Molecule 36 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SJ	72	Total	C	N	O		0	0
			609	385	114	110			

- Molecule 37 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SK	226	Total	C	N	O	S	0	0
			1721	1070	296	343	12		

- Molecule 38 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SL	243	Total	C	N	O	S	0	0
			1960	1254	344	356	6		

- Molecule 39 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SM	437	Total	C	N	O	S	0	0
			3452	2229	603	609	11		

- Molecule 40 is a protein called Probable rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SN	168	Total	C	N	O	S	0	0
			1308	821	247	235	5		

- Molecule 41 is a protein called Ribosome biogenesis protein BRX1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SO	307	Total	C	N	O	S	0	0
			2544	1637	458	434	15		

- Molecule 42 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SR	77	Total	C	N	O	S	0	0
			642	411	107	122	2		

- Molecule 43 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SS	235	Total	C	N	O	P S	0	0
			1955	1238	348	360	2 7		

- Molecule 44 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	ST	36	Total	C	N	O	S	0	0
			263	160	51	51	1		

- Molecule 45 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SV	137	Total	C	N	O	S	0	0
			1171	745	227	189	10		

- Molecule 46 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SW	445	Total	C	N	O	S	0	0
			3560	2288	609	646	17		

- Molecule 47 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SZ	160	Total	C	N	O	S	0	0
			1338	835	260	238	5		

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	L1	3	Total	Mg	0
			3	3	
48	L2	1	Total	Mg	0
			1	1	
48	L3	46	Total	Mg	0
			46	46	

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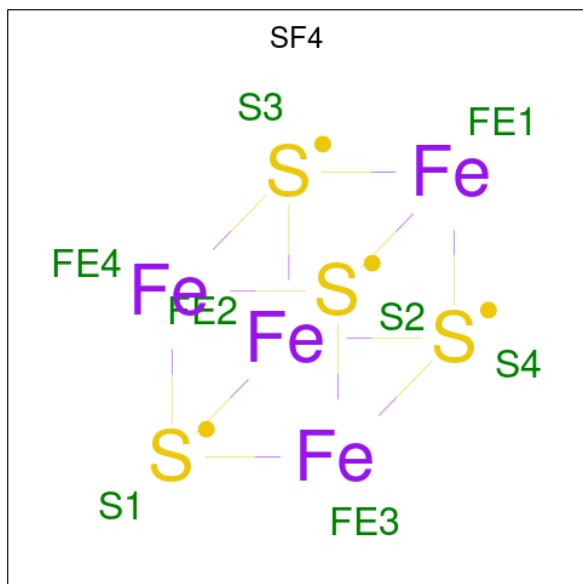
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Mol	Chain	Residues	Atoms		AltConf
48	L9	1	Total	Mg	0
			1	1	
48	LQ	1	Total	Mg	0
			1	1	
48	LT	1	Total	Mg	0
			1	1	
48	SA	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
49	LW	1	Total	Zn	0
			1	1	
49	SV	1	Total	Zn	0
			1	1	

- Molecule 50 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

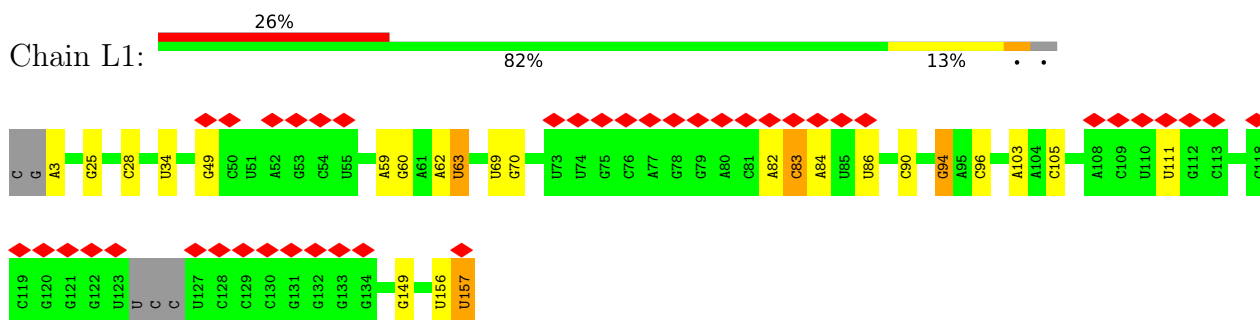


Mol	Chain	Residues	Atoms			AltConf
50	NM	1	Total	Fe	S	0
			8	4	4	

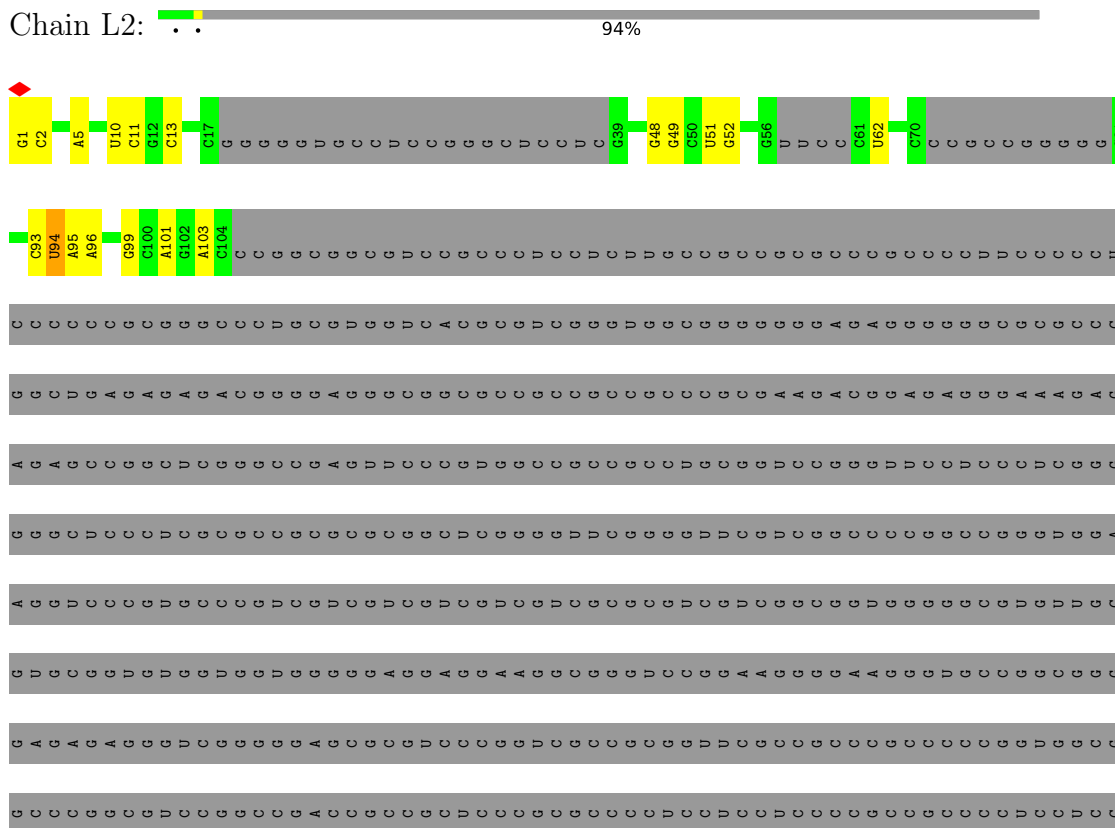
3 Residue-property plots [i](#)

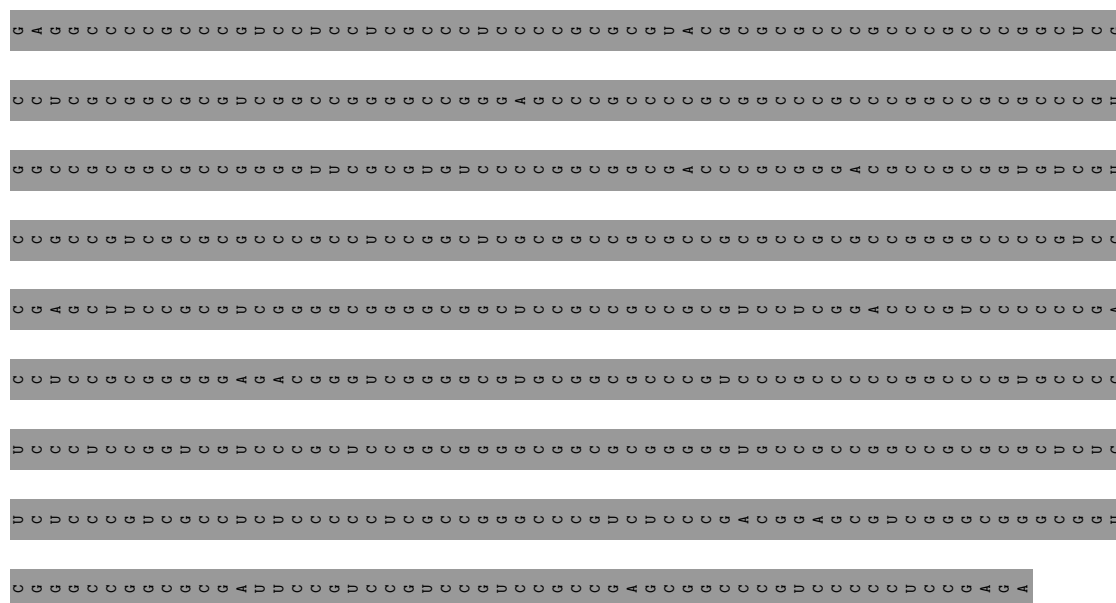
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 5.8S rRNA

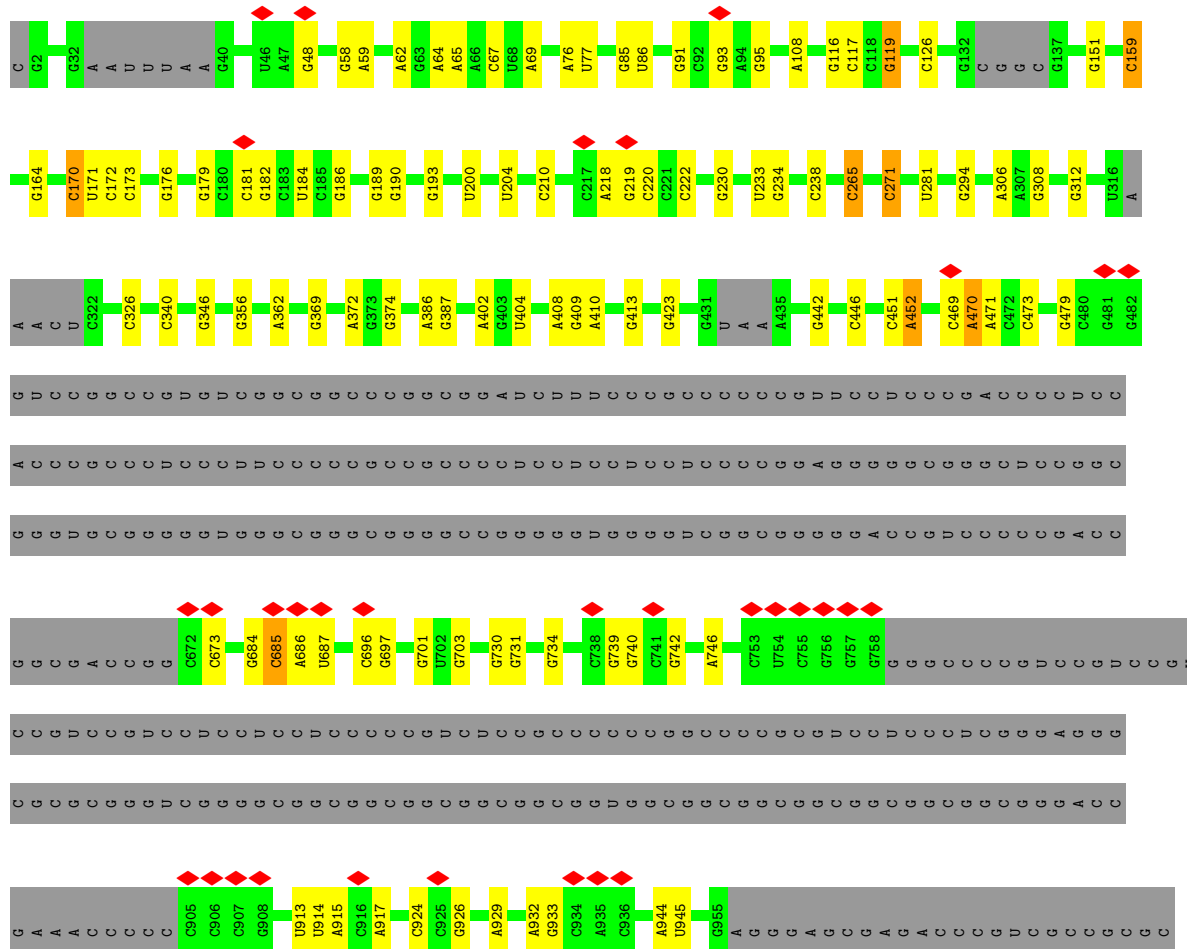


• Molecule 2: ITS2 rRNA

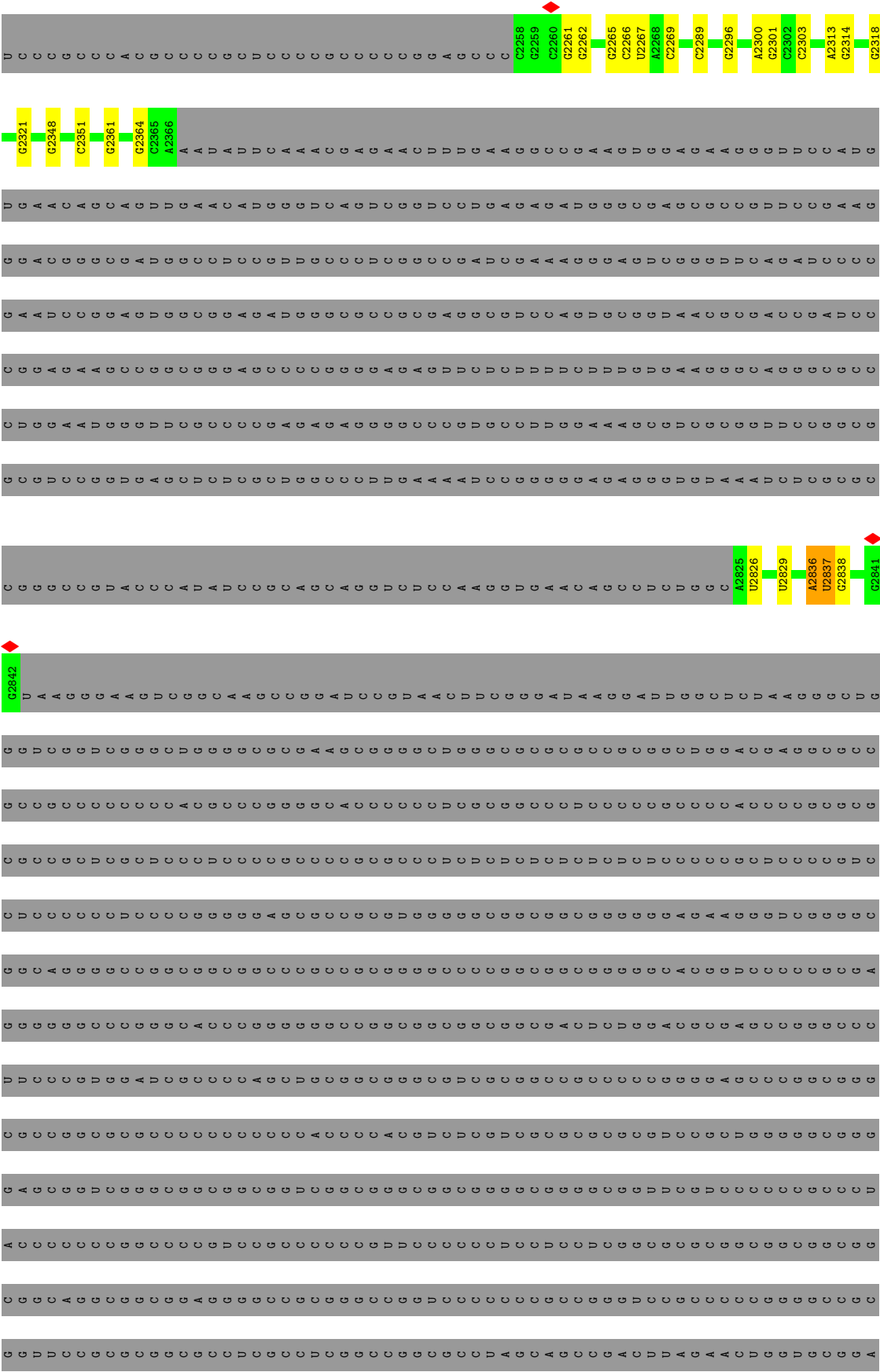


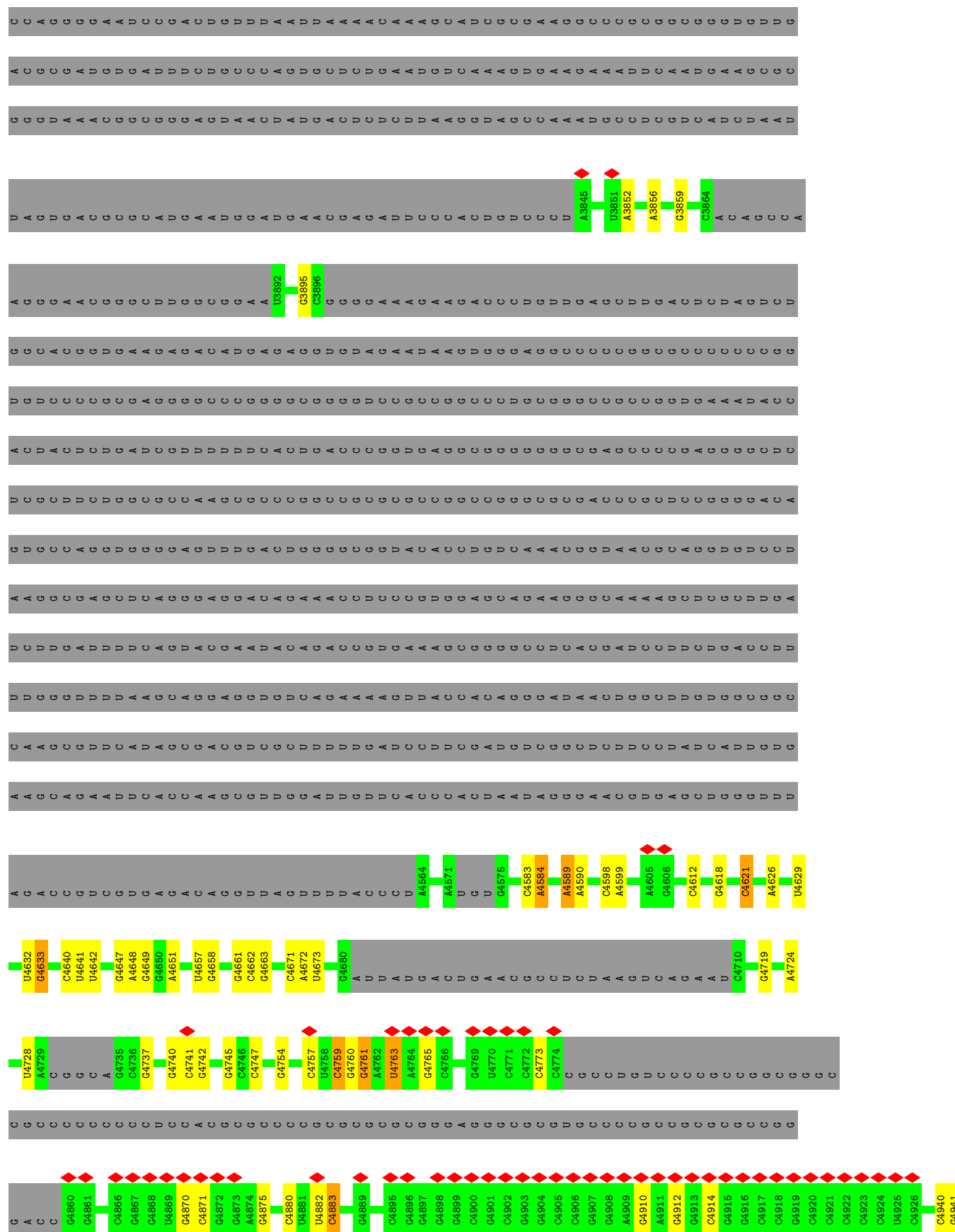


• Molecule 3: 28S rRNA

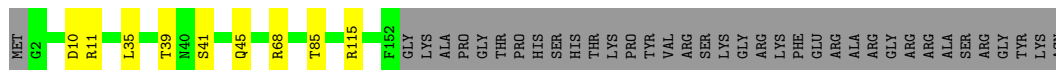
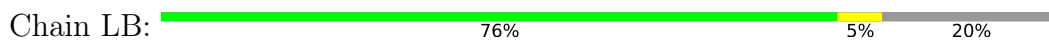




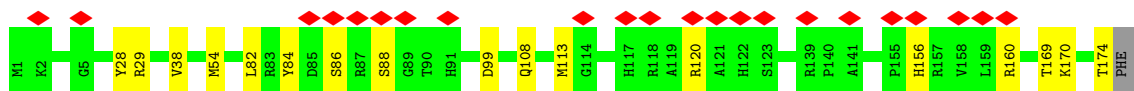
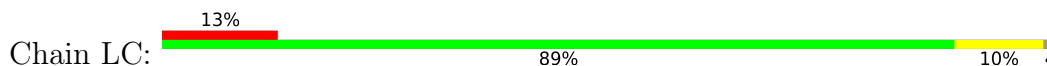




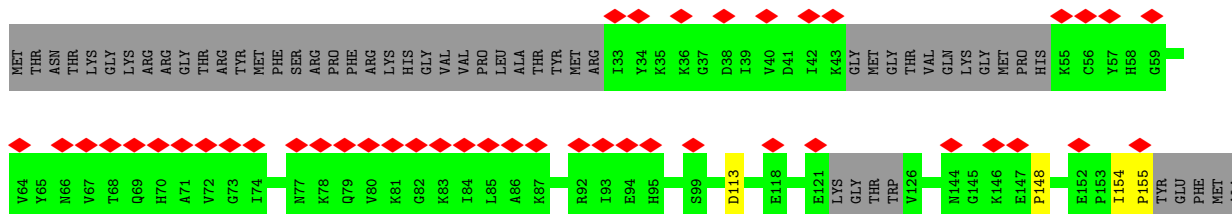
- Molecule 9: 60S ribosomal protein L18



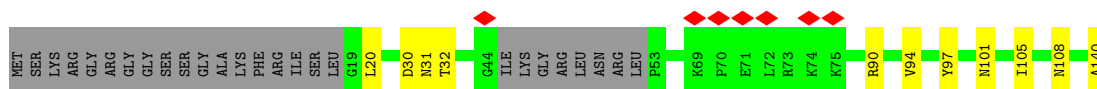
- Molecule 10: 60S ribosomal protein L18a



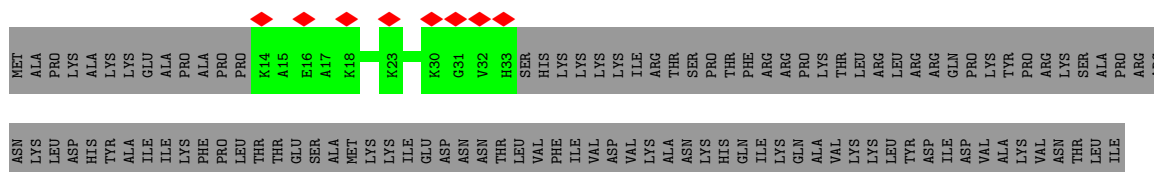
- Molecule 11: 60S ribosomal protein L21



- Molecule 12: 60S ribosomal protein L23



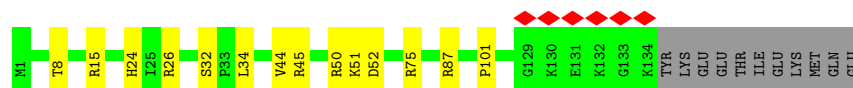
- Molecule 13: 60S ribosomal protein L23a



ARG
PRO
ASP
GLY
GLY
LYS
LYS
ALA
TYR
VAL
ARG
LEU
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PRO
ASP
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LEU
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VAL
ALA
ASN
LYS
ILE
GLY
ILE

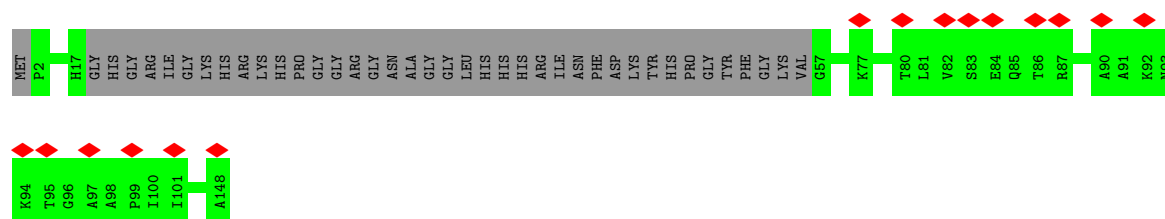
- Molecule 14: 60S ribosomal protein L26

Chain LI:  83% 10% 8%



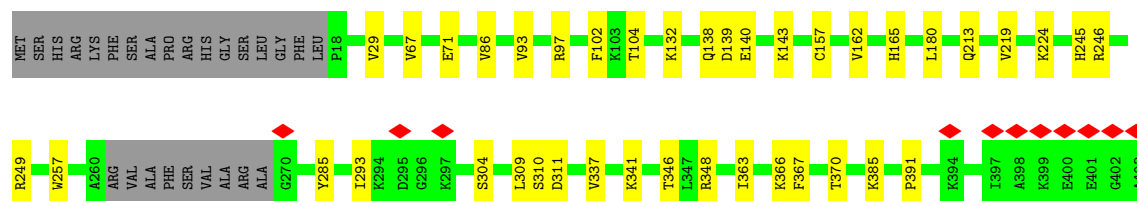
- Molecule 15: 60S ribosomal protein L27a

Chain LK:  10% 73% 27%

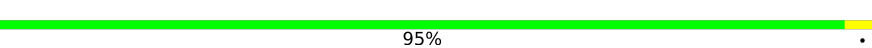


- Molecule 16: 60S ribosomal protein L3

Chain LN:  84% 10% 6%



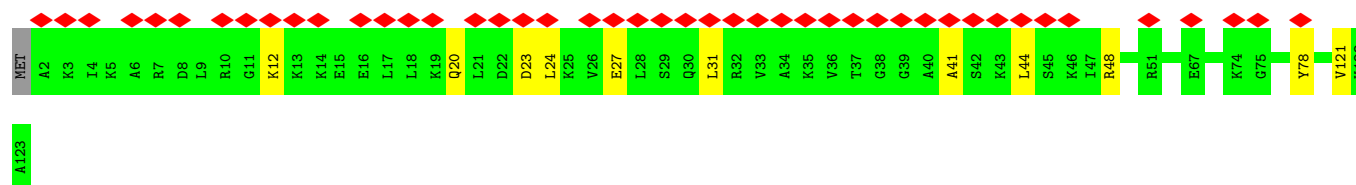
- Molecule 17: 60S ribosomal protein L32

Chain LQ:  95% 5% 0%

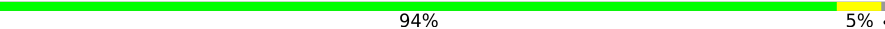


- Molecule 18: 60S ribosomal protein L35

Chain LS:  37% 90% 9% 0%

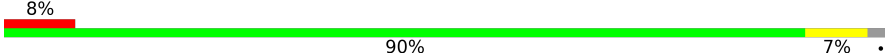


- Molecule 19: 60S ribosomal protein L35a

Chain LT:  94% 5% .



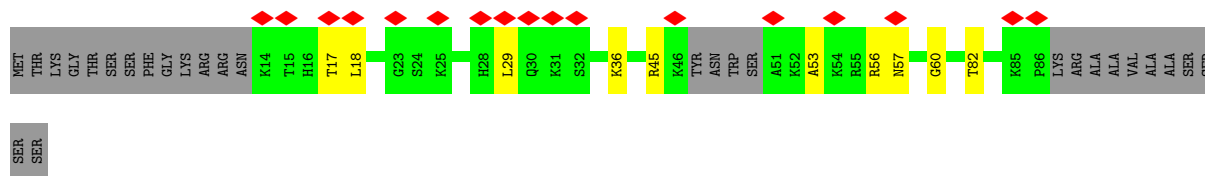
- Molecule 20: 60S ribosomal protein L36

Chain LU:  8% 90% 7% .

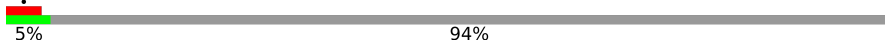


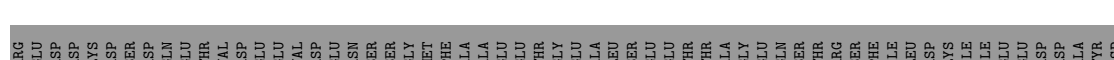
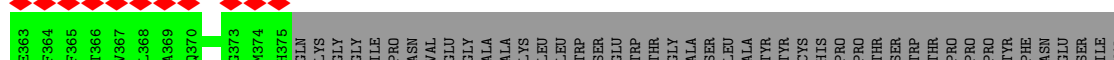
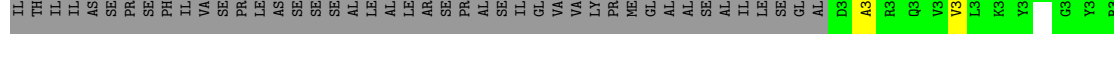
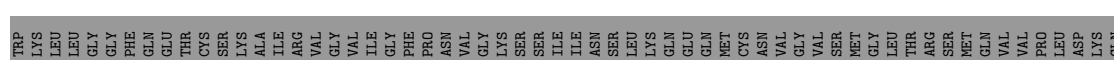
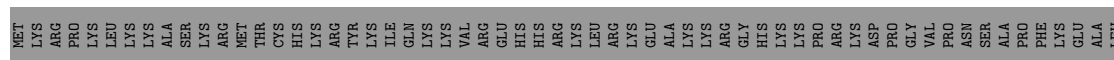
- Molecule 21: 60S ribosomal protein L37

Chain LW:  18% 61% 10% 29%

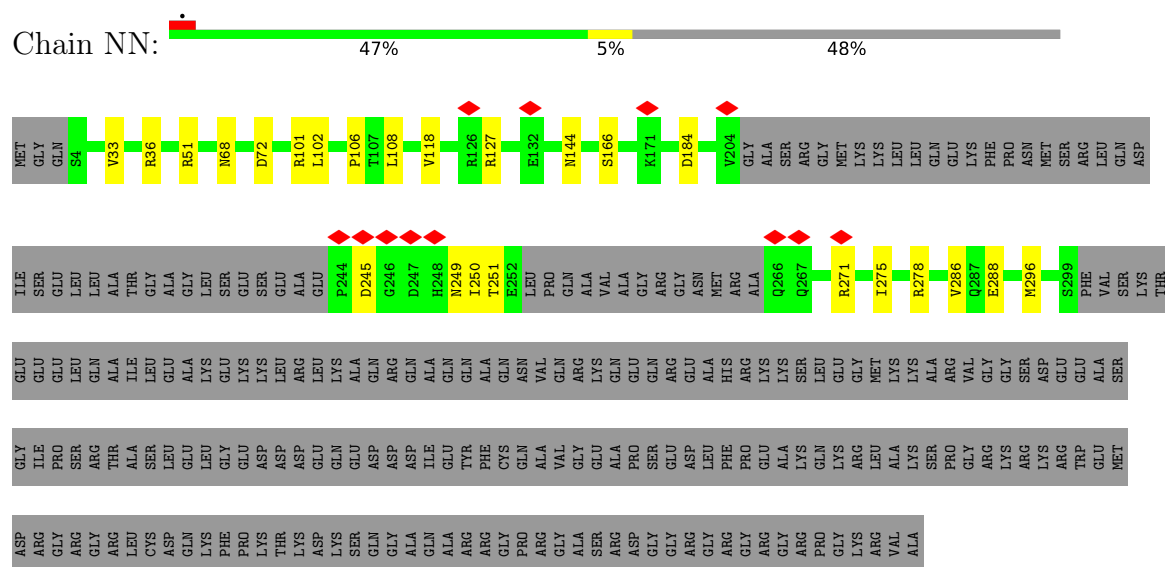


- Molecule 22: Guanine nucleotide-binding protein-like 3

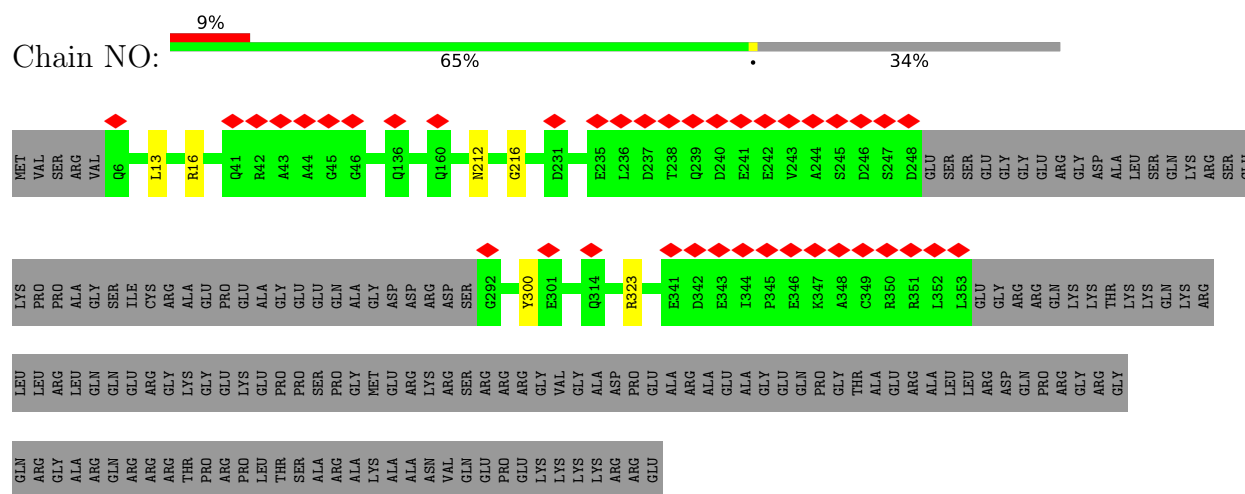
Chain NB:  5% 94%



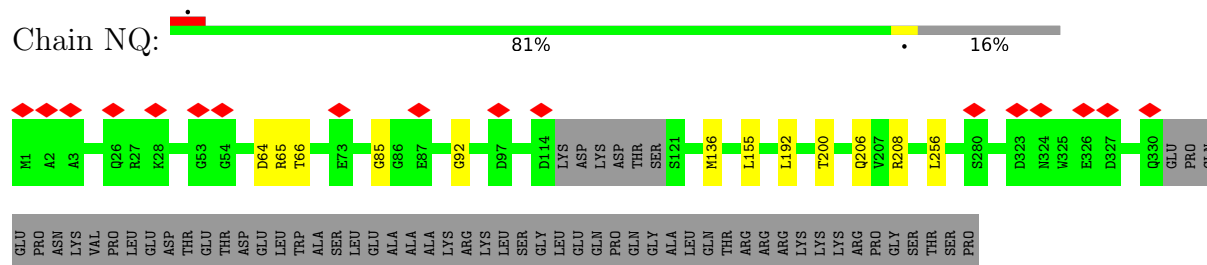
- Molecule 26: Suppressor of SWI4 1 homolog



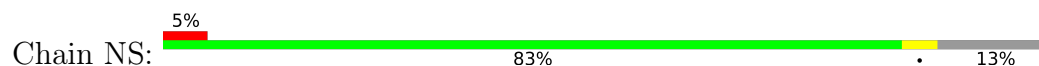
- Molecule 27: Ribosomal RNA processing protein 1 homolog A

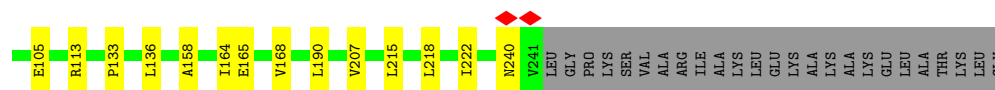


- Molecule 28: WD repeat-containing protein 74

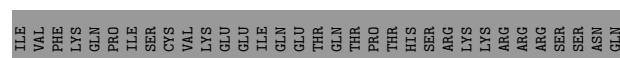
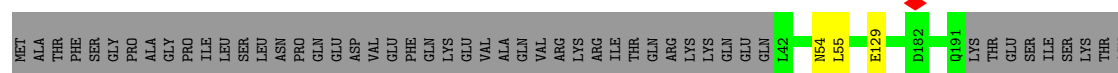


- Molecule 29: Ribosome production factor 1

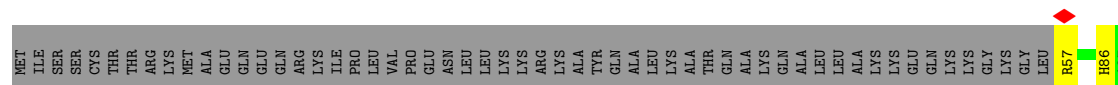




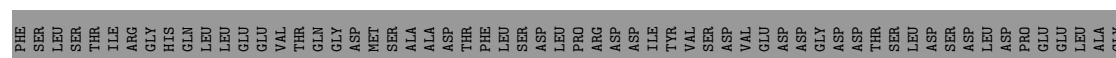
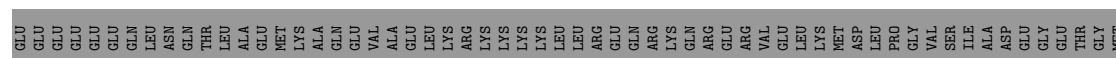
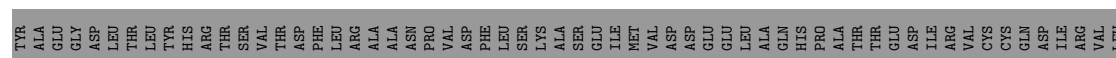
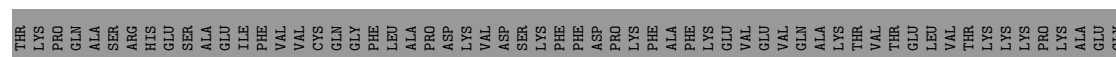
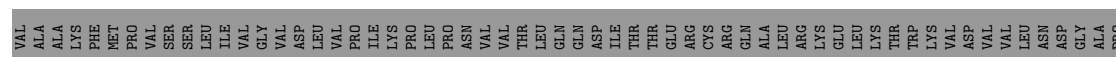
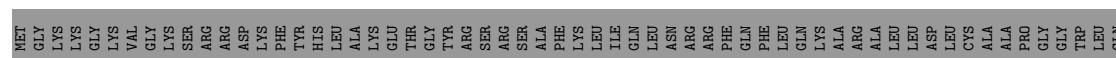
- Molecule 34: MKI67 FHA domain-interacting nucleolar phosphoprotein

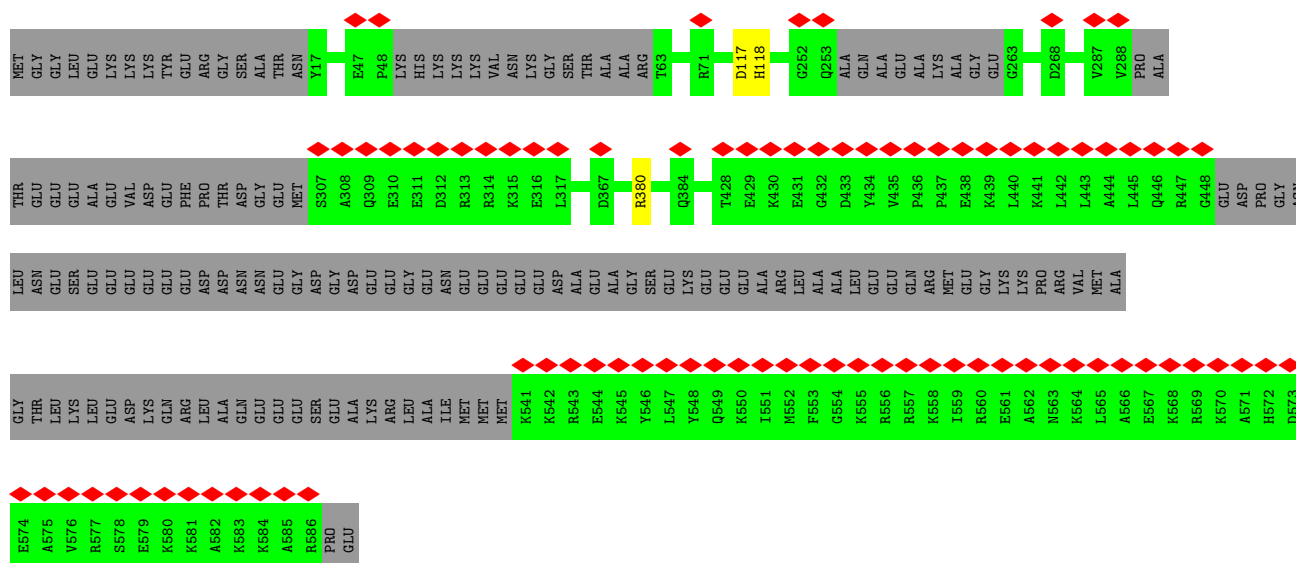


- Molecule 35: 60S ribosomal protein L7-like 1

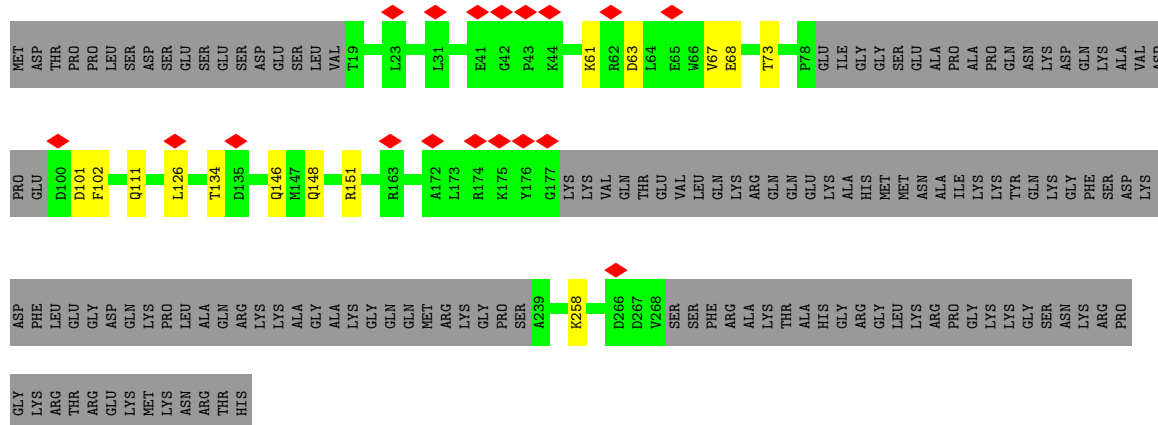


- Molecule 36: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3

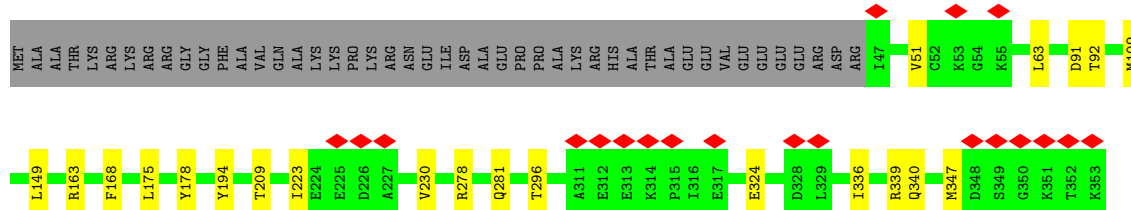
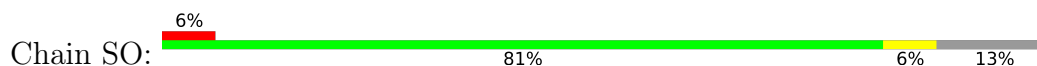




• Molecule 40: Probable rRNA-processing protein EBP2

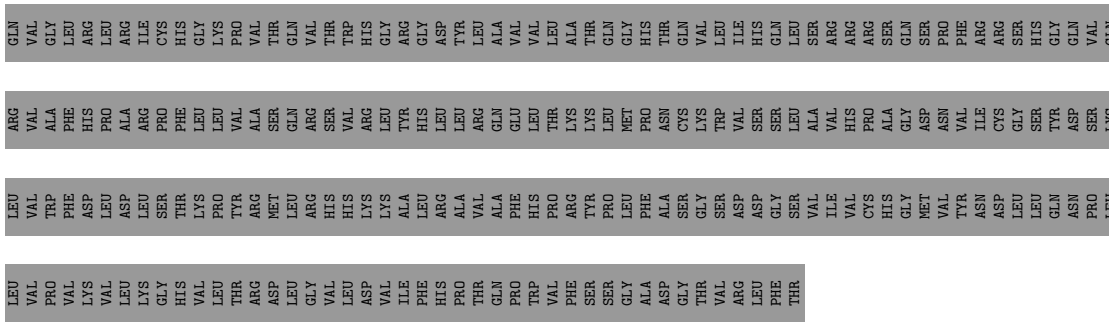


• Molecule 41: Ribosome biogenesis protein BRX1 homolog

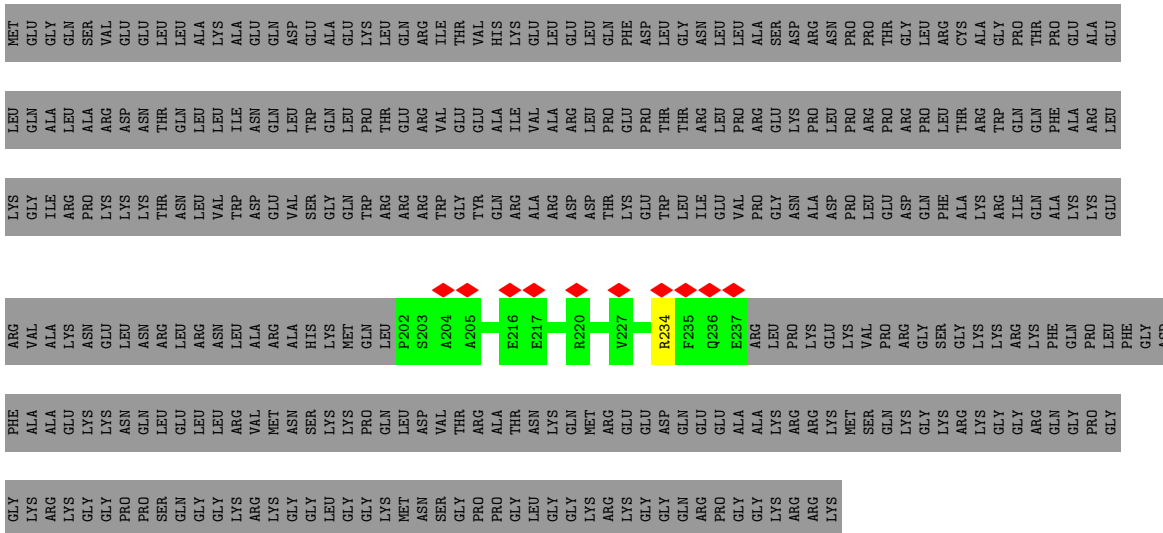


• Molecule 42: GTP-binding protein 4

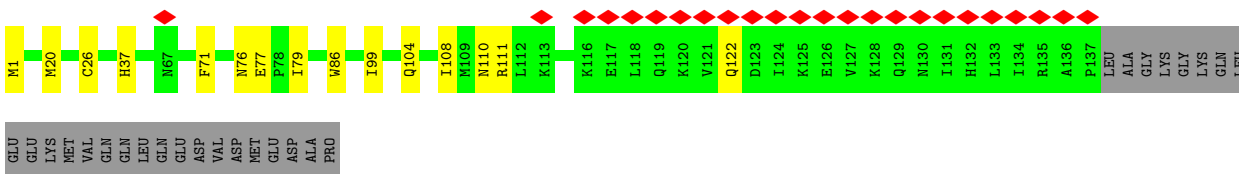
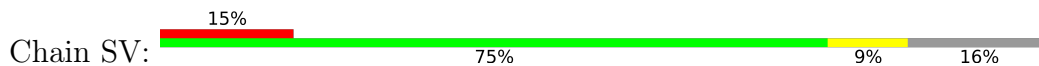




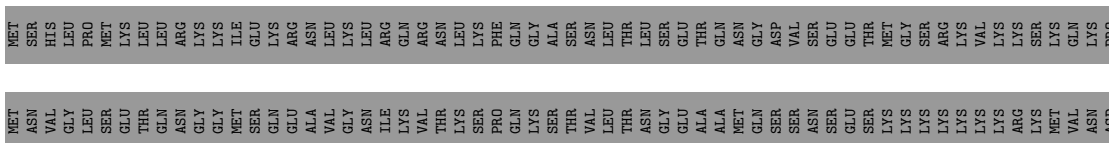
- Molecule 44: Ribosome biogenesis regulatory protein homolog



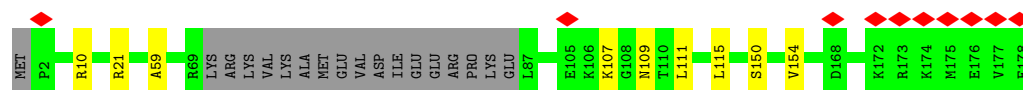
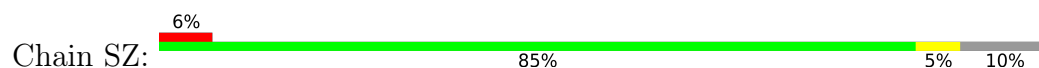
- Molecule 45: Probable ribosome biogenesis protein RLP24



- Molecule 46: ATP-dependent RNA helicase DDX18



- Molecule 47: Nucleolar protein 16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42413	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)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.947	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AME, ZN, SEP, MG, SF4, HIC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L1	0.20	0/3611	0.26	0/5623
2	L2	0.27	0/1634	0.30	0/2538
3	L3	0.23	0/36123	0.29	0/56296
4	L6	0.24	0/953	0.38	0/1276
5	L7	0.18	0/1534	0.34	0/2049
6	L8	0.17	0/1133	0.34	0/1516
7	L9	0.23	0/1584	0.36	0/2117
8	LA	0.18	0/1179	0.35	0/1575
9	LB	0.23	0/1239	0.37	0/1658
10	LC	0.21	0/1476	0.40	0/1981
11	LE	0.16	0/708	0.36	0/958
12	LG	0.20	0/856	0.37	0/1149
13	LH	0.16	0/146	0.28	0/190
14	LI	0.24	0/1132	0.37	0/1504
15	LK	0.18	0/648	0.41	0/880
16	LN	0.26	0/3092	0.38	0/4133
17	LQ	0.23	0/1114	0.34	0/1486
18	LS	0.18	0/1023	0.38	0/1351
19	LT	0.22	0/895	0.37	0/1198
20	LU	0.20	0/854	0.34	0/1129
21	LW	0.15	0/573	0.39	0/755
22	NB	0.13	0/262	0.26	0/352
23	NE	0.22	0/1339	0.39	0/1767
24	NG	0.16	0/743	0.32	0/986
25	NM	0.22	0/1566	0.31	0/2097
26	NN	0.28	0/1988	0.42	0/2678
27	NO	0.15	0/2530	0.28	0/3412
28	NQ	0.18	0/2556	0.32	0/3466
29	NS	0.19	0/2592	0.33	0/3487
30	SA	0.23	0/2705	0.34	0/3632
31	SC	0.16	0/1657	0.33	0/2219
32	SD	0.21	0/2022	0.34	0/2696

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	SE	0.23	0/1524	0.36	0/2056
34	SH	0.24	0/1298	0.32	0/1742
35	SI	0.21	0/1702	0.32	0/2289
36	SJ	0.17	0/623	0.31	0/836
37	SK	0.22	0/1745	0.43	0/2374
38	SL	0.24	0/1994	0.38	0/2684
39	SM	0.18	0/3530	0.27	0/4779
40	SN	0.16	0/1327	0.33	0/1774
41	SO	0.20	0/2608	0.32	0/3506
42	SR	0.24	0/657	0.48	0/887
43	SS	0.18	0/1994	0.32	0/2703
44	ST	0.14	0/267	0.31	0/357
45	SV	0.25	0/1194	0.44	0/1582
46	SW	0.18	0/3631	0.32	0/4900
47	SZ	0.20	0/1364	0.31	0/1826
All	All	0.21	0/106925	0.32	0/152449

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	3234	0	1639	14	0
2	L2	1468	0	755	8	0
3	L3	32319	0	16377	104	0
4	L6	936	0	1017	9	0
5	L7	1507	0	1649	11	0
6	L8	1111	0	1174	7	0
7	L9	1546	0	1585	6	0
8	LA	1161	0	1221	8	0
9	LB	1223	0	1330	7	0
10	LC	1438	0	1484	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	LE	702	0	561	4	0
12	LG	844	0	883	8	0
13	LH	146	0	176	0	0
14	LI	1115	0	1205	12	0
15	LK	642	0	455	0	0
16	LN	3044	0	3178	32	0
17	LQ	1096	0	1183	6	0
18	LS	1015	0	1148	9	0
19	LT	876	0	912	6	0
20	LU	840	0	930	6	0
21	LW	563	0	596	9	0
22	NB	257	0	259	1	0
23	NE	1331	0	1430	19	0
24	NG	738	0	786	4	0
25	NM	1550	0	1599	12	0
26	NN	1950	0	2005	17	0
27	NO	2487	0	2506	5	0
28	NQ	2502	0	2481	6	0
29	NS	2529	0	2563	10	0
30	SA	2656	0	2833	9	0
31	SC	1627	0	1751	17	0
32	SD	1985	0	2128	6	0
33	SE	1498	0	1601	10	0
34	SH	1267	0	1291	2	0
35	SI	1661	0	1752	11	0
36	SJ	609	0	600	2	0
37	SK	1721	0	1695	28	0
38	SL	1960	0	2052	8	0
39	SM	3452	0	3376	3	0
40	SN	1308	0	1286	10	0
41	SO	2544	0	2631	18	0
42	SR	642	0	630	12	0
43	SS	1955	0	1871	13	0
44	ST	263	0	260	1	0
45	SV	1171	0	1232	19	0
46	SW	3560	0	3641	14	0
47	SZ	1338	0	1352	8	0
48	L1	3	0	0	0	0
48	L2	1	0	0	0	0
48	L3	46	0	0	0	0
48	L9	1	0	0	0	0
48	LQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	LT	1	0	0	0	0
48	SA	1	0	0	0	0
49	LW	1	0	0	0	0
49	SV	1	0	0	0	0
50	NM	8	0	0	0	0
All	All	101451	0	85069	397	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 2.

All (397) 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)
8:LA:42:ARG:NH1	24:NG:195:MET:SD	2.49	0.85
3:L3:4598:C:O2	3:L3:4612:C:N4	2.13	0.82
30:SA:295:SER:OG	30:SA:297:GLU:OE1	1.96	0.82
30:SA:329:ASN:ND2	32:SD:188:GLU:OE1	2.12	0.82
7:L9:16:SER:OG	20:LU:48:CYS:SG	2.36	0.81
3:L3:271:C:OP1	46:SW:297:LYS:NZ	2.13	0.81
42:SR:453:LEU:HD21	45:SV:99:ILE:HD11	1.64	0.79
3:L3:2100:A:OP1	32:SD:29:LYS:NZ	2.15	0.79
3:L3:2084:C:O2	9:LB:45:GLN:NE2	2.16	0.78
3:L3:470:A:N6	3:L3:685:C:O2	2.16	0.77
3:L3:4940:C:OP1	31:SC:156:ARG:NH1	2.17	0.77
37:SK:95:ARG:NH1	45:SV:77:GLU:OE2	2.18	0.75
3:L3:306:A:OP1	20:LU:53:TYR:OH	2.04	0.75
3:L3:4946:U:HO2'	19:LT:2:SER:N	1.84	0.75
3:L3:116:G:O2'	43:SS:239:ARG:NH1	2.19	0.74
16:LN:304:SER:OG	16:LN:310:SER:O	2.06	0.74
3:L3:2836:A:O2'	3:L3:2837:U:O5'	2.04	0.73
37:SK:119:PRO:O	37:SK:139:ARG:NH2	2.21	0.73
23:NE:228:LEU:HD21	23:NE:271:THR:HG21	1.69	0.73
16:LN:309:LEU:HD11	42:SR:430:PRO:HB3	1.69	0.73
46:SW:241:ILE:HD11	46:SW:254:VAL:HG23	1.70	0.73
3:L3:62:A:N3	3:L3:77:U:O2'	2.22	0.73
3:L3:151:G:OP2	7:L9:4:TYR:OH	2.06	0.73
26:NN:36:ARG:NH1	26:NN:68:ASN:O	2.22	0.73
3:L3:126:C:OP1	18:LS:78:TYR:OH	2.07	0.72
3:L3:4598:C:OP2	3:L3:4599:A:O2'	2.06	0.72
3:L3:3856:A:OP1	8:LA:82:ARG:NE	2.23	0.71
3:L3:5058:A:OP1	26:NN:127:ARG:NH1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:NG:159:GLU:OE1	26:NN:278:ARG:NH2	2.24	0.71
1:L1:94:G:O2'	21:LW:82:THR:O	2.04	0.70
40:SN:67:VAL:HG22	40:SN:126:LEU:HD13	1.72	0.70
37:SK:201:ASP:OD1	37:SK:202:TRP:N	2.26	0.69
23:NE:275:TYR:HB2	23:NE:282:ILE:HD11	1.75	0.69
3:L3:2361:G:O2'	3:L3:3859:G:O6	2.09	0.69
3:L3:238:C:OP2	14:LI:45:ARG:NH2	2.26	0.68
3:L3:4763:U:C6	10:LC:174:THR:HA	2.27	0.68
3:L3:2054:U:O2'	5:L7:133:ARG:NH1	2.26	0.68
16:LN:165:HIS:HB3	16:LN:180:LEU:HD23	1.75	0.68
2:L2:10:U:OP2	38:SL:163:ARG:NH2	2.26	0.68
3:L3:423:G:OP1	8:LA:62:ARG:NH1	2.26	0.68
3:L3:1508:A:OP1	30:SA:110:ARG:NH2	2.27	0.68
3:L3:374:G:OP2	21:LW:56:ARG:NH1	2.26	0.67
3:L3:4759:C:O2	5:L7:165:LYS:NZ	2.15	0.67
3:L3:1922:G:OP1	10:LC:160:ARG:NH1	2.28	0.67
3:L3:182:G:N7	41:SO:339:ARG:NH1	2.43	0.67
7:L9:96:ARG:NH2	7:L9:104:GLU:OE1	2.28	0.67
16:LN:219:VAL:HG11	16:LN:337:VAL:HG21	1.75	0.67
31:SC:250:GLN:NE2	31:SC:254:ASP:OD1	2.28	0.67
1:L1:63:U:OP1	18:LS:48:ARG:NH2	2.28	0.67
26:NN:101:ARG:NH1	26:NN:102:LEU:O	2.28	0.67
35:SI:143:VAL:O	35:SI:147:VAL:HG12	1.94	0.66
3:L3:1833:G:N2	3:L3:1835:G:O4'	2.28	0.66
16:LN:138:GLN:O	16:LN:143:LYS:NZ	2.29	0.66
3:L3:308:G:OP2	3:L3:308:G:N2	2.21	0.66
37:SK:107:VAL:HG11	37:SK:121:LEU:HD21	1.77	0.65
9:LB:115:ARG:NH1	41:SO:296:THR:OG1	2.29	0.65
3:L3:1369:C:OP2	3:L3:1370:G:O2'	2.09	0.65
3:L3:4760:G:OP1	5:L7:117:ARG:NH2	2.29	0.65
18:LS:23:ASP:OD1	18:LS:24:LEU:N	2.30	0.65
20:LU:74:LYS:HD3	41:SO:109:MET:HE1	1.79	0.65
26:NN:245:ASP:OD1	26:NN:271:ARG:NH2	2.30	0.65
3:L3:369:G:N2	3:L3:372:A:OP2	2.21	0.64
46:SW:327:LEU:HD22	46:SW:354:LEU:HD22	1.79	0.64
35:SI:101:ARG:NH1	35:SI:122:LYS:O	2.31	0.64
9:LB:35:LEU:HD21	30:SA:298:ILE:HD11	1.80	0.64
3:L3:2062:C:OP1	10:LC:120:ARG:NH1	2.31	0.64
37:SK:112:ASP:OD2	37:SK:156:ASN:ND2	2.30	0.63
3:L3:402:A:O2'	29:NS:103:LYS:O	2.16	0.63
3:L3:4583:C:O4'	16:LN:97:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SW:182:LEU:HD22	46:SW:185:LEU:HD12	1.79	0.63
14:LI:32:SER:OG	14:LI:101:PRO:O	2.12	0.63
45:SV:110:ASN:OD1	45:SV:111:ARG:N	2.31	0.63
3:L3:184:U:O2'	3:L3:189:G:OP2	2.16	0.63
3:L3:404:U:O3'	14:LI:87:ARG:NH2	2.32	0.62
3:L3:1447:C:OP2	27:NO:323:ARG:NH2	2.32	0.62
11:LE:154:ILE:HD12	11:LE:155:PRO:HD2	1.81	0.62
12:LG:30:ASP:OD1	12:LG:31:ASN:N	2.31	0.62
4:L6:62:PRO:O	4:L6:63:THR:OG1	2.15	0.62
4:L6:100:PRO:O	20:LU:25[B]:ARG:NH2	2.33	0.61
37:SK:1:MET:N	37:SK:219:GLU:OE1	2.33	0.61
38:SL:57:LEU:HD11	46:SW:527:LEU:HD22	1.80	0.61
3:L3:230:G:OP1	14:LI:15:ARG:NH1	2.32	0.61
3:L3:471:A:N7	3:L3:684:G:N2	2.49	0.61
4:L6:50:PRO:HG3	18:LS:121:VAL:HG12	1.82	0.61
3:L3:222:C:OP2	30:SA:165:LYS:NZ	2.26	0.61
3:L3:4971:A:OP1	16:LN:246:ARG:NH1	2.33	0.61
23:NE:202:LYS:O	26:NN:166:SER:OG	2.16	0.60
37:SK:177:LEU:HD22	37:SK:181:LEU:HD21	1.83	0.60
16:LN:219:VAL:HG11	16:LN:337:VAL:CG2	2.32	0.60
46:SW:314:ASP:OD1	46:SW:318:ASN:ND2	2.35	0.60
3:L3:4763:U:O2'	10:LC:156:HIS:ND1	2.32	0.60
25:NM:13:ASN:OD1	25:NM:14:LYS:N	2.35	0.59
1:L1:157:U:OP2	35:SI:57:ARG:NH1	2.35	0.59
8:LA:158:PRO:O	29:NS:276:ARG:NH2	2.36	0.59
16:LN:257:TRP:N	26:NN:72:ASP:OD2	2.34	0.59
37:SK:142:VAL:HG23	37:SK:148:VAL:HG12	1.84	0.59
3:L3:2836:A:HO2'	3:L3:2837:U:P	2.26	0.59
40:SN:148:GLN:OE1	40:SN:151:ARG:NH2	2.35	0.59
3:L3:740:G:N2	3:L3:924:C:O2	2.35	0.59
12:LG:90:ARG:NH2	12:LG:140:ALA:OXT	2.33	0.59
31:SC:281:ILE:CG2	31:SC:286:LEU:HD11	2.33	0.59
37:SK:177:LEU:CD2	37:SK:181:LEU:HD21	2.33	0.58
18:LS:27:GLU:O	18:LS:31:LEU:HD23	2.02	0.58
21:LW:17:THR:OG1	21:LW:29:LEU:HD21	2.03	0.58
1:L1:94:G:H21	21:LW:82:THR:HG21	1.67	0.58
26:NN:249:ASN:OD1	26:NN:250:ILE:N	2.36	0.58
26:NN:250:ILE:HG23	26:NN:250:ILE:O	2.04	0.57
8:LA:94:MET:HG2	8:LA:148:MET:HE3	1.85	0.57
3:L3:452:A:N3	31:SC:226:ARG:NH2	2.53	0.57
3:L3:2318:G:N2	3:L3:2321:G:OP2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:4724:A:O2'	16:LN:104:THR:HG22	2.04	0.57
6:L8:62:LEU:HD21	6:L8:82:ILE:HD11	1.87	0.57
3:L3:119:G:OP2	43:SS:249:SER:OG	2.05	0.57
16:LN:309:LEU:HD11	42:SR:430:PRO:CB	2.35	0.57
29:NS:334:VAL:O	29:NS:340:MET:HE1	2.05	0.57
23:NE:275:TYR:CB	23:NE:282:ILE:HD11	2.34	0.56
18:LS:12:LYS:NZ	18:LS:20:GLN:OE1	2.39	0.56
14:LI:26:ARG:NH1	14:LI:75:ARG:O	2.39	0.56
32:SD:232:ASP:OD1	32:SD:236:ARG:NH2	2.39	0.56
3:L3:4972:U:OP1	16:LN:249:ARG:NH1	2.36	0.56
16:LN:86:VAL:HG13	16:LN:162:VAL:HG13	1.88	0.56
39:SM:117:ASP:OD1	39:SM:118:HIS:N	2.39	0.56
6:L8:15:VAL:HG22	6:L8:50:MET:HE1	1.88	0.55
40:SN:111:GLN:OE1	41:SO:209:THR:HG22	2.07	0.55
1:L1:3:A:O2'	8:LA:61:ARG:NH1	2.39	0.55
5:L7:141:LEU:O	5:L7:145:VAL:HG23	2.07	0.55
30:SA:204:ARG:NH1	30:SA:205:ARG:O	2.38	0.55
30:SA:211:TYR:OH	30:SA:218:ILE:HD11	2.06	0.55
34:SH:54:ASN:OD1	34:SH:55:LEU:HD12	2.06	0.55
12:LG:97:TYR:OH	45:SV:37:HIS:NE2	2.34	0.55
42:SR:453:LEU:HD21	45:SV:99:ILE:CD1	2.36	0.55
3:L3:265:C:N4	47:SZ:154:VAL:HG21	2.22	0.54
46:SW:285:ILE:HD11	46:SW:298:LEU:HD21	1.89	0.54
8:LA:53:LEU:O	8:LA:55:LYS:NZ	2.40	0.54
37:SK:107:VAL:CG1	37:SK:121:LEU:HD21	2.37	0.54
40:SN:146:GLN:NE2	41:SO:149:LEU:O	2.41	0.54
37:SK:72:VAL:HB	37:SK:76:THR:HG21	1.90	0.54
47:SZ:111:LEU:HD11	47:SZ:115:LEU:HD23	1.90	0.53
3:L3:5010:U:O2'	45:SV:122:GLN:OE1	2.27	0.53
5:L7:185:VAL:HG12	5:L7:185:VAL:O	2.09	0.53
16:LN:213:GLN:NE2	16:LN:285:TYR:O	2.41	0.53
46:SW:504:ASP:OD1	46:SW:505:ASP:N	2.42	0.53
23:NE:273:LEU:HD11	26:NN:296:MET:SD	2.49	0.53
25:NM:130:ARG:NH2	29:NS:177:GLY:O	2.42	0.53
31:SC:281:ILE:HG21	31:SC:286:LEU:HD11	1.91	0.53
37:SK:99:GLU:OE1	37:SK:125:THR:OG1	2.23	0.53
3:L3:76:A:N7	4:L6:74:ARG:NH2	2.55	0.53
3:L3:4875:G:H2'	10:LC:169:THR:HG22	1.90	0.53
24:NG:171:VAL:HG13	26:NN:251:THR:OG1	2.09	0.53
28:NQ:192:LEU:HD21	28:NQ:256:LEU:HD13	1.90	0.53
16:LN:93:VAL:HG12	16:LN:157:CYS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:NB:346:ALA:O	22:NB:350:VAL:HG23	2.09	0.52
40:SN:101:ASP:OD1	40:SN:102:PHE:N	2.42	0.52
3:L3:4589:A:N1	3:L3:4621:C:O2'	2.34	0.52
2:L2:1:G:O2'	2:L2:2:C:OP1	2.21	0.52
12:LG:94:VAL:HG11	45:SV:20:MET:HE3	1.92	0.52
23:NE:228:LEU:HD21	23:NE:271:THR:CG2	2.39	0.52
38:SL:67:MET:HE3	38:SL:212:SER:O	2.09	0.52
1:L1:49:G:H1'	18:LS:44:LEU:HD13	1.92	0.52
33:SE:164:ILE:O	33:SE:168:VAL:HG13	2.09	0.52
37:SK:155:SER:OG	37:SK:156:ASN:N	2.41	0.52
33:SE:218:LEU:O	33:SE:222:ILE:HD12	2.10	0.52
23:NE:258:GLU:OE1	23:NE:258:GLU:N	2.43	0.52
26:NN:118:VAL:HG23	26:NN:275:ILE:O	2.09	0.52
3:L3:346:G:OP1	14:LI:8:THR:HG23	2.10	0.52
3:L3:1311:G:OP2	40:SN:258:LYS:NZ	2.43	0.52
43:SS:296:HIS:NE2	43:SS:298:MET:O	2.43	0.52
7:L9:26:ARG:NH2	33:SE:165:GLU:OE1	2.42	0.51
23:NE:276:LYS:HG3	23:NE:282:ILE:HD12	1.93	0.51
35:SI:192:ILE:HD12	43:SS:351:ARG:NH1	2.25	0.51
3:L3:170:C:O2	47:SZ:109:ASN:ND2	2.39	0.51
14:LI:34:LEU:HD22	14:LI:44:VAL:HG13	1.92	0.51
35:SI:192:ILE:HD11	39:SM:380:ARG:HE	1.75	0.51
45:SV:104:GLN:O	45:SV:108:ILE:HG22	2.10	0.51
28:NQ:206:GLN:OE1	28:NQ:208:ARG:NH2	2.43	0.51
1:L1:90:C:O2'	14:LI:24:HIS:ND1	2.35	0.51
37:SK:28:ILE:HG23	37:SK:28:ILE:O	2.10	0.51
3:L3:4583:C:O2'	3:L3:4584:A:OP2	2.25	0.51
31:SC:47:ASN:ND2	31:SC:50:LEU:HD22	2.25	0.51
3:L3:2269:C:O2'	25:NM:13:ASN:ND2	2.45	0.50
25:NM:23:THR:OG1	25:NM:26:GLN:O	2.27	0.50
42:SR:453:LEU:HD22	45:SV:71:PHE:CE2	2.46	0.50
3:L3:1501:C:O2'	9:LB:68:ARG:NH1	2.44	0.50
31:SC:203:ILE:O	31:SC:203:ILE:HG22	2.12	0.50
3:L3:193:G:OP2	47:SZ:21:ARG:NH1	2.44	0.50
10:LC:86:SER:OG	10:LC:88:SER:O	2.30	0.50
3:L3:734:G:H22	3:L3:929:A:H2	1.57	0.50
12:LG:20:LEU:HD21	12:LG:101:ASN:CG	2.36	0.50
46:SW:316:MET:HE1	46:SW:350:ILE:HG23	1.94	0.50
3:L3:1364:U:OP2	4:L6:36:ARG:NH1	2.44	0.50
1:L1:25:G:N3	3:L3:356:G:O2'	2.44	0.50
33:SE:207:VAL:HG21	33:SE:215:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:SO:324:GLU:OE1	41:SO:324:GLU:N	2.45	0.50
8:LA:10:ASN:OD1	8:LA:12:THR:OG1	2.30	0.50
3:L3:4662:C:OP2	3:L3:4663:G:N2	2.46	0.49
10:LC:38:VAL:HG22	32:SD:237:GLU:OE1	2.12	0.49
37:SK:161:VAL:HG22	37:SK:162:HIS:H	1.76	0.49
46:SW:336:ASP:OD1	46:SW:337:ARG:N	2.43	0.49
3:L3:5005:G:N2	3:L3:5041:G:O2'	2.45	0.49
41:SO:347:MET:HE2	41:SO:347:MET:HA	1.95	0.49
25:NM:167:LEU:HD22	29:NS:300:GLU:O	2.12	0.49
3:L3:4993:G:H22	3:L3:5058:A:H2	1.60	0.49
9:LB:39:THR:HG22	9:LB:41:SER:H	1.78	0.49
16:LN:139:ASP:OD1	16:LN:140:GLU:N	2.46	0.49
35:SI:196:ASP:OD2	39:SM:380:ARG:NH2	2.46	0.49
3:L3:4728:U:OP2	16:LN:132:LYS:NZ	2.38	0.49
6:L8:131:GLN:O	6:L8:135:LEU:HD23	2.13	0.48
42:SR:432:ILE:HD13	45:SV:1:MET:HE3	1.95	0.48
3:L3:4940:C:OP2	31:SC:219:LYS:NZ	2.42	0.48
31:SC:201:ILE:HD11	31:SC:267:LEU:HD21	1.95	0.48
37:SK:103:ALA:O	37:SK:107:VAL:HG23	2.13	0.48
3:L3:4880:C:OP1	6:L8:124:LYS:NZ	2.28	0.48
3:L3:1881:C:O2'	3:L3:1882:U:O5'	2.27	0.48
29:NS:155:ARG:NH1	29:NS:231:GLU:OE2	2.41	0.48
43:SS:265:MET:HE2	43:SS:265:MET:N	2.28	0.48
26:NN:144:ASN:ND2	26:NN:184:ASP:OD1	2.47	0.48
37:SK:166:SER:OG	37:SK:168:GLU:OE2	2.31	0.48
37:SK:2:ALA:HB3	37:SK:215:LEU:HD11	1.96	0.48
41:SO:278:ARG:NH1	41:SO:281:GLN:OE1	2.46	0.48
9:LB:10:ASP:OD2	9:LB:11:ARG:N	2.47	0.48
16:LN:370:THR:O	16:LN:370:THR:HG22	2.14	0.47
35:SI:251:ILE:O	35:SI:255:ASN:N	2.47	0.47
3:L3:5052:C:H2'	3:L3:5053:U:O4'	2.14	0.47
10:LC:84:TYR:CD1	10:LC:113:MET:HE1	2.49	0.47
12:LG:20:LEU:HD21	12:LG:101:ASN:ND2	2.29	0.47
16:LN:29:VAL:HG23	16:LN:346:THR:HG21	1.96	0.47
28:NQ:65:ARG:NH1	28:NQ:85:GLY:O	2.46	0.47
28:NQ:64:ASP:O	28:NQ:66:THR:N	2.45	0.47
28:NQ:92:GLY:HA3	28:NQ:136:MET:HE3	1.96	0.47
37:SK:121:LEU:O	37:SK:139:ARG:NH2	2.48	0.47
33:SE:105:GLU:OE1	33:SE:113:ARG:NH1	2.48	0.47
21:LW:17:THR:HG22	21:LW:18:LEU:N	2.30	0.47
37:SK:173:LEU:O	37:SK:177:LEU:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:NM:132:ARG:NH2	29:NS:199:ASN:OD1	2.48	0.47
42:SR:442:ILE:CG2	45:SV:79:ILE:HD11	2.44	0.47
14:LI:52:ASP:O	14:LI:52:ASP:OD2	2.33	0.47
16:LN:367:PHE:HB2	45:SV:1:MET:HE1	1.97	0.47
29:NS:66:MET:SD	29:NS:69:ARG:NH2	2.88	0.47
40:SN:73:THR:HG22	41:SO:168:PHE:HB2	1.97	0.47
47:SZ:107:LYS:HE3	47:SZ:107:LYS:HA	1.95	0.47
2:L2:99:G:N2	34:SH:129:GLU:OE1	2.48	0.47
41:SO:223:ILE:HD11	41:SO:230:VAL:HG23	1.96	0.46
2:L2:13:C:OP1	35:SI:86:HIS:NE2	2.35	0.46
16:LN:29:VAL:HG13	16:LN:348:ARG:HD3	1.96	0.46
2:L2:5:A:N6	2:L2:95:A:O2'	2.49	0.46
23:NE:228:LEU:HD23	23:NE:228:LEU:H	1.81	0.46
23:NE:341:LEU:HD11	23:NE:351:LEU:HD13	1.97	0.46
25:NM:18:SER:OG	30:SA:139:SER:O	2.22	0.46
33:SE:99:ALA:HB1	33:SE:136:LEU:HD11	1.97	0.46
37:SK:53:ILE:HG23	37:SK:76:THR:HG22	1.96	0.46
41:SO:63:LEU:HD11	41:SO:91:ASP:HB2	1.98	0.46
16:LN:71:GLU:OE2	16:LN:366:LYS:NZ	2.27	0.46
23:NE:229:THR:OG1	23:NE:242:ARG:NH2	2.48	0.46
38:SL:67:MET:HE3	38:SL:67:MET:HA	1.97	0.46
3:L3:1925:G:OP1	6:L8:33:GLN:NE2	2.49	0.46
3:L3:4626:A:OP2	16:LN:224:LYS:NZ	2.38	0.46
17:LQ:84:GLU:OE1	25:NM:30:ARG:NH2	2.45	0.46
21:LW:36:LYS:O	21:LW:45:ARG:NH1	2.46	0.46
19:LT:37:ASP:OD1	19:LT:38:GLU:N	2.49	0.46
27:NO:13:LEU:HD23	27:NO:16:ARG:HH21	1.81	0.46
5:L7:178:ARG:NH1	6:L8:123:ILE:HG21	2.30	0.46
43:SS:150:VAL:HG23	43:SS:150:VAL:O	2.16	0.46
10:LC:38:VAL:HG13	32:SD:237:GLU:OE1	2.15	0.46
20:LU:77:VAL:HG11	20:LU:82:ARG:HB3	1.96	0.46
21:LW:53:ALA:O	21:LW:57:ASN:ND2	2.49	0.45
27:NO:300:TYR:CE2	31:SC:50:LEU:HD21	2.51	0.45
3:L3:1928:C:N4	3:L3:2054:U:O2	2.49	0.45
19:LT:108:SER:OG	31:SC:192:LYS:O	2.30	0.45
36:SJ:709:GLU:O	36:SJ:713:ARG:N	2.37	0.45
41:SO:91:ASP:OD1	41:SO:92:THR:N	2.48	0.45
3:L3:4632:U:H3'	3:L3:4633:G:H5''	1.98	0.45
16:LN:391:PRO:HD2	45:SV:108:ILE:HG21	1.97	0.45
40:SN:61:LYS:NZ	40:SN:63:ASP:OD1	2.48	0.45
3:L3:2303:C:OP1	17:LQ:107:ASN:ND2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:SK:100:ARG:NH1	45:SV:26:CYS:SG	2.90	0.45
42:SR:442:ILE:HD13	45:SV:86:TRP:CZ2	2.52	0.45
12:LG:32:THR:HG21	12:LG:105:ILE:HD12	1.98	0.45
37:SK:162:HIS:NE2	37:SK:191:GLU:OE2	2.49	0.45
7:L9:97:SER:O	7:L9:100:SER:OG	2.33	0.45
16:LN:29:VAL:CG2	16:LN:346:THR:HG21	2.47	0.45
16:LN:93:VAL:HG13	16:LN:102:PHE:HB2	1.99	0.45
38:SL:203:LEU:HD23	38:SL:214:ILE:HD13	1.98	0.45
1:L1:149:G:H21	33:SE:64:GLN:HE22	1.65	0.45
3:L3:4883:C:N4	31:SC:181:LEU:O	2.48	0.45
21:LW:60:GLY:O	47:SZ:10:ARG:NH1	2.50	0.45
23:NE:273:LEU:HD21	26:NN:288:GLU:HG2	1.97	0.45
6:L8:40:GLY:O	6:L8:43:THR:N	2.49	0.45
25:NM:41:ARG:NH1	25:NM:48:ASN:OD1	2.50	0.45
43:SS:368:LEU:HD22	43:SS:372:LEU:HD12	1.99	0.45
17:LQ:84:GLU:O	17:LQ:87:VAL:HG22	2.17	0.44
11:LE:154:ILE:HD12	11:LE:155:PRO:CD	2.47	0.44
18:LS:121:VAL:HG13	47:SZ:59:ALA:HB3	1.99	0.44
29:NS:176:ARG:NH2	31:SC:231:GLU:O	2.43	0.44
31:SC:235:THR:O	31:SC:235:THR:HG23	2.18	0.44
3:L3:442:G:OP1	19:LT:68:ARG:NH1	2.42	0.44
16:LN:311:ASP:OD1	16:LN:311:ASP:O	2.35	0.44
23:NE:273:LEU:HD22	26:NN:106:PRO:HG3	1.99	0.44
3:L3:67:C:OP2	3:L3:312:G:N2	2.45	0.44
3:L3:4761:G:O6	10:LC:170:LYS:NZ	2.50	0.44
19:LT:33:VAL:HG23	19:LT:38:GLU:HB2	1.99	0.44
3:L3:4626:A:OP1	16:LN:341:LYS:NZ	2.48	0.44
42:SR:418:ASP:C	42:SR:419:LEU:HD12	2.43	0.44
1:L1:28:C:O2'	3:L3:1371:A:N1	2.49	0.43
33:SE:158:ALA:HB2	33:SE:190:LEU:HD12	2.00	0.43
27:NO:212:ASN:O	27:NO:216:GLY:N	2.40	0.43
42:SR:453:LEU:HD22	45:SV:71:PHE:HE2	1.82	0.43
26:NN:108:LEU:HD22	26:NN:286:VAL:HG22	1.99	0.43
31:SC:214:ASP:OD1	31:SC:215:ALA:N	2.51	0.43
36:SJ:664:ASP:OD1	36:SJ:667:GLY:N	2.48	0.43
2:L2:93:C:O2'	2:L2:94:U:O5'	2.36	0.43
3:L3:1807:C:O2'	11:LE:113:ASP:OD2	2.31	0.43
3:L3:4763:U:H5	5:L7:126:VAL:HG21	1.82	0.43
16:LN:293:ILE:N	16:LN:293:ILE:HD12	2.34	0.43
37:SK:116:LEU:HD21	37:SK:176:LEU:HD22	2.00	0.43
3:L3:1854:G:H1'	3:L3:1855:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:SR:432:ILE:CD1	45:SV:1:MET:HE3	2.49	0.43
1:L1:83:C:H42	14:LI:50:ARG:NE	2.16	0.43
27:NO:13:LEU:HD23	27:NO:16:ARG:NH2	2.34	0.43
1:L1:60:G:O6	1:L1:96:C:O2'	2.31	0.42
3:L3:119:G:N3	3:L3:119:G:H2'	2.34	0.42
47:SZ:150:SER:O	47:SZ:154:VAL:HG23	2.18	0.42
1:L1:69:U:H2'	1:L1:70:G:O4'	2.19	0.42
5:L7:54:TYR:HD1	5:L7:145:VAL:HG21	1.84	0.42
17:LQ:118:LEU:HD12	25:NM:119:TYR:HE1	1.84	0.42
3:L3:116:G:H2'	3:L3:117:C:C6	2.54	0.42
3:L3:1887:G:H3'	3:L3:1888:A:C5'	2.48	0.42
3:L3:4761:G:OP1	5:L7:37:ARG:NH2	2.52	0.42
37:SK:107:VAL:HG12	37:SK:108:THR:HG23	2.00	0.42
3:L3:164:G:O2'	46:SW:577:LYS:NZ	2.41	0.42
10:LC:28:TYR:CD2	10:LC:54:MET:HE2	2.55	0.42
21:LW:17:THR:HG22	21:LW:18:LEU:H	1.84	0.42
41:SO:194:TYR:HA	43:SS:154:LEU:HD13	2.02	0.42
2:L2:52:G:N7	38:SL:171:ARG:NH1	2.68	0.42
16:LN:67:VAL:O	16:LN:67:VAL:HG22	2.19	0.42
46:SW:219:LEU:HD12	46:SW:384:LEU:O	2.19	0.42
3:L3:119:G:N2	33:SE:133:PRO:O	2.41	0.42
35:SI:135:GLN:OE1	35:SI:135:GLN:N	2.49	0.42
1:L1:83:C:N4	14:LI:50:ARG:HE	2.18	0.42
3:L3:5039:U:OP1	45:SV:111:ARG:NH1	2.52	0.42
12:LG:108:ASN:HD22	12:LG:108:ASN:C	2.25	0.42
10:LC:99:ASP:OD1	10:LC:108:GLN:NE2	2.53	0.42
29:NS:229:ARG:HE	29:NS:309:GLY:HA2	1.85	0.42
40:SN:68:GLU:O	41:SO:163:ARG:NH2	2.52	0.42
43:SS:298:MET:SD	43:SS:298:MET:N	2.93	0.42
38:SL:149:LEU:HD21	38:SL:176:ARG:HG3	2.01	0.42
23:NE:250:LEU:HD23	23:NE:264:LEU:HD23	2.02	0.42
35:SI:98:PHE:HB2	35:SI:152:PRO:HG3	2.02	0.42
3:L3:1353:G:O6	9:LB:85:THR:HG21	2.20	0.41
3:L3:4941:G:OP2	31:SC:188:ARG:NH2	2.50	0.41
3:L3:5001:U:OP1	16:LN:385:LYS:NZ	2.48	0.41
46:SW:284:LEU:HD12	46:SW:306:VAL:O	2.20	0.41
5:L7:20:ALA:HB3	5:L7:87:MET:HE1	2.02	0.41
38:SL:122:GLY:O	38:SL:124:LYS:NZ	2.50	0.41
2:L2:2:C:C6	35:SI:230:ARG:HD3	2.56	0.41
3:L3:159:C:O2	4:L6:88:LYS:NZ	2.47	0.41
10:LC:82:LEU:HD12	10:LC:82:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LI:50:ARG:NH1	14:LI:51:LYS:O	2.46	0.41
18:LS:41:ALA:HA	18:LS:44:LEU:HD12	2.01	0.41
23:NE:228:LEU:CD2	23:NE:271:THR:HG21	2.44	0.41
37:SK:96:ARG:O	45:SV:76:ASN:ND2	2.50	0.41
42:SR:369:ASP:OD2	42:SR:370:ASP:N	2.53	0.41
17:LQ:114:ARG:NH1	25:NM:119:TYR:OH	2.53	0.41
31:SC:281:ILE:HG23	31:SC:286:LEU:HD21	2.02	0.41
32:SD:147:LEU:O	32:SD:151:ASN:ND2	2.53	0.41
37:SK:199:VAL:HG21	37:SK:222:PHE:CE2	2.55	0.41
41:SO:175:LEU:HD12	41:SO:178:TYR:HD1	1.86	0.41
41:SO:336:ILE:HG23	41:SO:340:GLN:HB2	2.02	0.41
46:SW:209:SER:O	46:SW:213:LEU:HD13	2.21	0.41
17:LQ:118:LEU:HD12	25:NM:119:TYR:CE1	2.56	0.41
33:SE:240:ASN:O	33:SE:240:ASN:ND2	2.53	0.41
3:L3:2093:A:O2'	3:L3:2094:G:H4'	2.20	0.41
3:L3:2296:G:O2'	30:SA:242:PRO:O	2.37	0.41
23:NE:232:THR:HG21	23:NE:280:VAL:HG12	2.03	0.41
23:NE:253:LEU:HD12	23:NE:264:LEU:HD22	2.02	0.41
24:NG:187:LYS:HB3	24:NG:201:LEU:HD23	2.03	0.41
40:SN:134:THR:O	44:ST:234:ARG:NH2	2.45	0.41
43:SS:265:MET:HE2	43:SS:265:MET:CA	2.51	0.41
3:L3:1854:G:C8	3:L3:1855:G:N7	2.89	0.41
3:L3:2100:A:OP2	3:L3:2262:G:N2	2.54	0.41
3:L3:4763:U:C5	5:L7:126:VAL:HG21	2.56	0.41
3:L3:4946:U:O2'	19:LT:2:SER:N	2.50	0.41
41:SO:51:VAL:HG23	43:SS:132:ILE:O	2.21	0.41
41:SO:175:LEU:HD12	41:SO:178:TYR:CD1	2.56	0.41
37:SK:126:GLU:OE2	37:SK:139:ARG:NH1	2.54	0.40
4:L6:64:VAL:O	4:L6:67:HIS:ND1	2.54	0.40
20:LU:71:LYS:NZ	43:SS:127:SEP:O3P	2.39	0.40
23:NE:341:LEU:HD11	23:NE:351:LEU:CD1	2.51	0.40
43:SS:125:ASP:OD1	43:SS:126:SEP:N	2.55	0.40
7:L9:94:PHE:CE2	7:L9:96:ARG:HB2	2.56	0.40
10:LC:29:ARG:NH1	11:LE:148:PRO:O	2.54	0.40
26:NN:33:VAL:O	26:NN:51:ARG:NH2	2.52	0.40
28:NQ:155:LEU:HD22	28:NQ:200:THR:HG21	2.03	0.40
3:L3:1444:G:HO2'	3:L3:1448:G:HO2'	1.63	0.40
4:L6:63:THR:HG22	4:L6:64:VAL:N	2.36	0.40
4:L6:94:ILE:HD11	4:L6:96:ILE:HD12	2.02	0.40
16:LN:285:TYR:HA	16:LN:363:ILE:HD11	2.04	0.40
23:NE:350:ILE:HG21	23:NE:355:LEU:HD21	2.04	0.40

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	L6	112/211 (53%)	110 (98%)	2 (2%)	0	100	100
5	L7	180/203 (89%)	178 (99%)	2 (1%)	0	100	100
6	L8	133/215 (62%)	131 (98%)	2 (2%)	0	100	100
7	L9	179/204 (88%)	177 (99%)	2 (1%)	0	100	100
8	LA	137/184 (74%)	135 (98%)	2 (2%)	0	100	100
9	LB	149/188 (79%)	149 (100%)	0	0	100	100
10	LC	172/176 (98%)	169 (98%)	3 (2%)	0	100	100
11	LE	102/160 (64%)	102 (100%)	0	0	100	100
12	LG	110/140 (79%)	110 (100%)	0	0	100	100
13	LH	18/156 (12%)	18 (100%)	0	0	100	100
14	LI	132/145 (91%)	132 (100%)	0	0	100	100
15	LK	104/148 (70%)	100 (96%)	4 (4%)	0	100	100
16	LN	372/403 (92%)	365 (98%)	7 (2%)	0	100	100
17	LQ	131/135 (97%)	130 (99%)	1 (1%)	0	100	100
18	LS	120/123 (98%)	120 (100%)	0	0	100	100
19	LT	107/110 (97%)	107 (100%)	0	0	100	100
20	LU	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
21	LW	65/97 (67%)	64 (98%)	1 (2%)	0	100	100
22	NB	29/549 (5%)	29 (100%)	0	0	100	100
23	NE	152/361 (42%)	149 (98%)	3 (2%)	0	100	100
24	NG	87/282 (31%)	86 (99%)	1 (1%)	0	100	100
25	NM	180/300 (60%)	176 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	NN	238/473 (50%)	233 (98%)	5 (2%)	0	100	100
27	NO	301/461 (65%)	300 (100%)	1 (0%)	0	100	100
28	NQ	320/385 (83%)	315 (98%)	5 (2%)	0	100	100
29	NS	303/349 (87%)	302 (100%)	1 (0%)	0	100	100
30	SA	327/427 (77%)	323 (99%)	4 (1%)	0	100	100
31	SC	193/288 (67%)	188 (97%)	5 (3%)	0	100	100
32	SD	237/248 (96%)	232 (98%)	5 (2%)	0	100	100
33	SE	184/266 (69%)	182 (99%)	2 (1%)	0	100	100
34	SH	148/293 (50%)	147 (99%)	1 (1%)	0	100	100
35	SI	198/255 (78%)	195 (98%)	3 (2%)	0	100	100
36	SJ	70/847 (8%)	68 (97%)	2 (3%)	0	100	100
37	SK	224/245 (91%)	221 (99%)	3 (1%)	0	100	100
38	SL	241/490 (49%)	238 (99%)	3 (1%)	0	100	100
39	SM	427/588 (73%)	427 (100%)	0	0	100	100
40	SN	162/306 (53%)	161 (99%)	1 (1%)	0	100	100
41	SO	305/353 (86%)	302 (99%)	3 (1%)	0	100	100
42	SR	73/634 (12%)	71 (97%)	2 (3%)	0	100	100
43	SS	227/746 (30%)	227 (100%)	0	0	100	100
44	ST	34/365 (9%)	33 (97%)	1 (3%)	0	100	100
45	SV	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
46	SW	441/670 (66%)	434 (98%)	7 (2%)	0	100	100
47	SZ	156/178 (88%)	155 (99%)	1 (1%)	0	100	100
All	All	7816/13625 (57%)	7724 (99%)	92 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	L6	98/177 (55%)	98 (100%)	0	100	100
5	L7	157/174 (90%)	157 (100%)	0	100	100
6	L8	115/161 (71%)	115 (100%)	0	100	100
7	L9	155/172 (90%)	155 (100%)	0	100	100
8	LA	132/163 (81%)	132 (100%)	0	100	100
9	LB	136/165 (82%)	136 (100%)	0	100	100
10	LC	155/157 (99%)	155 (100%)	0	100	100
11	LE	47/140 (34%)	47 (100%)	0	100	100
12	LG	87/107 (81%)	87 (100%)	0	100	100
13	LH	13/133 (10%)	13 (100%)	0	100	100
14	LI	124/135 (92%)	124 (100%)	0	100	100
15	LK	29/121 (24%)	29 (100%)	0	100	100
16	LN	328/348 (94%)	328 (100%)	0	100	100
17	LQ	119/121 (98%)	119 (100%)	0	100	100
18	LS	109/110 (99%)	109 (100%)	0	100	100
19	LT	88/89 (99%)	88 (100%)	0	100	100
20	LU	87/89 (98%)	87 (100%)	0	100	100
21	LW	58/80 (72%)	58 (100%)	0	100	100
22	NB	27/485 (6%)	27 (100%)	0	100	100
23	NE	136/294 (46%)	136 (100%)	0	100	100
24	NG	83/246 (34%)	83 (100%)	0	100	100
25	NM	168/272 (62%)	168 (100%)	0	100	100
26	NN	218/398 (55%)	218 (100%)	0	100	100
27	NO	269/392 (69%)	269 (100%)	0	100	100
28	NQ	265/318 (83%)	265 (100%)	0	100	100
29	NS	276/305 (90%)	276 (100%)	0	100	100
30	SA	280/348 (80%)	280 (100%)	0	100	100
31	SC	178/252 (71%)	178 (100%)	0	100	100
32	SD	207/215 (96%)	207 (100%)	0	100	100
33	SE	159/223 (71%)	159 (100%)	0	100	100
34	SH	140/274 (51%)	140 (100%)	0	100	100
35	SI	182/228 (80%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	SJ	64/733 (9%)	64 (100%)	0	100	100
37	SK	196/213 (92%)	196 (100%)	0	100	100
38	SL	226/437 (52%)	226 (100%)	0	100	100
39	SM	350/509 (69%)	350 (100%)	0	100	100
40	SN	126/260 (48%)	126 (100%)	0	100	100
41	SO	283/319 (89%)	283 (100%)	0	100	100
42	SR	69/574 (12%)	69 (100%)	0	100	100
43	SS	208/648 (32%)	208 (100%)	0	100	100
44	ST	27/300 (9%)	27 (100%)	0	100	100
45	SV	127/149 (85%)	127 (100%)	0	100	100
46	SW	394/591 (67%)	394 (100%)	0	100	100
47	SZ	141/158 (89%)	141 (100%)	0	100	100
All	All	6836/11783 (58%)	6836 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
4	L6	104	ASN
5	L7	90	HIS
5	L7	199	HIS
6	L8	34	ASN
7	L9	8	GLN
7	L9	158	HIS
7	L9	201	HIS
9	LB	7	HIS
10	LC	37	HIS
10	LC	91	HIS
10	LC	122	HIS
14	LI	96	HIS
16	LN	68	ASN
16	LN	184	GLN
17	LQ	52	GLN
17	LQ	102	ASN
17	LQ	107	ASN
19	LT	21	GLN
19	LT	99	HIS

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Mol	Chain	Res	Type
20	LU	12	ASN
20	LU	15	HIS
20	LU	26	HIS
20	LU	36	HIS
23	NE	235	ASN
26	NN	170	HIS
28	NQ	113	HIS
29	NS	153	HIS
29	NS	162	GLN
29	NS	206	ASN
29	NS	257	HIS
29	NS	335	HIS
30	SA	38	ASN
30	SA	231	ASN
30	SA	245	HIS
31	SC	190	HIS
31	SC	227	HIS
32	SD	56	HIS
32	SD	99	ASN
32	SD	151	ASN
33	SE	64	GLN
33	SE	206	GLN
33	SE	208	ASN
33	SE	240	ASN
34	SH	51	HIS
34	SH	60	GLN
34	SH	119	HIS
35	SI	66	HIS
36	SJ	726	HIS
37	SK	68	HIS
37	SK	74	ASN
37	SK	79	GLN
37	SK	83	HIS
38	SL	35	GLN
38	SL	218	HIS
39	SM	191	GLN
39	SM	211	HIS
39	SM	253	GLN
39	SM	375	HIS
40	SN	113	GLN
40	SN	124	HIS
41	SO	340	GLN

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Mol	Chain	Res	Type
43	SS	211	GLN
46	SW	187	ASN
46	SW	525	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	150/157 (95%)	14 (9%)	0
2	L2	65/1167 (5%)	9 (13%)	0
3	L3	1477/5070 (29%)	208 (14%)	2 (0%)
All	All	1692/6394 (26%)	231 (13%)	2 (0%)

All (231) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	34	U
1	L1	59	A
1	L1	62	A
1	L1	63	U
1	L1	82	A
1	L1	83	C
1	L1	84	A
1	L1	86	U
1	L1	94	G
1	L1	103	A
1	L1	105	C
1	L1	111	U
1	L1	156	U
1	L1	157	U
2	L2	11	C
2	L2	48	G
2	L2	49	G
2	L2	51	U
2	L2	62	U
2	L2	94	U
2	L2	96	A
2	L2	101	A
2	L2	103	A
3	L3	48	G
3	L3	58	G
3	L3	59	A

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Mol	Chain	Res	Type
3	L3	64	A
3	L3	65	A
3	L3	69	A
3	L3	85	G
3	L3	86	U
3	L3	91	G
3	L3	93	G
3	L3	95	G
3	L3	108	A
3	L3	119	G
3	L3	159	C
3	L3	170	C
3	L3	171	U
3	L3	172	C
3	L3	173	C
3	L3	176	G
3	L3	179	G
3	L3	181	C
3	L3	186	G
3	L3	190	G
3	L3	200	U
3	L3	204	U
3	L3	210	C
3	L3	218	A
3	L3	219	G
3	L3	220	C
3	L3	233	U
3	L3	234	G
3	L3	265	C
3	L3	271	C
3	L3	281	U
3	L3	294	G
3	L3	326	C
3	L3	340	C
3	L3	362	A
3	L3	386	A
3	L3	387	G
3	L3	408	A
3	L3	409	G
3	L3	410	A
3	L3	413	G
3	L3	446	C

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Mol	Chain	Res	Type
3	L3	451	C
3	L3	452	A
3	L3	469	C
3	L3	470	A
3	L3	473	C
3	L3	479	G
3	L3	673	C
3	L3	685	C
3	L3	686	A
3	L3	687	U
3	L3	696	C
3	L3	697	G
3	L3	701	G
3	L3	703	G
3	L3	730	G
3	L3	731	G
3	L3	739	G
3	L3	742	G
3	L3	746	A
3	L3	913	U
3	L3	914	U
3	L3	915	A
3	L3	917	A
3	L3	926	G
3	L3	932	A
3	L3	933	G
3	L3	944	A
3	L3	945	U
3	L3	1296	G
3	L3	1297	U
3	L3	1301	C
3	L3	1313	C
3	L3	1314	C
3	L3	1315	C
3	L3	1328	G
3	L3	1330	A
3	L3	1337	A
3	L3	1354	A
3	L3	1358	G
3	L3	1359	G
3	L3	1445	U
3	L3	1502	G

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Mol	Chain	Res	Type
3	L3	1654	G
3	L3	1661	C
3	L3	1671	U
3	L3	1674	C
3	L3	1677	U
3	L3	1679	A
3	L3	1680	G
3	L3	1691	G
3	L3	1804	A
3	L3	1836	G
3	L3	1837	A
3	L3	1842	G
3	L3	1854	G
3	L3	1881	C
3	L3	1882	U
3	L3	1888	A
3	L3	1891	A
3	L3	1892	A
3	L3	1897	A
3	L3	1906	U
3	L3	1910	G
3	L3	1919	G
3	L3	1921	C
3	L3	1922	G
3	L3	2055	G
3	L3	2056	G
3	L3	2069	A
3	L3	2084	C
3	L3	2085	G
3	L3	2089	G
3	L3	2094	G
3	L3	2095	A
3	L3	2097	U
3	L3	2099	G
3	L3	2100	A
3	L3	2102	G
3	L3	2103	G
3	L3	2261	G
3	L3	2265	G
3	L3	2266	C
3	L3	2267	U
3	L3	2289	C

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Mol	Chain	Res	Type
3	L3	2300	A
3	L3	2301	G
3	L3	2313	A
3	L3	2314	G
3	L3	2348	G
3	L3	2351	C
3	L3	2364	G
3	L3	2826	U
3	L3	2829	U
3	L3	2836	A
3	L3	2837	U
3	L3	2838	G
3	L3	3852	A
3	L3	3895	G
3	L3	4584	A
3	L3	4589	A
3	L3	4590	A
3	L3	4618	G
3	L3	4621	C
3	L3	4629	U
3	L3	4633	G
3	L3	4640	C
3	L3	4641	U
3	L3	4642	U
3	L3	4647	G
3	L3	4648	A
3	L3	4649	G
3	L3	4651	A
3	L3	4657	U
3	L3	4658	G
3	L3	4661	G
3	L3	4671	C
3	L3	4672	A
3	L3	4673	U
3	L3	4719	G
3	L3	4737	G
3	L3	4740	G
3	L3	4741	C
3	L3	4742	G
3	L3	4745	G
3	L3	4747	C
3	L3	4754	G

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Mol	Chain	Res	Type
3	L3	4757	C
3	L3	4759	C
3	L3	4761	G
3	L3	4763	U
3	L3	4765	G
3	L3	4773	C
3	L3	4870	G
3	L3	4871	C
3	L3	4882	U
3	L3	4883	C
3	L3	4910	G
3	L3	4912	G
3	L3	4914	C
3	L3	4943	A
3	L3	4949	G
3	L3	4950	U
3	L3	4951	G
3	L3	4955	A
3	L3	4958	C
3	L3	4960	G
3	L3	4966	A
3	L3	4976	U
3	L3	5013	C
3	L3	5022	U
3	L3	5025	C
3	L3	5026	U
3	L3	5027	C
3	L3	5028	G
3	L3	5030	U
3	L3	5031	G
3	L3	5040	U
3	L3	5041	G
3	L3	5045	G
3	L3	5053	U
3	L3	5059	C
3	L3	5064	G
3	L3	5065	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L3	1880	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L3	2093	A

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

4 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
43	SEP	SS	127	43	8,9,10	1.57	1 (12%)	7,12,14	1.13	1 (14%)
16	HIC	LN	245	16	10,11,12	1.44	1 (10%)	9,14,16	1.19	2 (22%)
25	AME	NM	1	25	9,10,11	1.52	2 (22%)	9,11,13	1.37	1 (11%)
43	SEP	SS	126	43	8,9,10	1.57	1 (12%)	7,12,14	1.22	1 (14%)

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
43	SEP	SS	127	43	-	2/6/8/10	-
16	HIC	LN	245	16	-	0/5/6/8	0/1/1/1
25	AME	NM	1	25	-	1/9/10/12	-
43	SEP	SS	126	43	-	0/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	SS	126	SEP	P-O1P	3.47	1.61	1.50
43	SS	127	SEP	P-O1P	3.44	1.61	1.50
25	NM	1	AME	CT1-N	3.43	1.45	1.34
16	LN	245	HIC	CD2-CG	2.77	1.41	1.36
25	NM	1	AME	OT-CT1	-2.13	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	LN	245	HIC	NE2-CE1-ND1	-2.68	111.64	112.66
43	SS	126	SEP	OG-CB-CA	2.66	110.73	108.14
25	NM	1	AME	CT2-CT1-N	2.40	120.09	116.12
16	LN	245	HIC	CB-CG-CD2	-2.03	125.06	129.96
43	SS	127	SEP	OG-CB-CA	2.02	110.11	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	NM	1	AME	C-CA-N-CT1
43	SS	127	SEP	N-CA-CB-OG
43	SS	127	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	SS	127	SEP	1	0
43	SS	126	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 56 are monoatomic - leaving 1 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	$\# Z > 2$
50	SF4	NM	401	25	0,12,12	-	-	-		

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
50	SF4	NM	401	25	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

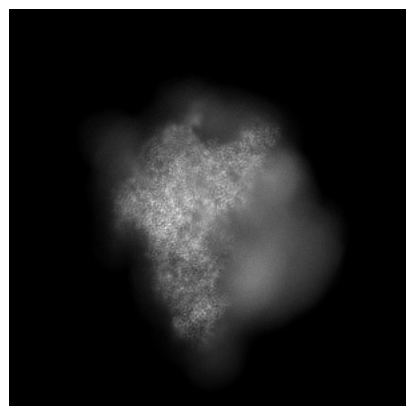
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29252. These allow visual inspection of the internal detail of the map and identification of artifacts.

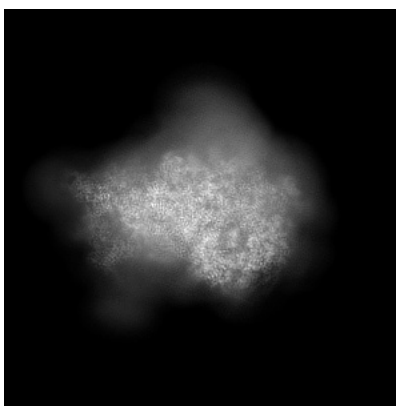
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

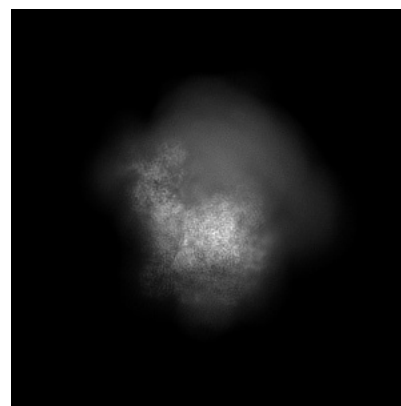
6.1.1 Primary map



X

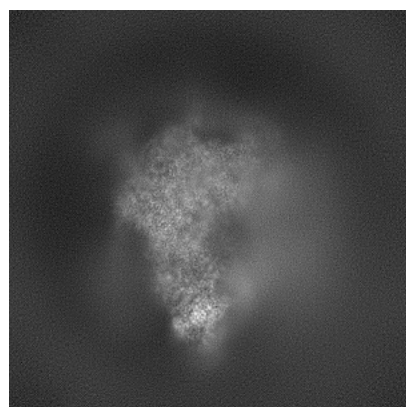


Y

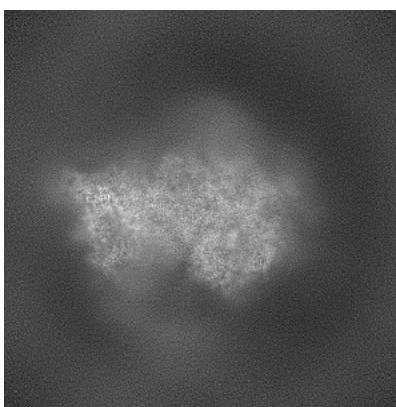


Z

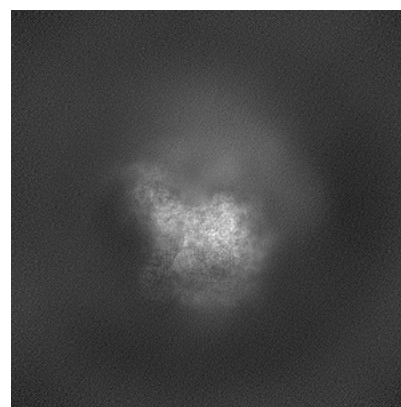
6.1.2 Raw map



X



Y

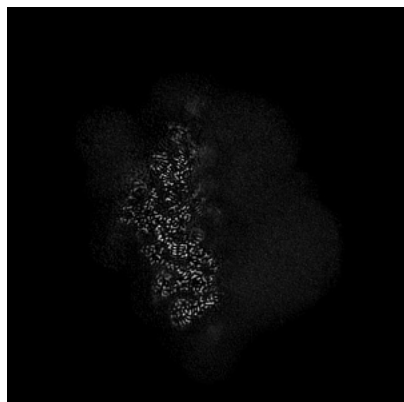


Z

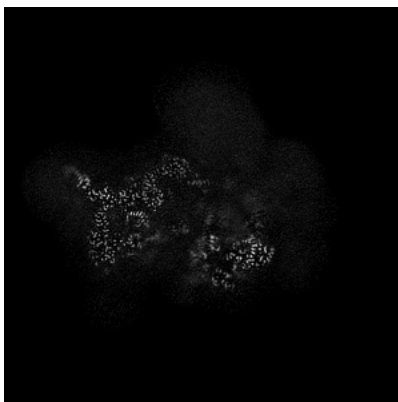
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

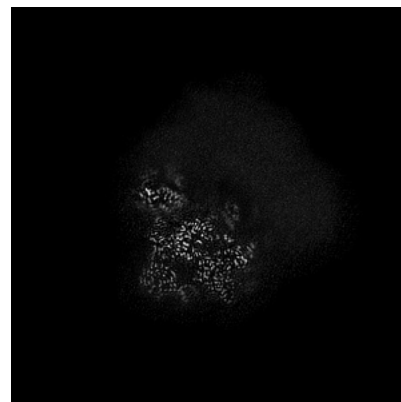
6.2.1 Primary map



X Index: 240

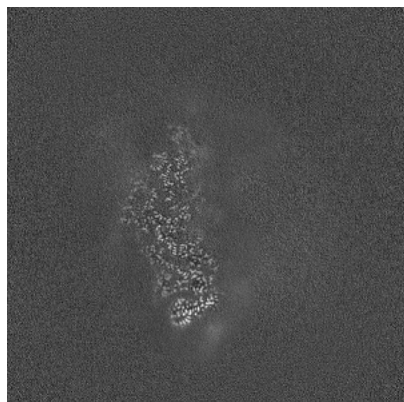


Y Index: 240

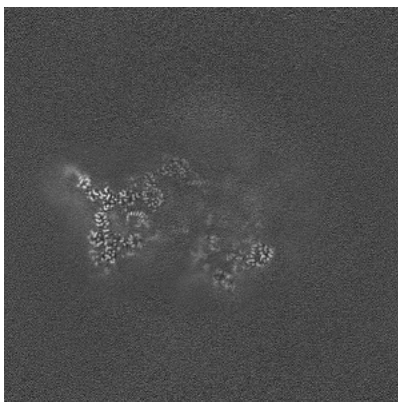


Z Index: 240

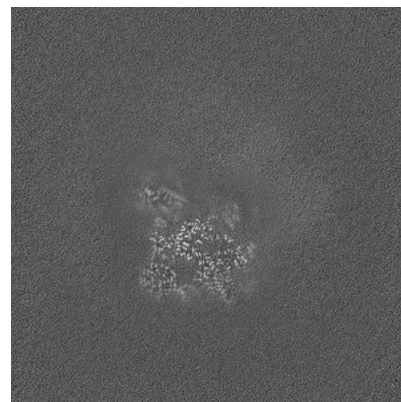
6.2.2 Raw map



X Index: 240



Y Index: 240

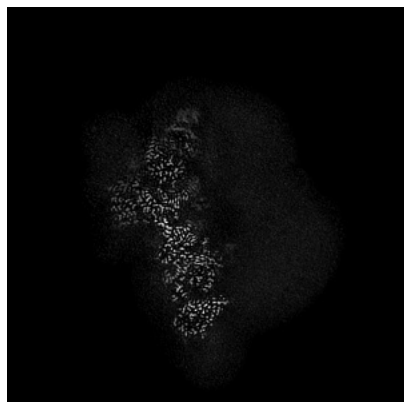


Z Index: 240

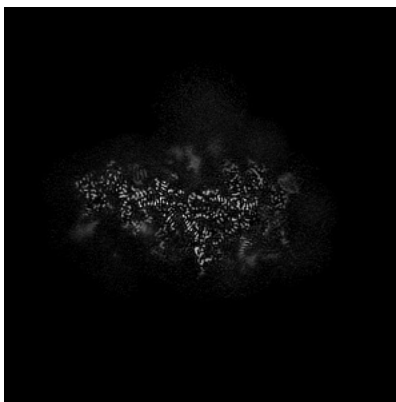
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

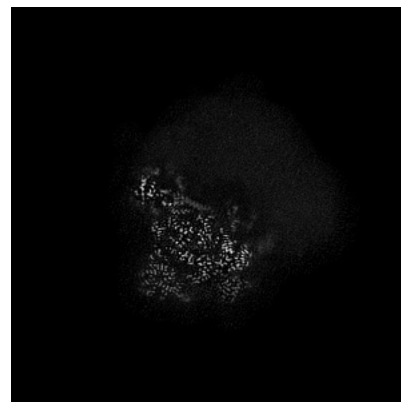
6.3.1 Primary map



X Index: 257

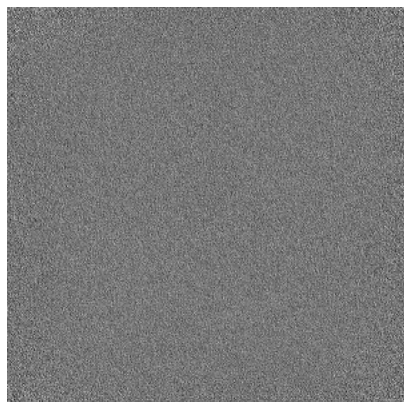


Y Index: 205

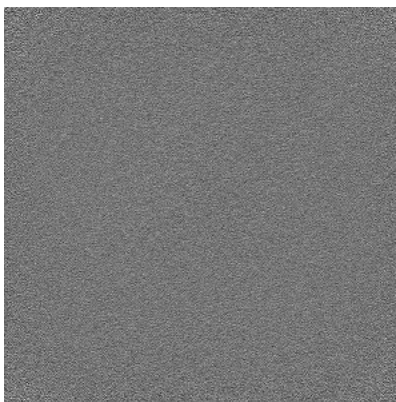


Z Index: 245

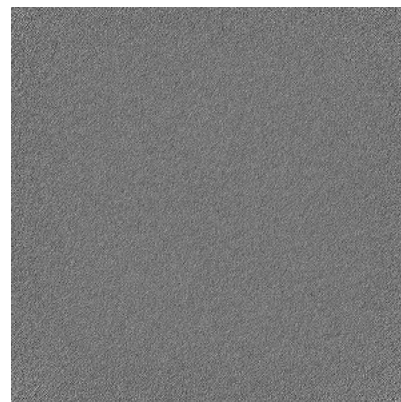
6.3.2 Raw map



X Index: 0



Y Index: 0

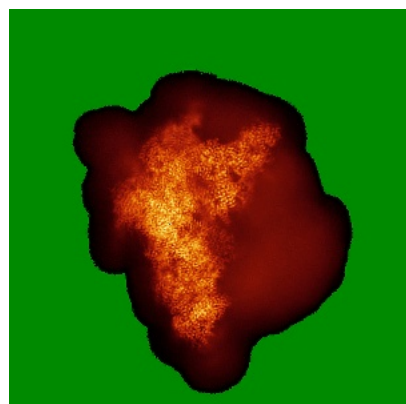


Z Index: 0

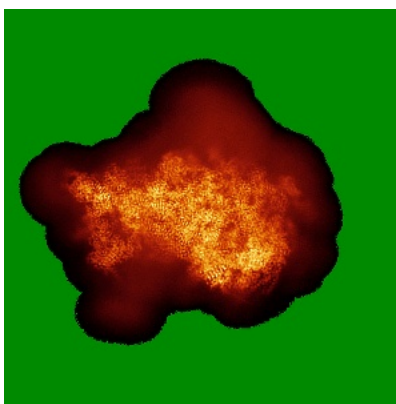
The images above show the largest variance slices of the map in three orthogonal directions.

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

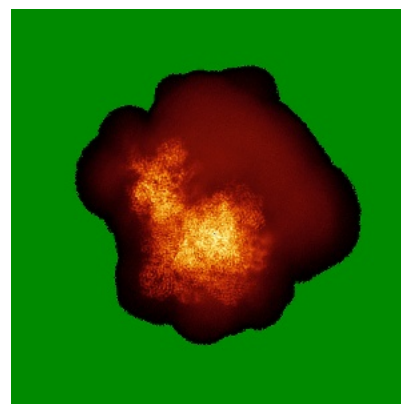
6.4.1 Primary map



X

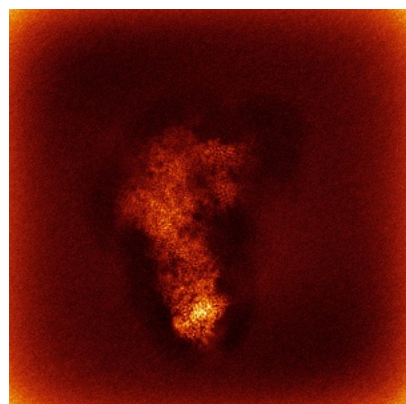


Y

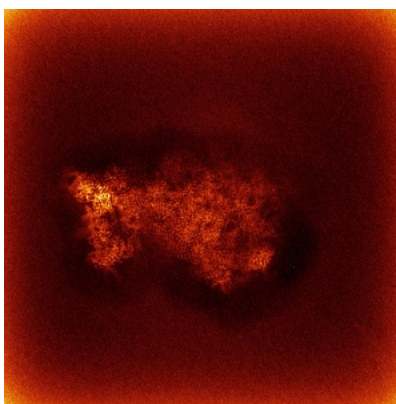


Z

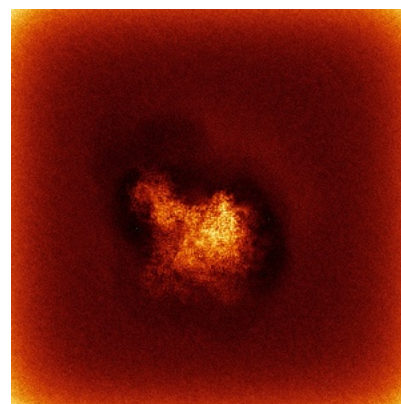
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

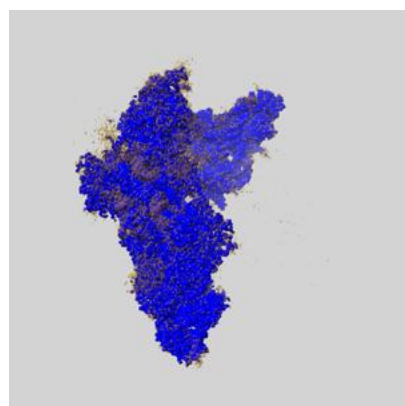
6.6 Mask visualisation [i](#)

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

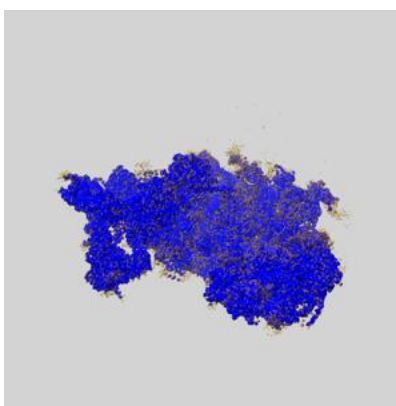
A mask typically either:

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

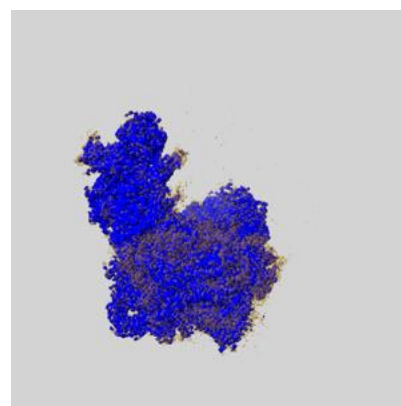
6.6.1 emd_29252_msk_1.map [i](#)



X



Y

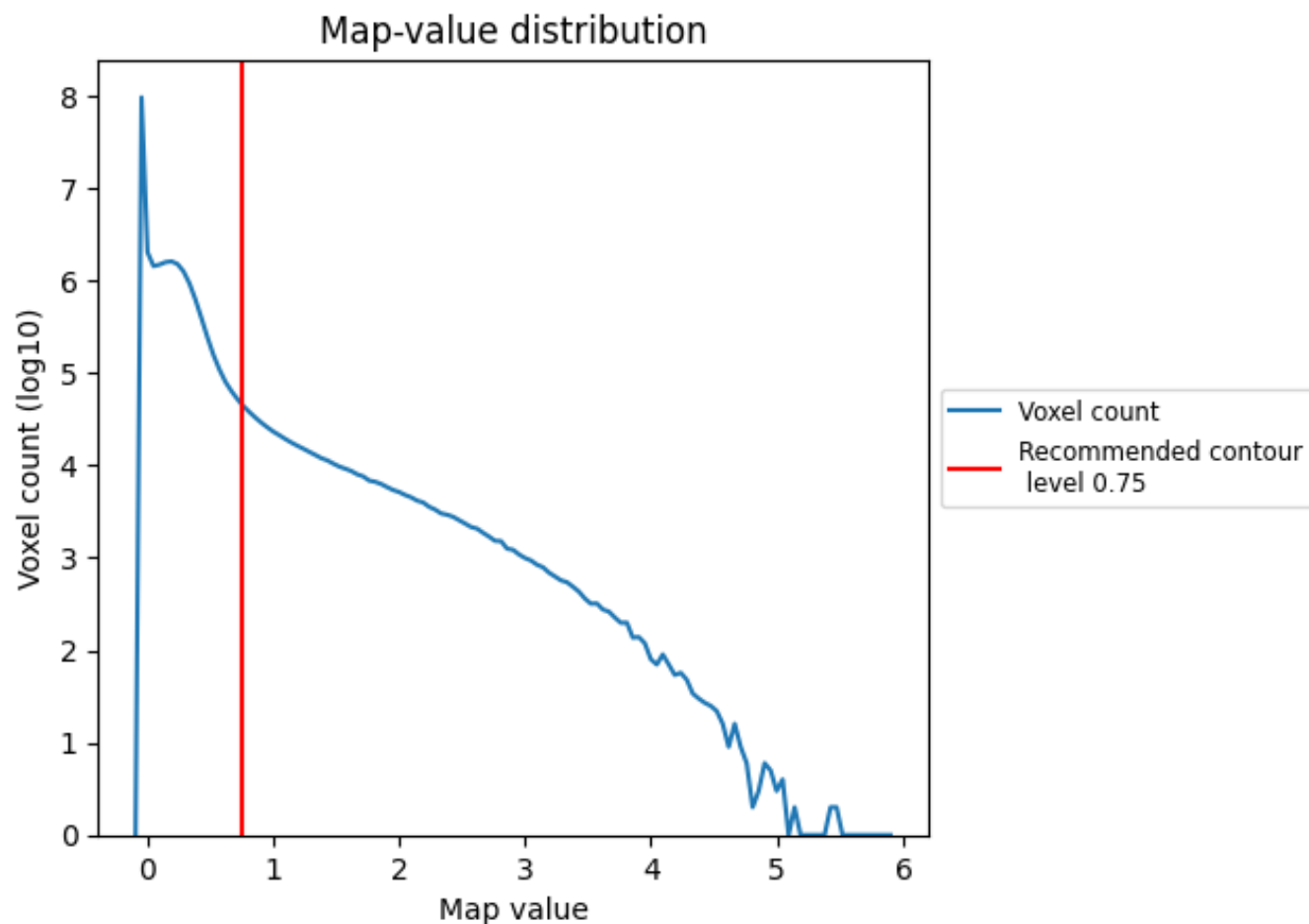


Z

7 Map analysis [i](#)

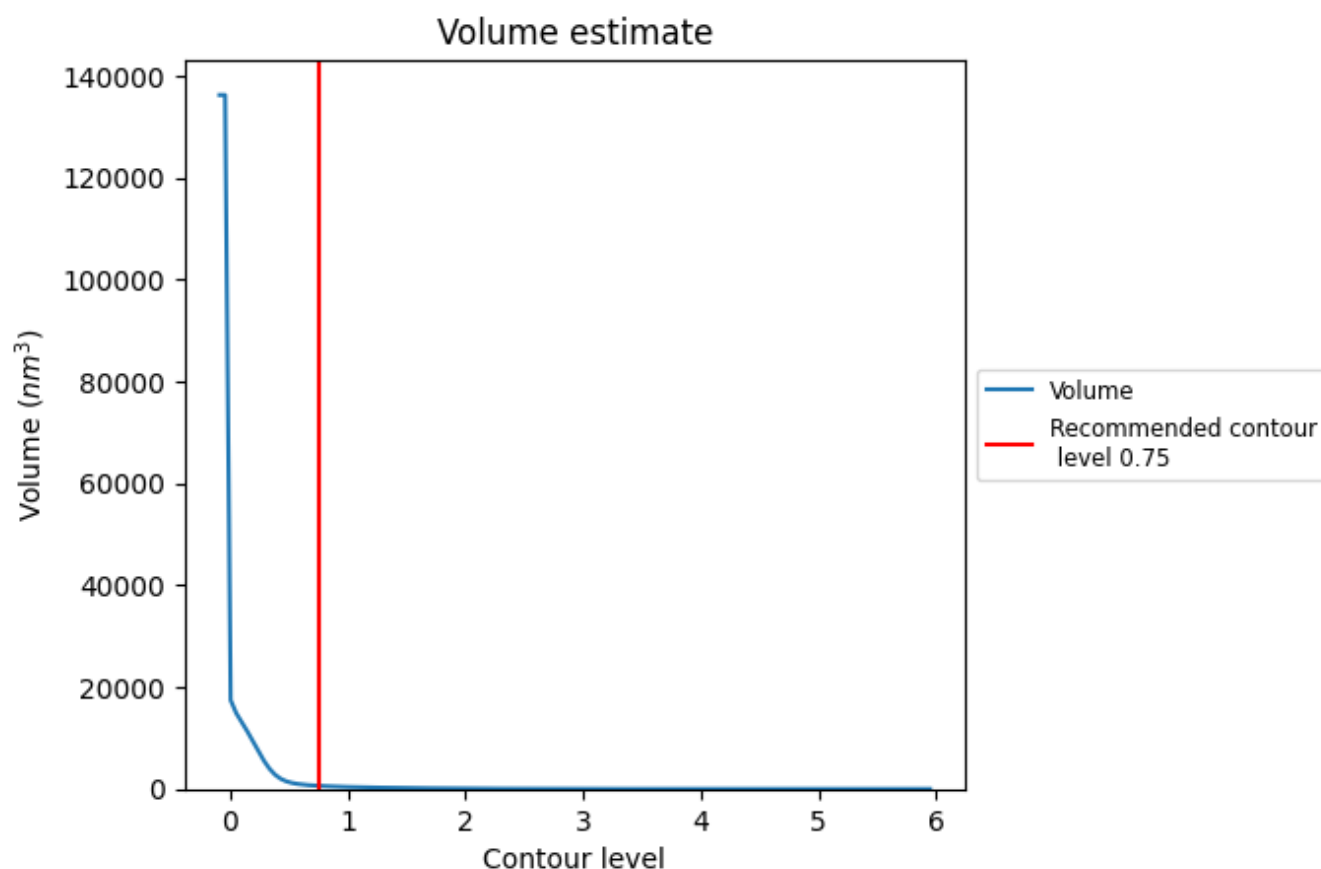
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

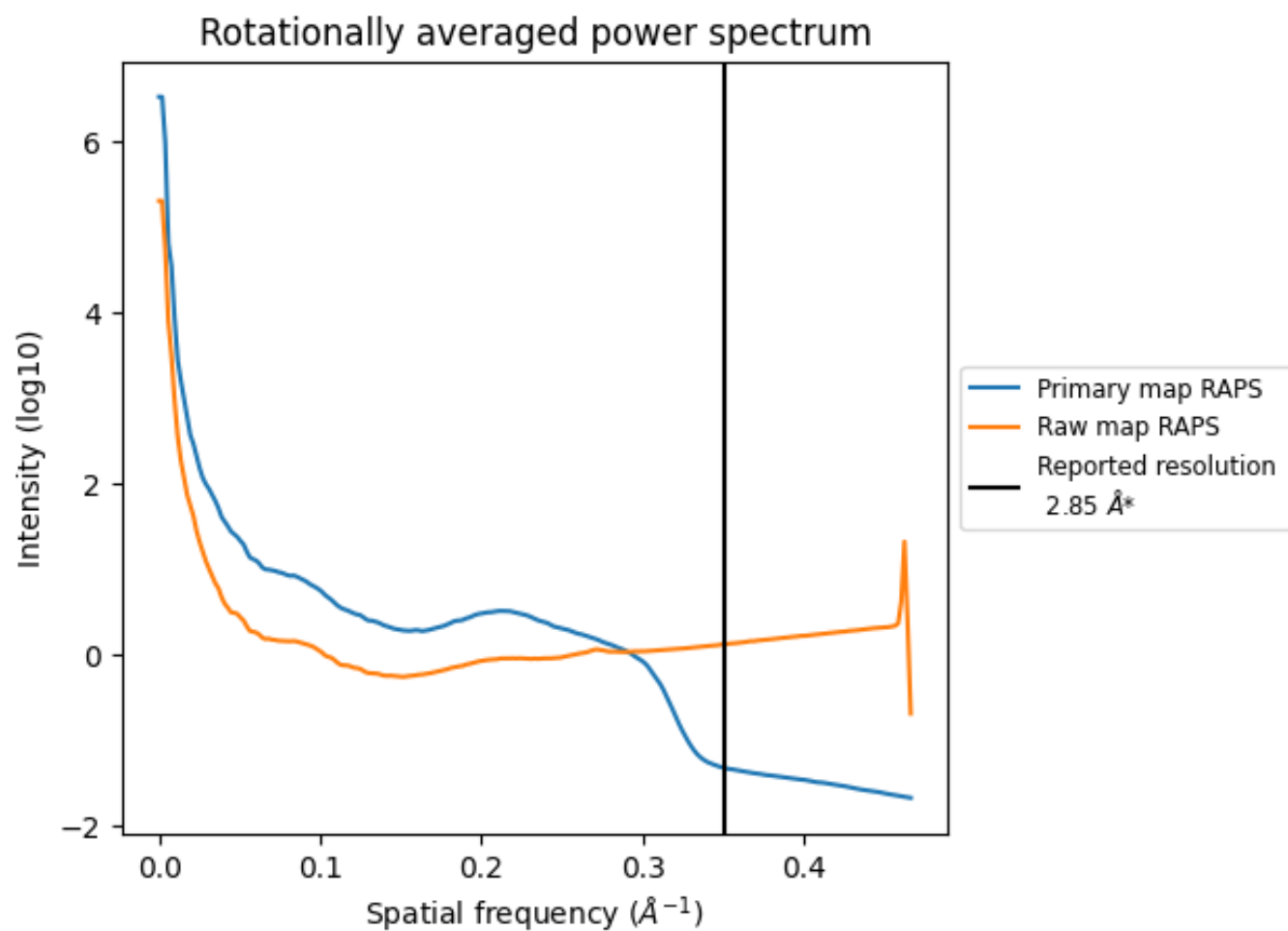
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621 nm³; this corresponds to an approximate mass of 561 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 ⓘ

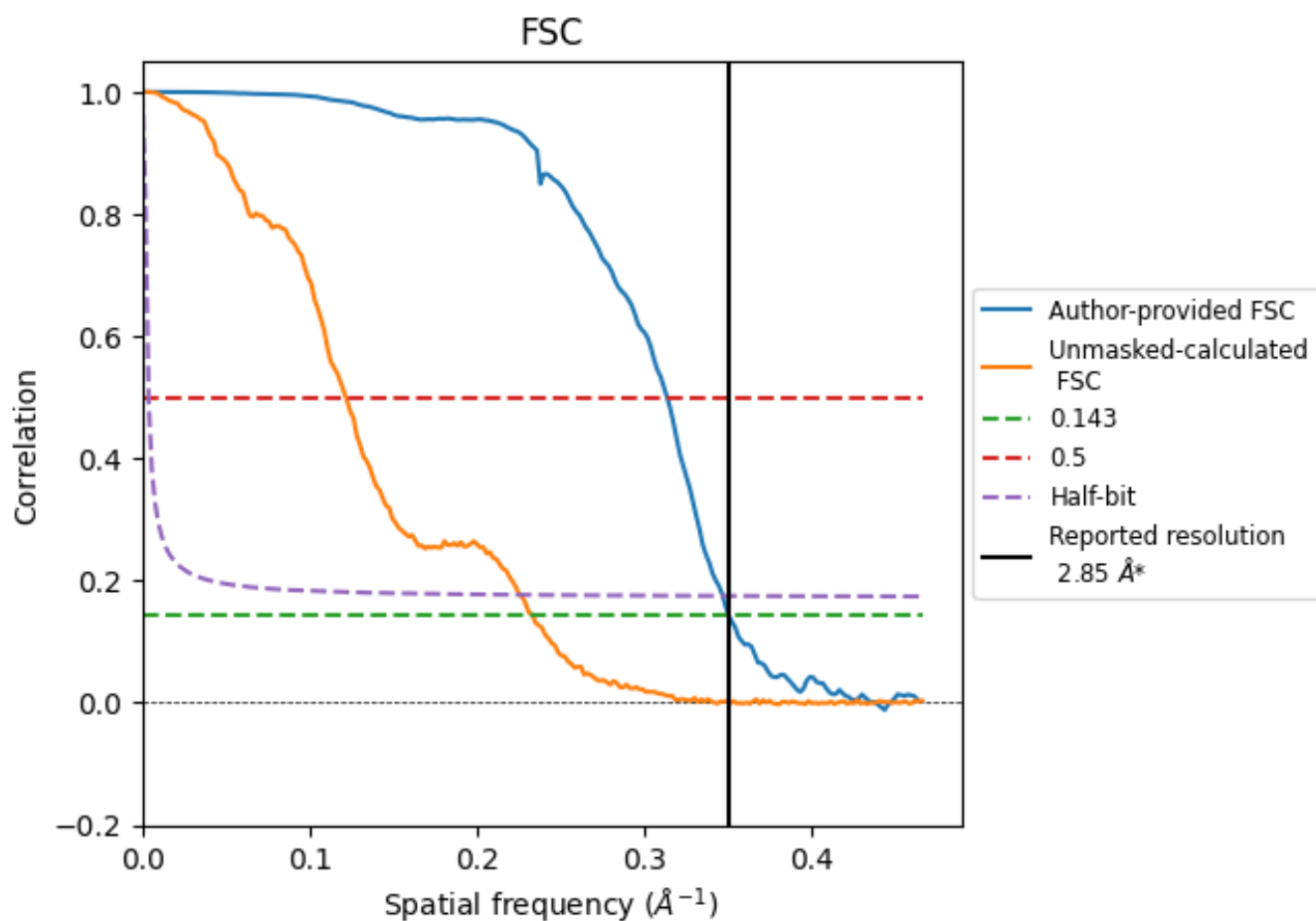


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.351 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

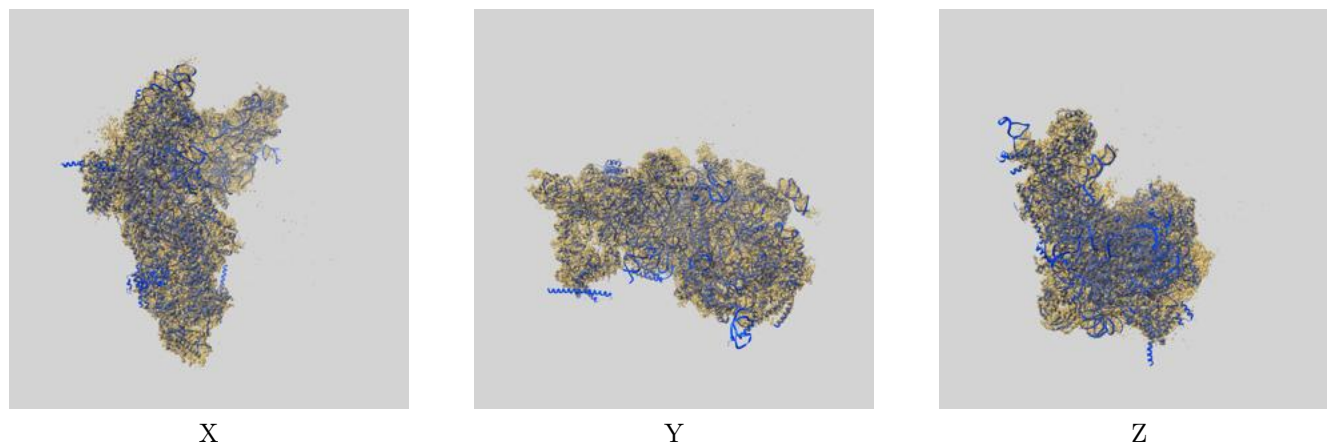
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.19	2.88
Unmasked-calculated*	4.28	8.21	4.43

*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 4.28 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

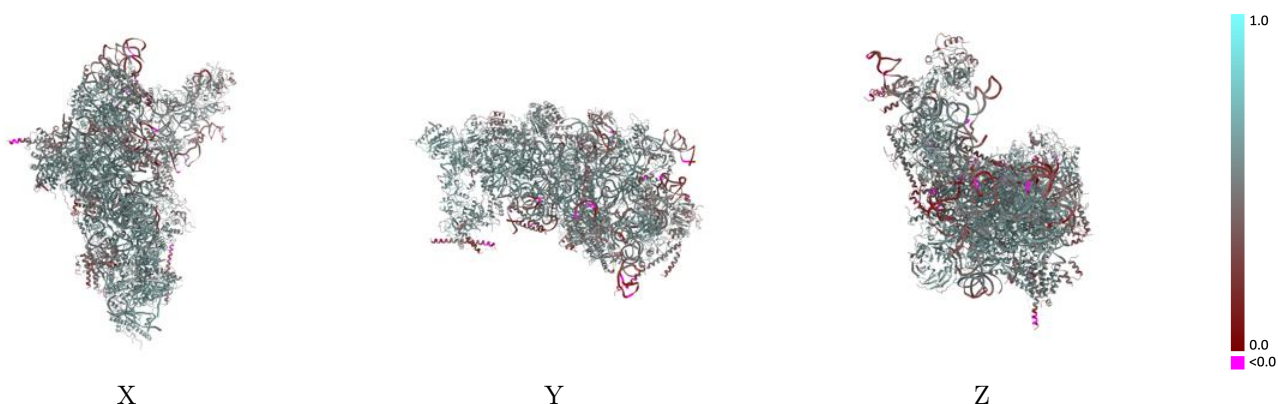
This section contains information regarding the fit between EMDB map EMD-29252 and PDB model 8FKP. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



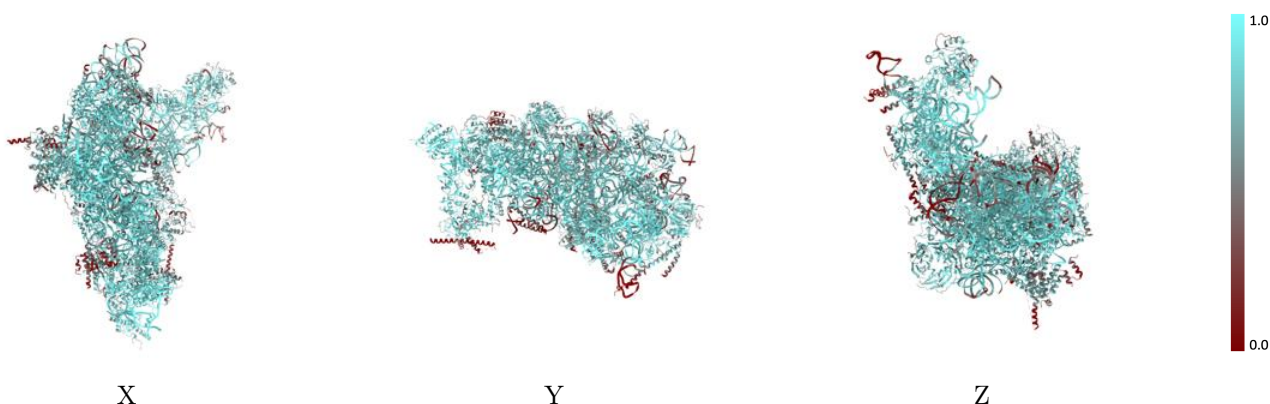
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



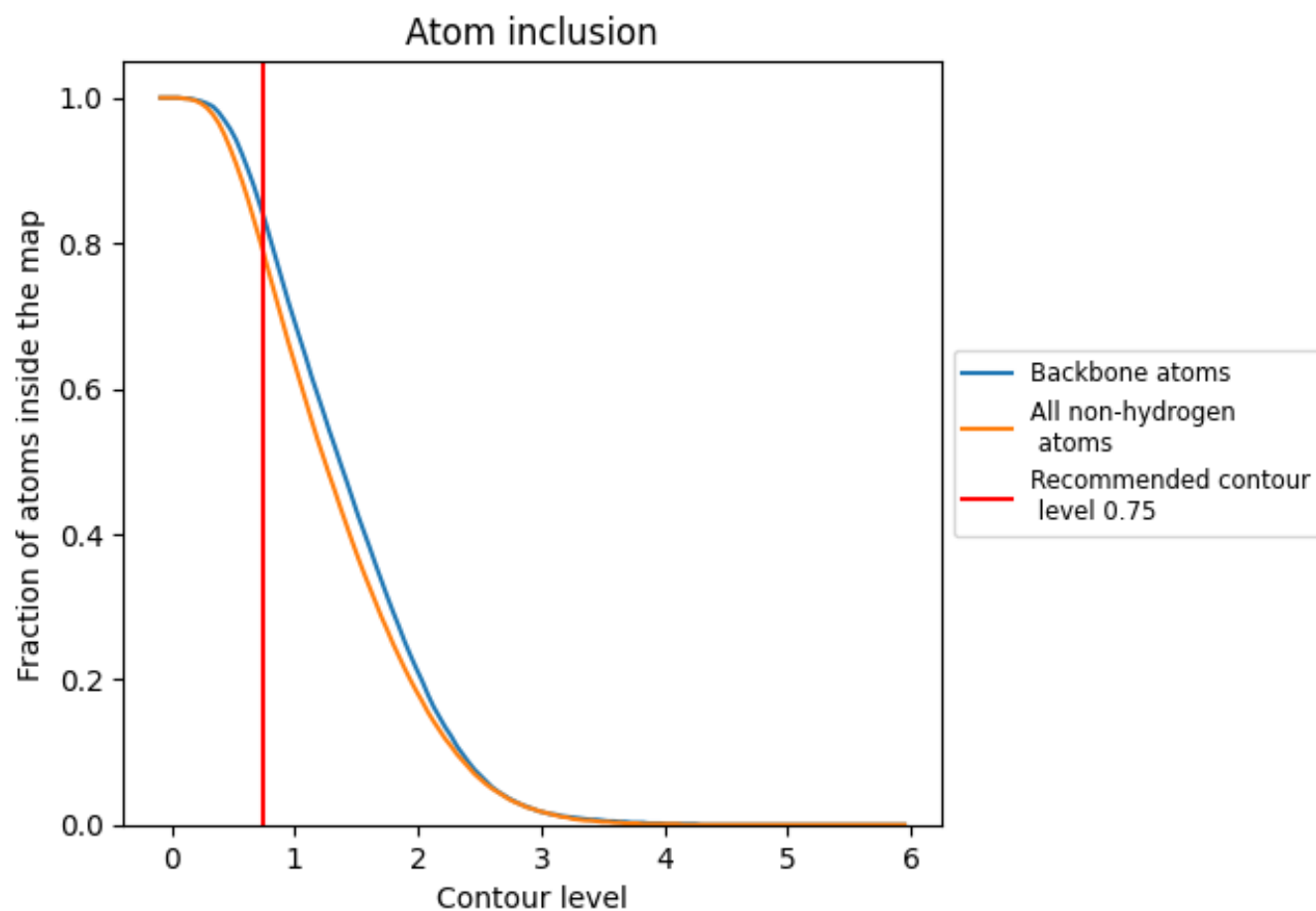
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 84% of all backbone atoms, 78% 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	 0.7850	 0.5210
L1	 0.6870	 0.4690
L2	 0.9420	 0.5730
L3	 0.8430	 0.5100
L6	 0.9290	 0.5970
L7	 0.7300	 0.5000
L8	 0.7170	 0.5030
L9	 0.9330	 0.6090
LA	 0.6360	 0.4950
LB	 0.9260	 0.6010
LC	 0.6930	 0.5140
LE	 0.5030	 0.4160
LG	 0.7450	 0.4930
LH	 0.4790	 0.5160
LI	 0.8440	 0.5840
LK	 0.7970	 0.4360
LN	 0.8600	 0.5490
LQ	 0.9020	 0.6020
LS	 0.5390	 0.4600
LT	 0.9240	 0.6090
LU	 0.7820	 0.5600
LW	 0.5850	 0.5180
NB	 0.1980	 0.3840
NE	 0.6460	 0.4130
NG	 0.4660	 0.3970
NM	 0.8390	 0.5810
NN	 0.8450	 0.5150
NO	 0.6770	 0.5150
NQ	 0.7730	 0.5540
NS	 0.7850	 0.5650
SA	 0.8830	 0.5900
SC	 0.7560	 0.5490
SD	 0.8510	 0.5740
SE	 0.9040	 0.5840
SH	 0.8660	 0.5770



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Continued from previous page...

Chain	Atom inclusion	Q-score
SI	 0.8180	 0.5770
SJ	 0.5700	 0.4960
SK	 0.7450	 0.4590
SL	 0.8320	 0.5630
SM	 0.6990	 0.5030
SN	 0.6670	 0.4780
SO	 0.7810	 0.5360
SR	 0.5710	 0.3990
SS	 0.6790	 0.5050
ST	 0.5100	 0.4710
SV	 0.6570	 0.4430
SW	 0.5790	 0.4790
SZ	 0.8110	 0.5460