



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 11:46 PM UTC

PDB ID : 8PV5 / pdb_00008pv5
EMDB ID : EMD-17954
Title : Chaetomium thermophilum pre-60S State 8 - pre-5S rotation without Foot - composite structure
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

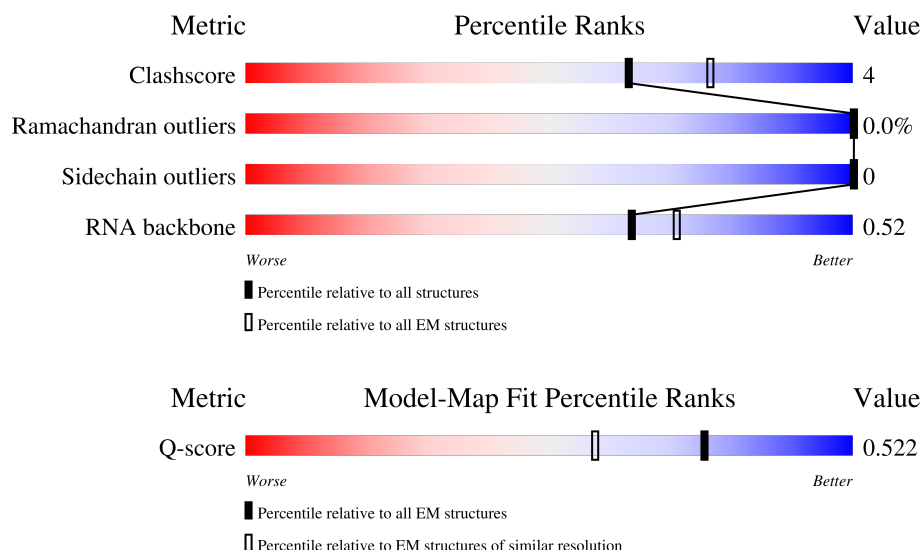
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

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	C1	3342	
2	C2	156	
3	C4	119	

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Mol	Chain	Length	Quality of chain
4	CF	270	
5	CH	661	
6	CK	261	
7	CL	558	
8	CN	246	
9	CO	120	
10	CQ	225	
11	Cb	117	
12	Cd	627	
13	Cf	350	
14	Cg	202	
15	Ch	517	
16	Cz	123	
17	LA	254	
18	LB	392	
19	LC	365	
20	LD	304	
21	LE	200	
22	LF	249	
23	LG	262	
24	LH	229	
25	LJ	173	
26	LK	165	
27	LL	213	
28	LM	142	

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Mol	Chain	Length	Quality of chain
29	LN	203	
30	LO	204	
31	LP	187	
32	LQ	213	
33	LR	2898	
34	LS	174	
35	LT	160	
36	LU	127	
37	LV	139	
38	LX	156	
39	LY	138	
40	LZ	135	
41	La	149	
42	Lc	108	
43	Ld	120	
44	Le	131	
45	Lf	109	
46	Lg	119	
47	Lh	935	
48	Li	110	
49	Lj	95	
50	Lk	94	
51	Ll	51	
52	Lp	92	
53	Lq	147	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 144398 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 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	3060	Total	C	N	O	P	0	0
			65497	29256	11853	21328	3060		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	152	Total	C	N	O	P	0	0
			3239	1448	579	1060	152		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C4	119	Total	C	N	O	P	0	0
			2536	1131	453	833	119		

- Molecule 4 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CF	245	Total	C	N	O	S	0	0
			1934	1215	350	360	9		

- Molecule 5 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CH	627	Total	C	N	O	S	0	0
			5053	3175	920	939	19		

- Molecule 6 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CK	237	Total	C	N	O	S	0	0
			1903	1198	368	333	4		

- Molecule 7 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	CL	79	Total	C	N	O	0	0
			622	389	125	108		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CN	246	Total	C	N	O	S	0	0
			1853	1156	322	368	7		

- Molecule 9 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 10 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CQ	183	Total	C	N	O	S	0	0
			1480	925	304	241	10		

- Molecule 11 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Cb	101	Total	C	N	O	S	0	0
			830	517	161	148	4		

- Molecule 12 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Cd	462	Total	C	N	O	S	0	0
			3691	2350	671	659	11		

- Molecule 13 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Cf	285	Total	C	N	O	S	0	0
			2282	1443	417	401	21		

- Molecule 14 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Cg	188	Total	C	N	O	S	0	0
			1478	924	283	270	1		

- Molecule 15 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ch	485	Total	C	N	O	S	1	0
			3812	2396	696	710	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	117	ASP	GLU	engineered mutation	UNP G0SC29

- Molecule 16 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Cz	101	Total	C	N	O	S	0	0
			869	541	180	144	4		

- Molecule 17 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LA	191	Total	C	N	O	S	0	0
			1454	917	278	256	3		

- Molecule 18 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LB	389	Total	C	N	O	S	0	0
			3104	1973	579	539	13		

- Molecule 19 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LC	363	Total	C	N	O	S	0	0
			2751	1737	527	478	9		

- Molecule 20 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LD	286	Total	C	N	O	S	0	0
			2266	1434	407	422	3		

- Molecule 21 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LE	191	Total	C	N	O	S	0	0
			1477	944	267	263	3		

- Molecule 22 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LF	248	Total	C	N	O	S	0	0
			2023	1297	377	346	3		

- Molecule 23 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LG	235	Total	C	N	O	S	0	0
			1885	1207	349	324	5		

- Molecule 24 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LH	190	Total	C	N	O	S	0	0
			1495	949	268	272	6		

- Molecule 25 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LJ	169	Total	C	N	O	S	0	0
			1357	850	266	235	6		

- Molecule 26 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LK	158	Total	C	N	O	S	0	0
			1184	743	215	224	2		

- Molecule 27 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LL	203	Total	C	N	O	S	0	0
			1587	989	325	271	2		

- Molecule 28 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LM	141	Total	C	N	O	S	0	0
			1126	714	216	195	1		

- Molecule 29 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LN	202	Total	C	N	O	S	0	0
			1704	1062	360	278	4		

- Molecule 30 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LO	203	Total	C	N	O	S	0	0
			1611	1034	305	267	5		

- Molecule 31 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LP	171	Total	C	N	O	S	0	0
			1343	834	274	232	3		

- Molecule 32 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LQ	150	Total	C	N	O	S	0	0
			1200	759	239	200	2		

- Molecule 33 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LR	152	Total	C	N	O	S	0	0
			1226	763	259	200	4		

- Molecule 34 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LS	174	Total	C	N	O	S	0	0
			1426	917	266	238	5		

- Molecule 35 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LT	129	Total	C	N	O	S	0	0
			1027	651	195	179	2		

- Molecule 36 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LU	105	Total	C	N	O	S	0	0
			846	548	146	151	1		

- Molecule 37 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LV	135	Total	C	N	O	S	0	0
			991	630	184	170	7		

- Molecule 38 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LX	122	Total	C	N	O		0	0
			959	614	174	171			

- Molecule 39 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LY	133	Total	C	N	O	S	0	0
			1056	658	213	183	2		

- Molecule 40 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LZ	135	Total	C	N	O	S	0	0
			1112	713	207	188	4		

- Molecule 41 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	La	108	Total	C	N	O	S	0	0
			872	556	168	147	1		

- Molecule 42 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lc	95	Total	C	N	O	S	0	0
			705	449	122	129	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ld	110	Total	C	N	O	S	0	0
			875	555	171	148	1		

- Molecule 44 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Le	126	Total	C	N	O	S	0	0
			1017	640	208	163	6		

- Molecule 45 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 46 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lg	118	Total	C	N	O	S	0	0
			914	567	186	157	4		

- Molecule 47 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Lh	118	Total	C	N	O	0	0
			981	626	194	161		

- Molecule 48 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Li	101	Total	C	N	O	S	0	0
			827	509	181	136	1		

- Molecule 49 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lj	88	Total	C	N	O	S	0	0
			698	427	154	112	5		

- Molecule 50 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lk	76	Total	C	N	O	S	0	0
			632	400	121	109	2		

- Molecule 51 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	Ll	50	Total	C	N	O	0	0
			436	275	97	64		

- Molecule 52 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lp	91	Total	C	N	O	S	0	0
			698	430	138	124	6		

- Molecule 53 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Lq	139	Total	C	N	O	0	0
			1049	657	204	188		

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

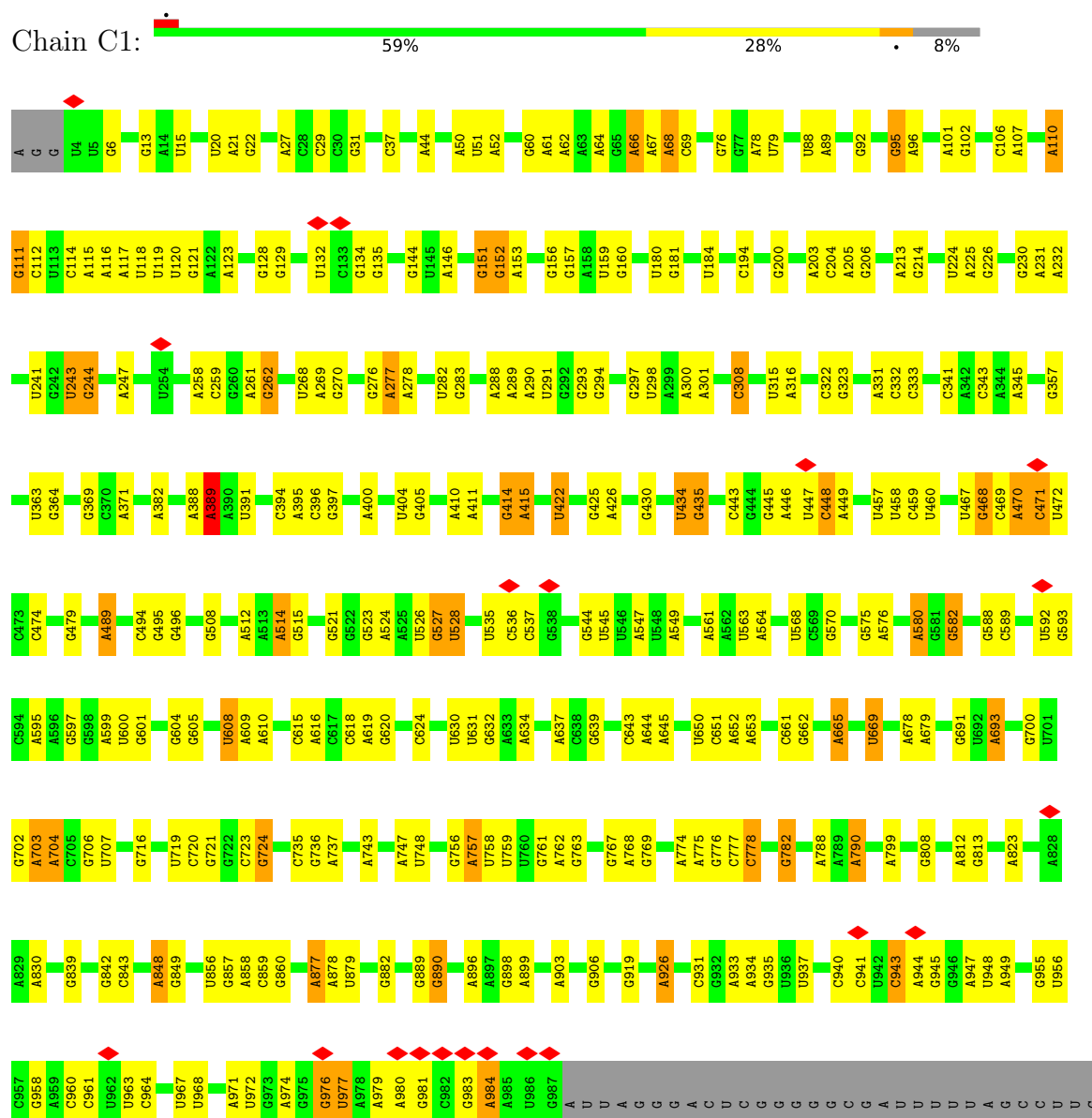
- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	CH	1	Total 1	O 1	0
57	Cd	2	Total 2	O 2	0

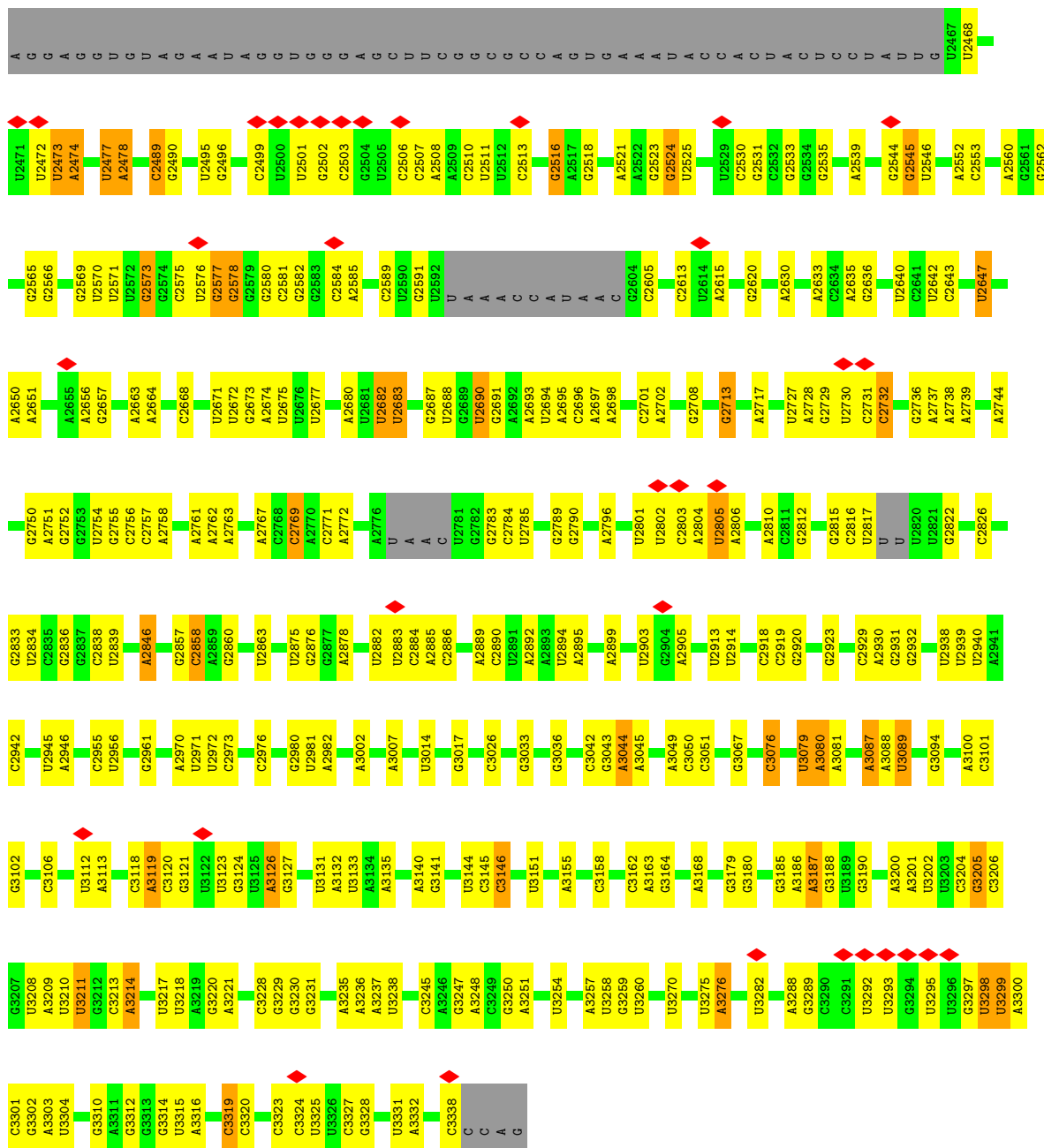
3 Residue-property plots

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

• Molecule 1: 26S rRNA

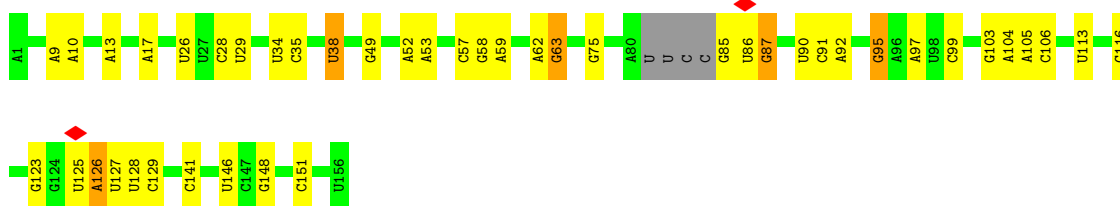




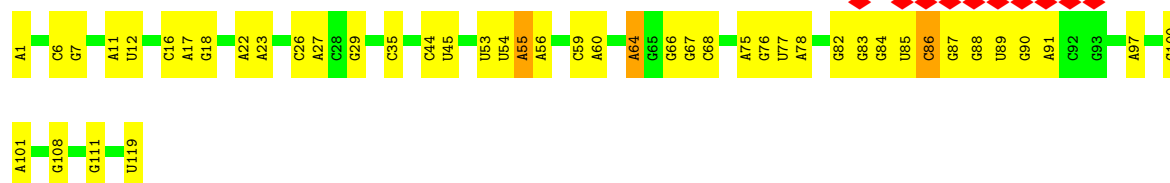


● Molecule 2: 5.8S rRNA

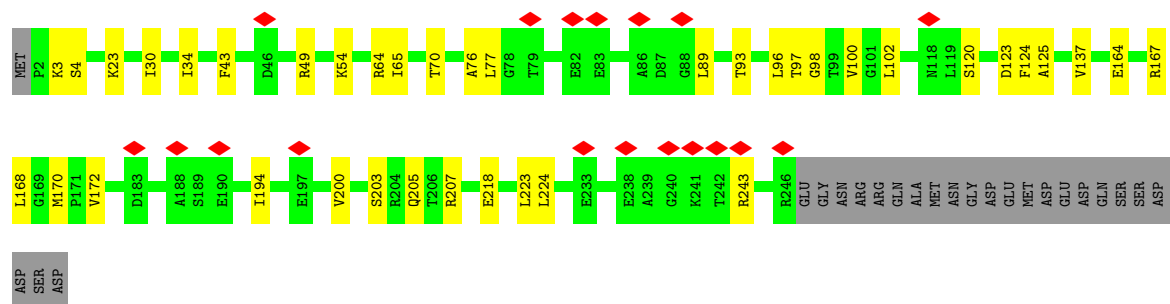
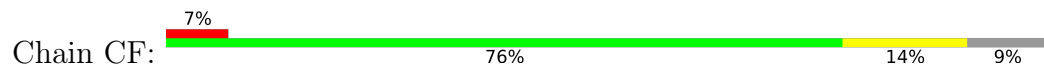
Chain C2: 69% 25%



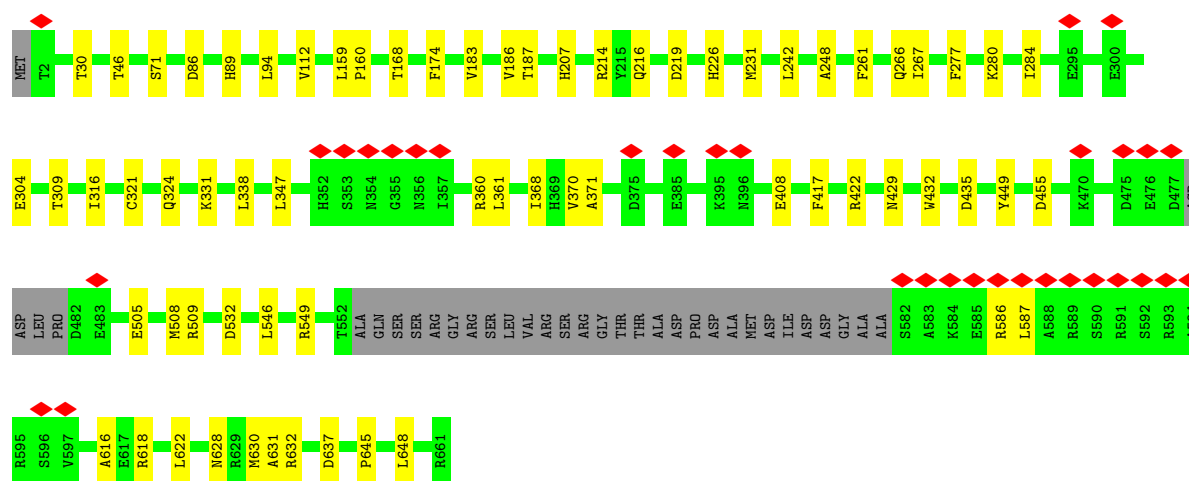
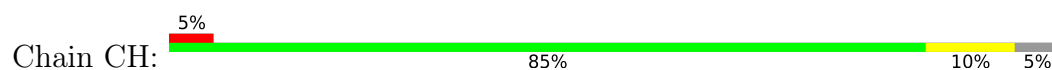
● Molecule 3: 5S rRNA



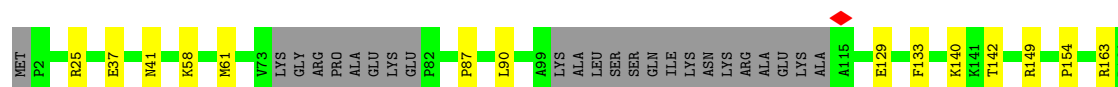
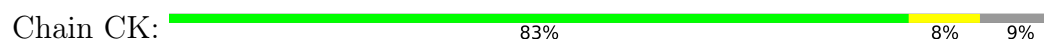
- Molecule 4: Large ribosomal subunit protein uL10

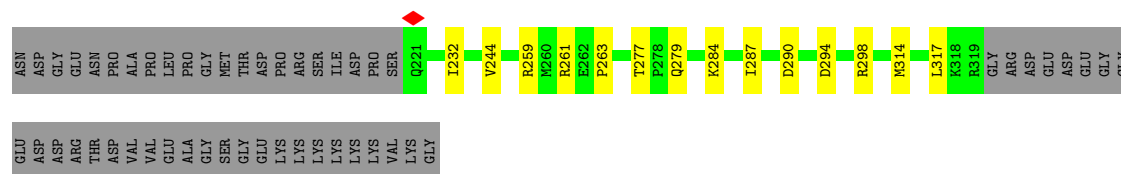


- Molecule 5: Nucleolar GTP-binding protein 1

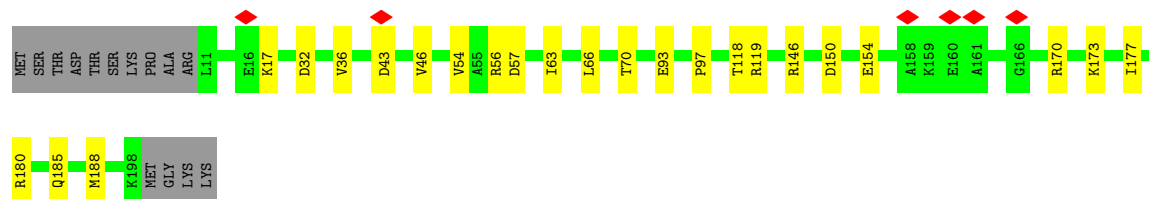
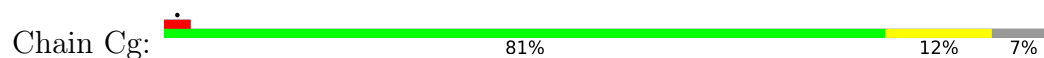


- Molecule 6: Ribosome biogenesis protein NSA2 homolog

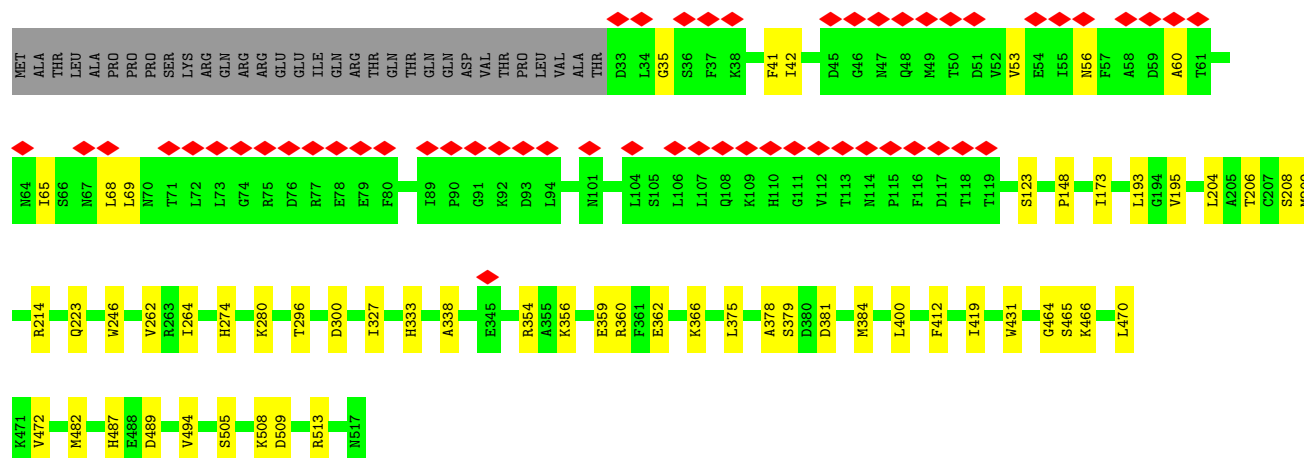
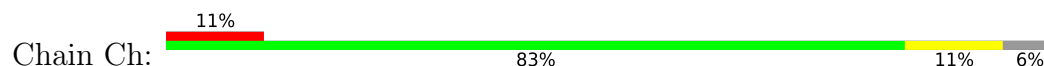




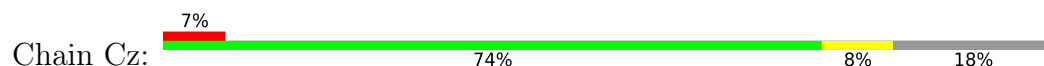
- Molecule 14: Ribosome biogenesis regulatory protein



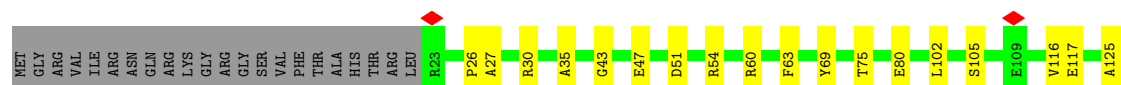
- Molecule 15: Ribosome assembly protein 4

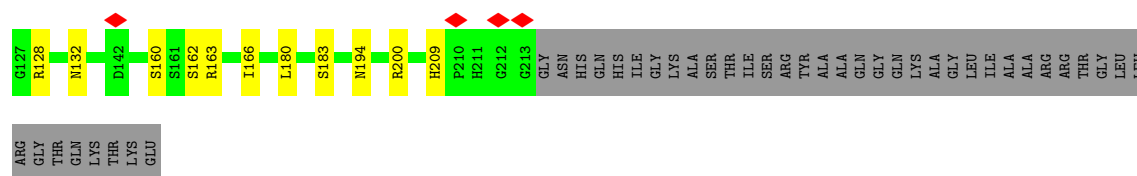


- Molecule 16: rRNA-processing protein

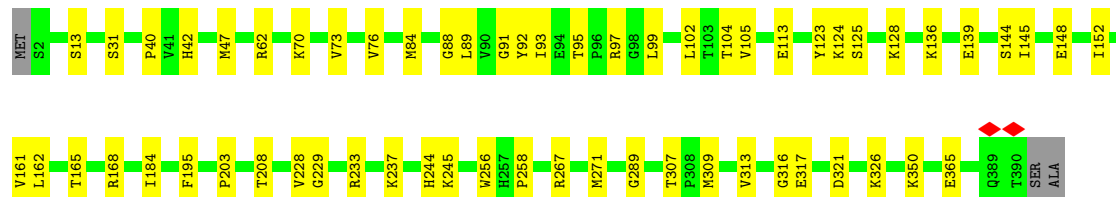
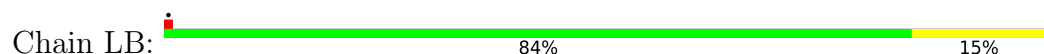


- Molecule 17: 60S ribosomal protein L2-like protein

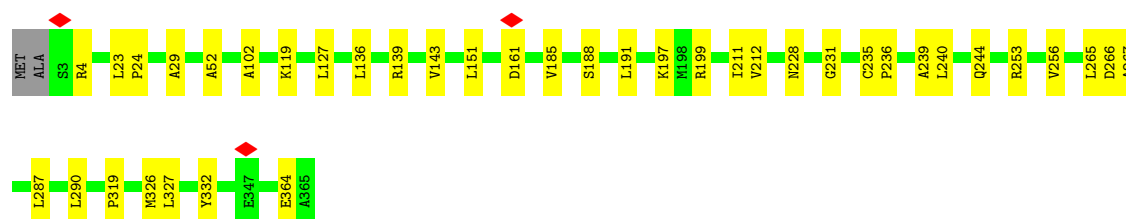




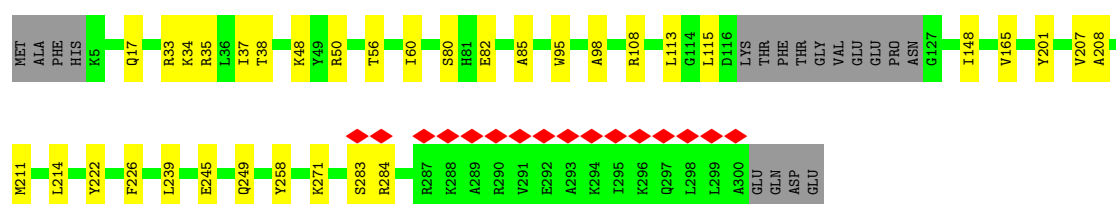
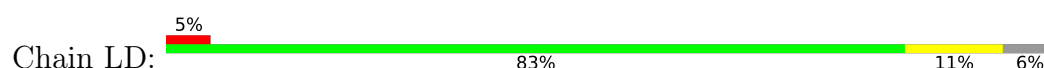
- Molecule 18: 60S ribosomal protein L3-like protein



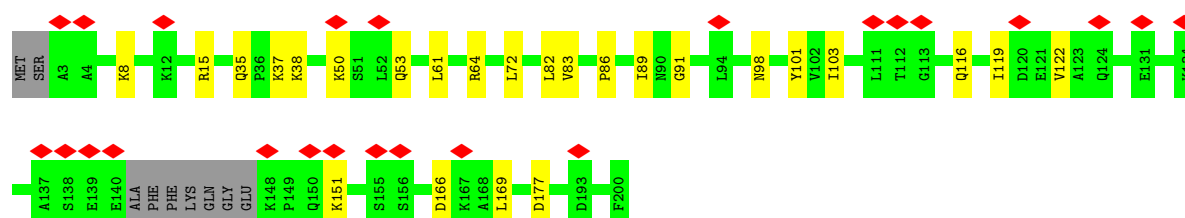
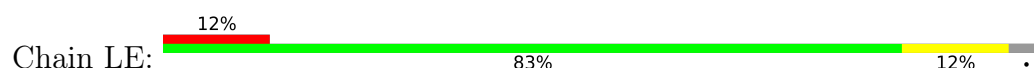
- Molecule 19: 60S ribosomal protein L4-like protein

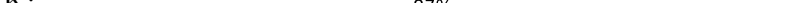


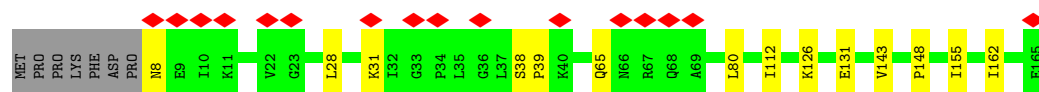
- Molecule 20: 60S ribosomal protein l5-like protein



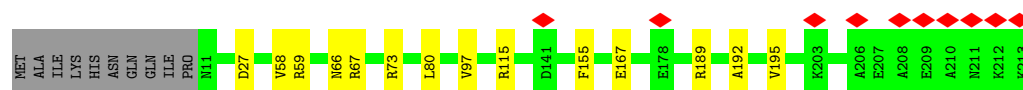
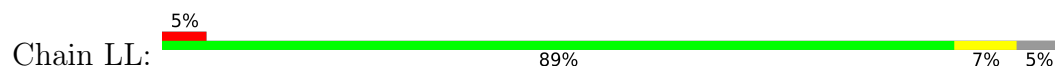
- Molecule 21: 60S ribosomal protein L6



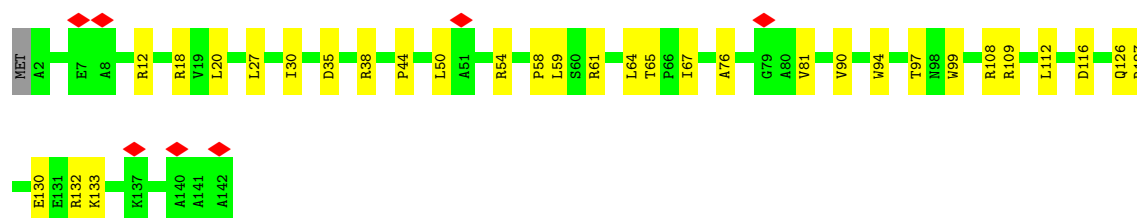
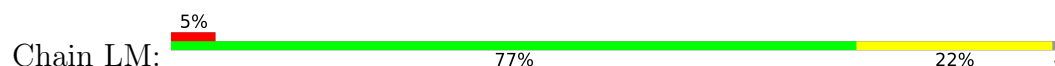
- Chain LK:  10% 87% 8%



- Molecule 27: 60S ribosomal protein L13



- Molecule 28: 60S ribosomal protein L14-like protein



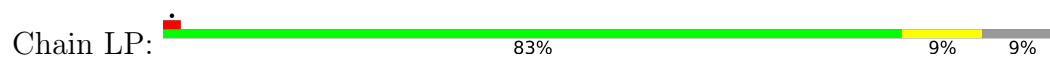
- Molecule 29: Ribosomal protein L15



- Molecule 30: 60S ribosomal protein L16-like protein

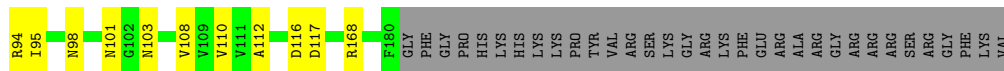


- Molecule 31: 60S ribosomal protein L17-like protein

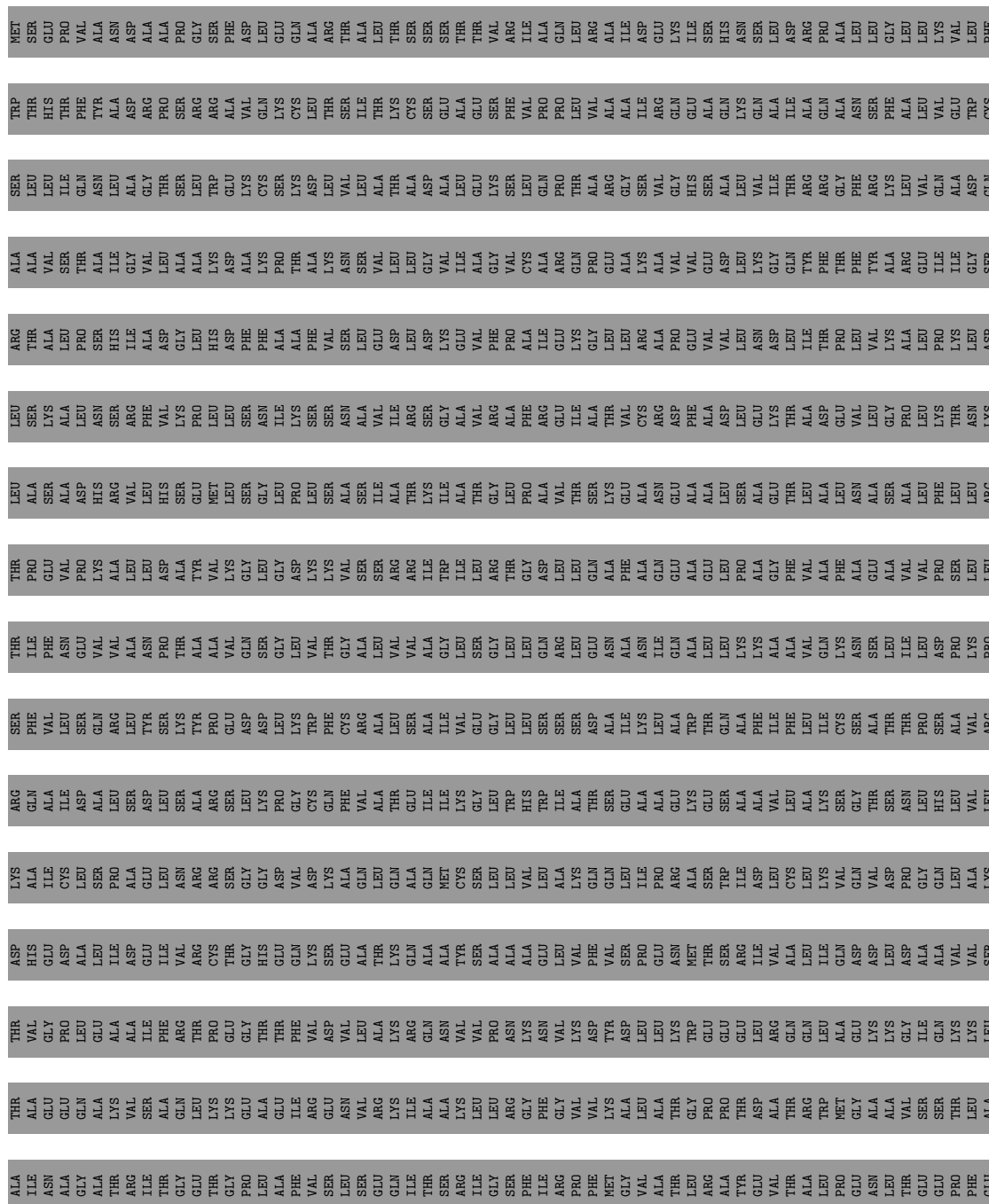


- Molecule 32: Ribosomal protein L18-like protein





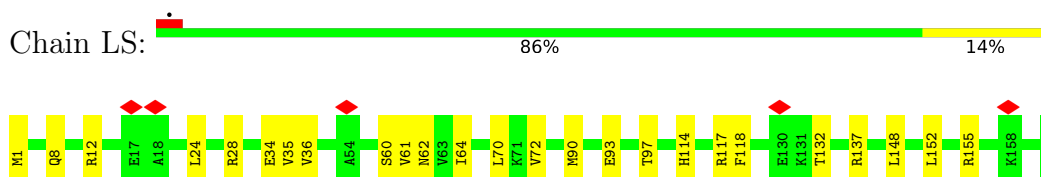
Chain LR: 5% 95%



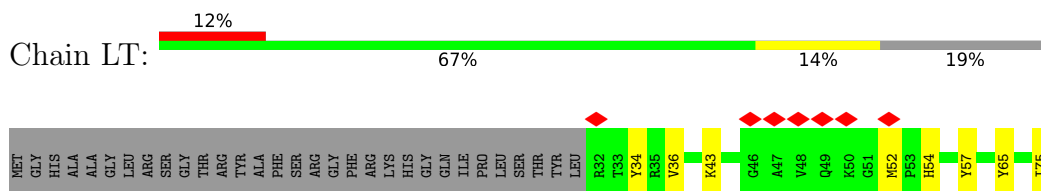


ALA
LYS
ARG
ALA
ALA
ARG
THR
LYS
ALA
ALA
ARG
GLU
ARG
LYS
GLN
GLU
ARG
GLN
ALA
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ALA
LEU
LEU
GLY
GLU
GLU
GLU
GLU
SER
LYS

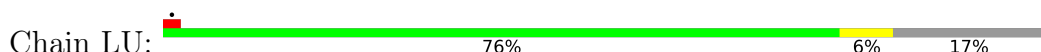
- Molecule 34: 60S ribosomal protein L20

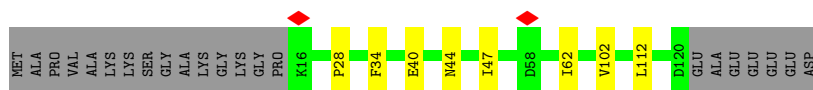


- Molecule 35: 60S ribosomal protein l21-like protein



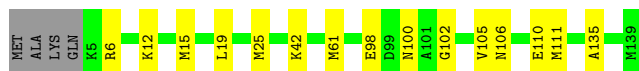
- Molecule 36: 60S ribosomal protein L22-like protein





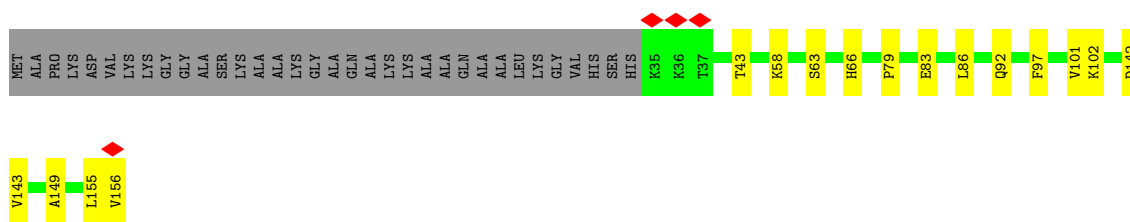
- Molecule 37: 60S ribosomal protein l23-like protein

Chain LV: 86% 11% .



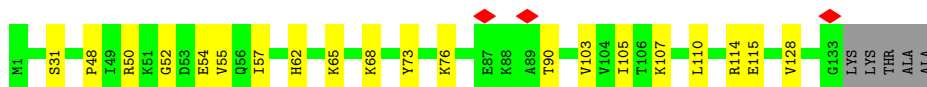
- Molecule 38: 60S ribosomal protein L25-like protein

Chain LX: 68% 10% 22%



- Molecule 39: 60S ribosomal protein L26-like protein

Chain LY: 82% 14% .



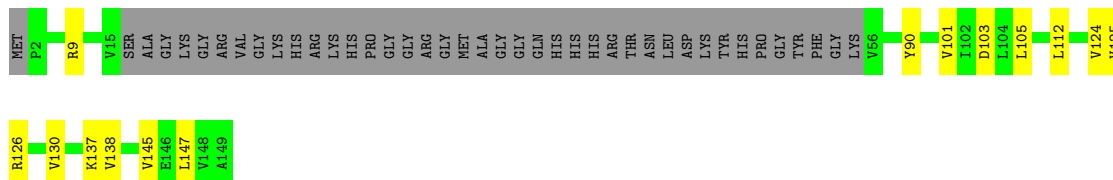
- Molecule 40: 60S ribosomal protein L27

Chain LZ: 7% 82% 18%



- Molecule 41: 60S ribosomal protein L28-like protein

Chain La: 63% 9% 28%

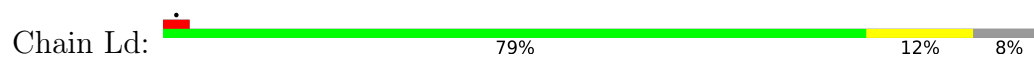


- Molecule 42: 60S ribosomal protein l30-like protein

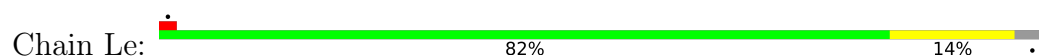
Chain Lc: 18% 70% 18% 12%



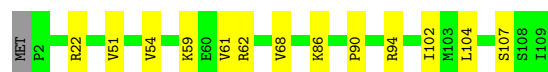
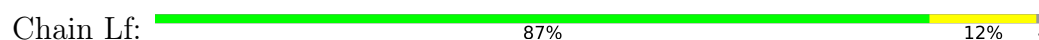
- Molecule 43: Putative 60S ribosomal protein



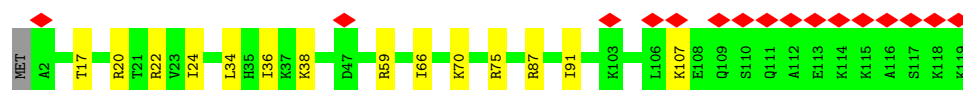
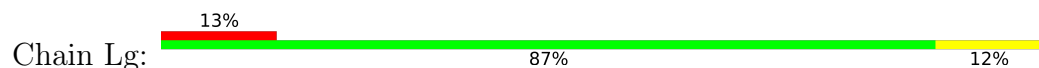
- Molecule 44: 60S ribosomal protein L32-like protein



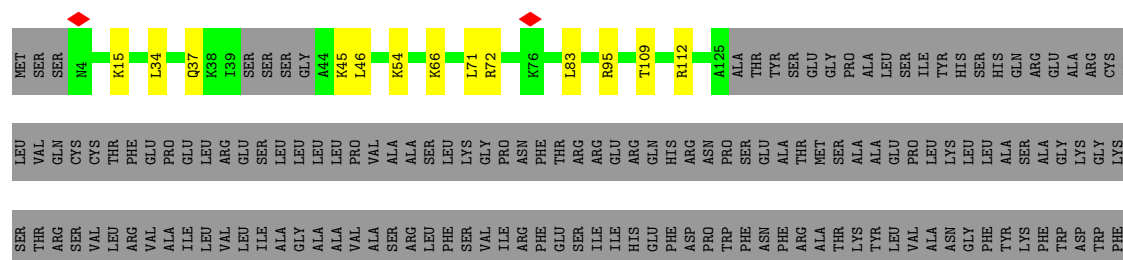
- Molecule 45: 60S ribosomal protein l33-like protein



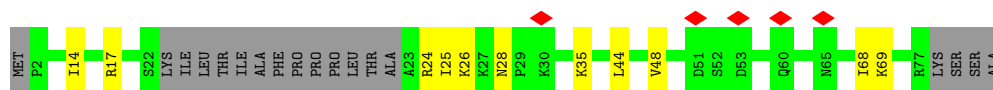
- Molecule 46: Ribosomal protein l34-like protein



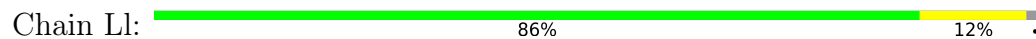
- Molecule 47: dolichyl-diphosphooligosaccharide--protein glycotransferase



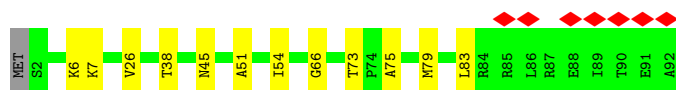
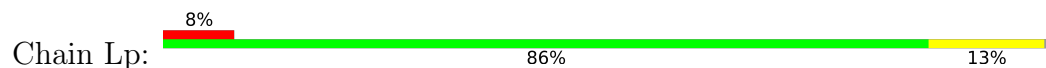




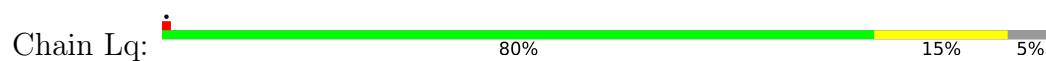
- Molecule 51: Ribosomal protein eL39



- Molecule 52: 60S ribosomal protein L43-like protein



- Molecule 53: Putative 60S ribosomal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88358	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 ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.628	Depositor
Minimum map value	-1.791	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, A2M, OMC, OMG, OMU, ZN, MG

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	C1	0.16	1/72444 (0.0%)	0.31	0/112946
2	C2	0.13	0/3621	0.29	0/5638
3	C4	0.14	0/2833	0.30	0/4414
4	CF	0.18	0/1972	0.43	0/2660
5	CH	0.17	0/5137	0.42	1/6915 (0.0%)
6	CK	0.15	0/1939	0.38	0/2608
7	CL	0.18	0/631	0.41	0/843
8	CN	0.19	0/1878	0.49	0/2555
9	CO	0.16	0/470	0.42	0/619
10	CQ	0.22	0/1504	0.55	1/2000 (0.1%)
11	Cb	0.16	0/845	0.40	0/1128
12	Cd	0.16	0/3770	0.39	0/5082
13	Cf	0.14	0/2326	0.39	0/3113
14	Cg	0.15	0/1508	0.36	0/2051
15	Ch	0.18	0/3914	0.45	0/5319
16	Cz	0.19	0/877	0.47	0/1148
17	LA	0.17	0/1488	0.44	0/2009
18	LB	0.19	0/3172	0.46	0/4260
19	LC	0.17	0/2808	0.40	0/3785
20	LD	0.15	0/2308	0.37	0/3105
21	LE	0.17	0/1504	0.46	2/2027 (0.1%)
22	LF	0.22	0/2061	0.54	0/2765
23	LG	0.17	0/1914	0.45	0/2561
24	LH	0.15	0/1515	0.40	0/2037
25	LJ	0.16	0/1379	0.43	0/1844
26	LK	0.18	0/1198	0.48	0/1611
27	LL	0.17	0/1614	0.39	0/2168
28	LM	0.22	0/1145	0.53	0/1539
29	LN	0.16	0/1741	0.38	0/2332
30	LO	0.18	0/1645	0.44	0/2205
31	LP	0.17	0/1364	0.42	0/1835
32	LQ	0.18	0/1218	0.45	1/1639 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LR	0.15	0/1245	0.39	0/1662
34	LS	0.17	0/1461	0.46	0/1966
35	LT	0.20	0/1046	0.53	0/1409
36	LU	0.16	0/859	0.42	0/1151
37	LV	0.16	0/1009	0.38	0/1357
38	LX	0.18	0/975	0.43	0/1317
39	LY	0.18	0/1070	0.46	0/1432
40	LZ	0.20	0/1135	0.46	0/1519
41	La	0.16	0/892	0.40	0/1200
42	Lc	0.17	0/714	0.48	0/960
43	Ld	0.17	0/889	0.38	0/1192
44	Le	0.18	0/1035	0.41	0/1379
45	Lf	0.16	0/883	0.44	0/1187
46	Lg	0.17	0/927	0.39	0/1244
47	Lh	0.15	0/991	0.36	0/1317
48	Li	0.14	0/834	0.36	0/1099
49	Lj	0.17	0/712	0.47	2/944 (0.2%)
50	Lk	0.17	0/640	0.47	0/850
51	Ll	0.13	0/446	0.30	0/593
52	Lp	0.16	0/706	0.47	0/940
53	Lq	0.18	0/1067	0.46	0/1442
All	All	0.16	1/153279 (0.0%)	0.37	7/222921 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1847	A2M	O3'-P	5.11	1.61	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	CQ	161	ARG	CB-CG-CD	7.69	128.99	111.30
49	Lj	69	THR	CA-C-N	5.56	123.74	120.24
49	Lj	69	THR	C-N-CA	5.56	123.74	120.24
5	CH	505	GLU	N-CA-CB	5.20	117.86	110.16
32	LQ	47	PRO	CA-N-CD	-5.07	104.91	112.00

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	C1	65497	0	33046	452	0
2	C2	3239	0	1637	24	0
3	C4	2536	0	1286	21	0
4	CF	1934	0	1945	26	0
5	CH	5053	0	5135	46	0
6	CK	1903	0	1990	16	0
7	CL	622	0	641	7	0
8	CN	1853	0	1852	26	0
9	CO	468	0	503	6	0
10	CQ	1480	0	1523	10	0
11	Cb	830	0	838	7	0
12	Cd	3691	0	3817	35	0
13	Cf	2282	0	2347	24	0
14	Cg	1478	0	1517	16	0
15	Ch	3812	0	3715	31	0
16	Cz	869	0	956	10	0
17	LA	1454	0	1490	22	0
18	LB	3104	0	3221	42	0
19	LC	2751	0	2875	30	0
20	LD	2266	0	2219	22	0
21	LE	1477	0	1567	21	0
22	LF	2023	0	2132	33	0
23	LG	1885	0	2032	18	0
24	LH	1495	0	1573	21	0
25	LJ	1357	0	1385	20	0
26	LK	1184	0	1249	8	0
27	LL	1587	0	1655	11	0
28	LM	1126	0	1198	21	0
29	LN	1704	0	1767	22	0
30	LO	1611	0	1702	16	0
31	LP	1343	0	1369	12	0
32	LQ	1200	0	1296	17	0
33	LR	1226	0	1292	16	0
34	LS	1426	0	1481	19	0
35	LT	1027	0	1076	14	0
36	LU	846	0	883	4	0
37	LV	991	0	1044	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LX	959	0	1018	12	0
39	LY	1056	0	1143	13	0
40	LZ	1112	0	1181	16	0
41	La	872	0	903	11	0
42	Lc	705	0	751	12	0
43	Ld	875	0	918	11	0
44	Le	1017	0	1092	15	0
45	Lf	862	0	891	9	0
46	Lg	914	0	960	12	0
47	Lh	981	0	1097	10	0
48	Li	827	0	906	11	0
49	Lj	698	0	726	10	0
50	Lk	632	0	693	6	0
51	Ll	436	0	473	6	0
52	Lp	698	0	737	7	0
53	Lq	1049	0	1075	15	0
54	CH	32	0	12	0	0
54	Cd	32	0	12	1	0
55	CH	1	0	0	0	0
55	Cd	2	0	0	0	0
56	CQ	1	0	0	0	0
56	Cb	1	0	0	0	0
56	Lg	1	0	0	0	0
56	Lj	1	0	0	0	0
56	Lp	1	0	0	0	0
57	CH	1	0	0	0	0
57	Cd	2	0	0	0	0
All	All	144398	0	111842	1052	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 4.

The worst 5 of 1052 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2400:G:H1	1:C1:2473:U:H3	1.05	0.93
1:C1:2389:U:H3	1:C1:2562:G:H1	1.20	0.90
1:C1:1054:U:H3	1:C1:1070:G:H1	0.85	0.85
18:LB:91:GLY:HA3	18:LB:152:ILE:HD11	1.60	0.82
1:C1:2327:G:H22	1:C1:2359:G:H1'	1.51	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CF	243/270 (90%)	242 (100%)	1 (0%)	0	100	100
5	CH	621/661 (94%)	616 (99%)	5 (1%)	0	100	100
6	CK	231/261 (88%)	224 (97%)	7 (3%)	0	100	100
7	CL	77/558 (14%)	76 (99%)	1 (1%)	0	100	100
8	CN	244/246 (99%)	239 (98%)	5 (2%)	0	100	100
9	CO	56/120 (47%)	55 (98%)	1 (2%)	0	100	100
10	CQ	181/225 (80%)	181 (100%)	0	0	100	100
11	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
12	Cd	458/627 (73%)	446 (97%)	12 (3%)	0	100	100
13	Cf	281/350 (80%)	277 (99%)	4 (1%)	0	100	100
14	Cg	186/202 (92%)	185 (100%)	1 (0%)	0	100	100
15	Ch	484/517 (94%)	469 (97%)	15 (3%)	0	100	100
16	Cz	99/123 (80%)	99 (100%)	0	0	100	100
17	LA	189/254 (74%)	185 (98%)	4 (2%)	0	100	100
18	LB	387/392 (99%)	381 (98%)	6 (2%)	0	100	100
19	LC	361/365 (99%)	354 (98%)	7 (2%)	0	100	100
20	LD	282/304 (93%)	280 (99%)	2 (1%)	0	100	100
21	LE	187/200 (94%)	182 (97%)	5 (3%)	0	100	100
22	LF	246/249 (99%)	240 (98%)	5 (2%)	1 (0%)	30	48
23	LG	233/262 (89%)	230 (99%)	3 (1%)	0	100	100
24	LH	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
25	LJ	167/173 (96%)	165 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LK	156/165 (94%)	154 (99%)	2 (1%)	0	100	100
27	LL	201/213 (94%)	199 (99%)	2 (1%)	0	100	100
28	LM	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
29	LN	200/203 (98%)	195 (98%)	5 (2%)	0	100	100
30	LO	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
31	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
32	LQ	148/213 (70%)	147 (99%)	1 (1%)	0	100	100
33	LR	150/2898 (5%)	148 (99%)	2 (1%)	0	100	100
34	LS	172/174 (99%)	167 (97%)	5 (3%)	0	100	100
35	LT	127/160 (79%)	124 (98%)	3 (2%)	0	100	100
36	LU	103/127 (81%)	99 (96%)	4 (4%)	0	100	100
37	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
38	LX	120/156 (77%)	117 (98%)	3 (2%)	0	100	100
39	LY	131/138 (95%)	125 (95%)	6 (5%)	0	100	100
40	LZ	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
41	La	104/149 (70%)	104 (100%)	0	0	100	100
42	Lc	93/108 (86%)	93 (100%)	0	0	100	100
43	Ld	108/120 (90%)	108 (100%)	0	0	100	100
44	Le	124/131 (95%)	121 (98%)	3 (2%)	0	100	100
45	Lf	106/109 (97%)	105 (99%)	1 (1%)	0	100	100
46	Lg	116/119 (98%)	113 (97%)	3 (3%)	0	100	100
47	Lh	114/935 (12%)	112 (98%)	2 (2%)	0	100	100
48	Li	99/110 (90%)	99 (100%)	0	0	100	100
49	Lj	86/95 (90%)	85 (99%)	1 (1%)	0	100	100
50	Lk	74/94 (79%)	73 (99%)	1 (1%)	0	100	100
51	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
52	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
53	Lq	137/147 (93%)	132 (96%)	5 (4%)	0	100	100
All	All	9079/14219 (64%)	8921 (98%)	157 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	LF	197	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	CF	212/236 (90%)	212 (100%)	0	100	100
5	CH	547/575 (95%)	547 (100%)	0	100	100
6	CK	206/225 (92%)	206 (100%)	0	100	100
7	CL	61/458 (13%)	61 (100%)	0	100	100
8	CN	205/206 (100%)	205 (100%)	0	100	100
9	CO	48/99 (48%)	48 (100%)	0	100	100
10	CQ	144/192 (75%)	144 (100%)	0	100	100
11	Cb	85/101 (84%)	85 (100%)	0	100	100
12	Cd	403/541 (74%)	403 (100%)	0	100	100
13	Cf	250/310 (81%)	250 (100%)	0	100	100
14	Cg	158/176 (90%)	158 (100%)	0	100	100
15	Ch	408/436 (94%)	408 (100%)	0	100	100
16	Cz	89/107 (83%)	89 (100%)	0	100	100
17	LA	150/198 (76%)	150 (100%)	0	100	100
18	LB	329/331 (99%)	329 (100%)	0	100	100
19	LC	282/285 (99%)	282 (100%)	0	100	100
20	LD	221/253 (87%)	221 (100%)	0	100	100
21	LE	157/166 (95%)	157 (100%)	0	100	100
22	LF	213/215 (99%)	213 (100%)	0	100	100
23	LG	199/222 (90%)	199 (100%)	0	100	100
24	LH	167/200 (84%)	167 (100%)	0	100	100
25	LJ	140/150 (93%)	140 (100%)	0	100	100
26	LK	127/136 (93%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	LL	158/176 (90%)	158 (100%)	0	100	100
28	LM	116/117 (99%)	116 (100%)	0	100	100
29	LN	179/180 (99%)	179 (100%)	0	100	100
30	LO	162/163 (99%)	162 (100%)	0	100	100
31	LP	133/152 (88%)	133 (100%)	0	100	100
32	LQ	128/178 (72%)	128 (100%)	0	100	100
33	LR	125/2396 (5%)	125 (100%)	0	100	100
34	LS	152/154 (99%)	152 (100%)	0	100	100
35	LT	110/135 (82%)	110 (100%)	0	100	100
36	LU	92/108 (85%)	92 (100%)	0	100	100
37	LV	98/102 (96%)	98 (100%)	0	100	100
38	LX	104/129 (81%)	104 (100%)	0	100	100
39	LY	116/119 (98%)	116 (100%)	0	100	100
40	LZ	121/121 (100%)	121 (100%)	0	100	100
41	La	93/122 (76%)	93 (100%)	0	100	100
42	Lc	76/88 (86%)	76 (100%)	0	100	100
43	Ld	90/105 (86%)	90 (100%)	0	100	100
44	Le	109/114 (96%)	109 (100%)	0	100	100
45	Lf	89/90 (99%)	89 (100%)	0	100	100
46	Lg	95/102 (93%)	95 (100%)	0	100	100
47	Lh	106/781 (14%)	106 (100%)	0	100	100
48	Li	85/93 (91%)	85 (100%)	0	100	100
49	Lj	72/78 (92%)	72 (100%)	0	100	100
50	Lk	73/88 (83%)	73 (100%)	0	100	100
51	Ll	45/46 (98%)	45 (100%)	0	100	100
52	Lp	73/74 (99%)	73 (100%)	0	100	100
53	Lq	104/112 (93%)	104 (100%)	0	100	100
All	All	7705/11941 (64%)	7705 (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. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
24	LH	95	HIS
53	Lq	43	HIS
32	LQ	73	ASN
51	Ll	33	ASN
49	Lj	13	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3051/3342 (91%)	580 (19%)	24 (0%)
2	C2	150/156 (96%)	22 (14%)	1 (0%)
3	C4	118/119 (99%)	19 (16%)	0
All	All	3319/3617 (91%)	621 (18%)	25 (0%)

5 of 621 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	G
1	C1	15	U
1	C1	27	A
1	C1	31	G
1	C1	44	A

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	2883	U
1	C1	3205	G
2	C2	127	U
1	C1	3132	A
1	C1	3210	U

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

34 non-standard protein/DNA/RNA residues are modelled in this entry.

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	C1	1868	1	19,22,23	3.12	6 (31%)	25,31,34	1.84	5 (20%)
1	OMC	C1	2300	1	19,22,23	0.52	0	25,31,34	0.70	0
1	OMU	C1	2277	1	19,22,23	3.11	6 (31%)	25,31,34	1.71	5 (20%)
1	OMG	C1	2774	1	23,26,27	0.46	0	32,38,41	0.49	0
1	OMG	C1	2881	1	23,26,27	0.45	0	32,38,41	0.48	0
1	OMU	C1	2688	1	19,22,23	3.12	6 (31%)	25,31,34	1.80	5 (20%)
1	OMG	C1	2876	1	23,26,27	0.47	0	32,38,41	0.48	0
1	A2M	C1	1432	1	22,25,26	4.01	12 (54%)	30,36,39	3.38	12 (40%)
1	OMG	C1	646	1	23,26,27	0.47	0	32,38,41	0.48	0
1	A2M	C1	1223	1	22,25,26	3.97	11 (50%)	30,36,39	3.37	13 (43%)
1	A2M	C1	1847	1	22,25,26	3.99	12 (54%)	30,36,39	3.49	14 (46%)
1	OMC	C1	2918	1	19,22,23	0.53	0	25,31,34	0.79	1 (4%)
1	OMG	C1	787	1	23,26,27	0.47	0	32,38,41	0.53	0
1	OMG	C1	2578	1	23,26,27	0.46	0	32,38,41	0.54	0
1	OMC	C1	1812	1	19,22,23	0.51	0	25,31,34	0.62	0
1	OMG	C1	1433	1	23,26,27	0.48	0	32,38,41	0.48	0
1	A2M	C1	389	1	22,25,26	4.00	12 (54%)	30,36,39	3.41	13 (43%)
1	OMU	C1	2380	1	19,22,23	3.11	6 (31%)	25,31,34	1.78	5 (20%)
1	OMU	C1	1917	1	19,22,23	3.14	6 (31%)	25,31,34	1.78	5 (20%)
1	OMG	C1	2358	1	23,26,27	0.48	0	32,38,41	0.50	0
1	A2M	C1	858	1	22,25,26	4.01	11 (50%)	30,36,39	3.41	13 (43%)
1	OMU	C1	2384	1	19,22,23	3.13	6 (31%)	25,31,34	1.77	4 (16%)
1	OMG	C1	385	1	23,26,27	0.47	0	32,38,41	0.57	0
1	OMU	C1	2683	1	19,22,23	3.10	6 (31%)	25,31,34	1.74	4 (16%)
1	A2M	C1	2289	1	22,25,26	4.01	11 (50%)	30,36,39	3.33	13 (43%)
1	OMC	C1	1491	1	19,22,23	0.52	0	25,31,34	0.72	0
1	OMC	C1	778	1	19,22,23	0.53	0	25,31,34	0.95	1 (4%)
1	OMU	C1	2690	1	19,22,23	3.11	6 (31%)	25,31,34	1.80	5 (20%)
1	OMG	C1	627	1	23,26,27	0.47	0	32,38,41	0.52	0
1	A2M	C1	848	1	22,25,26	4.00	12 (54%)	30,36,39	3.44	14 (46%)
1	A2M	C1	637	1	22,25,26	4.00	11 (50%)	30,36,39	3.46	13 (43%)
1	OMC	C1	1420	1	19,22,23	0.61	0	25,31,34	1.56	4 (16%)
1	OMC	C1	1836	1	19,22,23	0.54	0	25,31,34	0.89	1 (4%)
1	OMC	C1	2838	1	19,22,23	0.64	0	25,31,34	1.55	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2300	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2277	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2774	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	2881	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2876	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	1432	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	646	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	1223	1	-	2/9/27/28	0/3/3/3
1	A2M	C1	1847	1	-	3/9/27/28	0/3/3/3
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	787	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	2578	1	-	3/9/27/28	0/3/3/3
1	OMC	C1	1812	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	1433	1	-	2/9/27/28	0/3/3/3
1	A2M	C1	389	1	-	4/9/27/28	0/3/3/3
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	1917	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	2358	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	858	1	-	1/9/27/28	0/3/3/3
1	OMU	C1	2384	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	385	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	2289	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	1491	1	-	1/9/27/28	0/2/2/2
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	627	1	-	1/9/27/28	0/3/3/3
1	A2M	C1	848	1	-	1/9/27/28	0/3/3/3
1	A2M	C1	637	1	-	2/9/27/28	0/3/3/3
1	OMC	C1	1420	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	858	A2M	C3'-C2'	-13.07	1.24	1.53
1	C1	2289	A2M	C3'-C2'	-13.04	1.24	1.53
1	C1	848	A2M	C3'-C2'	-13.00	1.24	1.53
1	C1	1432	A2M	C3'-C2'	-12.99	1.24	1.53
1	C1	637	A2M	C3'-C2'	-12.96	1.24	1.53

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C8	-9.60	105.80	127.09
1	C1	637	A2M	C1'-N9-C8	-9.57	105.86	127.09
1	C1	389	A2M	C1'-N9-C8	-9.49	106.02	127.09
1	C1	1432	A2M	C1'-N9-C8	-9.38	106.28	127.09
1	C1	858	A2M	C1'-N9-C8	-9.31	106.43	127.09

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	389	A2M	O4'-C4'-C5'-O5'
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	858	A2M	C1'-C2'-O2'-CM'
1	C1	1223	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C1	2277	OMU	1	0
1	C1	2876	OMG	1	0
1	C1	1432	A2M	1	0
1	C1	2578	OMG	1	0
1	C1	389	A2M	1	0
1	C1	2384	OMU	1	0
1	C1	2683	OMU	2	0
1	C1	778	OMC	1	0
1	C1	848	A2M	1	0
1	C1	1420	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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$
54	GTP	Cd	1000	55	33,34,34	0.97	2 (6%)	50,54,54	1.59	8 (16%)
54	GTP	CH	701	55	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)

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
54	GTP	Cd	1000	55	-	5/22/38/38	0/3/3/3
54	GTP	CH	701	55	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CH	701	GTP	C2-N3	2.10	1.38	1.33
54	Cd	1000	GTP	PA-O3A	2.03	1.61	1.59
54	Cd	1000	GTP	C2-N3	2.02	1.38	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Cd	1000	GTP	C5-C4-N3	-4.96	120.49	128.39
54	CH	701	GTP	C5-C4-N3	-4.90	120.58	128.39
54	Cd	1000	GTP	C2-N3-C4	4.60	120.23	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CH	701	GTP	C2-N3-C4	4.53	120.10	112.30
54	Cd	1000	GTP	N9-C4-N3	3.12	132.20	125.95

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	CH	701	GTP	C5'-O5'-PA-O3A
54	CH	701	GTP	C5'-O5'-PA-O1A
54	Cd	1000	GTP	C5'-O5'-PA-O3A
54	Cd	1000	GTP	C5'-O5'-PA-O1A
54	Cd	1000	GTP	C5'-O5'-PA-O2A

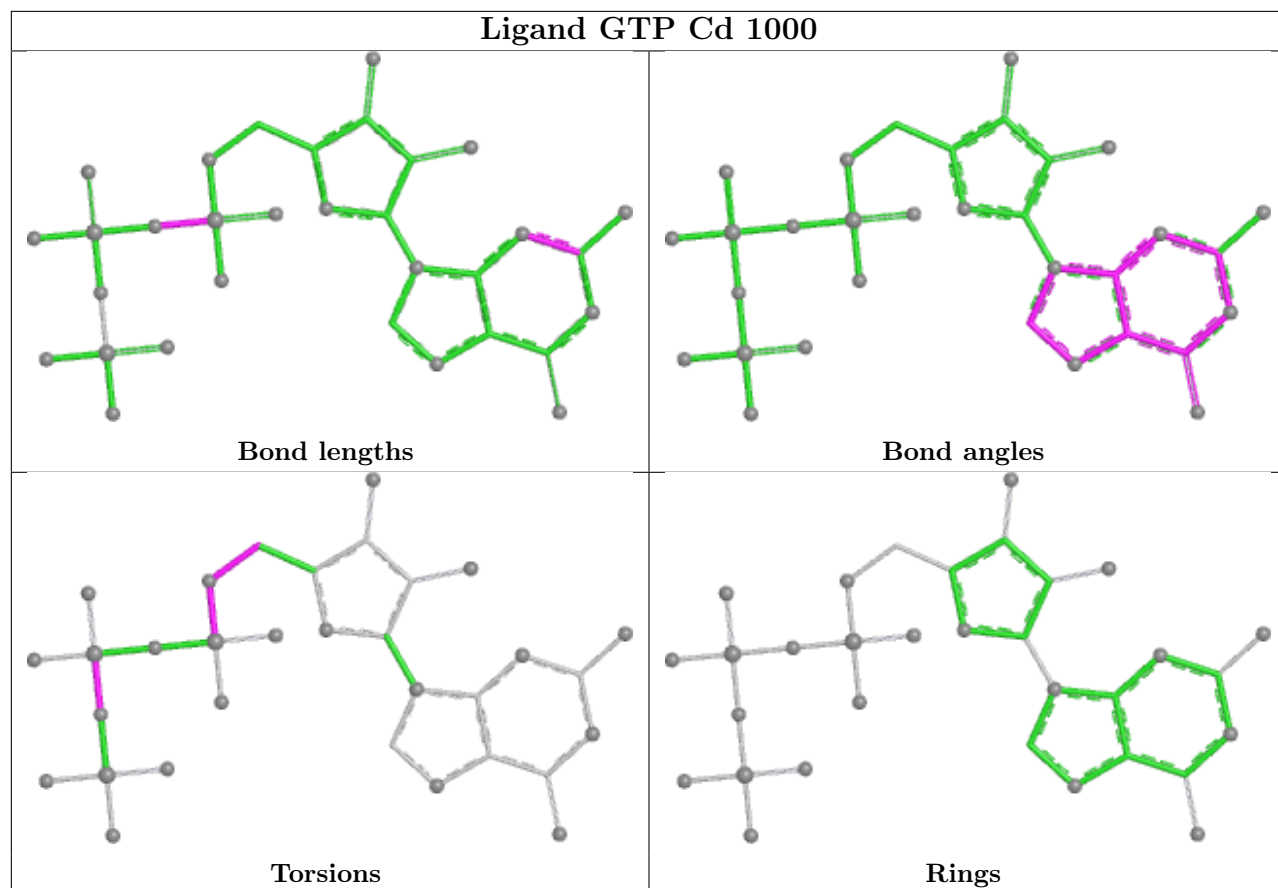
There are no ring outliers.

1 monomer is involved in 1 short contact:

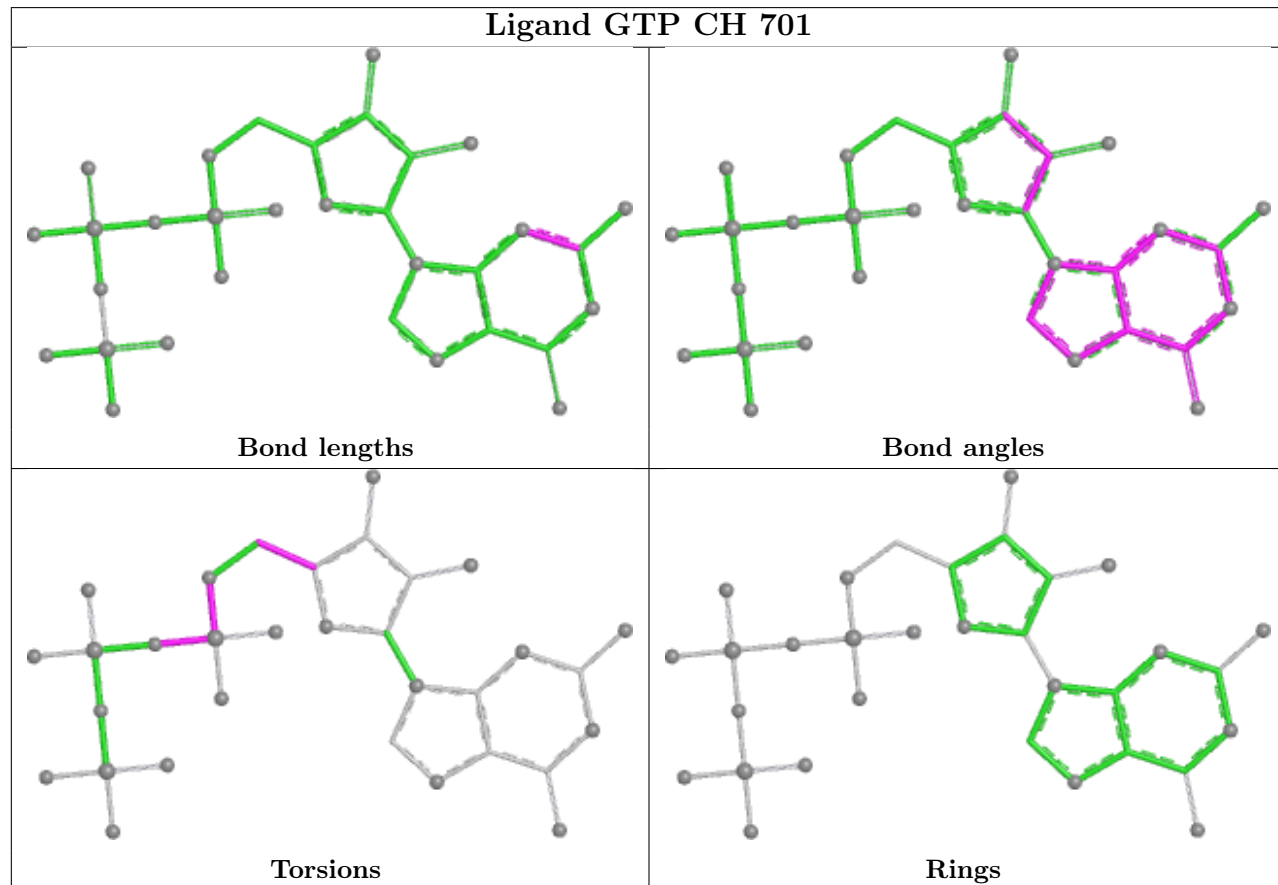
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	Cd	1000	GTP	1	0

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

Ligand GTP Cd 1000



Ligand GTP CH 701



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.

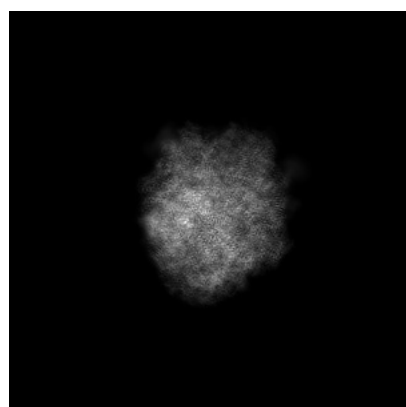
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17954. These allow visual inspection of the internal detail of the map and identification of artifacts.

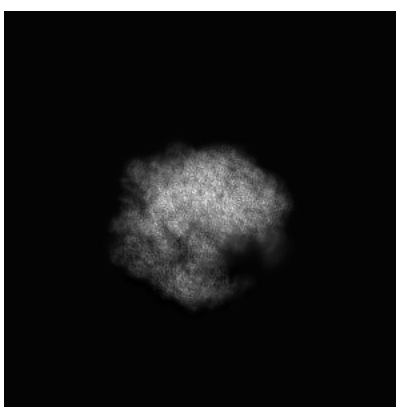
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

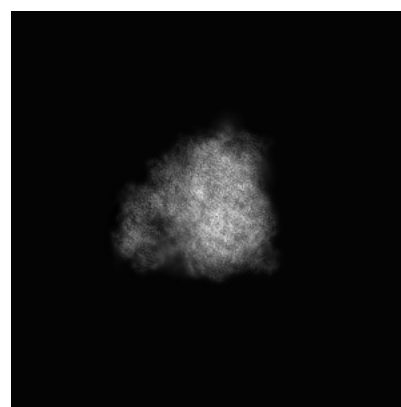
6.1.1 Primary map



X



Y

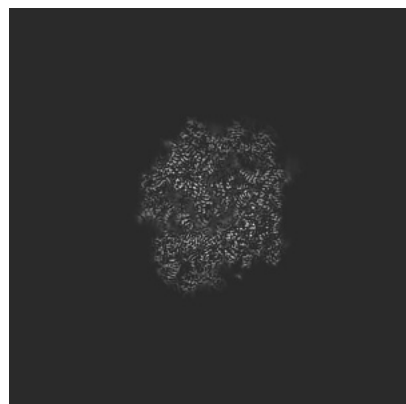


Z

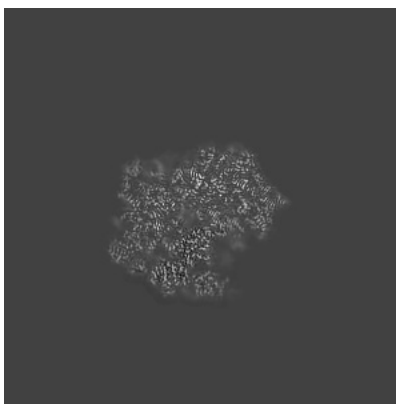
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

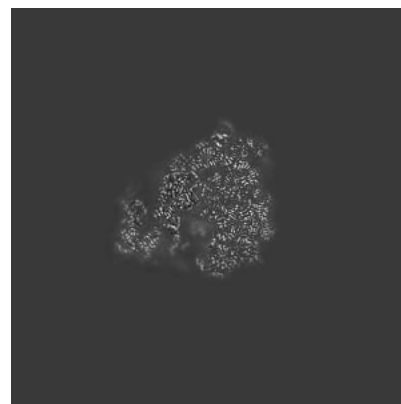
6.2.1 Primary map



X Index: 250



Y Index: 250

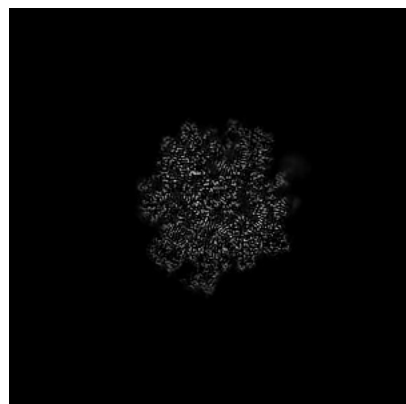


Z Index: 250

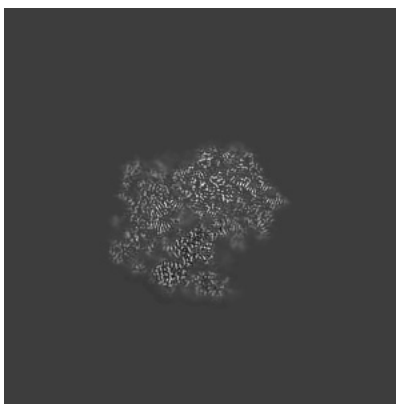
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

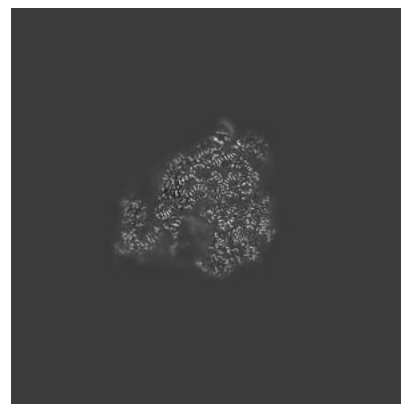
6.3.1 Primary map



X Index: 264



Y Index: 248

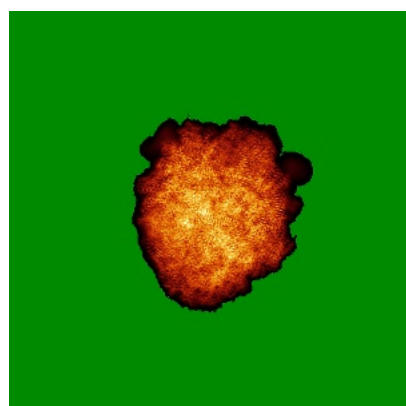


Z Index: 252

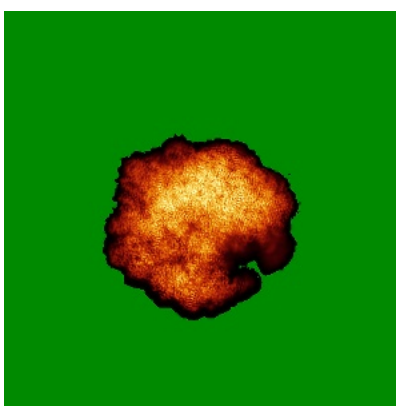
The images above show the largest variance slices of the map in three orthogonal directions.

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

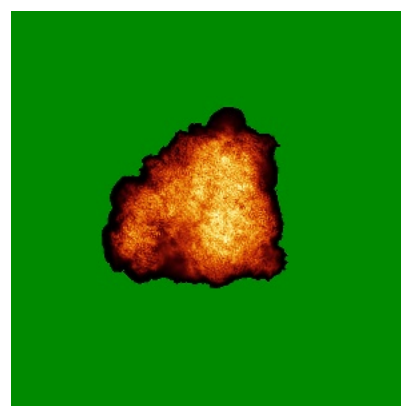
6.4.1 Primary map



X



Y

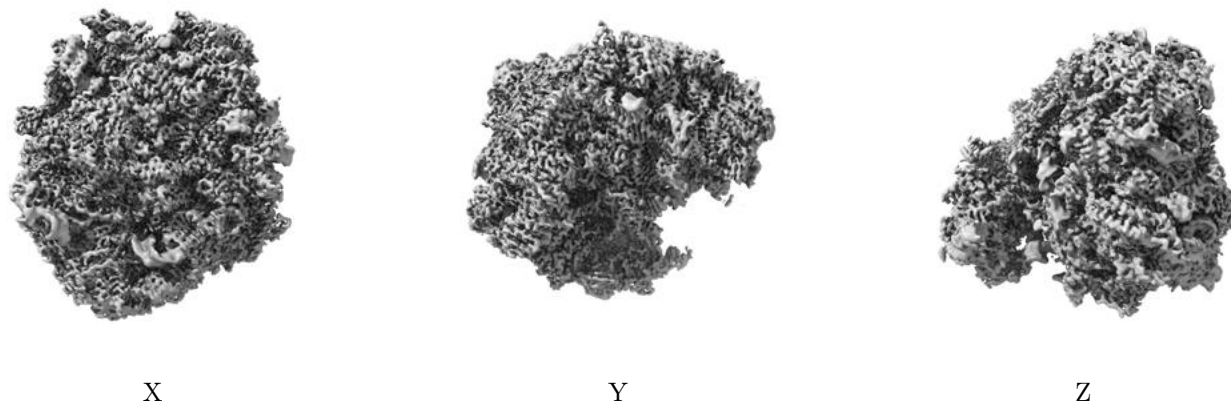


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

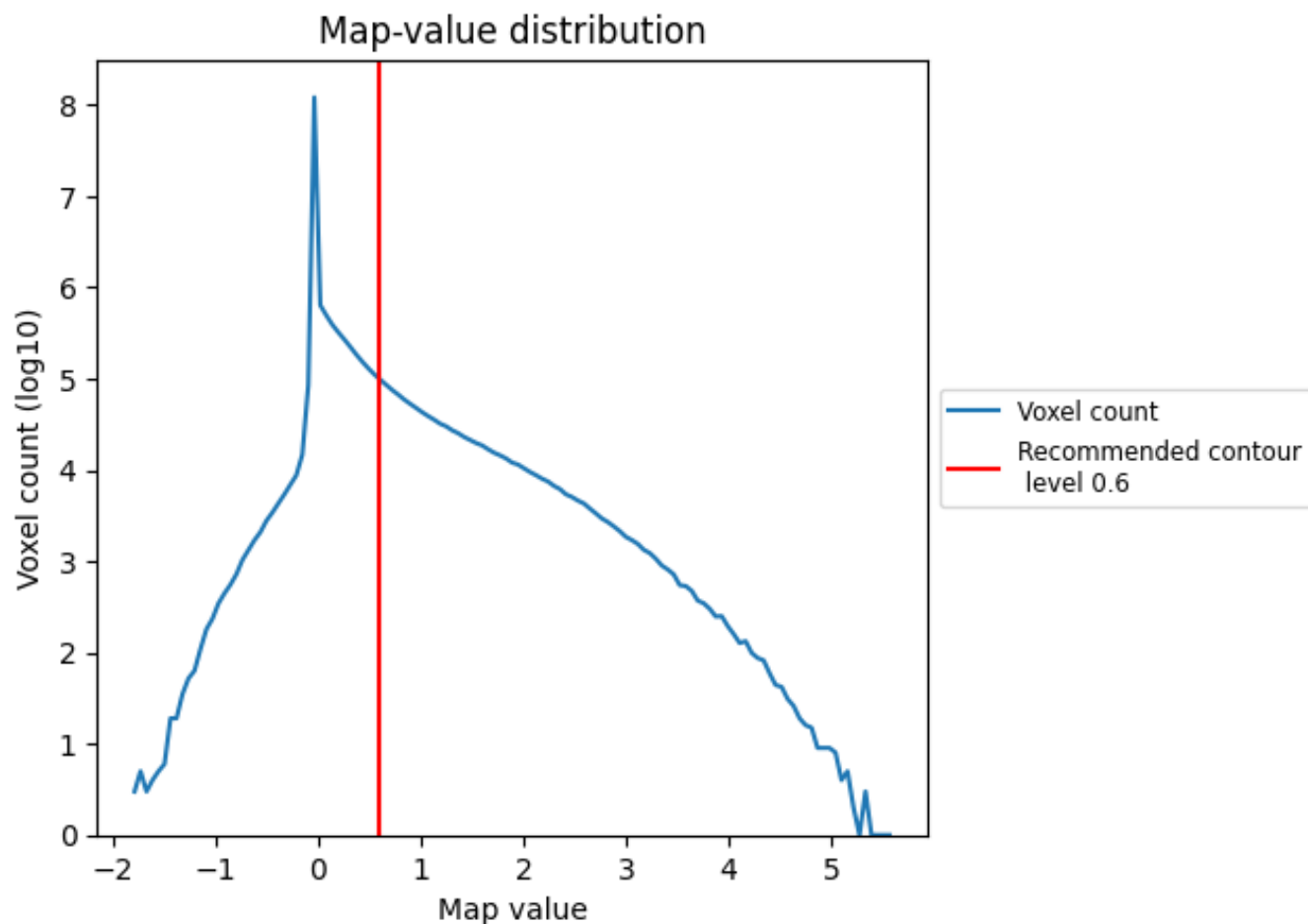
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

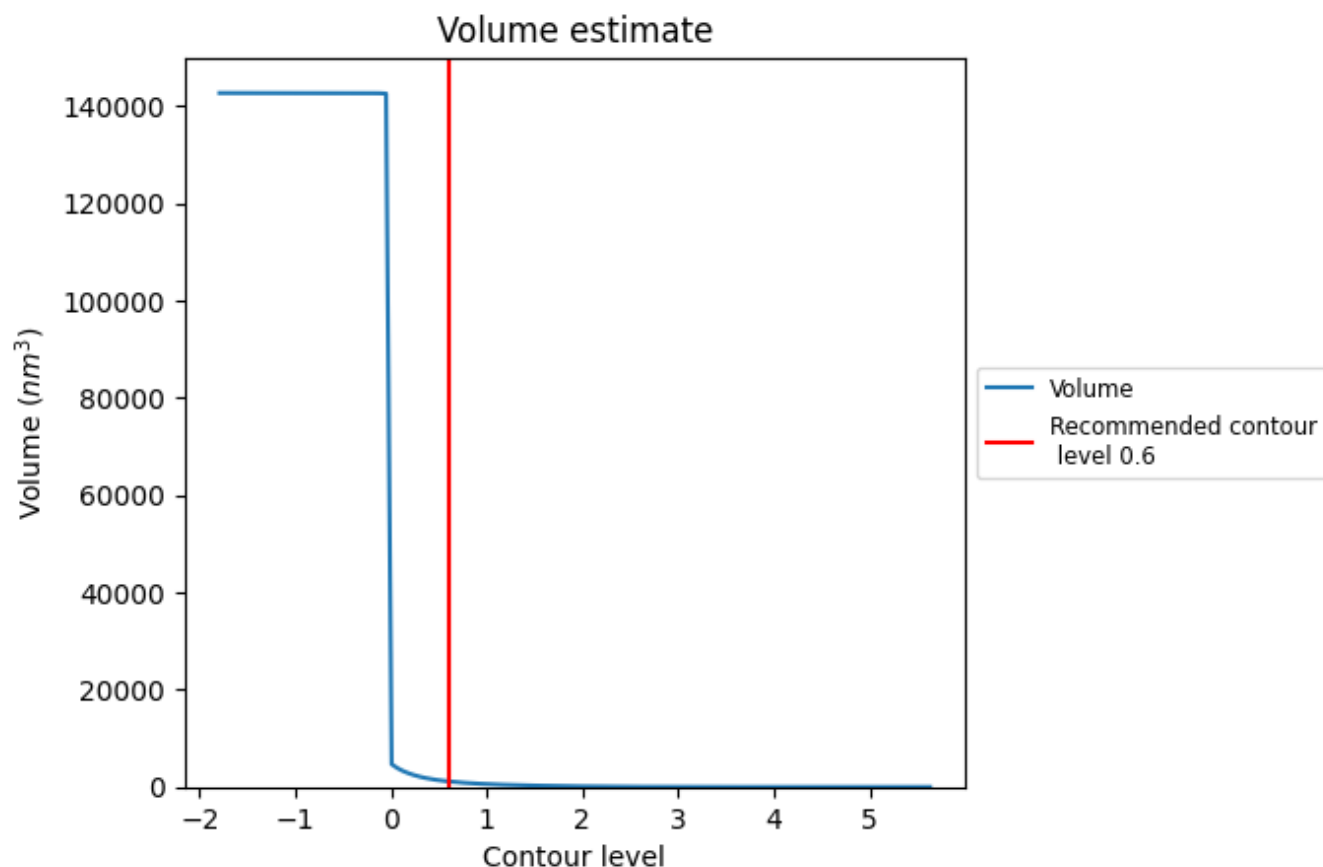
This section contains the results of statistical analysis of the map.

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.

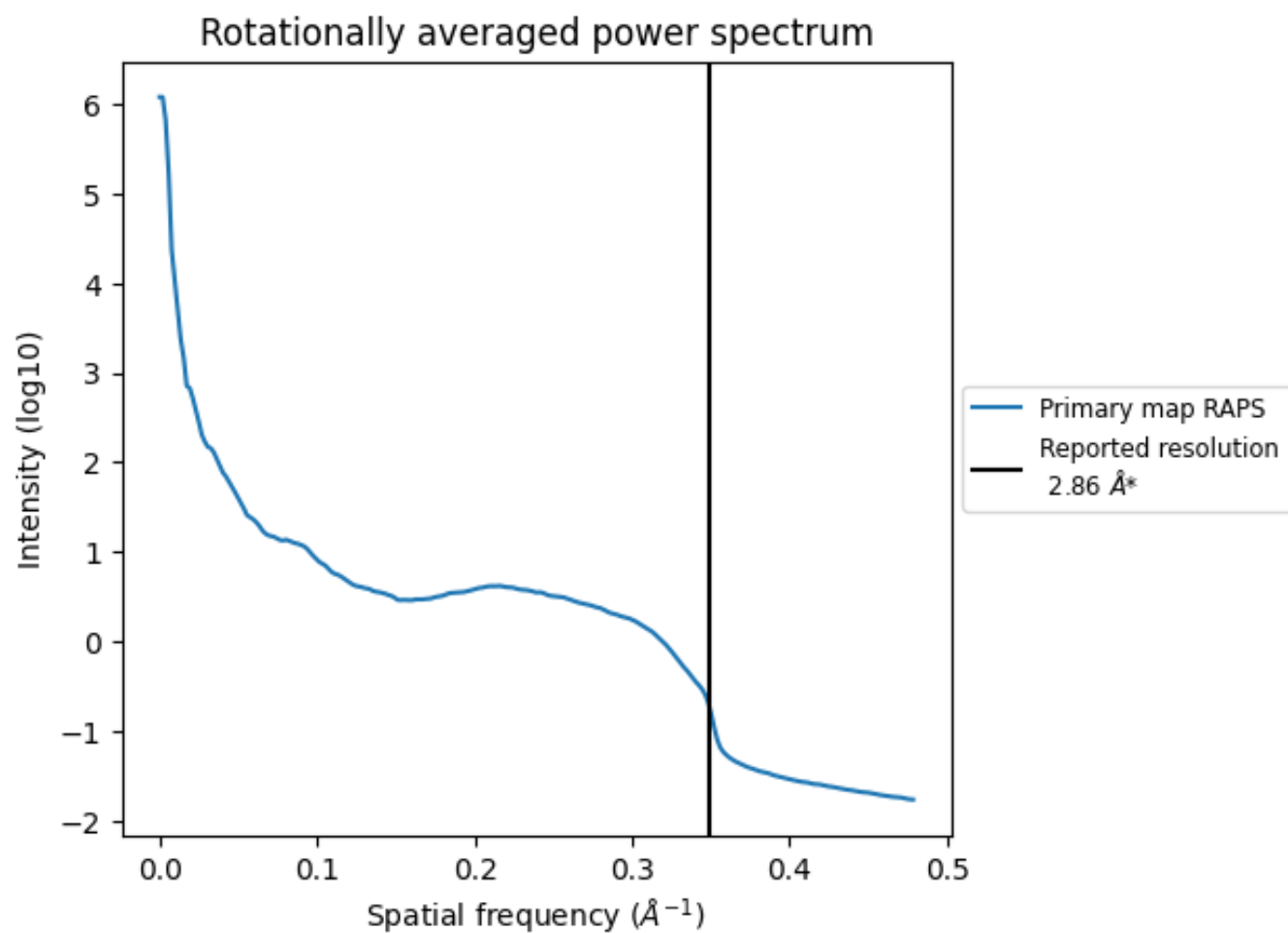
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1142 nm^3 ; this corresponds to an approximate mass of 1032 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 0.350 $\text{\AA}^{-1}$

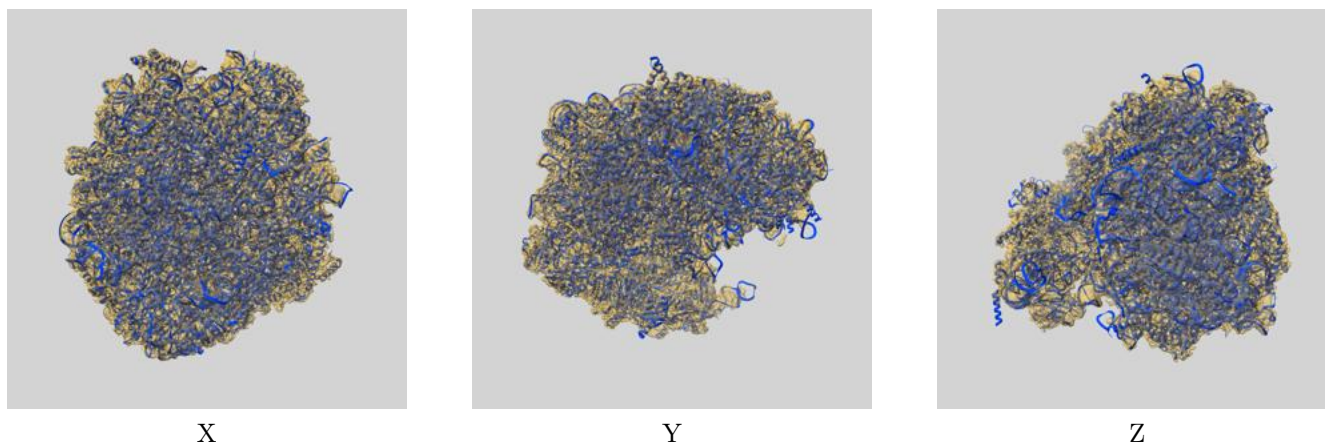
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

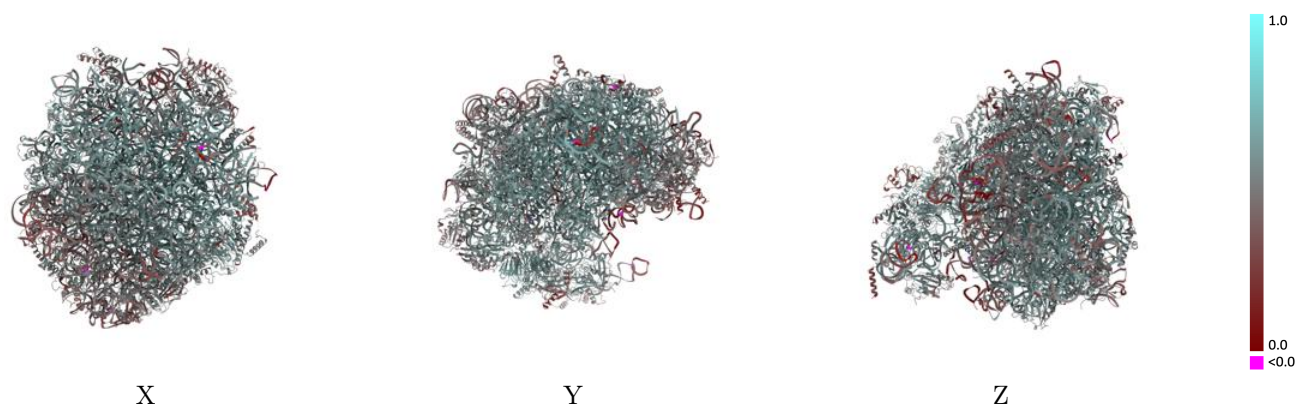
This section contains information regarding the fit between EMDB map EMD-17954 and PDB model 8PV5. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



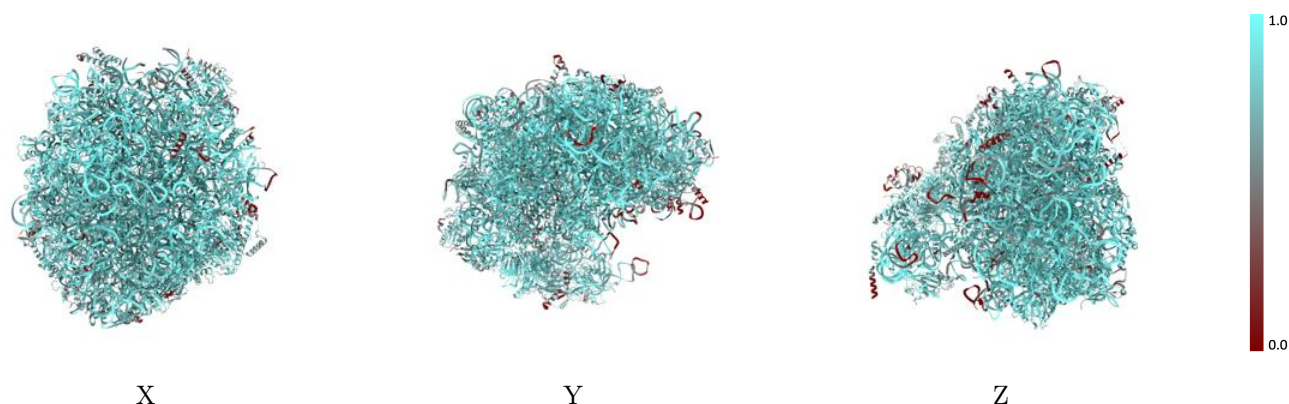
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



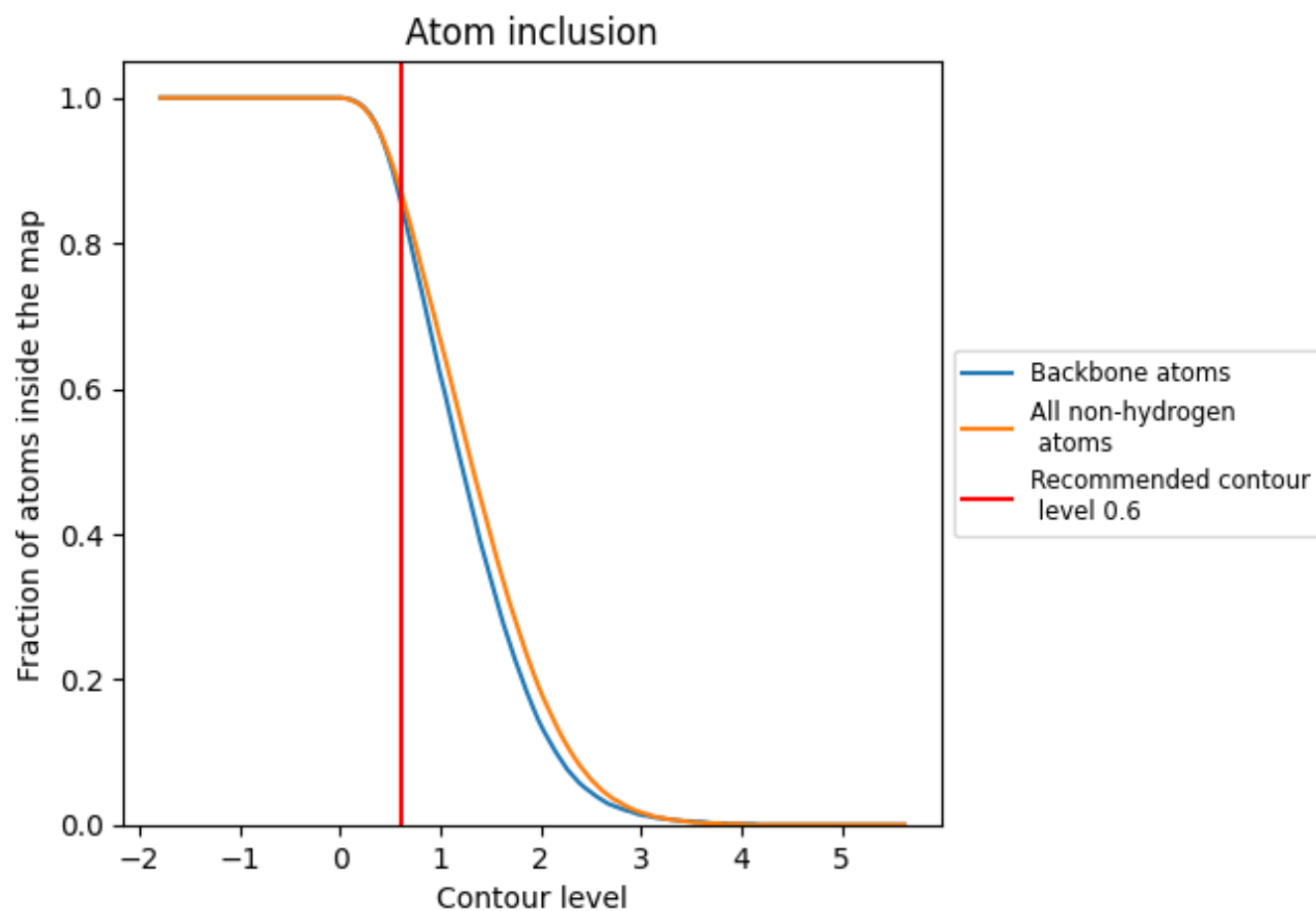
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 87% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5220
C1	 0.9120	 0.5220
C2	 0.9640	 0.5810
C4	 0.8710	 0.4960
CF	 0.7370	 0.4460
CH	 0.8320	 0.5440
CK	 0.9350	 0.5860
CL	 0.6160	 0.4490
CN	 0.8680	 0.5710
CO	 0.7460	 0.4820
CQ	 0.8180	 0.5360
Cb	 0.8680	 0.5740
Cd	 0.8970	 0.5640
Cf	 0.8730	 0.5440
Cg	 0.8490	 0.5300
Ch	 0.8250	 0.5380
Cz	 0.6850	 0.4190
LA	 0.8330	 0.4940
LB	 0.9190	 0.5540
LC	 0.9000	 0.5350
LD	 0.8680	 0.5390
LE	 0.7190	 0.4190
LF	 0.8260	 0.4470
LG	 0.7330	 0.4460
LH	 0.8280	 0.5050
LJ	 0.7900	 0.4790
LK	 0.7430	 0.4920
LL	 0.8750	 0.5660
LM	 0.7550	 0.4440
LN	 0.9310	 0.5840
LO	 0.8650	 0.4880
LP	 0.9090	 0.5440
LQ	 0.8350	 0.5030
LR	 0.8970	 0.5590
LS	 0.8430	 0.4710



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Chain	Atom inclusion	Q-score
LT	 0.6820	 0.4350
LU	 0.8580	 0.5430
LV	 0.9230	 0.6050
LX	 0.8800	 0.5570
LY	 0.8830	 0.5470
LZ	 0.7370	 0.4290
La	 0.8900	 0.5630
Lc	 0.6570	 0.4070
Ld	 0.9070	 0.5920
Le	 0.8810	 0.5020
Lf	 0.8950	 0.4740
Lg	 0.7950	 0.5030
Lh	 0.8570	 0.5330
Li	 0.8330	 0.5080
Lj	 0.9720	 0.6150
Lk	 0.7340	 0.5000
Ll	 0.9810	 0.6260
Lp	 0.8100	 0.4970
Lq	 0.8730	 0.4660