



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2023 – 03:20 pm GMT

PDB ID : 8PV4
EMDB ID : EMD-17953
Title : Chaetomium thermophilum pre-60S State 2 - pre-5S rotation with Rix1 complex - composite structure
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.90 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:

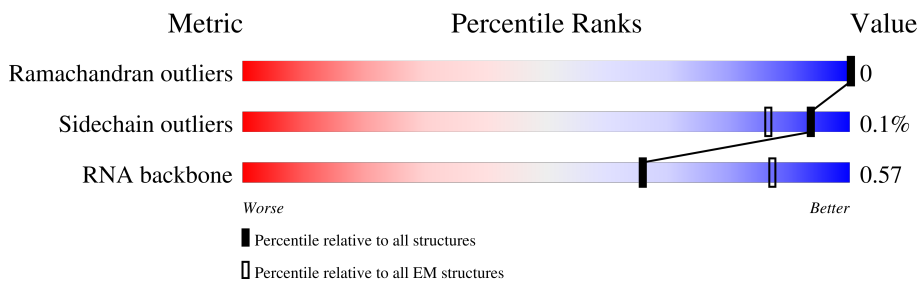
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







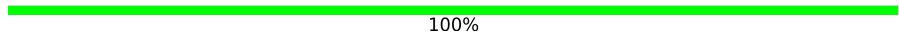
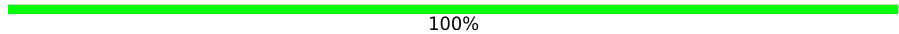












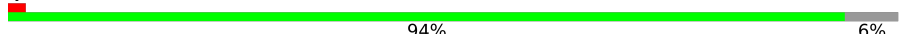


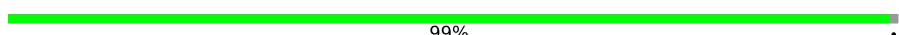
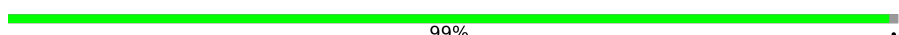
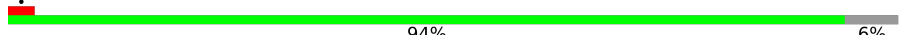
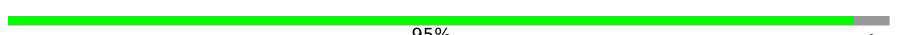
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	C3	162	
4	C4	119	
5	CB	391	
6	CF	270	
7	CH	661	
8	CI	414	

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Mol	Chain	Length	Quality of chain
9	CJ	679	 56% 44%
10	CK	261	 91% 9%
11	CL	558	 14% 86%
12	CM	249	 87% 13%
12	LF	249	 100%
13	CN	246	 100%
14	CO	120	 52% 48%
15	CQ	225	 81% 19%
16	CS	338	 79% 21%
17	CT	437	 90% 10%
17	CU	437	 90% 10%
18	CV	781	 70% 30%
18	CW	781	 70% 30%
19	Cb	117	 86% 14%
20	Cd	627	 74% 26%
21	Ce	443	 59% 41%
22	Cf	350	 81% 19%
23	Cg	202	 93% 7%
24	Ch	517	 94% 6%
25	Cz	123	 82% 18%
26	LA	254	 75% 25%
27	LB	392	 99%
28	LC	365	 99%
29	LD	304	 94% 6%
30	LE	200	 95%

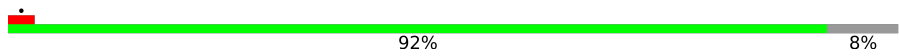
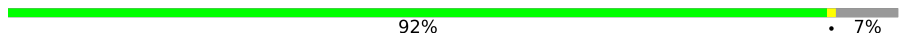

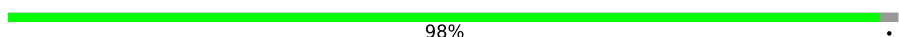

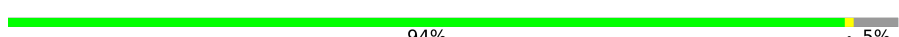


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Mol	Chain	Length	Quality of chain
31	LG	262	90% 10%
32	LH	229	83% 17%
33	LJ	173	98%
34	LK	165	96%
35	LL	213	95% 5%
36	LM	142	99%
37	LN	203	100%
38	LO	204	100%
39	LP	187	91% 9%
40	LQ	213	69% 30%
41	LR	2898	5% 95%
42	LS	174	100%
43	LT	160	80% 19%
44	LU	127	83% 17%
45	LV	139	97%
46	LX	156	91% 7%
47	LY	138	96%
48	LZ	135	100%
49	La	149	72% 28%
50	Lc	108	88% 12%
51	Ld	120	92% 8%
52	Le	131	96%
53	Lf	109	99%
54	Lg	119	6% 99%
55	Lh	935	13% 87%

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Mol	Chain	Length	Quality of chain
56	Li	110	 92% 8%
57	Lj	95	 92% 7%
58	Lk	94	 79% 19%
59	Ll	51	 98%
60	Lp	92	 99%
61	Lq	147	 94% 5%
62	Lr	217	 80% 99%
63	CR	767	 50% 49%

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 178878 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
			Total	C	N	O	P		
1	C1	3136	67131	29984	12153	21858	3136	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	156	3319	1484	589	1090	156	0	0

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C3	82	1754	780	316	576	82	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

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

- Molecule 5 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CB	265	2107	1351	371	382	3	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL10.

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

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	CH	627	5063	3181	924	939	19	0	0

- Molecule 8 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	CI	152	1234	791	230	208	5	0	0

- Molecule 9 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	CJ	382	3116	2008	548	550	10	0	0

- Molecule 10 is a protein called Ribosome biogenesis protein NSA2 homolog.

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

- Molecule 11 is a protein called Putative GTP binding protein.

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

- Molecule 12 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	CM	217	1773	1144	329	297	3	0	0
12	LF	248	2023	1297	377	346	3	0	0

- Molecule 13 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 14 is a protein called DUF2423 domain-containing protein.

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

- Molecule 15 is a protein called Ribosome biogenesis protein RLP24.

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

- Molecule 16 is a protein called Pre-rRNA-processing protein IPI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	CS	268	2063	1312	363	381	7	0	0

- Molecule 17 is a protein called Pre-rRNA-processing protein IPI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	CT	395	2953	1873	494	568	18	0	0
17	CU	395	2965	1881	496	570	18	0	0

- Molecule 18 is a protein called Pre-rRNA-processing protein RIX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CV	550	4217	2691	735	777	14	0	0
18	CW	550	4204	2685	729	776	14	0	0

- Molecule 19 is a protein called Zinc finger domain-containing protein.

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

- Molecule 20 is a protein called Nucleolar GTP-binding protein 2.

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

- Molecule 21 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Ce	262	2148	1337	413	394	4	0	0

- Molecule 22 is a protein called Ribosome production factor 2 homolog.

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

- Molecule 23 is a protein called Ribosome biogenesis regulatory protein.

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

- Molecule 24 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Ch	485	3809	2394	696	709	10	0	0

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 25 is a protein called rRNA-processing protein.

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

- Molecule 26 is a protein called 60S ribosomal protein L2-like protein.

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

- Molecule 27 is a protein called 60S ribosomal protein L3-like protein.

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

- Molecule 28 is a protein called 60S ribosomal protein L4-like protein.

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

- Molecule 29 is a protein called 60S ribosomal protein l5-like protein.

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

- Molecule 30 is a protein called 60S ribosomal protein L6.

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

- Molecule 31 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LG	235	Total	C	N	O	S	0	0
			1889	1210	350	324	5		

- Molecule 32 is a protein called 60S ribosomal protein l9-like protein.

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

- Molecule 33 is a protein called Putative ribosomal protein.

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

- Molecule 34 is a protein called 60S ribosomal protein L12-like protein.

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

- Molecule 35 is a protein called 60S ribosomal protein L13.

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

- Molecule 36 is a protein called 60S ribosomal protein L14-like protein.

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

- Molecule 37 is a protein called Ribosomal protein L15.

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

- Molecule 38 is a protein called 60S ribosomal protein L16-like protein.

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

- Molecule 39 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LP	171	1345	836	274	232	3	0	0

- Molecule 40 is a protein called Ribosomal protein L18-like protein.

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

- Molecule 41 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LR	155	1241	772	262	203	4	0	0

- Molecule 42 is a protein called 60S ribosomal protein L20.

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

- Molecule 43 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	LT	129	1021	647	194	178	2	0	0

- Molecule 44 is a protein called 60S ribosomal protein L22-like protein.

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

- Molecule 45 is a protein called 60S ribosomal protein l23-like protein.

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

- Molecule 46 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	LX	145	1133	723	211	199	0	0

- Molecule 47 is a protein called 60S ribosomal protein L26-like protein.

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

- Molecule 48 is a protein called 60S ribosomal protein L27.

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

- Molecule 49 is a protein called 60S ribosomal protein L28-like protein.

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

- Molecule 50 is a protein called 60S ribosomal protein l30-like protein.

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

- Molecule 51 is a protein called Putative 60S ribosomal protein.

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

- Molecule 52 is a protein called 60S ribosomal protein L32-like protein.

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

- Molecule 53 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 54 is a protein called Ribosomal protein l34-like protein.

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

- Molecule 55 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Lh	122	1003	637	198	168		0	0

- Molecule 56 is a protein called 60S ribosomal protein L36.

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

- Molecule 57 is a protein called Ribosomal protein L37.

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

- Molecule 58 is a protein called 60S ribosomal protein L38-like protein.

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

- Molecule 59 is a protein called Ribosomal protein eL39.

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

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

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

- Molecule 61 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
61	Lq	139	1073	672	213	188	0	0

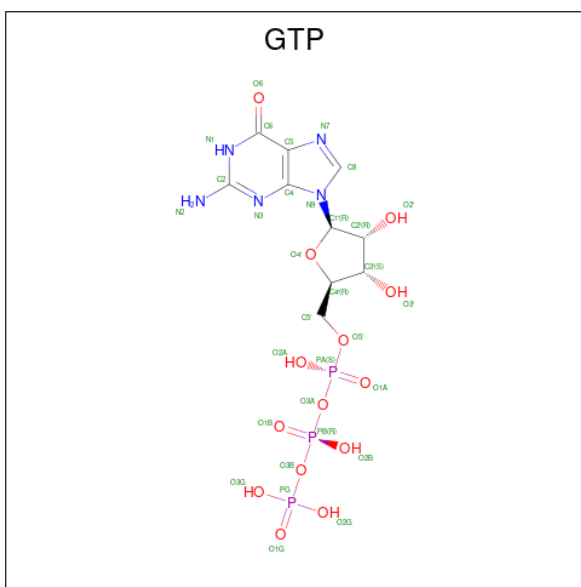
- Molecule 62 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	Lr	214	1056	628	214	214	0	0

- Molecule 63 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	CR	390	2934	1879	517	526	12	0	0

- Molecule 64 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	CH	1	32	10	5	14	3	0
64	Cd	1	32	10	5	14	3	0

- Molecule 65 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
65	CH	1	Total Mg 1 1	0
65	Cd	2	Total Mg 2 2	0

- Molecule 66 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
66	CQ	1	Total Zn 1 1	0
66	Cb	1	Total Zn 1 1	0
66	Lg	1	Total Zn 1 1	0
66	Lj	1	Total Zn 1 1	0
66	Lp	1	Total Zn 1 1	0

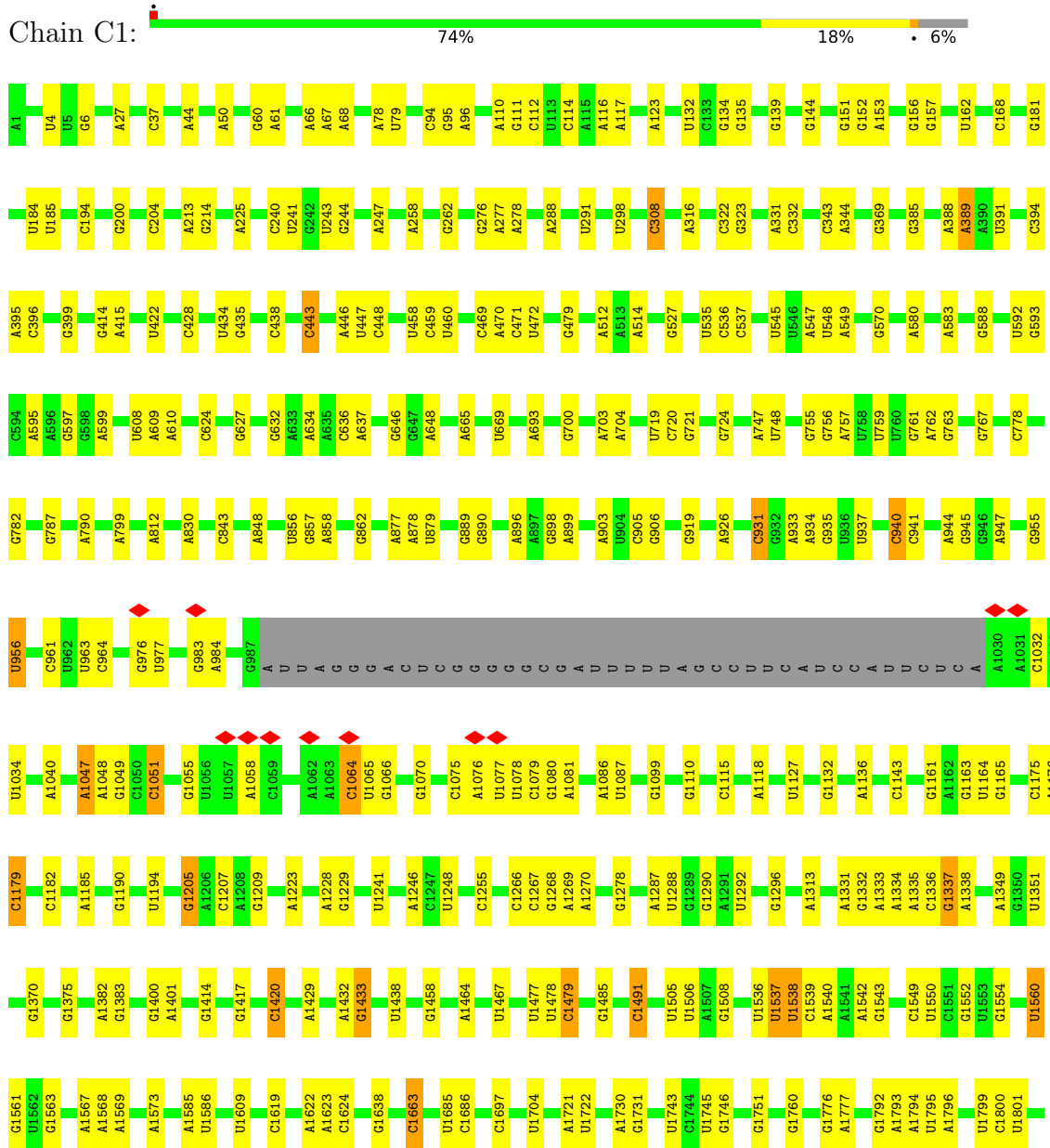
- Molecule 67 is water.

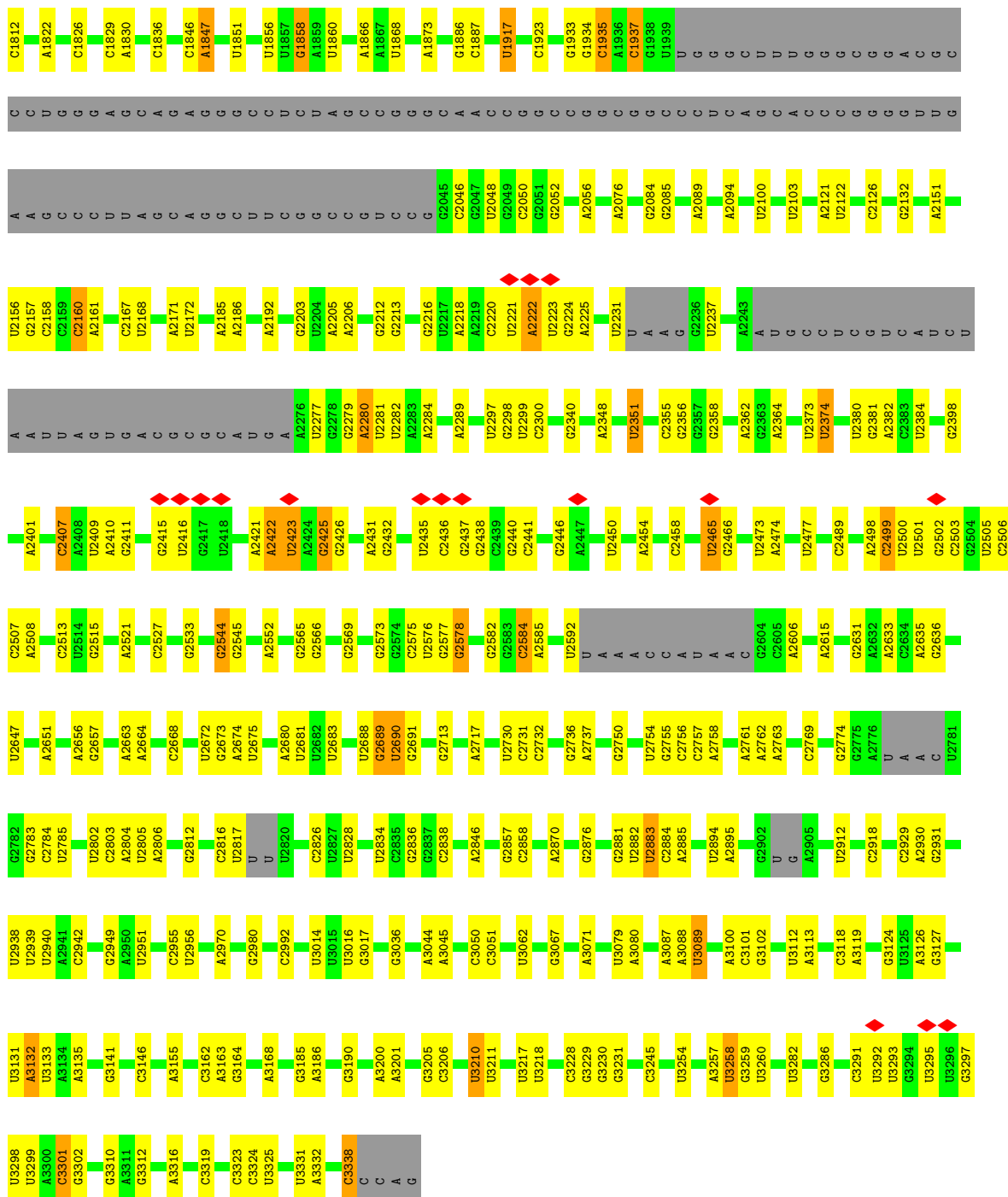
Mol	Chain	Residues	Atoms	AltConf
67	CH	1	Total O 1 1	0
67	Cd	2	Total O 2 2	0

3 Residue-property plots i

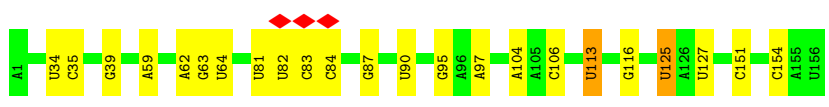
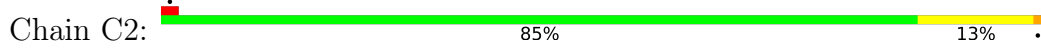
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 26S rRNA

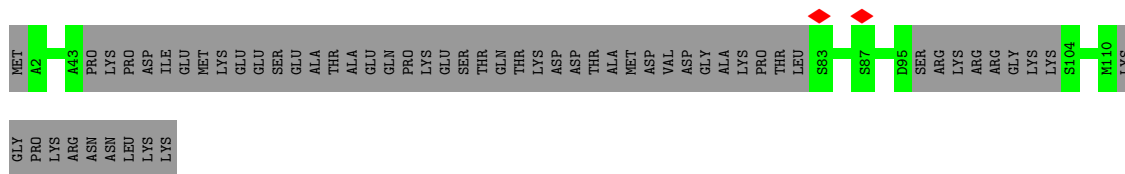




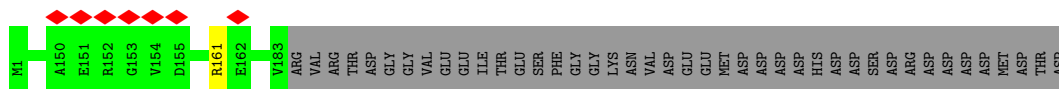
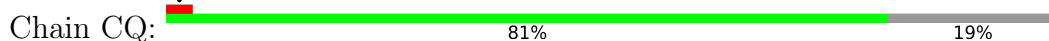
• Molecule 2: 5.8S rRNA



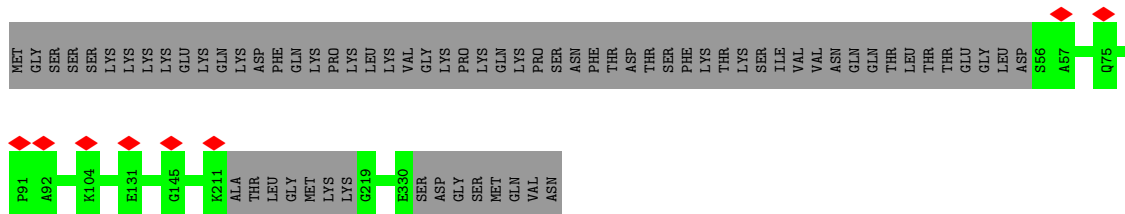
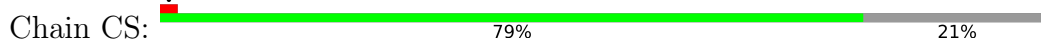
• Molecule 3: ITS2



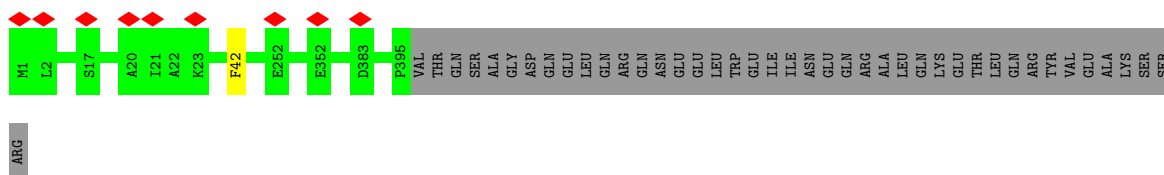
- Molecule 15: Ribosome biogenesis protein RLP24



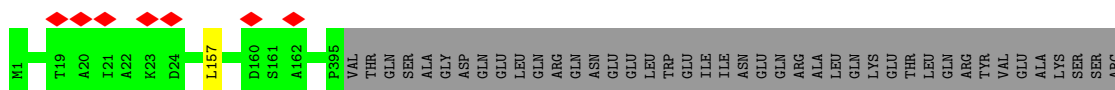
- Molecule 16: Pre-rRNA-processing protein IPI1



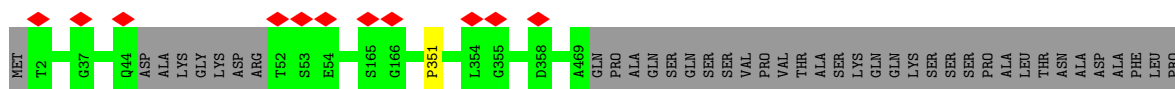
- Molecule 17: Pre-rRNA-processing protein IPI3

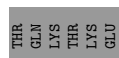
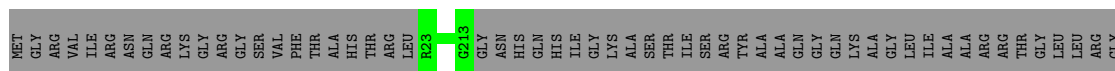


- Molecule 17: Pre-rRNA-processing protein IPI3

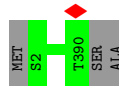


- Molecule 18: Pre-rRNA-processing protein RIX1

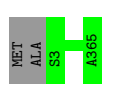




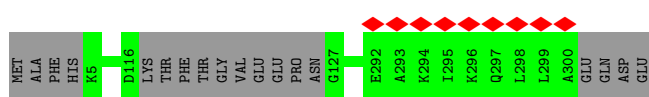
- Molecule 27: 60S ribosomal protein L3-like protein



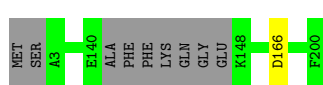
- Molecule 28: 60S ribosomal protein L4-like protein



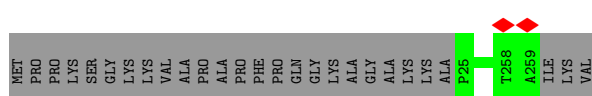
- Molecule 29: 60S ribosomal protein l5-like protein



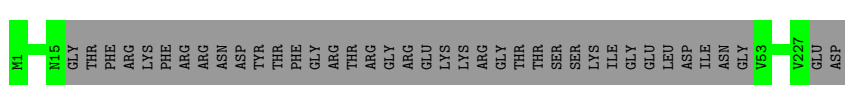
- Molecule 30: 60S ribosomal protein L6



- Molecule 31: 60S ribosomal protein L8

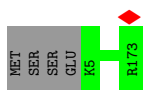


- Molecule 32: 60S ribosomal protein l9-like protein



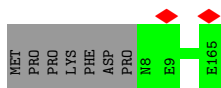
- Molecule 33: Putative ribosomal protein

Chain LJ:  98%



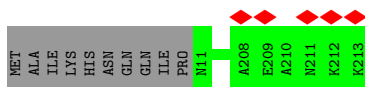
- Molecule 34: 60S ribosomal protein L12-like protein

Chain LK:  96%



- Molecule 35: 60S ribosomal protein L13

Chain LL:  95% 5%



- Molecule 36: 60S ribosomal protein L14-like protein

Chain LM:  99%



- Molecule 37: Ribosomal protein L15

Chain LN:  100%



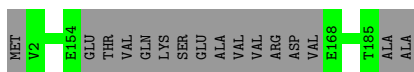
- Molecule 38: 60S ribosomal protein L16-like protein

Chain LO:  100%



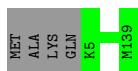
- Molecule 39: 60S ribosomal protein l17-like protein

Chain LP:  91% 9%



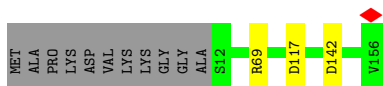
- Molecule 40: Ribosomal protein L18-like protein

Chain LV:  97%



- Molecule 46: 60S ribosomal protein L25-like protein

Chain LX:  91% 7%



- Molecule 47: 60S ribosomal protein L26-like protein

Chain LY:  96%



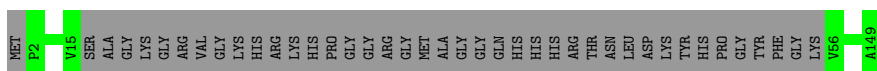
- Molecule 48: 60S ribosomal protein L27

Chain LZ:  100%


There are no outlier residues recorded for this chain.

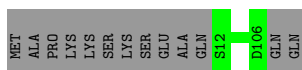
- Molecule 49: 60S ribosomal protein L28-like protein

Chain La:  72% 28%



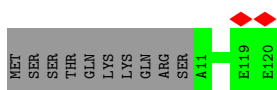
- Molecule 50: 60S ribosomal protein l30-like protein

Chain Lc:  88% 12%



- Molecule 51: Putative 60S ribosomal protein

Chain Ld:  92% 8%



- Molecule 52: 60S ribosomal protein L32-like protein

Chain Le:  96%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25363	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 ($e^-/\text{\AA}^2$)	45.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.938	Depositor
Minimum map value	0.000	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.153	Depositor
Recommended contour level	0.5	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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C1	0.27	0/74274	0.90	103/115802 (0.1%)
2	C2	0.26	0/3710	0.87	5/5778 (0.1%)
3	C3	0.26	0/1958	0.96	4/3050 (0.1%)
4	C4	0.29	0/2833	1.00	11/4414 (0.2%)
5	CB	0.27	0/2153	0.55	0/2926
6	CF	0.26	0/1972	0.55	0/2660
7	CH	0.26	0/5147	0.53	0/6926
8	CI	0.28	0/1265	0.61	0/1702
9	CJ	0.26	0/3196	0.51	0/4319
10	CK	0.26	0/1939	0.53	0/2608
11	CL	0.26	0/631	0.57	0/843
12	CM	0.27	0/1805	0.55	0/2417
12	LF	0.28	0/2061	0.54	0/2765
13	CN	0.25	0/1878	0.55	0/2555
14	CO	0.25	0/470	0.51	0/619
15	CQ	0.28	0/1504	0.62	1/2000 (0.1%)
16	CS	0.27	0/2109	0.53	0/2871
17	CT	0.26	0/3022	0.55	0/4132
17	CU	0.27	0/3034	0.58	1/4147 (0.0%)
18	CV	0.27	0/4312	0.55	2/5897 (0.0%)
18	CW	0.26	0/4299	0.51	0/5882
19	Cb	0.27	0/845	0.59	0/1128
20	Cd	0.25	0/3770	0.51	0/5082
21	Ce	0.26	0/2173	0.56	2/2890 (0.1%)
22	Cf	0.26	0/2326	0.54	0/3113
23	Cg	0.26	0/1508	0.54	0/2051
24	Ch	0.25	0/3908	0.54	0/5311
25	Cz	0.27	0/877	0.60	0/1148
26	LA	0.27	0/1488	0.57	0/2009
27	LB	0.26	0/3172	0.54	0/4260
28	LC	0.26	0/2808	0.52	0/3785
29	LD	0.26	0/2308	0.51	0/3105

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	LE	0.26	0/1504	0.53	1/2027 (0.0%)
31	LG	0.27	0/1918	0.52	0/2565
32	LH	0.25	0/1515	0.52	0/2037
33	LJ	0.25	0/1379	0.60	0/1844
34	LK	0.26	0/1198	0.57	0/1611
35	LL	0.25	0/1614	0.56	0/2168
36	LM	0.29	0/1145	0.57	0/1539
37	LN	0.25	0/1741	0.59	0/2332
38	LO	0.28	0/1645	0.53	0/2205
39	LP	0.25	0/1367	0.57	0/1840
40	LQ	0.26	0/1218	0.60	1/1639 (0.1%)
41	LR	0.25	0/1260	0.53	0/1683
42	LS	0.27	0/1461	0.54	0/1966
43	LT	0.26	0/1040	0.59	1/1401 (0.1%)
44	LU	0.27	0/859	0.50	0/1151
45	LV	0.27	0/1009	0.52	0/1357
46	LX	0.27	0/1151	0.58	2/1547 (0.1%)
47	LY	0.25	0/1070	0.58	0/1432
48	LZ	0.26	0/1135	0.54	0/1519
49	La	0.25	0/892	0.52	0/1200
50	Lc	0.27	0/714	0.54	0/960
51	Ld	0.25	0/889	0.55	0/1192
52	Le	0.24	0/1035	0.53	0/1379
53	Lf	0.26	0/883	0.56	0/1187
54	Lg	0.26	0/927	0.58	0/1244
55	Lh	0.29	0/1014	0.58	0/1349
56	Li	0.26	0/834	0.61	0/1099
57	Lj	0.26	0/712	0.61	0/944
58	Lk	0.29	0/640	0.61	1/850 (0.1%)
59	Ll	0.23	0/446	0.55	0/593
60	Lp	0.29	0/706	0.67	0/940
61	Lq	0.26	0/1091	0.56	0/1468
62	Lr	0.23	0/1055	0.41	0/1467
63	CR	0.27	0/2990	0.58	2/4073 (0.0%)
All	All	0.27	0/188812	0.74	137/272003 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	CT	0	1

There are no bond length outliers.

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	CV	351	PRO	CA-N-CD	-9.38	98.37	111.50
1	C1	1179	C	C2-N1-C1'	9.09	128.79	118.80
1	C1	1179	C	N1-C2-O2	9.05	124.33	118.90
1	C1	1935	C	C2-N1-C1'	8.82	128.50	118.80
1	C1	1478	U	C2-N1-C1'	8.82	128.28	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	CT	42	PHE	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
5	CB	259/391 (66%)	255 (98%)	4 (2%)	0	100	100
6	CF	243/270 (90%)	240 (99%)	3 (1%)	0	100	100
7	CH	621/661 (94%)	615 (99%)	6 (1%)	0	100	100
8	CI	150/414 (36%)	147 (98%)	3 (2%)	0	100	100
9	CJ	376/679 (55%)	373 (99%)	3 (1%)	0	100	100
10	CK	231/261 (88%)	226 (98%)	5 (2%)	0	100	100
11	CL	77/558 (14%)	76 (99%)	1 (1%)	0	100	100
12	CM	211/249 (85%)	206 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	LF	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
13	CN	244/246 (99%)	236 (97%)	8 (3%)	0	100	100
14	CO	56/120 (47%)	56 (100%)	0	0	100	100
15	CQ	181/225 (80%)	180 (99%)	1 (1%)	0	100	100
16	CS	264/338 (78%)	262 (99%)	2 (1%)	0	100	100
17	CT	393/437 (90%)	383 (98%)	10 (2%)	0	100	100
17	CU	393/437 (90%)	382 (97%)	11 (3%)	0	100	100
18	CV	544/781 (70%)	535 (98%)	9 (2%)	0	100	100
18	CW	544/781 (70%)	536 (98%)	8 (2%)	0	100	100
19	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
20	Cd	458/627 (73%)	449 (98%)	9 (2%)	0	100	100
21	Ce	252/443 (57%)	250 (99%)	2 (1%)	0	100	100
22	Cf	281/350 (80%)	279 (99%)	2 (1%)	0	100	100
23	Cg	186/202 (92%)	185 (100%)	1 (0%)	0	100	100
24	Ch	483/517 (93%)	469 (97%)	14 (3%)	0	100	100
25	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
26	LA	189/254 (74%)	183 (97%)	6 (3%)	0	100	100
27	LB	387/392 (99%)	380 (98%)	7 (2%)	0	100	100
28	LC	361/365 (99%)	357 (99%)	4 (1%)	0	100	100
29	LD	282/304 (93%)	280 (99%)	2 (1%)	0	100	100
30	LE	187/200 (94%)	183 (98%)	4 (2%)	0	100	100
31	LG	233/262 (89%)	230 (99%)	3 (1%)	0	100	100
32	LH	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
33	LJ	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
34	LK	156/165 (94%)	156 (100%)	0	0	100	100
35	LL	201/213 (94%)	200 (100%)	1 (0%)	0	100	100
36	LM	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
37	LN	200/203 (98%)	194 (97%)	6 (3%)	0	100	100
38	LO	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
39	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
40	LQ	148/213 (70%)	145 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
42	LS	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
43	LT	127/160 (79%)	126 (99%)	1 (1%)	0	100	100
44	LU	103/127 (81%)	102 (99%)	1 (1%)	0	100	100
45	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
46	LX	143/156 (92%)	139 (97%)	4 (3%)	0	100	100
47	LY	131/138 (95%)	128 (98%)	3 (2%)	0	100	100
48	LZ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
49	La	104/149 (70%)	104 (100%)	0	0	100	100
50	Lc	93/108 (86%)	93 (100%)	0	0	100	100
51	Ld	108/120 (90%)	107 (99%)	1 (1%)	0	100	100
52	Le	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
53	Lf	106/109 (97%)	106 (100%)	0	0	100	100
54	Lg	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
55	Lh	120/935 (13%)	116 (97%)	4 (3%)	0	100	100
56	Li	99/110 (90%)	98 (99%)	1 (1%)	0	100	100
57	Lj	86/95 (90%)	84 (98%)	2 (2%)	0	100	100
58	Lk	74/94 (79%)	73 (99%)	1 (1%)	0	100	100
59	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
60	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
61	Lq	137/147 (93%)	132 (96%)	5 (4%)	0	100	100
62	Lr	212/217 (98%)	207 (98%)	5 (2%)	0	100	100
63	CR	386/767 (50%)	379 (98%)	7 (2%)	0	100	100
All	All	13094/20153 (65%)	12881 (98%)	213 (2%)	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	
5	CB	227/329 (69%)	226 (100%)	1 (0%)	91	97
6	CF	212/236 (90%)	212 (100%)	0	100	100
7	CH	549/575 (96%)	549 (100%)	0	100	100
8	CI	124/336 (37%)	123 (99%)	1 (1%)	81	94
9	CJ	331/579 (57%)	331 (100%)	0	100	100
10	CK	206/225 (92%)	206 (100%)	0	100	100
11	CL	61/458 (13%)	61 (100%)	0	100	100
12	CM	185/215 (86%)	185 (100%)	0	100	100
12	LF	213/215 (99%)	213 (100%)	0	100	100
13	CN	205/206 (100%)	205 (100%)	0	100	100
14	CO	48/99 (48%)	48 (100%)	0	100	100
15	CQ	144/192 (75%)	144 (100%)	0	100	100
16	CS	216/291 (74%)	216 (100%)	0	100	100
17	CT	324/376 (86%)	324 (100%)	0	100	100
17	CU	328/376 (87%)	328 (100%)	0	100	100
18	CV	472/675 (70%)	472 (100%)	0	100	100
18	CW	469/675 (70%)	467 (100%)	2 (0%)	91	97
19	Cb	85/101 (84%)	85 (100%)	0	100	100
20	Cd	403/541 (74%)	402 (100%)	1 (0%)	93	98
21	Ce	223/383 (58%)	223 (100%)	0	100	100
22	Cf	250/310 (81%)	250 (100%)	0	100	100
23	Cg	158/176 (90%)	158 (100%)	0	100	100
24	Ch	407/436 (93%)	407 (100%)	0	100	100
25	Cz	89/107 (83%)	89 (100%)	0	100	100
26	LA	150/198 (76%)	150 (100%)	0	100	100
27	LB	329/331 (99%)	329 (100%)	0	100	100
28	LC	282/285 (99%)	282 (100%)	0	100	100
29	LD	221/253 (87%)	221 (100%)	0	100	100
30	LE	157/166 (95%)	157 (100%)	0	100	100
31	LG	200/222 (90%)	200 (100%)	0	100	100
32	LH	167/200 (84%)	167 (100%)	0	100	100
33	LJ	140/150 (93%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	LK	127/136 (93%)	127 (100%)	0	100	100
35	LL	158/176 (90%)	158 (100%)	0	100	100
36	LM	116/117 (99%)	116 (100%)	0	100	100
37	LN	179/180 (99%)	179 (100%)	0	100	100
38	LO	162/163 (99%)	162 (100%)	0	100	100
39	LP	134/152 (88%)	134 (100%)	0	100	100
40	LQ	128/178 (72%)	127 (99%)	1 (1%)	81	94
41	LR	125/2396 (5%)	125 (100%)	0	100	100
42	LS	152/154 (99%)	152 (100%)	0	100	100
43	LT	108/135 (80%)	108 (100%)	0	100	100
44	LU	92/108 (85%)	92 (100%)	0	100	100
45	LV	98/102 (96%)	98 (100%)	0	100	100
46	LX	122/129 (95%)	121 (99%)	1 (1%)	81	94
47	LY	116/119 (98%)	115 (99%)	1 (1%)	78	93
48	LZ	121/121 (100%)	121 (100%)	0	100	100
49	La	93/122 (76%)	93 (100%)	0	100	100
50	Lc	76/88 (86%)	76 (100%)	0	100	100
51	Ld	90/105 (86%)	90 (100%)	0	100	100
52	Le	109/114 (96%)	109 (100%)	0	100	100
53	Lf	89/90 (99%)	89 (100%)	0	100	100
54	Lg	95/102 (93%)	95 (100%)	0	100	100
55	Lh	109/781 (14%)	109 (100%)	0	100	100
56	Li	85/93 (91%)	85 (100%)	0	100	100
57	Lj	72/78 (92%)	71 (99%)	1 (1%)	67	89
58	Lk	73/88 (83%)	72 (99%)	1 (1%)	67	89
59	Ll	45/46 (98%)	45 (100%)	0	100	100
60	Lp	73/74 (99%)	73 (100%)	0	100	100
61	Lq	109/112 (97%)	108 (99%)	1 (1%)	78	93
63	CR	293/663 (44%)	292 (100%)	1 (0%)	92	98
All	All	10924/16839 (65%)	10912 (100%)	12 (0%)	93	98

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	LY	2	LYS
57	Lj	84	LYS
63	CR	436	LYS
58	Lk	18	LYS
18	CW	554	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
19	Cb	68	HIS
32	LH	5	HIS
55	Lh	37	GLN
37	LN	91	GLN
17	CU	30	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3127/3342 (93%)	587 (18%)	23 (0%)
2	C2	155/156 (99%)	22 (14%)	0
3	C3	80/162 (49%)	21 (26%)	0
4	C4	118/119 (99%)	24 (20%)	1 (0%)
All	All	3480/3779 (92%)	654 (18%)	24 (0%)

5 of 654 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	4	U
1	C1	6	G
1	C1	27	A
1	C1	44	A
1	C1	50	A

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	3079	U
1	C1	3210	U
1	C1	3205	G
1	C1	3230	G
1	C1	1267	C

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

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	OMC	C1	778	1	19,22,23	0.58	0	26,31,34	0.95	1 (3%)
1	OMG	C1	2881	1	18,26,27	1.12	2 (11%)	19,38,41	0.83	1 (5%)
1	OMG	C1	787	1	18,26,27	1.14	2 (11%)	19,38,41	0.89	1 (5%)
1	OMG	C1	2358	1	18,26,27	1.15	2 (11%)	19,38,41	0.85	1 (5%)
1	A2M	C1	1223	1	18,25,26	4.31	9 (50%)	18,36,39	3.84	4 (22%)
1	A2M	C1	389	1	18,25,26	4.33	9 (50%)	18,36,39	3.80	4 (22%)
1	OMG	C1	646	1	18,26,27	1.14	2 (11%)	19,38,41	0.88	2 (10%)
1	OMC	C1	1420	1	19,22,23	0.62	0	26,31,34	1.42	4 (15%)
1	OMU	C1	1868	1	19,22,23	3.09	6 (31%)	26,31,34	1.73	5 (19%)
1	OMU	C1	2277	1	19,22,23	3.07	6 (31%)	26,31,34	1.65	4 (15%)
1	A2M	C1	1847	1	18,25,26	4.35	9 (50%)	18,36,39	3.93	4 (22%)
1	OMG	C1	1433	1	18,26,27	1.13	2 (11%)	19,38,41	0.84	1 (5%)
1	OMU	C1	2380	1	19,22,23	3.06	6 (31%)	26,31,34	1.69	5 (19%)
1	OMC	C1	2918	1	19,22,23	0.57	0	26,31,34	0.81	1 (3%)
1	OMC	C1	1812	1	19,22,23	0.56	0	26,31,34	1.07	2 (7%)
1	OMG	C1	2578	1	18,26,27	1.14	2 (11%)	19,38,41	0.89	1 (5%)
1	OMU	C1	2688	1	19,22,23	3.08	6 (31%)	26,31,34	1.68	5 (19%)
1	OMG	C1	385	1	18,26,27	1.12	2 (11%)	19,38,41	0.83	1 (5%)
1	A2M	C1	1432	1	18,25,26	4.36	9 (50%)	18,36,39	3.84	4 (22%)
1	OMG	C1	2876	1	18,26,27	1.13	2 (11%)	19,38,41	0.85	1 (5%)
1	A2M	C1	637	1	18,25,26	4.33	9 (50%)	18,36,39	3.89	4 (22%)
1	A2M	C1	858	1	18,25,26	4.37	9 (50%)	18,36,39	3.85	4 (22%)
1	OMG	C1	2774	1	18,26,27	1.12	2 (11%)	19,38,41	0.87	1 (5%)
1	OMC	C1	2838	1	19,22,23	0.68	0	26,31,34	1.50	4 (15%)
1	OMU	C1	2690	1	19,22,23	3.05	6 (31%)	26,31,34	1.69	5 (19%)
1	OMU	C1	2384	1	19,22,23	3.06	6 (31%)	26,31,34	1.66	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	C1	848	1	18,25,26	4.34	9 (50%)	18,36,39	3.79	4 (22%)
1	OMC	C1	1491	1	19,22,23	0.55	0	26,31,34	0.80	1 (3%)
1	OMU	C1	1917	1	19,22,23	3.09	6 (31%)	26,31,34	1.73	5 (19%)
1	OMC	C1	2300	1	19,22,23	0.53	0	26,31,34	0.73	1 (3%)
1	OMU	C1	2683	1	19,22,23	3.03	6 (31%)	26,31,34	1.62	5 (19%)
1	OMC	C1	1836	1	19,22,23	0.57	0	26,31,34	0.80	1 (3%)
1	A2M	C1	2289	1	18,25,26	4.36	9 (50%)	18,36,39	3.76	4 (22%)
1	OMG	C1	627	1	18,26,27	1.15	2 (11%)	19,38,41	0.88	1 (5%)

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	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2881	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	787	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	2358	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	1223	1	-	1/5/27/28	0/3/3/3
1	A2M	C1	389	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	646	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	1420	1	-	3/9/27/28	0/2/2/2
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2277	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	1847	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	1433	1	-	2/5/27/28	0/3/3/3
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1812	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	2578	1	-	3/5/27/28	0/3/3/3
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	385	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	1432	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	2876	1	-	1/5/27/28	0/3/3/3
1	A2M	C1	637	1	-	1/5/27/28	0/3/3/3
1	A2M	C1	858	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	2774	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMU	C1	2384	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	848	1	-	1/5/27/28	0/3/3/3
1	OMC	C1	1491	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	1917	1	-	3/9/27/28	0/2/2/2
1	OMC	C1	2300	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	2289	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	627	1	-	0/5/27/28	0/3/3/3

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'	-12.81	1.24	1.52
1	C1	2289	A2M	C3'-C2'	-12.80	1.24	1.52
1	C1	848	A2M	C3'-C2'	-12.71	1.24	1.52
1	C1	1432	A2M	C3'-C2'	-12.69	1.24	1.52
1	C1	1847	A2M	C3'-C2'	-12.67	1.24	1.52

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C4	10.92	145.83	126.64
1	C1	637	A2M	C1'-N9-C4	10.78	145.57	126.64
1	C1	1432	A2M	C1'-N9-C4	10.52	145.12	126.64
1	C1	858	A2M	C1'-N9-C4	10.50	145.09	126.64
1	C1	1223	A2M	C1'-N9-C4	10.40	144.91	126.64

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	637	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'
1	C1	1812	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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$
64	GTP	CH	701	65	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
64	GTP	Cd	1000	65	26,34,34	1.15	2 (7%)	32,54,54	1.54	6 (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
64	GTP	CH	701	65	-	3/18/38/38	0/3/3/3
64	GTP	Cd	1000	65	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	Cd	1000	GTP	C5-C6	-4.13	1.39	1.47
64	CH	701	GTP	C5-C6	-4.04	1.39	1.47
64	CH	701	GTP	C2-N3	2.17	1.38	1.33
64	Cd	1000	GTP	C2-N3	2.09	1.38	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	CH	701	GTP	PB-O3B-PG	-3.73	120.03	132.83
64	Cd	1000	GTP	PB-O3B-PG	-3.47	120.90	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	CH	701	GTP	PA-O3A-PB	-3.42	121.11	132.83
64	CH	701	GTP	C5-C6-N1	3.22	119.63	113.95
64	Cd	1000	GTP	C5-C6-N1	3.21	119.63	113.95

There are no chirality outliers.

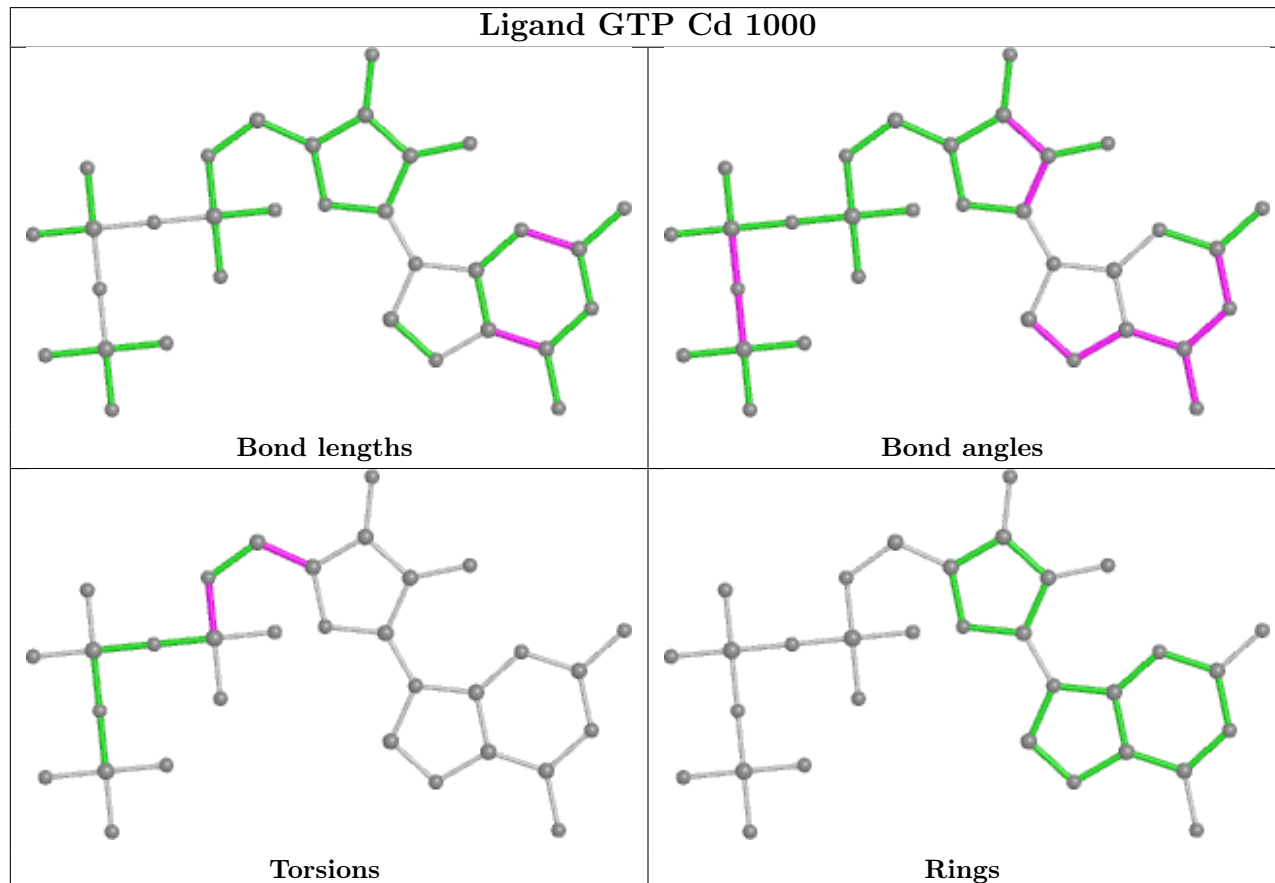
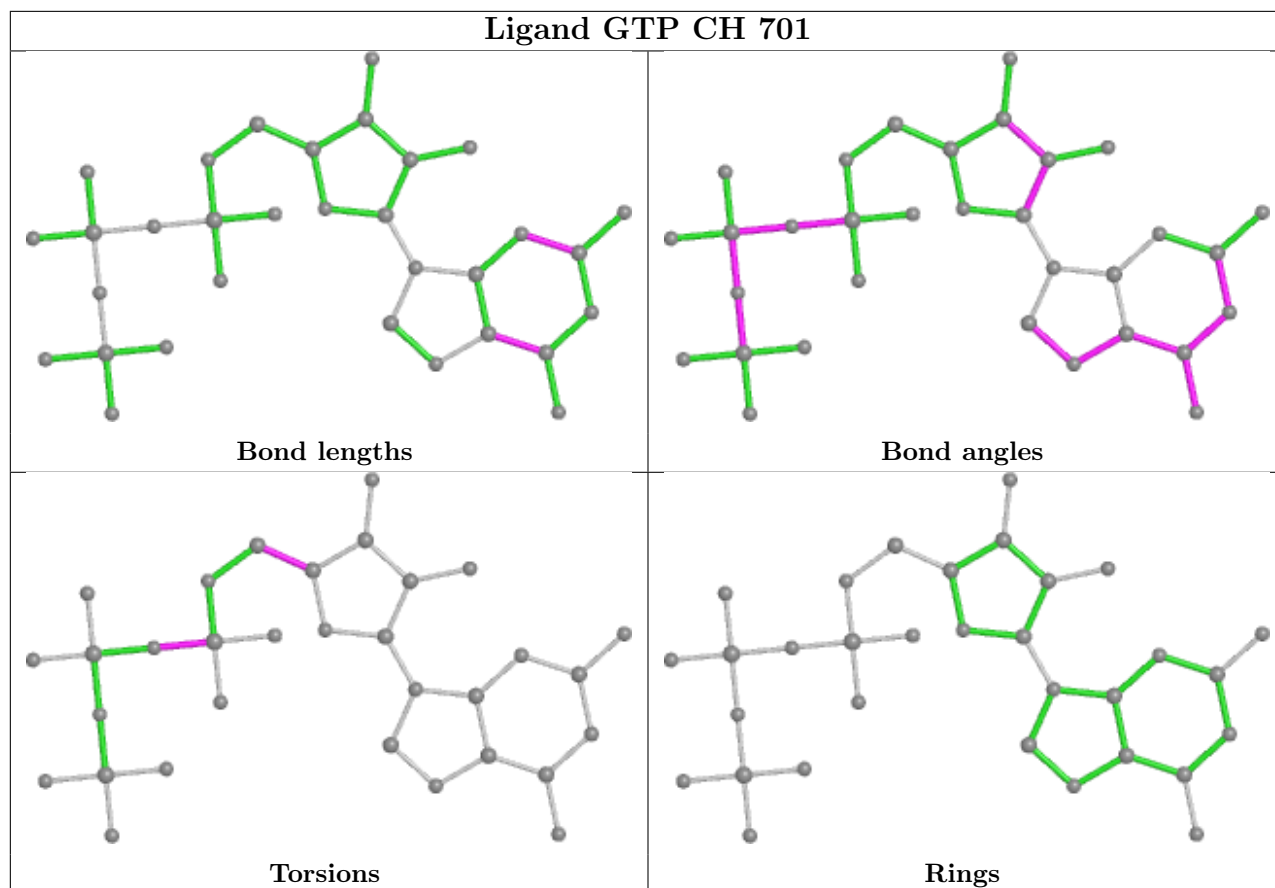
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	Cd	1000	GTP	C5'-O5'-PA-O1A
64	Cd	1000	GTP	C3'-C4'-C5'-O5'
64	Cd	1000	GTP	O4'-C4'-C5'-O5'
64	CH	701	GTP	O4'-C4'-C5'-O5'
64	CH	701	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

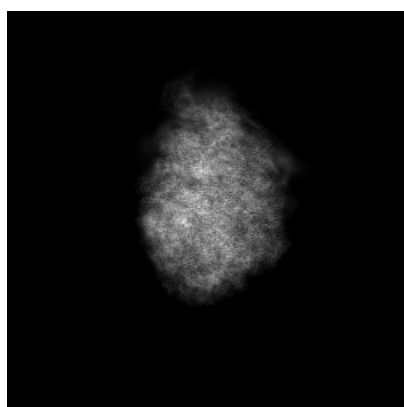
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17953. These allow visual inspection of the internal detail of the map and identification of artifacts.

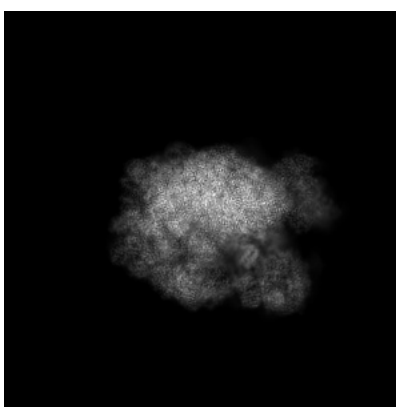
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

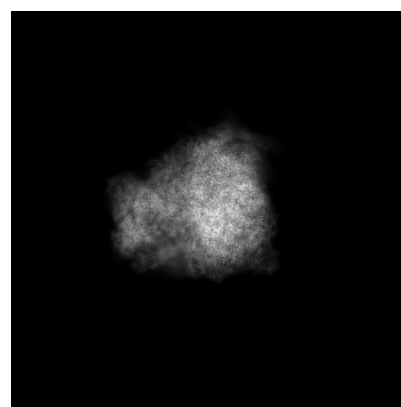
6.1.1 Primary map



X



Y



Z

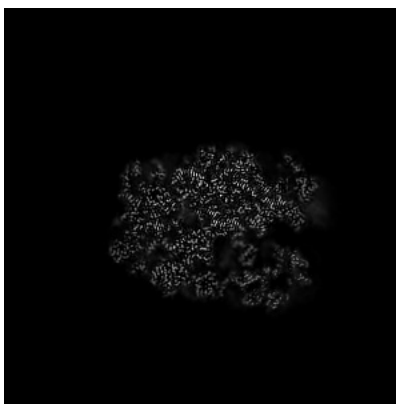
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

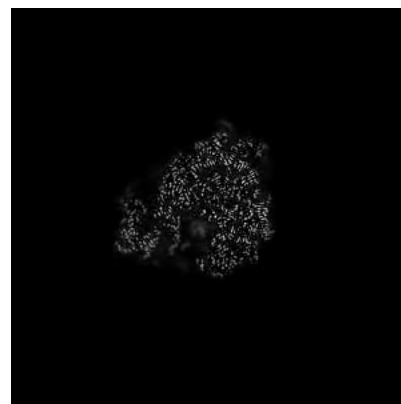
6.2.1 Primary map



X Index: 250



Y Index: 250

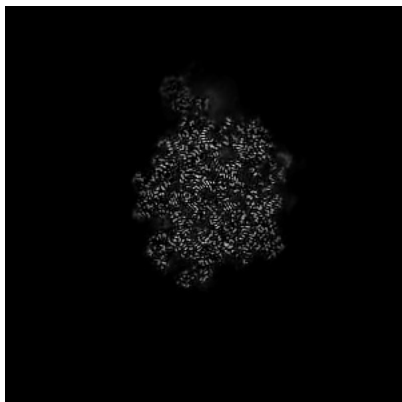


Z Index: 250

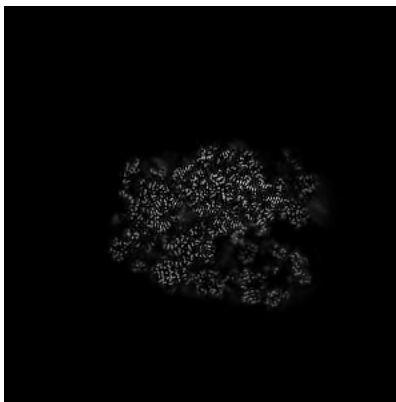
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

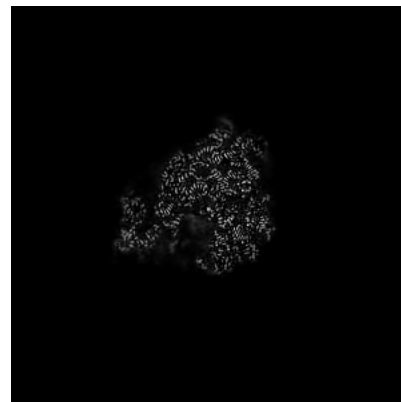
6.3.1 Primary map



X Index: 259



Y Index: 248

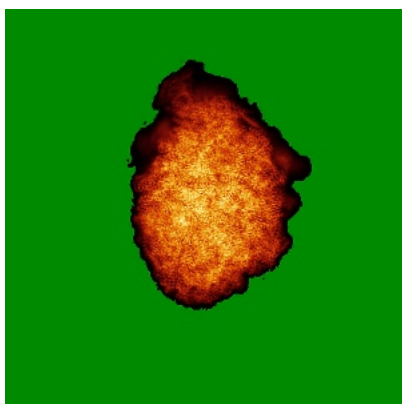


Z Index: 252

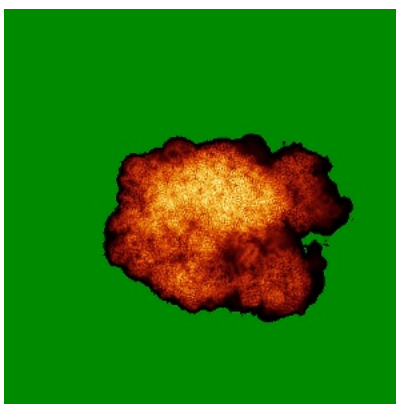
The images above show the largest variance slices of the map in three orthogonal directions.

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

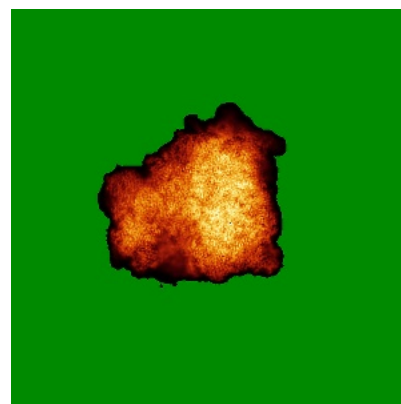
6.4.1 Primary map



X



Y

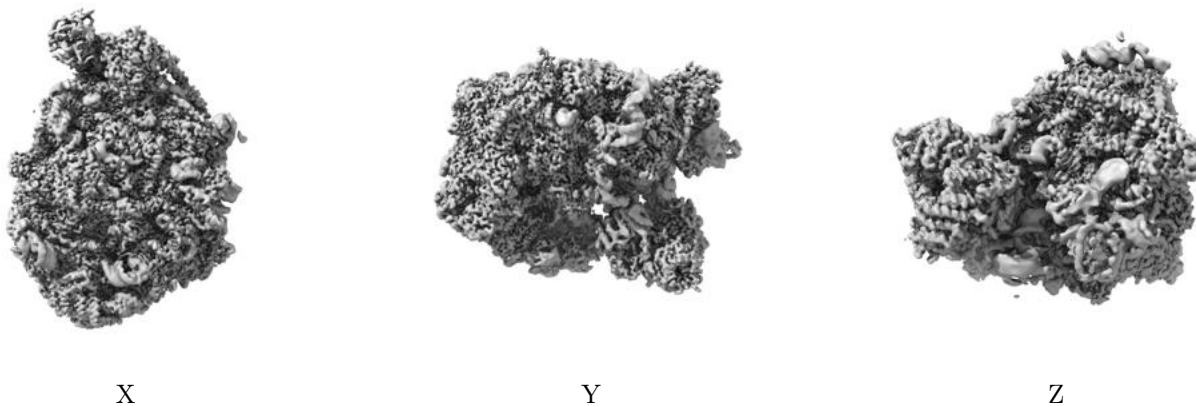


Z

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 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

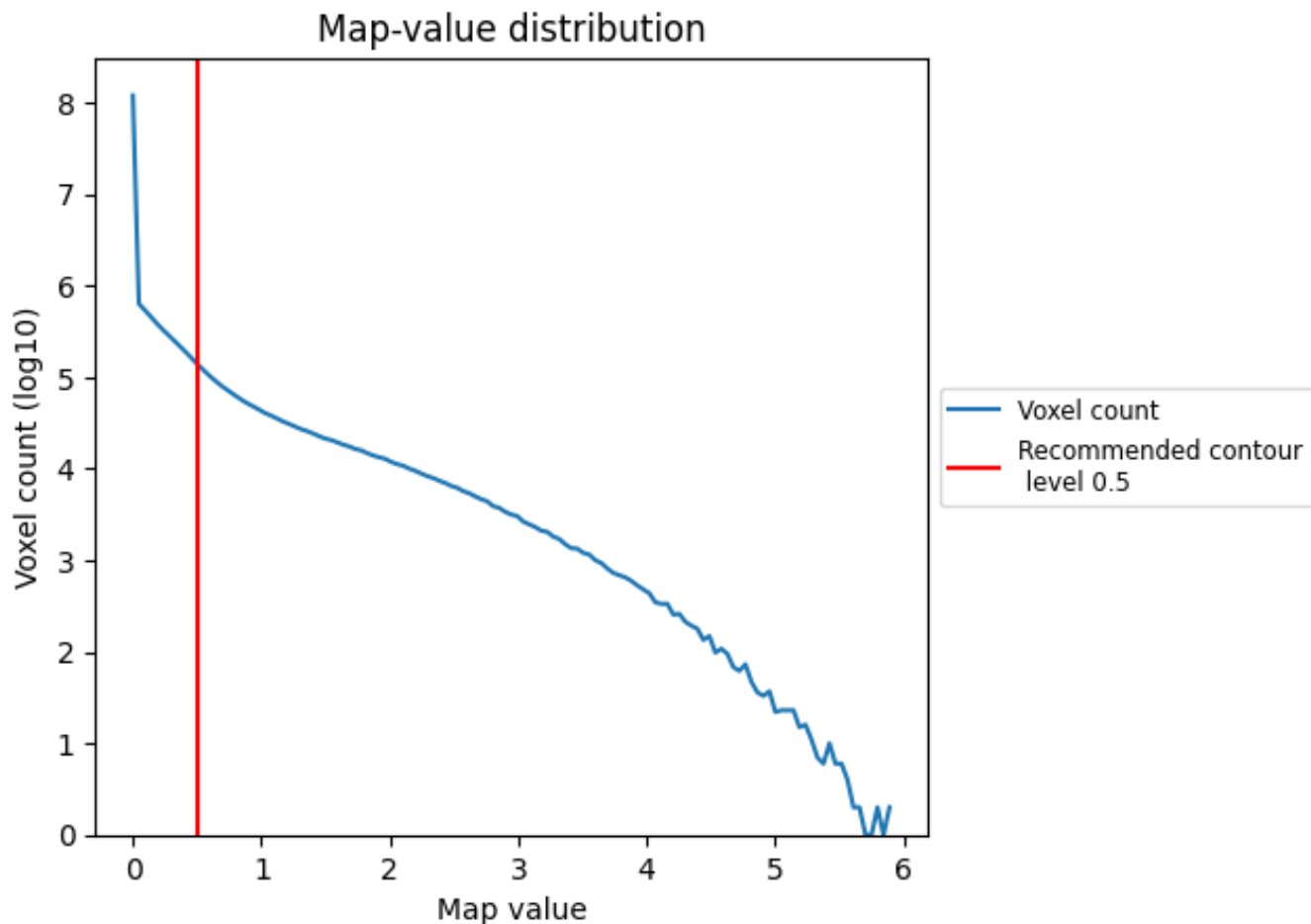
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

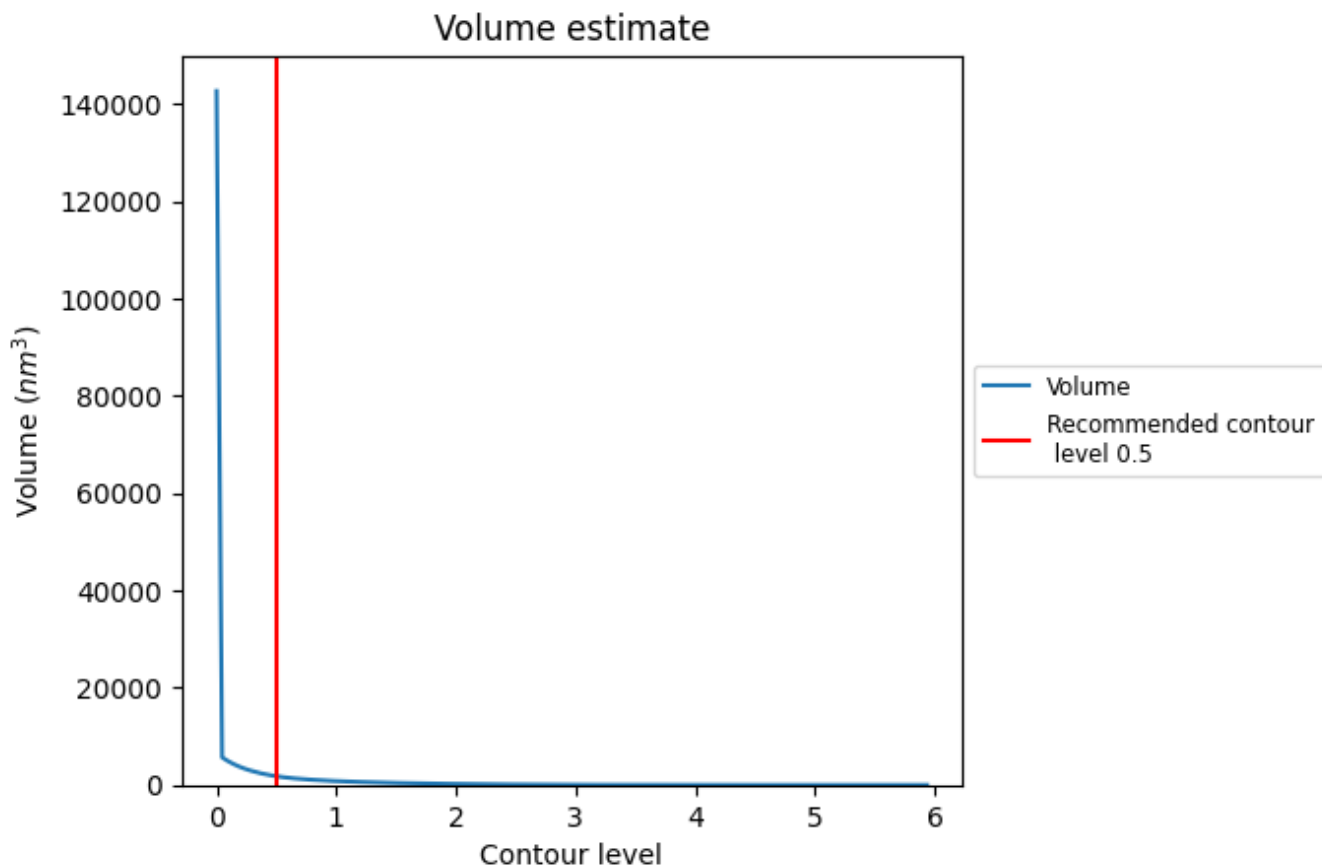
This section contains the results of statistical analysis of the map.

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.

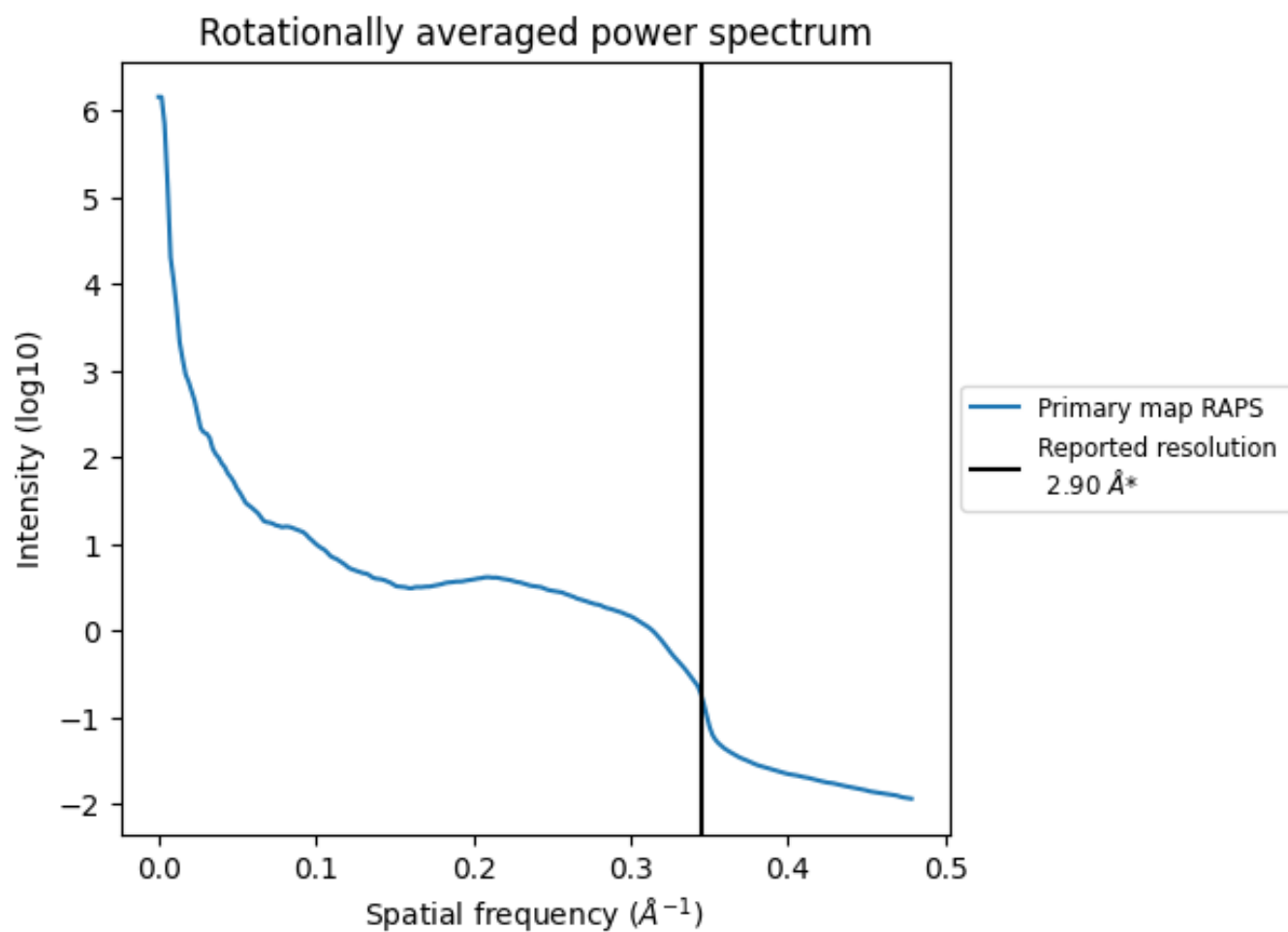
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1795 nm³; this corresponds to an approximate mass of 1622 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

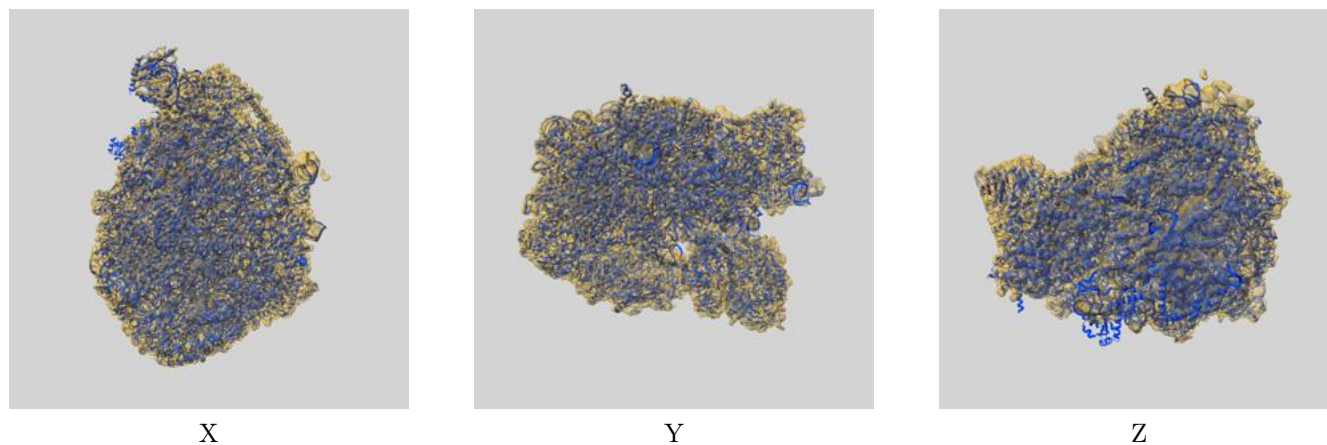
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

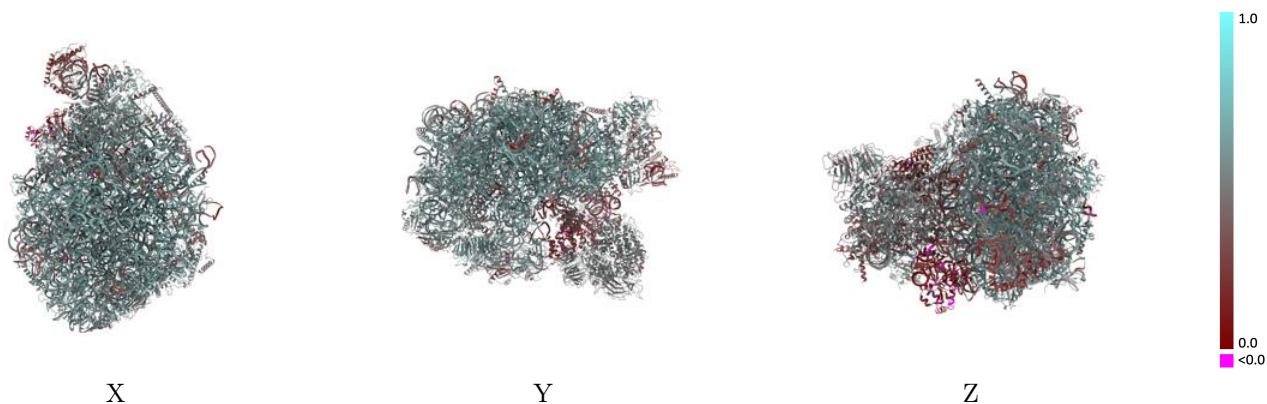
This section contains information regarding the fit between EMDB map EMD-17953 and PDB model 8PV4. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



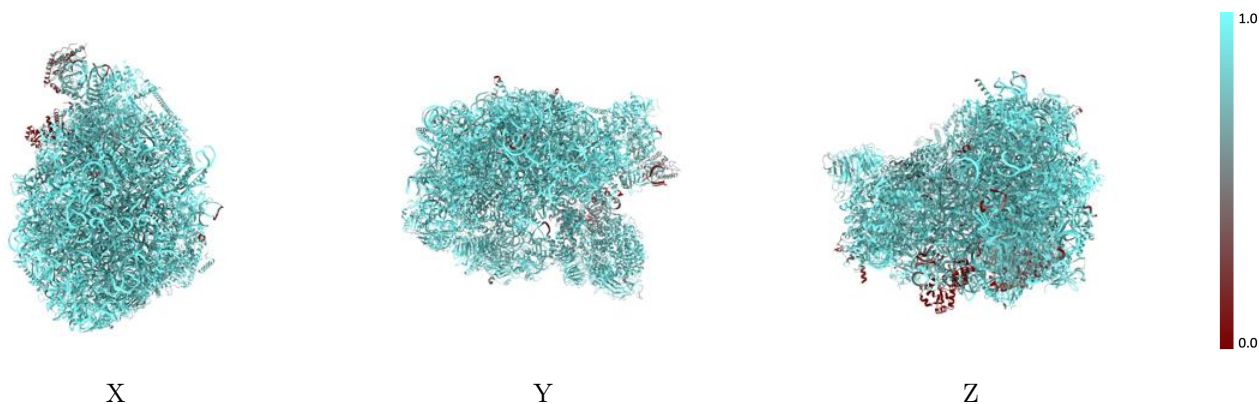
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



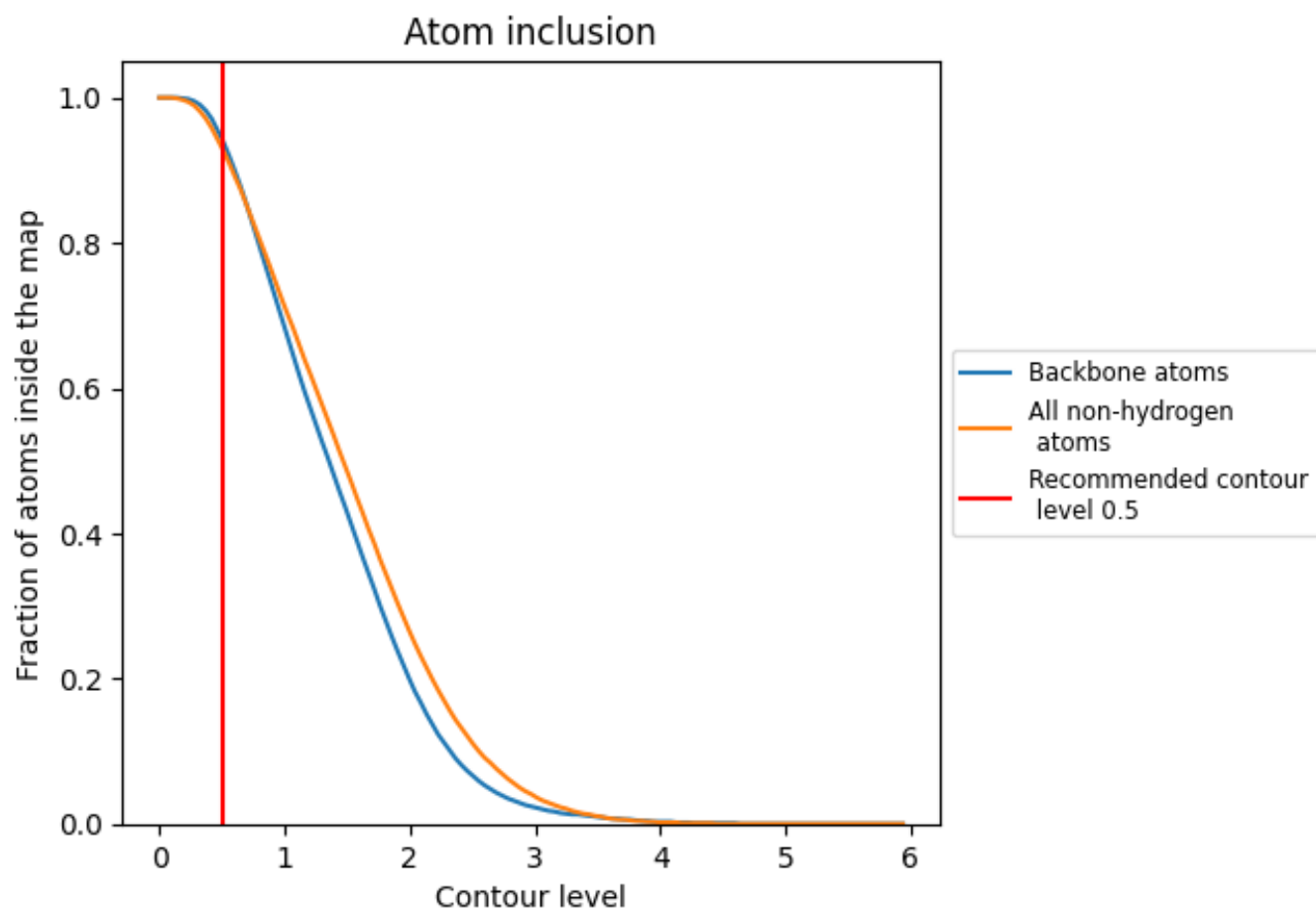
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9310	 0.5350
C1	 0.9750	 0.5590
C2	 0.9770	 0.5980
C3	 0.7060	 0.3310
C4	 0.9720	 0.5060
CB	 0.5850	 0.3470
CF	 0.9140	 0.5230
CH	 0.9130	 0.5410
CI	 0.7490	 0.4200
CJ	 0.9590	 0.5600
CK	 0.9700	 0.5960
CL	 0.9170	 0.5060
CM	 0.8960	 0.4900
CN	 0.9460	 0.5630
CO	 0.9010	 0.5510
CQ	 0.8990	 0.5410
CR	 0.7680	 0.2830
CS	 0.7710	 0.2640
CT	 0.8610	 0.4660
CU	 0.9010	 0.4720
CV	 0.8630	 0.4530
CW	 0.8840	 0.4640
Cb	 0.9530	 0.5560
Cd	 0.9540	 0.5690
Ce	 0.8550	 0.4760
Cf	 0.9500	 0.5510
Cg	 0.9320	 0.5280
Ch	 0.9180	 0.5350
Cz	 0.8370	 0.4620
LA	 0.9820	 0.5900
LB	 0.9720	 0.6040
LC	 0.9650	 0.5970
LD	 0.9260	 0.5320
LE	 0.9320	 0.5540
LF	 0.9410	 0.5710



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Chain	Atom inclusion	Q-score
LG	 0.9560	 0.5670
LH	 0.9450	 0.5740
LJ	 0.9120	 0.4830
LK	 0.8650	 0.4690
LL	 0.9430	 0.5680
LM	 0.9470	 0.5740
LN	 0.9900	 0.6170
LO	 0.9760	 0.6050
LP	 0.9780	 0.6040
LQ	 0.9360	 0.5680
LR	 0.9710	 0.5860
LS	 0.9640	 0.5840
LT	 0.8910	 0.4810
LU	 0.9160	 0.5320
LV	 0.9770	 0.6000
LX	 0.9510	 0.5660
LY	 0.9480	 0.5750
LZ	 0.9660	 0.5760
La	 0.9590	 0.5830
Lc	 0.9380	 0.5520
Ld	 0.9560	 0.5960
Le	 0.9730	 0.6050
Lf	 0.9860	 0.6210
Lg	 0.9200	 0.5770
Lh	 0.9470	 0.5430
Li	 0.9440	 0.5300
Lj	 0.9900	 0.6260
Lk	 0.9210	 0.5400
Ll	 0.9930	 0.6360
Lp	 0.9350	 0.5460
Lq	 0.9590	 0.5760
Lr	 0.1740	 0.1330