



Full wwPDB EM Validation Report ⓘ

Nov 7, 2023 – 05:10 am GMT

PDB ID : 8PV3
EMDB ID : EMD-17952
Title : Chaetomium thermophilum pre-60S State 9 - pre-5S rotation - immature
H68/H69 - composite structure
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

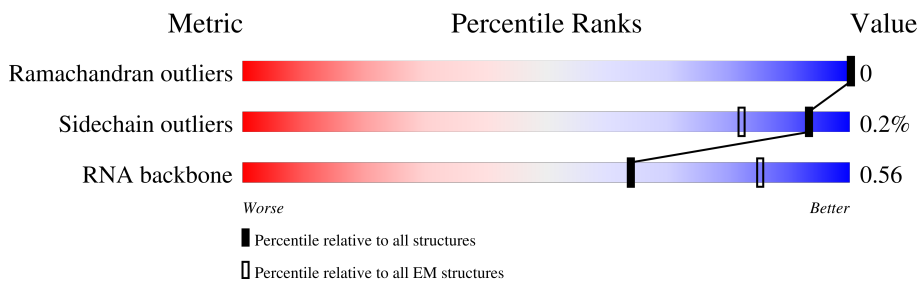
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 2.80 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.




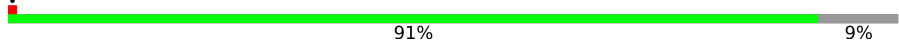


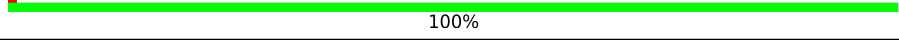
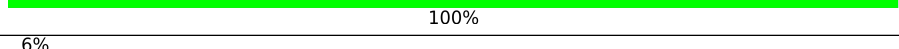

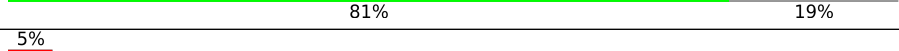
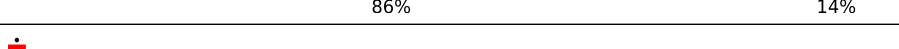
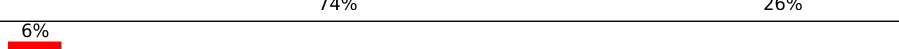
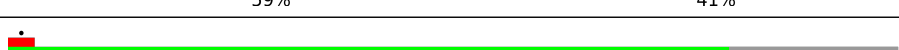

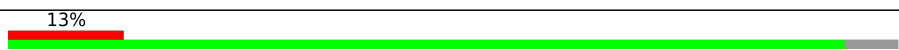

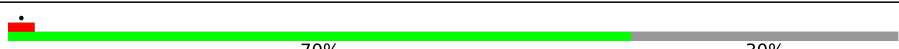
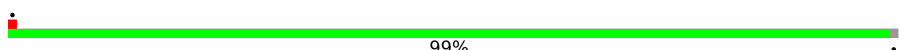
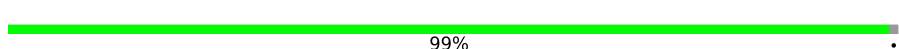
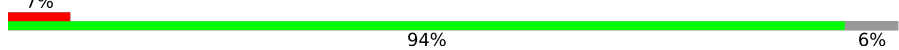
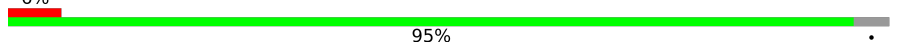

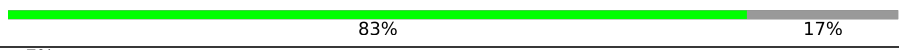
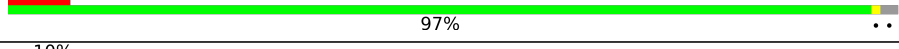
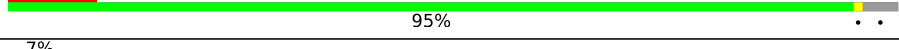
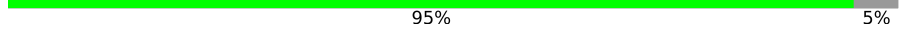

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	71% 17% 10%
2	C2	156	83% 15%
3	C3	162	36% 14% 49%
4	C4	119	76% 23%
5	CB	391	68% 32%
6	CF	270	91% 9%
7	CH	661	95% 5%
8	CI	414	36% 63%

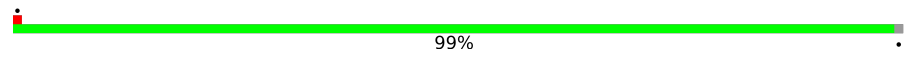
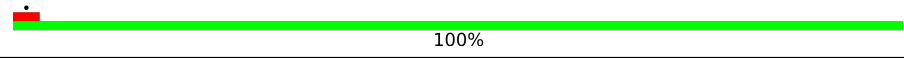
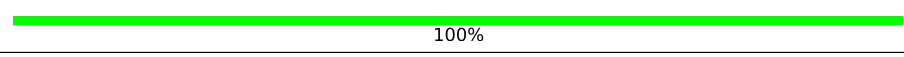
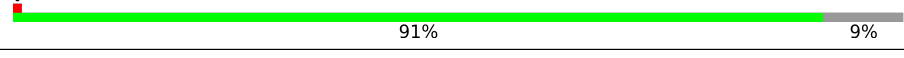
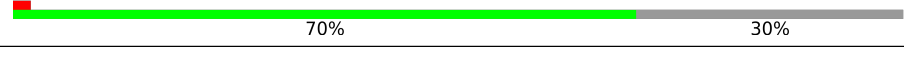
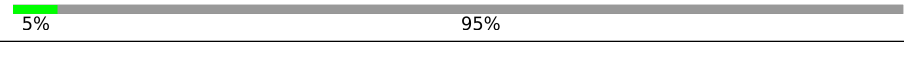
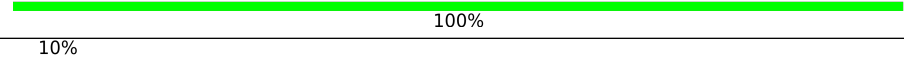
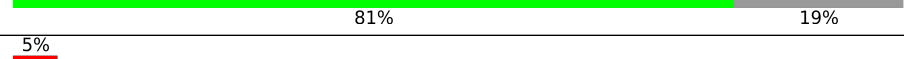

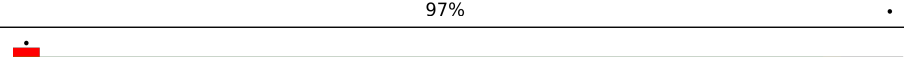
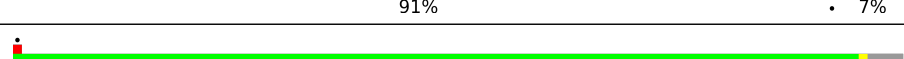
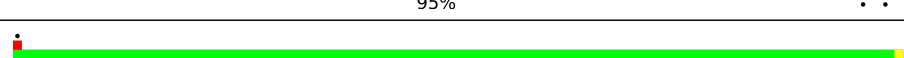
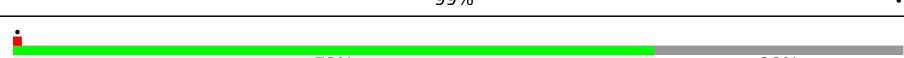
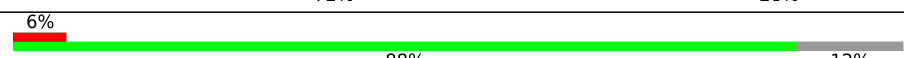
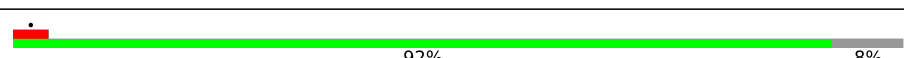
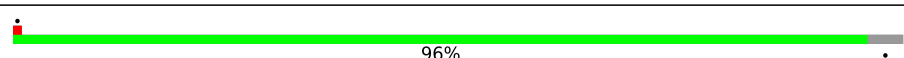
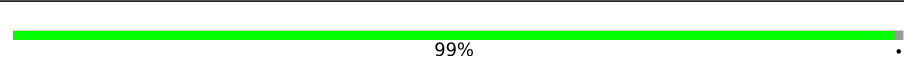
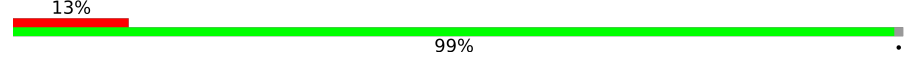

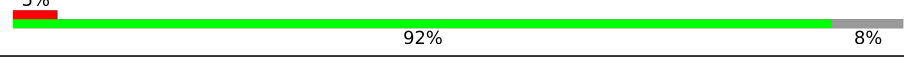
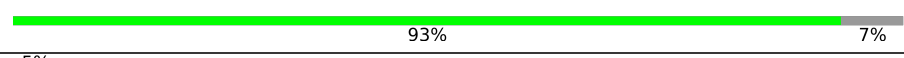

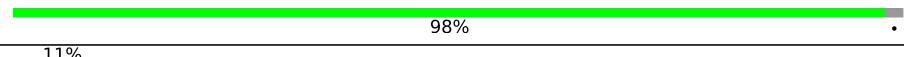
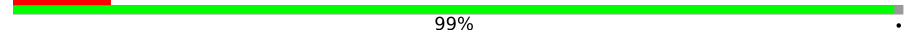

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Mol	Chain	Length	Quality of chain
9	CJ	679	 56% 44%
10	CK	261	 91% 9%
11	CL	558	 14% 86%
12	CM	249	 8% 87% 13%
12	LF	249	 100%
13	CN	246	 100%
14	CO	120	 6% 52% 48%
15	CQ	225	 12% 81% 19%
16	Cb	117	 5% 86% 14%
17	Cd	627	 74% 26%
18	Ce	443	 6% 59% 41%
19	Cf	350	 81% 19%
20	Cg	202	 8% 93% 7%
21	Ch	517	 13% 94% 6%
22	Cz	123	 8% 80% 18% 2%
23	LA	254	 70% 30%
24	LB	392	 99%
25	LC	365	 99%
26	LD	304	 7% 94% 6%
27	LE	200	 6% 95% 1%
28	LG	262	 5% 90% 10%
29	LH	229	 83% 17%
30	LJ	173	 7% 97% 2% 2%
31	LK	165	 10% 95% 1% 2%
32	LL	213	 7% 95% 5%

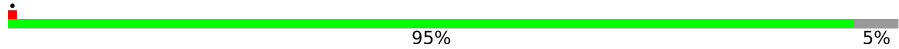
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Mol	Chain	Length	Quality of chain
33	LM	142	 99%
34	LN	203	 100%
35	LO	204	 100%
36	LP	187	 91% 9%
37	LQ	213	 70% 30%
38	LR	2898	 5% 95%
39	LS	174	 100%
40	LT	160	 10% 81% 19%
41	LU	127	 5% 83% 17%
42	LV	139	 97%
43	LX	156	 91% 7%
44	LY	138	 95%
45	LZ	135	 99%
46	La	149	 72% 28%
47	Lc	108	 6% 88% 12%
48	Ld	120	 92% 8%
49	Le	131	 96%
50	Lf	109	 99%
51	Lg	119	 13% 99%
52	Lh	935	 13% 87%
53	Li	110	 5% 92% 8%
54	Lj	95	 93% 7%
55	Lk	94	 5% 80% 19%
56	Ll	51	 98%
57	Lp	92	 11% 99%

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Mol	Chain	Length	Quality of chain
58	Lq	147	 A horizontal bar chart representing the quality of the chain. The bar is 95% green and 5% grey. The green portion is labeled '95%' and the grey portion is labeled '5%'. A small red dot is visible at the beginning of the bar.

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 155443 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	2998	64177	28664	11614	20901	2998	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	267	2119	1359	373	384	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 Zinc finger domain-containing protein.

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

- Molecule 17 is a protein called Nucleolar GTP-binding protein 2.

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

- Molecule 18 is a protein called Ribosome biogenesis protein NOP53.

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

- Molecule 19 is a protein called Ribosome production factor 2 homolog.

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

- Molecule 20 is a protein called Ribosome biogenesis regulatory protein.

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

- Molecule 21 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Ch	485	3812	2396	696	710	10	1	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 22 is a protein called rRNA-processing protein.

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

- Molecule 23 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LA	178	1365	863	260	240	2	0	0

- Molecule 24 is a protein called 60S ribosomal protein L3-like protein.

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

- Molecule 25 is a protein called 60S ribosomal protein L4-like protein.

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

- Molecule 26 is a protein called 60S ribosomal protein l5-like protein.

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

- Molecule 27 is a protein called 60S ribosomal protein L6.

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

- Molecule 28 is a protein called 60S ribosomal protein L8.

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

- Molecule 29 is a protein called 60S ribosomal protein L9-like protein.

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

- Molecule 30 is a protein called Putative ribosomal protein.

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

- Molecule 31 is a protein called 60S ribosomal protein L12-like protein.

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

- Molecule 32 is a protein called 60S ribosomal protein L13.

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

- Molecule 33 is a protein called 60S ribosomal protein L14-like protein.

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

- Molecule 34 is a protein called Ribosomal protein L15.

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

- Molecule 35 is a protein called 60S ribosomal protein L16-like protein.

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

- Molecule 36 is a protein called 60S ribosomal protein l17-like protein.

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

- Molecule 37 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LQ	150	Total	C	N	O	S	0	0
			1181	745	234	200	2		

- Molecule 38 is a protein called Ribosomal protein L19.

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

- Molecule 39 is a protein called 60S ribosomal protein L20.

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

- Molecule 40 is a protein called 60S ribosomal protein l21-like protein.

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

- Molecule 41 is a protein called 60S ribosomal protein L22-like protein.

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

- Molecule 42 is a protein called 60S ribosomal protein l23-like protein.

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

- Molecule 43 is a protein called 60S ribosomal protein L25-like protein.

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

- Molecule 44 is a protein called 60S ribosomal protein L26-like protein.

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

- Molecule 45 is a protein called 60S ribosomal protein L27.

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

- Molecule 46 is a protein called 60S ribosomal protein L28-like protein.

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

- Molecule 47 is a protein called 60S ribosomal protein l30-like protein.

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

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

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

- Molecule 49 is a protein called 60S ribosomal protein L32-like protein.

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

- Molecule 50 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 51 is a protein called Ribosomal protein l34-like protein.

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

- Molecule 52 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

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

- Molecule 53 is a protein called 60S ribosomal protein L36.

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

- Molecule 54 is a protein called Ribosomal protein L37.

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

- Molecule 55 is a protein called 60S ribosomal protein L38-like protein.

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

- Molecule 56 is a protein called Ribosomal protein eL39.

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

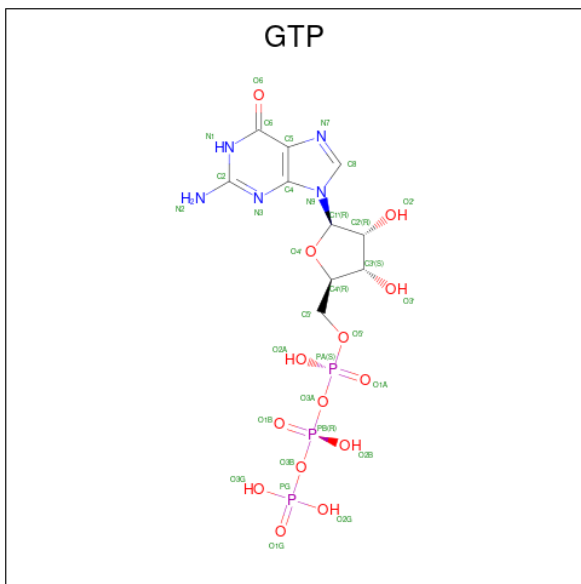
- Molecule 57 is a protein called 60S ribosomal protein L43-like protein.

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

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

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

- Molecule 59 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	
59	CH	1	32	10	5	14	3	0

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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

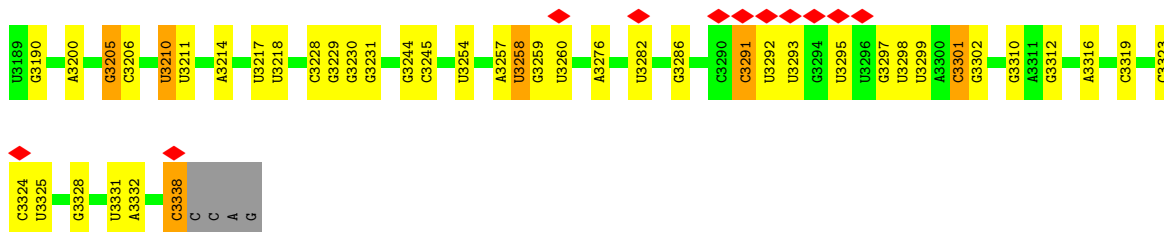
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	CH	1	1	1	0
60	Cd	2	2	2	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

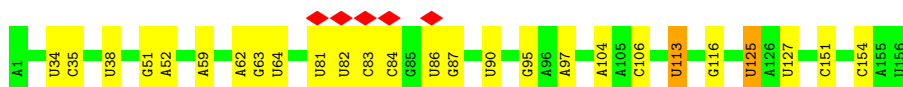
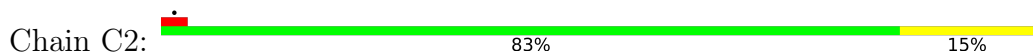
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
61	CQ	1	1	1	0
61	Cb	1	1	1	0
61	Lg	1	1	1	0
61	Lj	1	1	1	0
61	Lp	1	1	1	0

- Molecule 62 is water.

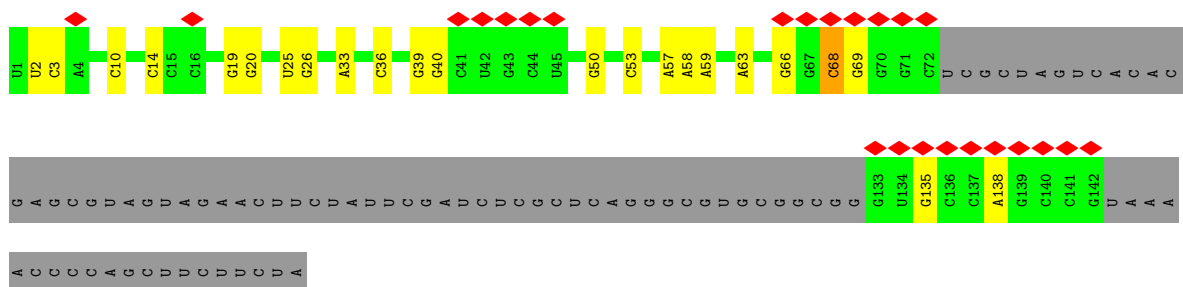
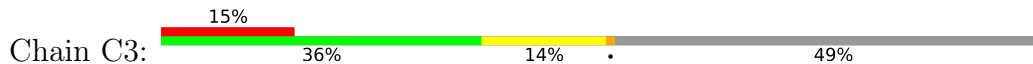
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
62	CH	1	1	1	0
62	Cd	2	2	2	0



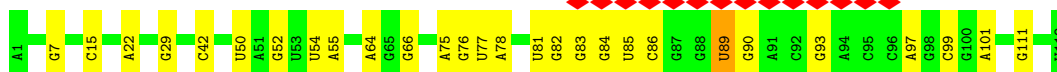
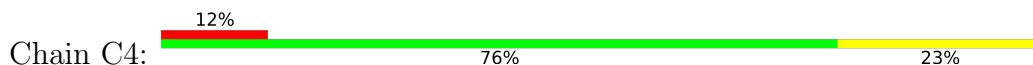
• Molecule 2: 5.8S rRNA



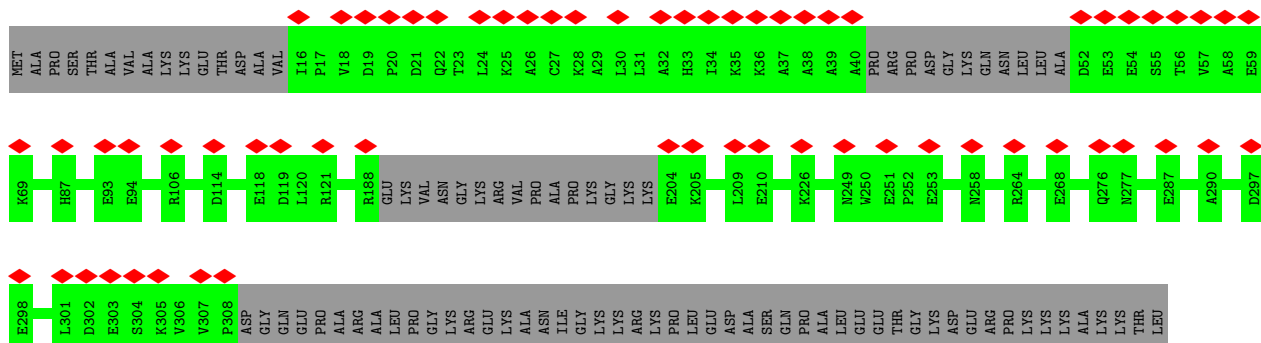
• Molecule 3: ITS2

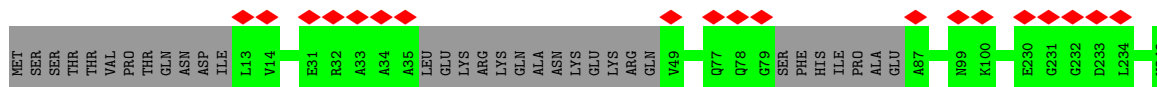
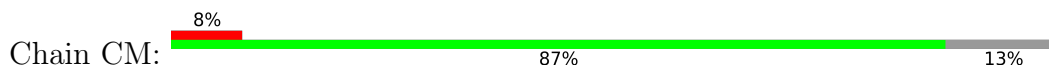


• Molecule 4: 5S rRNA

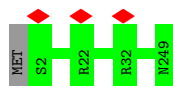


• Molecule 5: Utp30

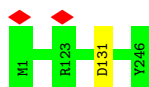




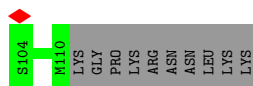
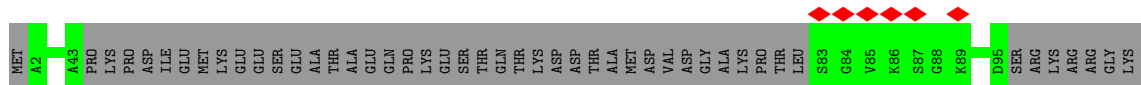
- Molecule 12: 60S ribosomal protein l7-like protein



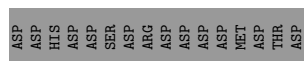
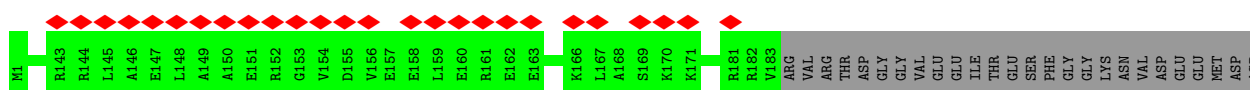
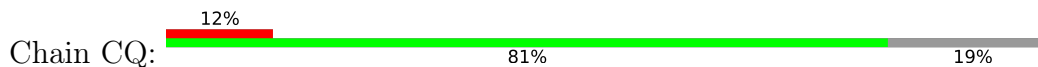
- Molecule 13: Eukaryotic translation initiation factor 6



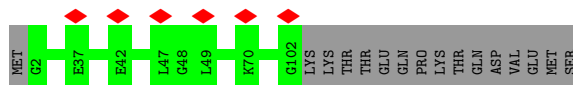
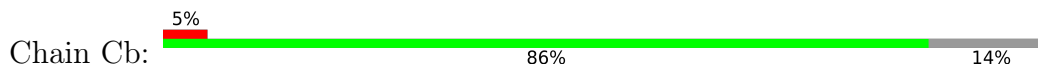
- Molecule 14: DUF2423 domain-containing protein

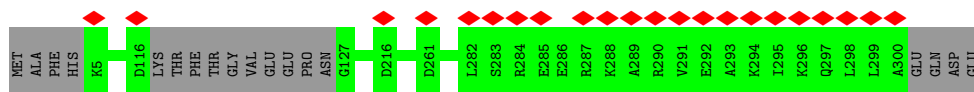


- Molecule 15: Ribosome biogenesis protein RLP24

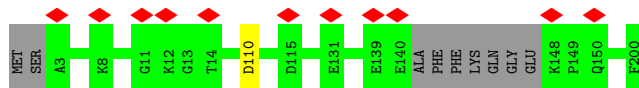


- Molecule 16: Zinc finger domain-containing protein

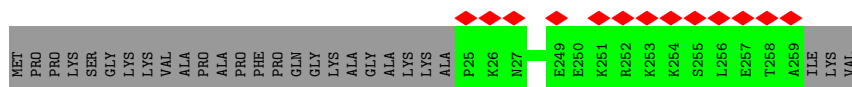




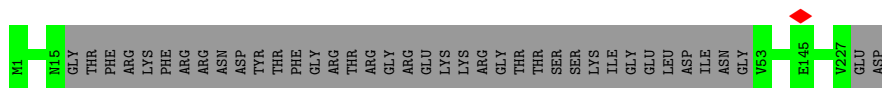
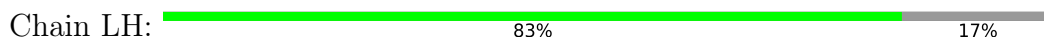
- Molecule 27: 60S ribosomal protein L6



- Molecule 28: 60S ribosomal protein L8



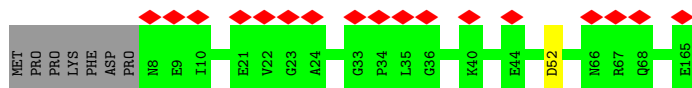
- Molecule 29: 60S ribosomal protein L9-like protein



- Molecule 30: Putative ribosomal protein



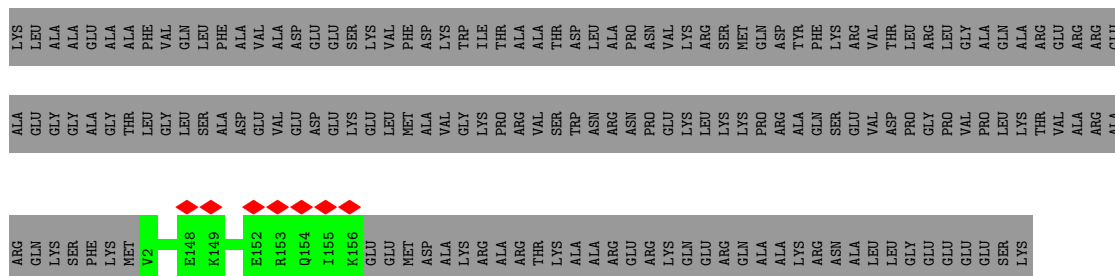
- Molecule 31: 60S ribosomal protein L12-like protein



- Molecule 32: 60S ribosomal protein L13



- Molecule 33: 60S ribosomal protein L14-like protein



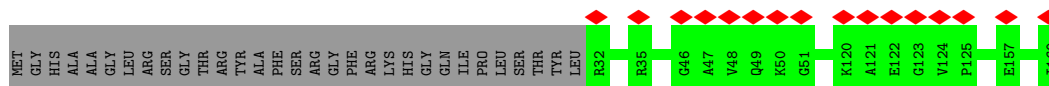
- Molecule 39: 60S ribosomal protein L20

Chain LS: 100%

There are no outlier residues recorded for this chain.

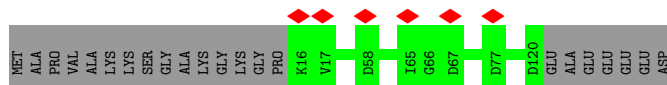
- Molecule 40: 60S ribosomal protein l21-like protein

Chain LT: 10% 81% 19%



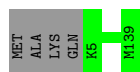
- Molecule 41: 60S ribosomal protein L22-like protein

Chain LU: 5% 83% 17%



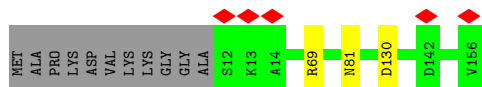
- Molecule 42: 60S ribosomal protein l23-like protein

Chain LV: 97%



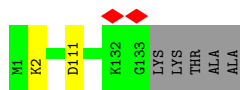
- Molecule 43: 60S ribosomal protein L25-like protein

Chain LX: 91% 7%

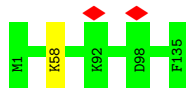


- Molecule 44: 60S ribosomal protein L26-like protein

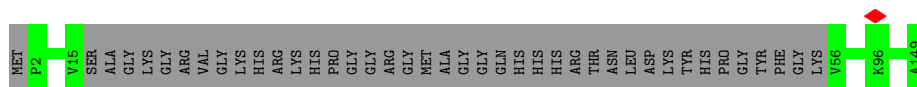
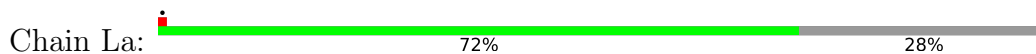
Chain LY: 95%



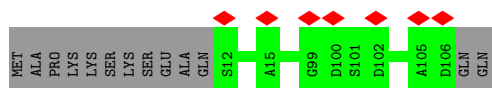
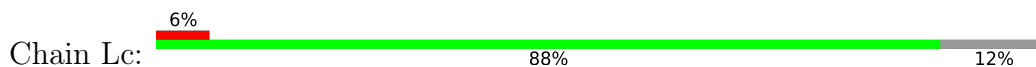
- Molecule 45: 60S ribosomal protein L27



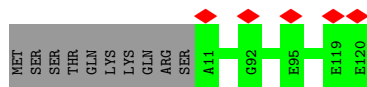
- Molecule 46: 60S ribosomal protein L28-like protein



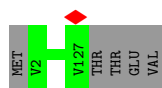
- Molecule 47: 60S ribosomal protein l30-like protein



- Molecule 48: Putative 60S ribosomal protein



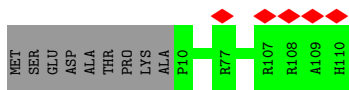
- Molecule 49: 60S ribosomal protein L32-like protein



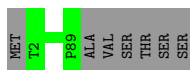
- Molecule 50: 60S ribosomal protein l33-like protein



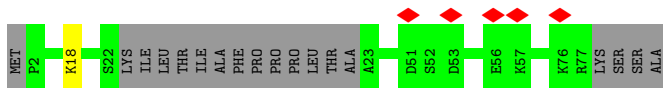
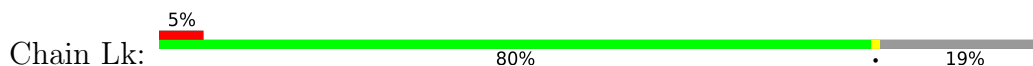
- Molecule 51: Ribosomal protein l34-like protein



- Molecule 54: Ribosomal protein L37



- Molecule 55: 60S ribosomal protein L38-like protein



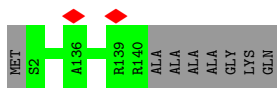
- Molecule 56: Ribosomal protein eL39



- Molecule 57: 60S ribosomal protein L43-like protein



- Molecule 58: 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	35432	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	7.243	Depositor
Minimum map value	0.000	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.147	Depositor
Recommended contour level	0.7	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: OMG, GTP, OMC, OMU, A2M, 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	0.35	0/70966	0.91	93/110644 (0.1%)
2	C2	0.34	0/3710	0.87	4/5778 (0.1%)
3	C3	0.27	0/1958	0.94	3/3050 (0.1%)
4	C4	0.31	0/2833	0.98	8/4414 (0.2%)
5	CB	0.26	0/2166	0.53	0/2945
6	CF	0.28	0/1972	0.56	0/2660
7	CH	0.27	0/5147	0.55	0/6926
8	CI	0.31	0/1265	0.66	0/1702
9	CJ	0.28	0/3196	0.52	1/4319 (0.0%)
10	CK	0.27	0/1939	0.55	0/2608
11	CL	0.26	0/631	0.56	0/843
12	CM	0.27	0/1805	0.54	0/2417
12	LF	0.29	0/2061	0.54	0/2765
13	CN	0.27	0/1878	0.58	1/2555 (0.0%)
14	CO	0.28	0/470	0.60	0/619
15	CQ	0.28	0/1504	0.61	0/2000
16	Cb	0.29	0/845	0.61	0/1128
17	Cd	0.26	0/3770	0.52	0/5082
18	Ce	0.26	0/2173	0.58	1/2890 (0.0%)
19	Cf	0.26	0/2326	0.53	0/3113
20	Cg	0.26	0/1508	0.55	1/2051 (0.0%)
21	Ch	0.27	0/3914	0.56	0/5319
22	Cz	0.32	0/877	0.72	1/1148 (0.1%)
23	LA	0.28	0/1395	0.59	0/1881
24	LB	0.29	0/3172	0.57	0/4260
25	LC	0.27	0/2808	0.52	0/3785
26	LD	0.27	0/2308	0.51	0/3105
27	LE	0.27	0/1504	0.54	1/2027 (0.0%)
28	LG	0.27	0/1918	0.53	0/2565
29	LH	0.28	0/1515	0.54	0/2037
30	LJ	0.28	0/1379	0.62	1/1844 (0.1%)
31	LK	0.27	0/1198	0.61	1/1611 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LL	0.26	0/1614	0.57	0/2168
33	LM	0.26	0/1145	0.54	0/1539
34	LN	0.27	0/1741	0.58	0/2332
35	LO	0.30	0/1645	0.55	0/2205
36	LP	0.27	0/1364	0.57	0/1835
37	LQ	0.26	0/1197	0.56	0/1612
38	LR	0.26	0/1260	0.57	0/1683
39	LS	0.28	0/1461	0.55	0/1966
40	LT	0.29	0/1046	0.61	0/1409
41	LU	0.28	0/859	0.51	0/1151
42	LV	0.32	0/1009	0.58	0/1357
43	LX	0.28	0/1151	0.57	1/1547 (0.1%)
44	LY	0.26	0/1070	0.62	1/1432 (0.1%)
45	LZ	0.30	0/1135	0.60	0/1519
46	La	0.26	0/892	0.53	0/1200
47	Lc	0.27	0/714	0.50	0/960
48	Ld	0.27	0/889	0.55	0/1192
49	Le	0.27	0/1035	0.56	0/1379
50	Lf	0.29	0/883	0.57	0/1187
51	Lg	0.28	0/927	0.63	0/1244
52	Lh	0.25	0/1014	0.55	0/1349
53	Li	0.26	0/834	0.62	0/1099
54	Lj	0.27	0/712	0.61	0/944
55	Lk	0.27	0/640	0.56	0/850
56	Ll	0.24	0/446	0.58	0/593
57	Lp	0.26	0/706	0.60	0/940
58	Lq	0.27	0/1091	0.56	0/1468
All	All	0.31	0/164591	0.77	118/238251 (0.0%)

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1538	U	N1-C2-O2	8.91	129.04	122.80
1	C1	1538	U	N3-C2-O2	-8.65	116.14	122.20
1	C1	1935	C	C2-N1-C1'	8.50	128.15	118.80
1	C1	1179	C	C2-N1-C1'	8.45	128.10	118.80
1	C1	1478	U	C2-N1-C1'	8.37	127.74	117.70
1	C1	1179	C	N1-C2-O2	8.27	123.86	118.90
1	C1	2681	U	N3-C2-O2	-8.26	116.42	122.20
1	C1	2730	U	C2-N1-C1'	8.26	127.61	117.70
1	C1	1538	U	C2-N1-C1'	8.22	127.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2730	U	N1-C2-O2	8.20	128.54	122.80
18	Ce	387	ASP	CB-CG-OD2	8.08	125.58	118.30
1	C1	2730	U	N3-C2-O2	-7.73	116.79	122.20
1	C1	1478	U	N1-C2-O2	7.48	128.03	122.80
43	LX	130	ASP	CB-CG-OD1	7.44	125.00	118.30
9	CJ	363	PRO	CA-N-CD	-7.28	101.31	111.50
1	C1	2351	U	N3-C2-O2	-7.05	117.26	122.20
1	C1	1478	U	N3-C2-O2	-6.99	117.31	122.20
1	C1	1479	C	C2-N1-C1'	6.95	126.44	118.80
4	C4	50	U	N1-C2-O2	6.76	127.53	122.80
1	C1	2681	U	N1-C2-O2	6.76	127.53	122.80
1	C1	399	G	O4'-C1'-N9	6.68	113.54	108.20
1	C1	103	C	N1-C2-O2	6.64	122.88	118.90
1	C1	3089	U	C2-N1-C1'	6.62	125.64	117.70
3	C3	14	C	C2-N1-C1'	6.55	126.01	118.80
13	CN	131	ASP	CB-CG-OD2	6.54	124.18	118.30
44	LY	111	ASP	CB-CG-OD1	6.52	124.17	118.30
1	C1	1179	C	N3-C2-O2	-6.51	117.34	121.90
1	C1	1851	U	N3-C2-O2	-6.50	117.65	122.20
1	C1	1064	C	P-O3'-C3'	6.44	127.43	119.70
1	C1	2544	G	N3-C4-C5	-6.44	125.38	128.60
1	C1	308	C	C2-N1-C1'	6.38	125.82	118.80
27	LE	110	ASP	CB-CG-OD2	6.35	124.02	118.30
1	C1	1537	U	P-O3'-C3'	6.31	127.27	119.70
1	C1	2544	G	C4-N9-C1'	6.29	134.68	126.50
4	C4	50	U	N3-C2-O2	-6.29	117.80	122.20
1	C1	79	U	N3-C2-O2	-6.28	117.80	122.20
1	C1	3258	U	P-O3'-C3'	6.26	127.21	119.70
1	C1	2689	G	C4-N9-C1'	6.18	134.54	126.50
3	C3	68	C	C2-N1-C1'	6.17	125.58	118.80
1	C1	3016	U	C2-N1-C1'	6.14	125.07	117.70
2	C2	113	U	C2-N1-C1'	6.13	125.06	117.70
1	C1	2499	C	C2-N1-C1'	6.11	125.52	118.80
1	C1	2100	U	C2-N1-C1'	6.08	124.99	117.70
1	C1	940	C	C2-N1-C1'	6.04	125.44	118.80
1	C1	2544	G	N3-C4-N9	6.03	129.62	126.00
1	C1	3338	C	N1-C2-O2	6.02	122.51	118.90
1	C1	1179	C	C6-N1-C1'	-6.00	113.60	120.80
1	C1	1935	C	C6-N1-C1'	-5.96	113.65	120.80
1	C1	940	C	N1-C2-O2	5.96	122.48	118.90
1	C1	443	C	C2-N1-C1'	5.94	125.33	118.80
1	C1	2501	U	N1-C2-O2	5.92	126.95	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	103	C	N3-C2-O2	-5.91	117.76	121.90
31	LK	52	ASP	CB-CG-OD1	5.85	123.56	118.30
4	C4	42	C	N1-C2-O2	5.83	122.40	118.90
1	C1	3338	C	C2-N1-C1'	5.82	125.20	118.80
1	C1	1337	G	C4-N9-C1'	5.81	134.06	126.50
1	C1	2351	U	N1-C2-O2	5.81	126.86	122.80
20	Cg	77	ASP	CB-CG-OD2	5.76	123.49	118.30
1	C1	2883	U	P-O3'-C3'	5.72	126.57	119.70
1	C1	1051	C	C2-N1-C1'	5.68	125.05	118.80
1	C1	2374	U	N3-C2-O2	-5.68	118.22	122.20
1	C1	1663	C	N1-C2-O2	5.68	122.31	118.90
1	C1	1478	U	C6-N1-C1'	-5.61	113.34	121.20
1	C1	1560	U	C2-N1-C1'	5.59	124.41	117.70
1	C1	1935	C	C6-N1-C2	-5.56	118.08	120.30
1	C1	2689	G	N3-C4-N9	5.56	129.33	126.00
1	C1	2992	C	N1-C2-O2	5.55	122.23	118.90
1	C1	1851	U	N1-C2-O2	5.54	126.68	122.80
1	C1	3016	U	N1-C2-O2	5.54	126.68	122.80
1	C1	2501	U	N3-C2-O2	-5.50	118.35	122.20
1	C1	2499	C	N1-C2-O2	5.47	122.18	118.90
4	C4	50	U	C2-N1-C1'	5.46	124.25	117.70
1	C1	2584	C	C2-N1-C1'	5.44	124.79	118.80
22	Cz	79	ARG	CA-CB-CG	5.44	125.36	113.40
1	C1	3301	C	P-O3'-C3'	5.38	126.15	119.70
2	C2	64	U	N3-C2-O2	-5.37	118.44	122.20
1	C1	2501	U	C2-N1-C1'	5.36	124.13	117.70
1	C1	114	C	C2-N1-C1'	5.35	124.69	118.80
1	C1	2280	A	P-O3'-C3'	5.35	126.12	119.70
1	C1	1560	U	N1-C2-O2	5.35	126.54	122.80
1	C1	1937	C	C2-N1-C1'	5.33	124.67	118.80
1	C1	2689	G	N3-C4-C5	-5.33	125.93	128.60
1	C1	636	C	N1-C2-O2	5.32	122.09	118.90
1	C1	1351	U	N1-C2-O2	5.32	126.52	122.80
1	C1	1047	A	P-O3'-C3'	5.31	126.07	119.70
3	C3	53	C	C2-N1-C1'	5.28	124.61	118.80
1	C1	2730	U	C6-N1-C1'	-5.27	113.82	121.20
1	C1	3132	A	P-O3'-C3'	5.26	126.02	119.70
1	C1	2374	U	N1-C2-O2	5.26	126.48	122.80
2	C2	113	U	N1-C2-O2	5.26	126.48	122.80
4	C4	99	C	C2-N1-C1'	5.26	124.59	118.80
1	C1	1560	U	N3-C2-O2	-5.26	118.52	122.20
1	C1	443	C	N1-C2-O2	5.26	122.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2689	G	C8-N9-C1'	-5.25	120.17	127.00
1	C1	1205	G	O4'-C1'-N9	5.25	112.40	108.20
1	C1	1479	C	C6-N1-C2	-5.24	118.20	120.30
1	C1	961	C	C2-N1-C1'	5.23	124.56	118.80
1	C1	168	C	C2-N1-C1'	5.21	124.53	118.80
4	C4	15	C	N3-C2-O2	-5.21	118.26	121.90
1	C1	3210	U	P-O3'-C3'	5.20	125.94	119.70
1	C1	2584	C	N1-C2-O2	5.19	122.02	118.90
1	C1	2544	G	C8-N9-C1'	-5.16	120.30	127.00
1	C1	3291	C	C6-N1-C2	-5.14	118.24	120.30
1	C1	1337	G	C8-N9-C1'	-5.13	120.33	127.00
30	LJ	81	LEU	CA-CB-CG	5.12	127.08	115.30
1	C1	1508	G	C4-N9-C1'	5.12	133.15	126.50
1	C1	1538	U	C6-N1-C1'	-5.12	114.04	121.20
1	C1	103	C	C6-N1-C2	-5.08	118.27	120.30
4	C4	89	U	C2-N1-C1'	5.05	123.77	117.70
4	C4	89	U	N1-C2-O2	5.05	126.34	122.80
1	C1	1858	G	C4-N9-C1'	5.05	133.06	126.50
1	C1	2575	C	P-O3'-C3'	5.04	125.75	119.70
2	C2	125	U	C2-N1-C1'	5.02	123.73	117.70
1	C1	2668	C	C2-N1-C1'	5.02	124.32	118.80
1	C1	103	C	C2-N1-C1'	5.02	124.32	118.80
1	C1	1856	U	C2-N1-C1'	5.01	123.71	117.70
1	C1	2513	C	N1-C2-O2	5.00	121.90	118.90
1	C1	3205	G	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

There are no planarity outliers.

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	261/391 (67%)	256 (98%)	5 (2%)	0	100	100
6	CF	243/270 (90%)	241 (99%)	2 (1%)	0	100	100
7	CH	621/661 (94%)	614 (99%)	7 (1%)	0	100	100
8	CI	150/414 (36%)	149 (99%)	1 (1%)	0	100	100
9	CJ	376/679 (55%)	372 (99%)	4 (1%)	0	100	100
10	CK	231/261 (88%)	225 (97%)	6 (3%)	0	100	100
11	CL	77/558 (14%)	76 (99%)	1 (1%)	0	100	100
12	CM	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
12	LF	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
13	CN	244/246 (99%)	239 (98%)	5 (2%)	0	100	100
14	CO	56/120 (47%)	56 (100%)	0	0	100	100
15	CQ	181/225 (80%)	179 (99%)	2 (1%)	0	100	100
16	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
17	Cd	458/627 (73%)	451 (98%)	7 (2%)	0	100	100
18	Ce	252/443 (57%)	251 (100%)	1 (0%)	0	100	100
19	Cf	281/350 (80%)	277 (99%)	4 (1%)	0	100	100
20	Cg	186/202 (92%)	183 (98%)	3 (2%)	0	100	100
21	Ch	484/517 (94%)	471 (97%)	13 (3%)	0	100	100
22	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
23	LA	176/254 (69%)	172 (98%)	4 (2%)	0	100	100
24	LB	387/392 (99%)	380 (98%)	7 (2%)	0	100	100
25	LC	361/365 (99%)	356 (99%)	5 (1%)	0	100	100
26	LD	282/304 (93%)	280 (99%)	2 (1%)	0	100	100
27	LE	187/200 (94%)	183 (98%)	4 (2%)	0	100	100
28	LG	233/262 (89%)	228 (98%)	5 (2%)	0	100	100
29	LH	188/229 (82%)	186 (99%)	2 (1%)	0	100	100
30	LJ	167/173 (96%)	167 (100%)	0	0	100	100
31	LK	156/165 (94%)	156 (100%)	0	0	100	100
32	LL	201/213 (94%)	198 (98%)	3 (2%)	0	100	100
33	LM	139/142 (98%)	136 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	LN	200/203 (98%)	195 (98%)	5 (2%)	0	100	100
35	LO	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
36	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
37	LQ	148/213 (70%)	147 (99%)	1 (1%)	0	100	100
38	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
39	LS	172/174 (99%)	168 (98%)	4 (2%)	0	100	100
40	LT	127/160 (79%)	126 (99%)	1 (1%)	0	100	100
41	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
42	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
43	LX	143/156 (92%)	139 (97%)	4 (3%)	0	100	100
44	LY	131/138 (95%)	128 (98%)	3 (2%)	0	100	100
45	LZ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
46	La	104/149 (70%)	102 (98%)	2 (2%)	0	100	100
47	Lc	93/108 (86%)	93 (100%)	0	0	100	100
48	Ld	108/120 (90%)	107 (99%)	1 (1%)	0	100	100
49	Le	124/131 (95%)	124 (100%)	0	0	100	100
50	Lf	106/109 (97%)	106 (100%)	0	0	100	100
51	Lg	116/119 (98%)	115 (99%)	1 (1%)	0	100	100
52	Lh	120/935 (13%)	117 (98%)	3 (2%)	0	100	100
53	Li	99/110 (90%)	99 (100%)	0	0	100	100
54	Lj	86/95 (90%)	85 (99%)	1 (1%)	0	100	100
55	Lk	74/94 (79%)	74 (100%)	0	0	100	100
56	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
57	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
58	Lq	137/147 (93%)	134 (98%)	3 (2%)	0	100	100
All	All	10348/16395 (63%)	10194 (98%)	154 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	228/329 (69%)	228 (100%)	0	100	100
6	CF	212/236 (90%)	212 (100%)	0	100	100
7	CH	549/575 (96%)	548 (100%)	1 (0%)	93	98
8	CI	124/336 (37%)	122 (98%)	2 (2%)	62	88
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	Cb	85/101 (84%)	85 (100%)	0	100	100
17	Cd	403/541 (74%)	402 (100%)	1 (0%)	93	98
18	Ce	223/383 (58%)	223 (100%)	0	100	100
19	Cf	250/310 (81%)	250 (100%)	0	100	100
20	Cg	158/176 (90%)	158 (100%)	0	100	100
21	Ch	408/436 (94%)	408 (100%)	0	100	100
22	Cz	89/107 (83%)	87 (98%)	2 (2%)	52	83
23	LA	141/198 (71%)	141 (100%)	0	100	100
24	LB	329/331 (99%)	328 (100%)	1 (0%)	92	98
25	LC	282/285 (99%)	281 (100%)	1 (0%)	91	97
26	LD	221/253 (87%)	221 (100%)	0	100	100
27	LE	157/166 (95%)	157 (100%)	0	100	100
28	LG	200/222 (90%)	200 (100%)	0	100	100
29	LH	167/200 (84%)	167 (100%)	0	100	100
30	LJ	140/150 (93%)	139 (99%)	1 (1%)	84	95
31	LK	127/136 (93%)	127 (100%)	0	100	100
32	LL	158/176 (90%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	LM	116/117 (99%)	116 (100%)	0	100	100
34	LN	179/180 (99%)	179 (100%)	0	100	100
35	LO	162/163 (99%)	162 (100%)	0	100	100
36	LP	133/152 (88%)	133 (100%)	0	100	100
37	LQ	125/178 (70%)	125 (100%)	0	100	100
38	LR	125/2396 (5%)	125 (100%)	0	100	100
39	LS	152/154 (99%)	152 (100%)	0	100	100
40	LT	110/135 (82%)	110 (100%)	0	100	100
41	LU	92/108 (85%)	92 (100%)	0	100	100
42	LV	98/102 (96%)	98 (100%)	0	100	100
43	LX	122/129 (95%)	120 (98%)	2 (2%)	62	88
44	LY	116/119 (98%)	115 (99%)	1 (1%)	78	94
45	LZ	121/121 (100%)	120 (99%)	1 (1%)	81	94
46	La	93/122 (76%)	93 (100%)	0	100	100
47	Lc	76/88 (86%)	76 (100%)	0	100	100
48	Ld	90/105 (86%)	90 (100%)	0	100	100
49	Le	109/114 (96%)	109 (100%)	0	100	100
50	Lf	89/90 (99%)	89 (100%)	0	100	100
51	Lg	95/102 (93%)	95 (100%)	0	100	100
52	Lh	109/781 (14%)	109 (100%)	0	100	100
53	Li	85/93 (91%)	85 (100%)	0	100	100
54	Lj	72/78 (92%)	72 (100%)	0	100	100
55	Lk	73/88 (83%)	72 (99%)	1 (1%)	67	90
56	Ll	45/46 (98%)	45 (100%)	0	100	100
57	Lp	73/74 (99%)	73 (100%)	0	100	100
58	Lq	109/112 (97%)	109 (100%)	0	100	100
All	All	8813/13783 (64%)	8799 (100%)	14 (0%)	93	98

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	CH	391	LYS
8	CI	308	LYS

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Mol	Chain	Res	Type
8	CI	333	LYS
17	Cd	298	ARG
22	Cz	78	LYS
22	Cz	79	ARG
24	LB	245	LYS
25	LC	139	ARG
30	LJ	162	ARG
43	LX	69	ARG
43	LX	81	ASN
44	LY	2	LYS
45	LZ	58	LYS
55	Lk	18	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
7	CH	490	GLN
8	CI	301	GLN
16	Cb	68	HIS
18	Ce	216	ASN
31	LK	65	GLN
31	LK	66	ASN
34	LN	32	GLN
34	LN	87	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2989/3342 (89%)	553 (18%)	20 (0%)
2	C2	155/156 (99%)	25 (16%)	0
3	C3	80/162 (49%)	21 (26%)	0
4	C4	118/119 (99%)	24 (20%)	0
All	All	3342/3779 (88%)	623 (18%)	20 (0%)

All (623) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	C1	44	A
1	C1	50	A
1	C1	60	G
1	C1	61	A
1	C1	66	A
1	C1	67	A
1	C1	68	A
1	C1	94	C
1	C1	95	G
1	C1	96	A
1	C1	110	A
1	C1	111	G
1	C1	116	A
1	C1	117	A
1	C1	123	A
1	C1	132	U
1	C1	134	G
1	C1	135	G
1	C1	139	G
1	C1	146	A
1	C1	152	G
1	C1	153	A
1	C1	157	G
1	C1	181	G
1	C1	184	U
1	C1	185	U
1	C1	193	A
1	C1	194	C
1	C1	200	G
1	C1	204	C
1	C1	213	A
1	C1	214	G
1	C1	225	A
1	C1	240	C
1	C1	241	U
1	C1	242	G
1	C1	244	G
1	C1	247	A
1	C1	258	A
1	C1	259	C
1	C1	262	G
1	C1	276	G

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Mol	Chain	Res	Type
1	C1	277	A
1	C1	288	A
1	C1	291	U
1	C1	298	U
1	C1	308	C
1	C1	316	A
1	C1	322	C
1	C1	323	G
1	C1	332	C
1	C1	342	A
1	C1	343	C
1	C1	369	G
1	C1	388	A
1	C1	389	A2M
1	C1	391	U
1	C1	392	A
1	C1	394	C
1	C1	395	A
1	C1	396	C
1	C1	414	G
1	C1	415	A
1	C1	430	G
1	C1	434	U
1	C1	435	G
1	C1	443	C
1	C1	446	A
1	C1	447	U
1	C1	448	C
1	C1	458	U
1	C1	459	C
1	C1	460	U
1	C1	469	C
1	C1	470	A
1	C1	471	C
1	C1	472	U
1	C1	479	G
1	C1	512	A
1	C1	514	A
1	C1	527	G
1	C1	535	U
1	C1	536	C
1	C1	537	C

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Mol	Chain	Res	Type
1	C1	545	U
1	C1	547	A
1	C1	549	A
1	C1	550	G
1	C1	559	G
1	C1	561	A
1	C1	570	G
1	C1	583	A
1	C1	588	G
1	C1	592	U
1	C1	593	G
1	C1	595	A
1	C1	597	G
1	C1	599	A
1	C1	608	U
1	C1	609	A
1	C1	610	A
1	C1	624	C
1	C1	632	G
1	C1	634	A
1	C1	648	A
1	C1	650	U
1	C1	665	A
1	C1	669	U
1	C1	678	A
1	C1	693	A
1	C1	700	G
1	C1	703	A
1	C1	719	U
1	C1	720	C
1	C1	721	G
1	C1	743	A
1	C1	747	A
1	C1	748	U
1	C1	756	G
1	C1	757	A
1	C1	759	U
1	C1	761	G
1	C1	762	A
1	C1	763	G
1	C1	766	G
1	C1	767	G

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Mol	Chain	Res	Type
1	C1	782	G
1	C1	790	A
1	C1	799	A
1	C1	812	A
1	C1	830	A
1	C1	843	C
1	C1	856	U
1	C1	857	G
1	C1	862	G
1	C1	877	A
1	C1	889	G
1	C1	890	G
1	C1	891	G
1	C1	896	A
1	C1	898	G
1	C1	899	A
1	C1	905	C
1	C1	906	G
1	C1	915	A
1	C1	919	G
1	C1	926	A
1	C1	931	C
1	C1	933	A
1	C1	934	A
1	C1	935	G
1	C1	937	U
1	C1	940	C
1	C1	941	C
1	C1	944	A
1	C1	945	G
1	C1	947	A
1	C1	955	G
1	C1	956	U
1	C1	963	U
1	C1	964	C
1	C1	976	G
1	C1	977	U
1	C1	983	G
1	C1	984	A
1	C1	1032	C
1	C1	1034	U
1	C1	1040	A

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Mol	Chain	Res	Type
1	C1	1047	A
1	C1	1048	A
1	C1	1049	G
1	C1	1051	C
1	C1	1055	G
1	C1	1058	A
1	C1	1059	C
1	C1	1064	C
1	C1	1065	U
1	C1	1066	G
1	C1	1070	G
1	C1	1075	C
1	C1	1076	A
1	C1	1077	U
1	C1	1078	U
1	C1	1079	C
1	C1	1080	G
1	C1	1081	A
1	C1	1086	A
1	C1	1099	G
1	C1	1109	G
1	C1	1110	G
1	C1	1115	C
1	C1	1118	A
1	C1	1127	U
1	C1	1132	G
1	C1	1136	A
1	C1	1143	C
1	C1	1161	G
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1169	G
1	C1	1175	C
1	C1	1176	A
1	C1	1179	C
1	C1	1182	C
1	C1	1185	A
1	C1	1187	A
1	C1	1194	U
1	C1	1205	G
1	C1	1209	G

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Mol	Chain	Res	Type
1	C1	1228	A
1	C1	1241	U
1	C1	1242	A
1	C1	1246	A
1	C1	1248	U
1	C1	1255	C
1	C1	1268	G
1	C1	1269	A
1	C1	1270	A
1	C1	1284	A
1	C1	1287	A
1	C1	1288	U
1	C1	1290	G
1	C1	1292	U
1	C1	1296	G
1	C1	1313	A
1	C1	1331	A
1	C1	1332	G
1	C1	1333	A
1	C1	1334	A
1	C1	1335	A
1	C1	1336	C
1	C1	1337	G
1	C1	1369	A
1	C1	1370	G
1	C1	1375	G
1	C1	1382	A
1	C1	1383	G
1	C1	1400	G
1	C1	1401	A
1	C1	1413	U
1	C1	1417	G
1	C1	1420	OMC
1	C1	1429	A
1	C1	1433	OMG
1	C1	1438	U
1	C1	1458	G
1	C1	1464	A
1	C1	1467	U
1	C1	1477	U
1	C1	1485	G
1	C1	1491	OMC

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Mol	Chain	Res	Type
1	C1	1498	A
1	C1	1505	U
1	C1	1506	U
1	C1	1522	A
1	C1	1536	U
1	C1	1538	U
1	C1	1539	C
1	C1	1540	A
1	C1	1542	A
1	C1	1543	G
1	C1	1549	C
1	C1	1550	U
1	C1	1554	G
1	C1	1560	U
1	C1	1561	G
1	C1	1563	G
1	C1	1567	A
1	C1	1568	A
1	C1	1569	A
1	C1	1570	G
1	C1	1573	A
1	C1	1585	A
1	C1	1586	U
1	C1	1609	U
1	C1	1619	C
1	C1	1622	A
1	C1	1623	A
1	C1	1624	C
1	C1	1638	G
1	C1	1685	U
1	C1	1696	A
1	C1	1697	C
1	C1	1704	U
1	C1	1721	A
1	C1	1722	U
1	C1	1730	A
1	C1	1731	G
1	C1	1745	U
1	C1	1746	G
1	C1	1751	G
1	C1	1760	G
1	C1	1776	G

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Mol	Chain	Res	Type
1	C1	1777	A
1	C1	1788	G
1	C1	1792	G
1	C1	1793	A
1	C1	1794	A
1	C1	1795	U
1	C1	1796	A
1	C1	1799	U
1	C1	1800	C
1	C1	1801	U
1	C1	1822	A
1	C1	1826	C
1	C1	1829	C
1	C1	1846	C
1	C1	1847	A2M
1	C1	1856	U
1	C1	1858	G
1	C1	1860	U
1	C1	1866	A
1	C1	1886	G
1	C1	1887	C
1	C1	1933	G
1	C1	1934	G
1	C1	1935	C
1	C1	1937	C
1	C1	2046	C
1	C1	2048	U
1	C1	2050	C
1	C1	2052	G
1	C1	2054	U
1	C1	2056	A
1	C1	2076	A
1	C1	2084	G
1	C1	2085	G
1	C1	2089	A
1	C1	2094	A
1	C1	2103	U
1	C1	2121	A
1	C1	2126	C
1	C1	2132	G
1	C1	2137	G
1	C1	2151	A

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Mol	Chain	Res	Type
1	C1	2237	U
1	C1	2279	G
1	C1	2281	U
1	C1	2282	U
1	C1	2284	A
1	C1	2297	U
1	C1	2298	G
1	C1	2299	U
1	C1	2310	U
1	C1	2326	A
1	C1	2328	C
1	C1	2340	G
1	C1	2348	A
1	C1	2351	U
1	C1	2355	C
1	C1	2356	G
1	C1	2362	A
1	C1	2364	A
1	C1	2373	U
1	C1	2374	U
1	C1	2381	G
1	C1	2382	A
1	C1	2398	G
1	C1	2401	A
1	C1	2403	A
1	C1	2470	U
1	C1	2473	U
1	C1	2474	A
1	C1	2477	U
1	C1	2478	A
1	C1	2489	C
1	C1	2499	C
1	C1	2500	U
1	C1	2501	U
1	C1	2502	G
1	C1	2503	C
1	C1	2506	C
1	C1	2507	C
1	C1	2508	A
1	C1	2513	C
1	C1	2515	G
1	C1	2521	A

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Mol	Chain	Res	Type
1	C1	2526	C
1	C1	2527	C
1	C1	2533	G
1	C1	2544	G
1	C1	2545	G
1	C1	2552	A
1	C1	2565	G
1	C1	2566	G
1	C1	2573	G
1	C1	2575	C
1	C1	2576	U
1	C1	2577	G
1	C1	2578	OMG
1	C1	2582	G
1	C1	2584	C
1	C1	2585	A
1	C1	2606	A
1	C1	2613	C
1	C1	2615	A
1	C1	2631	G
1	C1	2633	A
1	C1	2635	A
1	C1	2636	G
1	C1	2639	A
1	C1	2647	U
1	C1	2651	A
1	C1	2656	A
1	C1	2657	G
1	C1	2663	A
1	C1	2664	A
1	C1	2667	C
1	C1	2672	U
1	C1	2673	G
1	C1	2674	A
1	C1	2675	U
1	C1	2680	A
1	C1	2682	U
1	C1	2690	OMU
1	C1	2691	G
1	C1	2713	G
1	C1	2717	A
1	C1	2731	C

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Mol	Chain	Res	Type
1	C1	2732	C
1	C1	2736	G
1	C1	2737	A
1	C1	2754	U
1	C1	2755	G
1	C1	2756	C
1	C1	2757	C
1	C1	2758	A
1	C1	2761	A
1	C1	2762	A
1	C1	2763	A
1	C1	2769	C
1	C1	2773	G
1	C1	2783	G
1	C1	2784	C
1	C1	2785	U
1	C1	2802	U
1	C1	2803	C
1	C1	2804	A
1	C1	2805	U
1	C1	2806	A
1	C1	2812	G
1	C1	2815	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	U
1	C1	2831	A
1	C1	2834	U
1	C1	2836	G
1	C1	2846	A
1	C1	2857	G
1	C1	2858	C
1	C1	2882	U
1	C1	2883	U
1	C1	2884	C
1	C1	2885	A
1	C1	2894	U
1	C1	2895	A
1	C1	2900	A
1	C1	2903	U
1	C1	2905	A

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Mol	Chain	Res	Type
1	C1	2929	C
1	C1	2930	A
1	C1	2931	G
1	C1	2938	U
1	C1	2939	U
1	C1	2940	U
1	C1	2942	C
1	C1	2951	U
1	C1	2955	C
1	C1	2956	U
1	C1	2964	A
1	C1	2970	A
1	C1	2980	G
1	C1	3014	U
1	C1	3017	G
1	C1	3032	G
1	C1	3036	G
1	C1	3044	A
1	C1	3045	A
1	C1	3049	A
1	C1	3050	C
1	C1	3051	C
1	C1	3067	G
1	C1	3080	A
1	C1	3087	A
1	C1	3088	A
1	C1	3089	U
1	C1	3100	A
1	C1	3101	C
1	C1	3102	G
1	C1	3112	U
1	C1	3113	A
1	C1	3119	A
1	C1	3124	G
1	C1	3125	U
1	C1	3126	A
1	C1	3127	G
1	C1	3131	U
1	C1	3133	U
1	C1	3135	A
1	C1	3141	G
1	C1	3146	C

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Mol	Chain	Res	Type
1	C1	3155	A
1	C1	3162	C
1	C1	3163	A
1	C1	3164	G
1	C1	3185	G
1	C1	3186	A
1	C1	3188	G
1	C1	3190	G
1	C1	3200	A
1	C1	3206	C
1	C1	3210	U
1	C1	3211	U
1	C1	3214	A
1	C1	3217	U
1	C1	3218	U
1	C1	3228	C
1	C1	3229	G
1	C1	3231	G
1	C1	3244	G
1	C1	3245	C
1	C1	3254	U
1	C1	3257	A
1	C1	3258	U
1	C1	3259	G
1	C1	3260	U
1	C1	3276	A
1	C1	3282	U
1	C1	3286	G
1	C1	3291	C
1	C1	3292	U
1	C1	3293	U
1	C1	3295	U
1	C1	3297	G
1	C1	3299	U
1	C1	3302	G
1	C1	3310	G
1	C1	3312	G
1	C1	3316	A
1	C1	3319	C
1	C1	3323	C
1	C1	3324	C
1	C1	3325	U

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Mol	Chain	Res	Type
1	C1	3328	G
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	38	U
2	C2	51	G
2	C2	52	A
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	83	C
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	97	A
2	C2	104	A
2	C2	106	C
2	C2	113	U
2	C2	116	G
2	C2	125	U
2	C2	127	U
2	C2	151	C
2	C2	154	C
3	C3	2	U
3	C3	3	C
3	C3	10	C
3	C3	19	G
3	C3	20	G
3	C3	25	U
3	C3	26	G
3	C3	33	A
3	C3	36	C
3	C3	39	G
3	C3	40	G
3	C3	50	G
3	C3	57	A

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Mol	Chain	Res	Type
3	C3	58	A
3	C3	59	A
3	C3	63	A
3	C3	66	G
3	C3	68	C
3	C3	69	G
3	C3	135	G
3	C3	138	A
4	C4	7	G
4	C4	22	A
4	C4	29	G
4	C4	52	G
4	C4	54	U
4	C4	55	A
4	C4	64	A
4	C4	66	G
4	C4	75	A
4	C4	76	G
4	C4	77	U
4	C4	78	A
4	C4	81	U
4	C4	82	G
4	C4	83	G
4	C4	84	G
4	C4	85	U
4	C4	86	C
4	C4	89	U
4	C4	90	G
4	C4	93	G
4	C4	97	A
4	C4	101	A
4	C4	111	G

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	151	G
1	C1	243	U
1	C1	898	G
1	C1	1047	A
1	C1	1064	C
1	C1	1077	U

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Mol	Chain	Res	Type
1	C1	1267	C
1	C1	1537	U
1	C1	2280	A
1	C1	2575	C
1	C1	2883	U
1	C1	3079	U
1	C1	3132	A
1	C1	3205	G
1	C1	3210	U
1	C1	3230	G
1	C1	3258	U
1	C1	3298	U
1	C1	3301	C
1	C1	3324	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	OMG	C1	2774	1	18,26,27	1.13	2 (11%)	19,38,41	0.88	1 (5%)
1	OMG	C1	2881	1	18,26,27	1.13	2 (11%)	19,38,41	0.83	1 (5%)
1	OMU	C1	1868	1	19,22,23	3.05	6 (31%)	26,31,34	1.74	4 (15%)
1	A2M	C1	858	1	18,25,26	4.36	8 (44%)	18,36,39	3.89	4 (22%)
1	OMU	C1	2277	1	19,22,23	3.07	6 (31%)	26,31,34	1.63	4 (15%)
1	OMC	C1	778	1	19,22,23	0.60	0	26,31,34	0.89	1 (3%)
1	A2M	C1	1223	1	18,25,26	4.31	9 (50%)	18,36,39	3.84	4 (22%)
1	A2M	C1	1847	1	18,25,26	4.35	9 (50%)	18,36,39	3.96	4 (22%)
1	OMC	C1	1836	1	19,22,23	0.60	0	26,31,34	0.82	1 (3%)
1	OMU	C1	2384	1	19,22,23	3.10	6 (31%)	26,31,34	1.69	5 (19%)
1	OMC	C1	1491	1	19,22,23	0.60	0	26,31,34	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	C1	627	1	18,26,27	1.18	2 (11%)	19,38,41	0.94	1 (5%)
1	A2M	C1	2289	1	18,25,26	4.38	8 (44%)	18,36,39	3.77	4 (22%)
1	OMU	C1	2688	1	19,22,23	3.06	6 (31%)	26,31,34	1.70	5 (19%)
1	OMC	C1	2300	1	19,22,23	0.58	0	26,31,34	0.80	1 (3%)
1	A2M	C1	637	1	18,25,26	4.32	9 (50%)	18,36,39	3.85	4 (22%)
1	OMC	C1	2918	1	19,22,23	0.57	0	26,31,34	0.76	0
1	OMC	C1	1812	1	19,22,23	0.61	0	26,31,34	0.73	0
1	OMU	C1	2683	1	19,22,23	3.05	6 (31%)	26,31,34	1.68	4 (15%)
1	OMG	C1	2876	1	18,26,27	1.14	2 (11%)	19,38,41	0.85	1 (5%)
1	A2M	C1	389	1	18,25,26	4.37	9 (50%)	18,36,39	3.94	4 (22%)
1	OMU	C1	1917	1	19,22,23	3.05	6 (31%)	26,31,34	1.72	5 (19%)
1	OMG	C1	646	1	18,26,27	1.19	2 (11%)	19,38,41	0.88	2 (10%)
1	OMG	C1	2578	1	18,26,27	1.14	2 (11%)	19,38,41	0.92	1 (5%)
1	OMG	C1	385	1	18,26,27	1.13	2 (11%)	19,38,41	0.82	1 (5%)
1	OMU	C1	2380	1	19,22,23	3.07	6 (31%)	26,31,34	1.69	5 (19%)
1	A2M	C1	1432	1	18,25,26	4.33	9 (50%)	18,36,39	3.91	4 (22%)
1	A2M	C1	848	1	18,25,26	4.35	9 (50%)	18,36,39	3.83	4 (22%)
1	OMC	C1	1420	1	19,22,23	0.64	0	26,31,34	1.39	4 (15%)
1	OMG	C1	787	1	18,26,27	1.16	2 (11%)	19,38,41	0.88	1 (5%)
1	OMG	C1	1433	1	18,26,27	1.15	2 (11%)	19,38,41	0.87	1 (5%)
1	OMU	C1	2690	1	19,22,23	3.04	6 (31%)	26,31,34	1.70	5 (19%)
1	OMG	C1	2358	1	18,26,27	1.16	2 (11%)	19,38,41	0.90	1 (5%)
1	OMC	C1	2838	1	19,22,23	0.67	0	26,31,34	1.53	4 (15%)

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	OMG	C1	2774	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	2881	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	858	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	2277	1	-	1/9/27/28	0/2/2/2
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	1223	1	-	1/5/27/28	0/3/3/3
1	A2M	C1	1847	1	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2384	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1491	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	627	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	2289	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2300	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	637	1	-	1/5/27/28	0/3/3/3
1	OMC	C1	2918	1	-	1/9/27/28	0/2/2/2
1	OMC	C1	1812	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	2876	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	389	1	-	3/5/27/28	0/3/3/3
1	OMU	C1	1917	1	-	3/9/27/28	0/2/2/2
1	OMG	C1	646	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	2578	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	385	1	-	2/5/27/28	0/3/3/3
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	1432	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	848	1	-	2/5/27/28	0/3/3/3
1	OMC	C1	1420	1	-	3/9/27/28	0/2/2/2
1	OMG	C1	787	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	1433	1	-	2/5/27/28	0/3/3/3
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	2358	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C3'-C2'	-12.87	1.24	1.52
1	C1	1432	A2M	C3'-C2'	-12.75	1.24	1.52
1	C1	858	A2M	C3'-C2'	-12.74	1.24	1.52
1	C1	389	A2M	C3'-C2'	-12.72	1.24	1.52
1	C1	848	A2M	C3'-C2'	-12.71	1.24	1.52
1	C1	1847	A2M	C3'-C2'	-12.69	1.24	1.52
1	C1	637	A2M	C3'-C2'	-12.67	1.24	1.52
1	C1	1223	A2M	C3'-C2'	-12.65	1.24	1.52
1	C1	1847	A2M	O4'-C1'	8.13	1.52	1.41
1	C1	2289	A2M	O4'-C1'	8.06	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	848	A2M	O4'-C1'	7.99	1.52	1.41
1	C1	858	A2M	O4'-C1'	7.99	1.52	1.41
1	C1	389	A2M	O4'-C1'	7.94	1.52	1.41
1	C1	1432	A2M	O4'-C1'	7.82	1.52	1.41
1	C1	637	A2M	O4'-C1'	7.81	1.52	1.41
1	C1	1223	A2M	O4'-C1'	7.73	1.51	1.41
1	C1	2384	OMU	C2-N1	7.45	1.50	1.38
1	C1	2277	OMU	C2-N1	7.35	1.50	1.38
1	C1	1917	OMU	C2-N1	7.34	1.50	1.38
1	C1	1868	OMU	C2-N1	7.30	1.50	1.38
1	C1	2380	OMU	C2-N1	7.28	1.50	1.38
1	C1	2683	OMU	C2-N1	7.25	1.50	1.38
1	C1	2688	OMU	C2-N1	7.22	1.50	1.38
1	C1	2690	OMU	C2-N1	7.16	1.49	1.38
1	C1	2384	OMU	C2-N3	7.14	1.50	1.38
1	C1	2380	OMU	C2-N3	7.13	1.50	1.38
1	C1	2277	OMU	C2-N3	7.11	1.50	1.38
1	C1	1868	OMU	C2-N3	7.08	1.50	1.38
1	C1	2688	OMU	C2-N3	7.08	1.50	1.38
1	C1	2683	OMU	C2-N3	7.07	1.50	1.38
1	C1	2690	OMU	C2-N3	7.01	1.50	1.38
1	C1	1917	OMU	C2-N3	6.97	1.50	1.38
1	C1	389	A2M	O4'-C4'	-6.72	1.30	1.45
1	C1	637	A2M	O4'-C4'	-6.60	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.54	1.30	1.45
1	C1	1847	A2M	O4'-C4'	-6.49	1.30	1.45
1	C1	1432	A2M	O4'-C4'	-6.48	1.30	1.45
1	C1	858	A2M	O4'-C4'	-6.46	1.30	1.45
1	C1	848	A2M	O4'-C4'	-6.40	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.38	1.30	1.45
1	C1	2688	OMU	C6-C5	6.21	1.49	1.35
1	C1	2683	OMU	C6-C5	6.19	1.49	1.35
1	C1	2277	OMU	C6-C5	6.18	1.49	1.35
1	C1	2384	OMU	C6-C5	6.18	1.49	1.35
1	C1	2380	OMU	C6-C5	6.17	1.49	1.35
1	C1	2690	OMU	C6-C5	6.16	1.49	1.35
1	C1	1917	OMU	C6-C5	6.14	1.49	1.35
1	C1	1868	OMU	C6-C5	6.11	1.49	1.35
1	C1	858	A2M	C3'-C4'	5.33	1.66	1.53
1	C1	2289	A2M	C3'-C4'	5.25	1.66	1.53
1	C1	848	A2M	C3'-C4'	5.20	1.66	1.53
1	C1	1223	A2M	C3'-C4'	5.16	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1432	A2M	C3'-C4'	5.11	1.66	1.53
1	C1	637	A2M	C3'-C4'	5.07	1.65	1.53
1	C1	1847	A2M	C3'-C4'	5.04	1.65	1.53
1	C1	389	A2M	C3'-C4'	4.94	1.65	1.53
1	C1	2384	OMU	C4-N3	4.30	1.46	1.38
1	C1	2688	OMU	C4-N3	4.27	1.46	1.38
1	C1	2380	OMU	C4-N3	4.25	1.46	1.38
1	C1	2690	OMU	C4-N3	4.21	1.46	1.38
1	C1	2683	OMU	C4-N3	4.21	1.46	1.38
1	C1	2277	OMU	C4-N3	4.18	1.46	1.38
1	C1	1917	OMU	C4-N3	4.16	1.46	1.38
1	C1	1868	OMU	C4-N3	4.16	1.46	1.38
1	C1	389	A2M	O2'-C2'	3.77	1.52	1.42
1	C1	637	A2M	O2'-C2'	3.48	1.51	1.42
1	C1	848	A2M	O2'-C2'	3.45	1.51	1.42
1	C1	858	A2M	O2'-C2'	3.45	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.45	1.51	1.42
1	C1	1432	A2M	O2'-C2'	3.43	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.43	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.36	1.51	1.42
1	C1	848	A2M	C6-N6	3.14	1.45	1.34
1	C1	2289	A2M	C6-N6	3.14	1.45	1.34
1	C1	389	A2M	C6-N6	3.12	1.45	1.34
1	C1	1223	A2M	C6-N6	3.12	1.45	1.34
1	C1	858	A2M	C6-N6	3.10	1.45	1.34
1	C1	637	A2M	C6-N6	3.09	1.45	1.34
1	C1	1847	A2M	C6-N6	3.09	1.45	1.34
1	C1	1432	A2M	C6-N6	3.09	1.45	1.34
1	C1	1433	OMG	C8-N7	-2.97	1.30	1.35
1	C1	385	OMG	C8-N7	-2.96	1.30	1.35
1	C1	627	OMG	C8-N7	-2.94	1.30	1.35
1	C1	646	OMG	C8-N7	-2.92	1.30	1.35
1	C1	2578	OMG	C8-N7	-2.88	1.30	1.35
1	C1	2876	OMG	C8-N7	-2.88	1.30	1.35
1	C1	2881	OMG	C8-N7	-2.82	1.30	1.35
1	C1	848	A2M	C5-C4	-2.81	1.33	1.40
1	C1	787	OMG	C8-N7	-2.79	1.30	1.35
1	C1	2358	OMG	C8-N7	-2.78	1.30	1.35
1	C1	1432	A2M	C5-C4	-2.78	1.33	1.40
1	C1	2289	A2M	C5-C4	-2.77	1.33	1.40
1	C1	2690	OMU	C6-N1	2.76	1.44	1.38
1	C1	1223	A2M	C5-C4	-2.74	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	389	A2M	C5-C4	-2.74	1.33	1.40
1	C1	2774	OMG	C8-N7	-2.73	1.30	1.35
1	C1	858	A2M	C5-C4	-2.73	1.33	1.40
1	C1	2277	OMU	C6-N1	2.73	1.44	1.38
1	C1	2380	OMU	C6-N1	2.73	1.44	1.38
1	C1	2384	OMU	C6-N1	2.71	1.44	1.38
1	C1	1917	OMU	C6-N1	2.70	1.44	1.38
1	C1	637	A2M	C5-C4	-2.70	1.33	1.40
1	C1	2683	OMU	C6-N1	2.68	1.44	1.38
1	C1	2688	OMU	C6-N1	2.67	1.44	1.38
1	C1	1847	A2M	C5-C4	-2.67	1.33	1.40
1	C1	1868	OMU	C6-N1	2.61	1.44	1.38
1	C1	646	OMG	C5-C6	-2.54	1.42	1.47
1	C1	2358	OMG	C5-C6	-2.49	1.42	1.47
1	C1	2578	OMG	C5-C6	-2.38	1.42	1.47
1	C1	627	OMG	C5-C6	-2.38	1.42	1.47
1	C1	787	OMG	C5-C6	-2.36	1.42	1.47
1	C1	1433	OMG	C5-C6	-2.36	1.42	1.47
1	C1	2881	OMG	C5-C6	-2.34	1.42	1.47
1	C1	2876	OMG	C5-C6	-2.33	1.42	1.47
1	C1	2688	OMU	C5-C4	2.31	1.48	1.43
1	C1	2774	OMG	C5-C6	-2.30	1.42	1.47
1	C1	2380	OMU	C5-C4	2.28	1.48	1.43
1	C1	385	OMG	C5-C6	-2.27	1.42	1.47
1	C1	2277	OMU	C5-C4	2.26	1.48	1.43
1	C1	1868	OMU	C5-C4	2.26	1.48	1.43
1	C1	1847	A2M	O3'-C3'	2.24	1.48	1.43
1	C1	2690	OMU	C5-C4	2.23	1.48	1.43
1	C1	2384	OMU	C5-C4	2.22	1.48	1.43
1	C1	2683	OMU	C5-C4	2.21	1.48	1.43
1	C1	848	A2M	O3'-C3'	2.19	1.48	1.43
1	C1	1432	A2M	O3'-C3'	2.15	1.48	1.43
1	C1	2289	A2M	O3'-C3'	2.14	1.48	1.43
1	C1	1847	A2M	C2-N3	2.14	1.35	1.32
1	C1	1917	OMU	C5-C4	2.14	1.48	1.43
1	C1	848	A2M	C2-N3	2.14	1.35	1.32
1	C1	858	A2M	O3'-C3'	2.12	1.48	1.43
1	C1	389	A2M	C2-N3	2.07	1.35	1.32
1	C1	1223	A2M	C2-N3	2.07	1.35	1.32
1	C1	637	A2M	O3'-C3'	2.06	1.47	1.43
1	C1	637	A2M	C2-N3	2.05	1.35	1.32
1	C1	1432	A2M	C2-N3	2.04	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1223	A2M	O3'-C3'	2.03	1.47	1.43
1	C1	389	A2M	O3'-C3'	2.01	1.47	1.43

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	389	A2M	C1'-N9-C4	10.97	145.92	126.64
1	C1	1847	A2M	C1'-N9-C4	10.83	145.67	126.64
1	C1	637	A2M	C1'-N9-C4	10.60	145.26	126.64
1	C1	1432	A2M	C1'-N9-C4	10.57	145.22	126.64
1	C1	1223	A2M	C1'-N9-C4	10.21	144.58	126.64
1	C1	848	A2M	C1'-N9-C4	10.16	144.50	126.64
1	C1	858	A2M	C1'-N9-C4	10.16	144.50	126.64
1	C1	2289	A2M	C1'-N9-C4	9.83	143.91	126.64
1	C1	858	A2M	C5-C6-N6	9.27	134.44	120.35
1	C1	1432	A2M	C5-C6-N6	9.15	134.25	120.35
1	C1	1847	A2M	C5-C6-N6	9.12	134.21	120.35
1	C1	1223	A2M	C5-C6-N6	9.07	134.14	120.35
1	C1	2289	A2M	C5-C6-N6	9.01	134.05	120.35
1	C1	848	A2M	C5-C6-N6	8.97	133.99	120.35
1	C1	389	A2M	C5-C6-N6	8.89	133.86	120.35
1	C1	637	A2M	C5-C6-N6	8.85	133.79	120.35
1	C1	1432	A2M	N6-C6-N1	-6.23	105.65	118.57
1	C1	858	A2M	N6-C6-N1	-6.21	105.69	118.57
1	C1	1847	A2M	N6-C6-N1	-6.21	105.69	118.57
1	C1	848	A2M	N6-C6-N1	-6.15	105.81	118.57
1	C1	1223	A2M	N6-C6-N1	-6.08	105.96	118.57
1	C1	2289	A2M	N6-C6-N1	-6.05	106.01	118.57
1	C1	389	A2M	N6-C6-N1	-5.95	106.23	118.57
1	C1	637	A2M	N6-C6-N1	-5.91	106.30	118.57
1	C1	858	A2M	N3-C2-N1	-5.87	119.50	128.68
1	C1	1847	A2M	N3-C2-N1	-5.79	119.62	128.68
1	C1	2289	A2M	N3-C2-N1	-5.72	119.74	128.68
1	C1	848	A2M	N3-C2-N1	-5.71	119.75	128.68
1	C1	1432	A2M	N3-C2-N1	-5.66	119.83	128.68
1	C1	637	A2M	N3-C2-N1	-5.65	119.86	128.68
1	C1	1223	A2M	N3-C2-N1	-5.62	119.90	128.68
1	C1	389	A2M	N3-C2-N1	-5.56	119.99	128.68
1	C1	1868	OMU	C4-N3-C2	-5.35	119.53	126.58
1	C1	2688	OMU	C4-N3-C2	-5.30	119.59	126.58
1	C1	2690	OMU	C4-N3-C2	-5.25	119.65	126.58
1	C1	2683	OMU	C4-N3-C2	-5.18	119.75	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2380	OMU	C4-N3-C2	-5.17	119.76	126.58
1	C1	1917	OMU	C4-N3-C2	-5.09	119.86	126.58
1	C1	2384	OMU	C4-N3-C2	-4.98	120.01	126.58
1	C1	2277	OMU	C4-N3-C2	-4.91	120.10	126.58
1	C1	2838	OMC	C1'-N1-C2	4.82	129.17	118.42
1	C1	1420	OMC	C1'-N1-C2	4.16	127.71	118.42
1	C1	1868	OMU	N3-C2-N1	3.93	120.11	114.89
1	C1	1917	OMU	N3-C2-N1	3.88	120.05	114.89
1	C1	2688	OMU	N3-C2-N1	3.85	120.00	114.89
1	C1	2384	OMU	N3-C2-N1	3.84	119.98	114.89
1	C1	2690	OMU	N3-C2-N1	3.80	119.94	114.89
1	C1	2380	OMU	N3-C2-N1	3.77	119.89	114.89
1	C1	2683	OMU	N3-C2-N1	3.73	119.84	114.89
1	C1	2277	OMU	N3-C2-N1	3.63	119.71	114.89
1	C1	2838	OMC	C1'-N1-C6	-3.54	113.12	120.84
1	C1	2683	OMU	C5-C4-N3	3.42	119.95	114.84
1	C1	2690	OMU	C5-C4-N3	3.38	119.90	114.84
1	C1	2380	OMU	C5-C4-N3	3.33	119.82	114.84
1	C1	2688	OMU	C5-C4-N3	3.32	119.81	114.84
1	C1	1868	OMU	C5-C4-N3	3.27	119.73	114.84
1	C1	1917	OMU	C5-C4-N3	3.23	119.67	114.84
1	C1	2277	OMU	C5-C4-N3	3.21	119.64	114.84
1	C1	2384	OMU	C5-C4-N3	3.15	119.56	114.84
1	C1	1420	OMC	C1'-N1-C6	-2.97	114.37	120.84
1	C1	2380	OMU	O4-C4-C5	-2.91	120.05	125.16
1	C1	2683	OMU	O4-C4-C5	-2.89	120.08	125.16
1	C1	1868	OMU	O4-C4-C5	-2.85	120.15	125.16
1	C1	2384	OMU	O4-C4-C5	-2.85	120.15	125.16
1	C1	1917	OMU	O4-C4-C5	-2.82	120.20	125.16
1	C1	2690	OMU	O4-C4-C5	-2.81	120.22	125.16
1	C1	2688	OMU	O4-C4-C5	-2.77	120.28	125.16
1	C1	2277	OMU	O4-C4-C5	-2.77	120.28	125.16
1	C1	2838	OMC	O2-C2-N3	-2.66	118.01	122.33
1	C1	1433	OMG	O6-C6-C5	2.50	129.25	124.37
1	C1	778	OMC	C1'-N1-C2	2.48	123.94	118.42
1	C1	2578	OMG	O6-C6-C5	2.47	129.19	124.37
1	C1	2358	OMG	O6-C6-C5	2.43	129.12	124.37
1	C1	627	OMG	O6-C6-C5	2.42	129.09	124.37
1	C1	787	OMG	O6-C6-C5	2.41	129.08	124.37
1	C1	2774	OMG	O6-C6-C5	2.41	129.08	124.37
1	C1	2881	OMG	O6-C6-C5	2.39	129.05	124.37
1	C1	385	OMG	O6-C6-C5	2.38	129.01	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1420	OMC	O2-C2-N1	2.34	123.72	118.89
1	C1	2384	OMU	C1'-N1-C2	2.34	121.80	117.57
1	C1	646	OMG	O6-C6-C5	2.33	128.93	124.37
1	C1	2300	OMC	C1'-N1-C2	2.32	123.60	118.42
1	C1	2876	OMG	O6-C6-C5	2.32	128.91	124.37
1	C1	1836	OMC	C1'-N1-C2	2.31	123.58	118.42
1	C1	1917	OMU	C1'-N1-C2	2.23	121.60	117.57
1	C1	2838	OMC	O2-C2-N1	2.19	123.42	118.89
1	C1	1420	OMC	O2-C2-N3	-2.19	118.77	122.33
1	C1	646	OMG	C5-C6-N1	-2.08	110.28	113.95
1	C1	2688	OMU	O2-C2-N1	-2.06	120.05	122.79
1	C1	2380	OMU	O2-C2-N1	-2.05	120.06	122.79
1	C1	2690	OMU	O2-C2-N1	-2.03	120.09	122.79

There are no chirality outliers.

All (31) 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	1433	OMG	C3'-C4'-C5'-O5'
1	C1	1917	OMU	C1'-C2'-O2'-CM2
1	C1	2277	OMU	C1'-C2'-O2'-CM2
1	C1	2578	OMG	O4'-C4'-C5'-O5'
1	C1	2578	OMG	C3'-C4'-C5'-O5'
1	C1	2683	OMU	C1'-C2'-O2'-CM2
1	C1	2690	OMU	C3'-C4'-C5'-O5'
1	C1	2690	OMU	O4'-C4'-C5'-O5'
1	C1	2838	OMC	O4'-C1'-N1-C2
1	C1	2838	OMC	O4'-C1'-N1-C6
1	C1	389	A2M	C3'-C4'-C5'-O5'
1	C1	1491	OMC	O4'-C4'-C5'-O5'
1	C1	848	A2M	O4'-C4'-C5'-O5'
1	C1	385	OMG	C3'-C4'-C5'-O5'
1	C1	1223	A2M	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C3'-C4'-C5'-O5'
1	C1	1917	OMU	O4'-C4'-C5'-O5'
1	C1	2578	OMG	C4'-C5'-O5'-P
1	C1	385	OMG	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	C1	1420	OMC	C2'-C1'-N1-C6
1	C1	1420	OMC	O4'-C4'-C5'-O5'
1	C1	2918	OMC	C1'-C2'-O2'-CM2
1	C1	1420	OMC	C2'-C1'-N1-C2
1	C1	848	A2M	C3'-C4'-C5'-O5'
1	C1	1847	A2M	O4'-C4'-C5'-O5'
1	C1	1917	OMU	C3'-C4'-C5'-O5'

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
59	GTP	Cd	1003	60	26,34,34	1.18	2 (7%)	32,54,54	1.53	7 (21%)
59	GTP	CH	701	60	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)

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
59	GTP	Cd	1003	60	-	6/18/38/38	0/3/3/3
59	GTP	CH	701	60	-	5/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Cd	1003	GTP	C5-C6	-4.26	1.38	1.47
59	CH	701	GTP	C5-C6	-4.06	1.39	1.47
59	CH	701	GTP	C2-N3	2.14	1.38	1.33
59	Cd	1003	GTP	C2-N3	2.11	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Cd	1003	GTP	PB-O3B-PG	-3.37	121.28	132.83
59	CH	701	GTP	PA-O3A-PB	-3.34	121.37	132.83
59	Cd	1003	GTP	C5-C6-N1	3.28	119.75	113.95
59	CH	701	GTP	C5-C6-N1	3.27	119.73	113.95
59	CH	701	GTP	PB-O3B-PG	-3.21	121.82	132.83
59	CH	701	GTP	C3'-C2'-C1'	3.03	105.54	100.98
59	CH	701	GTP	C8-N7-C5	2.98	108.67	102.99
59	Cd	1003	GTP	C8-N7-C5	2.94	108.59	102.99
59	Cd	1003	GTP	C2-N1-C6	-2.92	119.72	125.10
59	CH	701	GTP	C2-N1-C6	-2.88	119.80	125.10
59	Cd	1003	GTP	C3'-C2'-C1'	2.70	105.04	100.98
59	Cd	1003	GTP	O6-C6-C5	-2.27	119.93	124.37
59	Cd	1003	GTP	PA-O3A-PB	-2.23	125.19	132.83
59	CH	701	GTP	O6-C6-C5	-2.16	120.16	124.37

There are no chirality outliers.

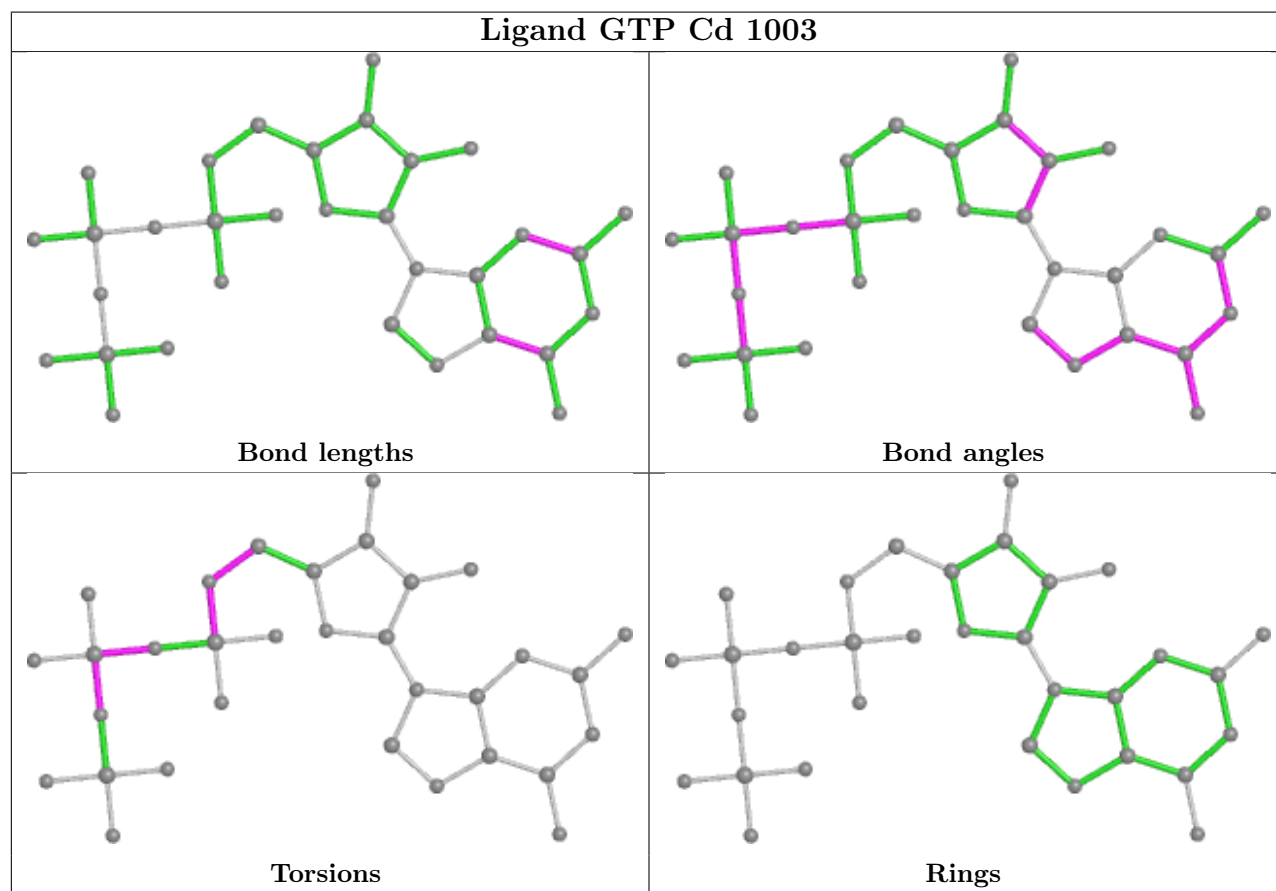
All (11) torsion outliers are listed below:

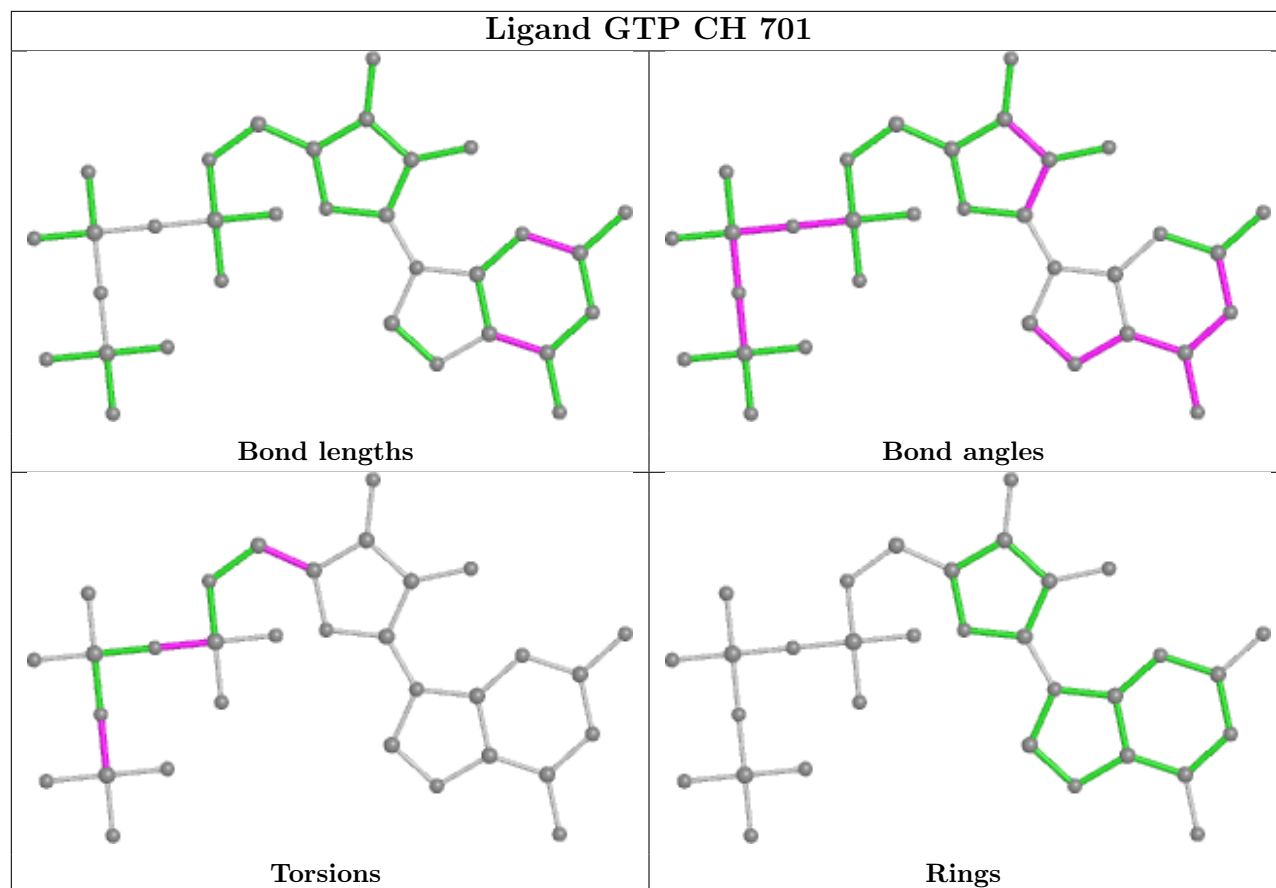
Mol	Chain	Res	Type	Atoms
59	Cd	1003	GTP	C5'-O5'-PA-O1A
59	Cd	1003	GTP	C5'-O5'-PA-O2A
59	CH	701	GTP	PB-O3B-PG-O2G
59	Cd	1003	GTP	PG-O3B-PB-O1B
59	CH	701	GTP	C3'-C4'-C5'-O5'
59	CH	701	GTP	PB-O3A-PA-O2A
59	Cd	1003	GTP	C4'-C5'-O5'-PA
59	CH	701	GTP	O4'-C4'-C5'-O5'
59	Cd	1003	GTP	PA-O3A-PB-O1B
59	CH	701	GTP	PB-O3B-PG-O3G
59	Cd	1003	GTP	C5'-O5'-PA-O3A

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.

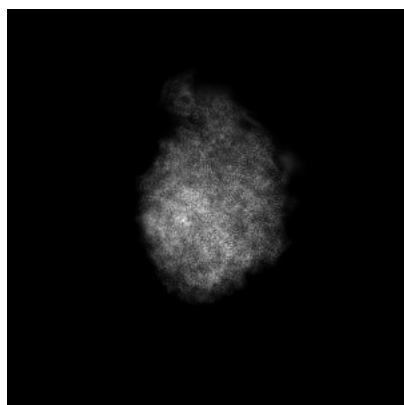
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17952. These allow visual inspection of the internal detail of the map and identification of artifacts.

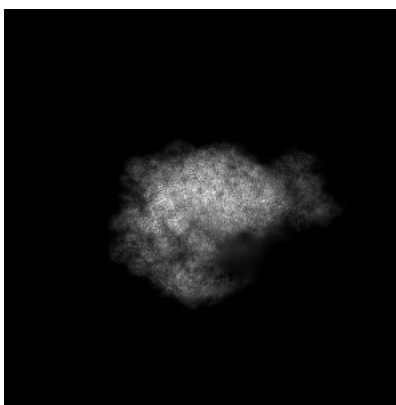
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

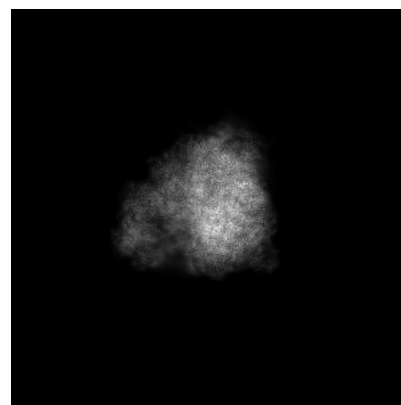
6.1.1 Primary map



X



Y

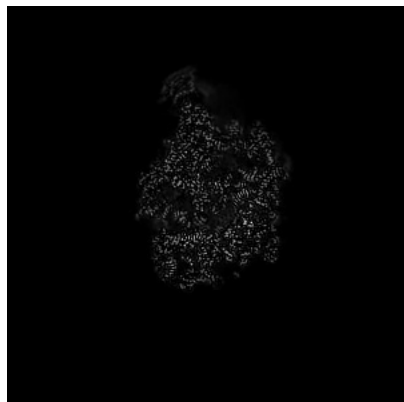


Z

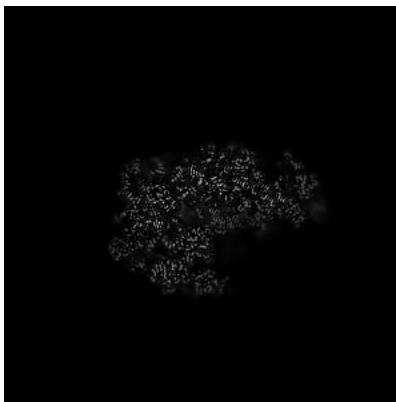
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

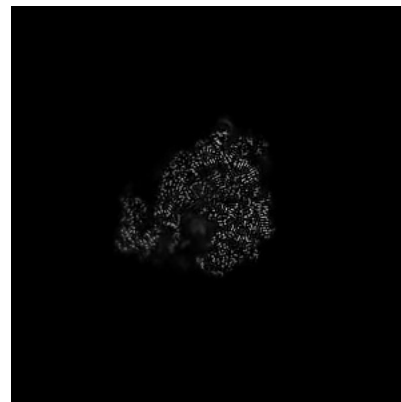
6.2.1 Primary map



X Index: 250



Y Index: 250

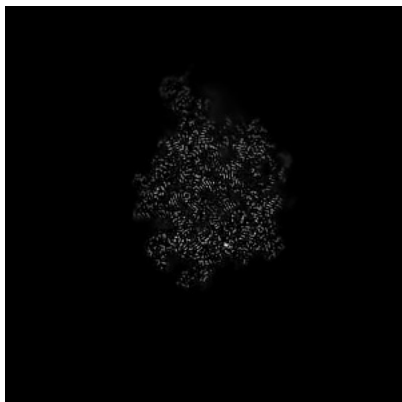


Z Index: 250

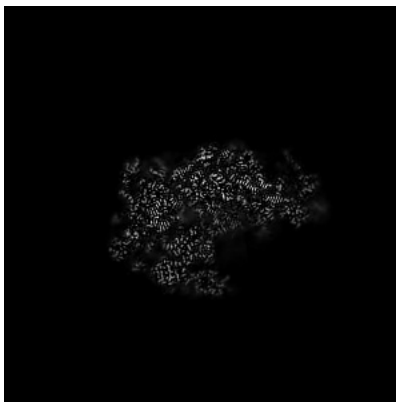
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

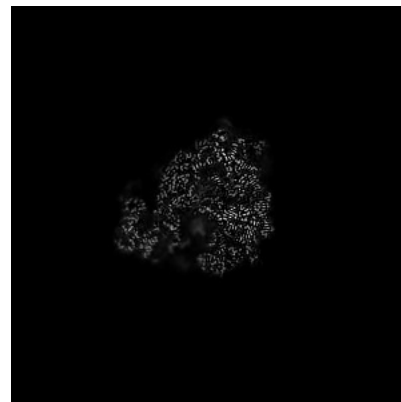
6.3.1 Primary map



X Index: 259



Y Index: 248

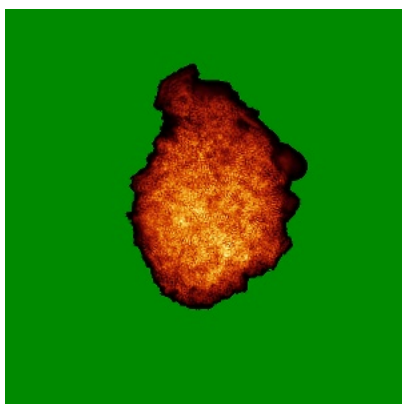


Z Index: 248

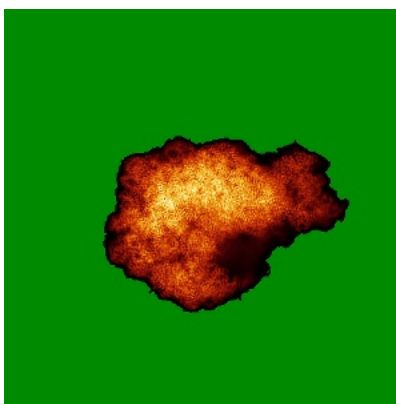
The images above show the largest variance slices of the map in three orthogonal directions.

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

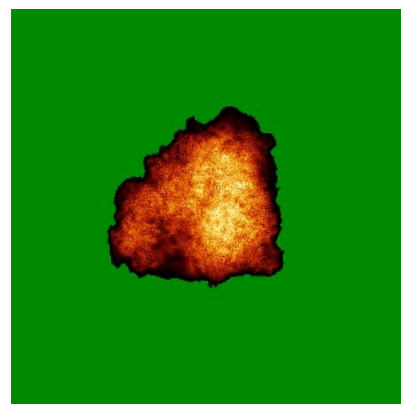
6.4.1 Primary map



X



Y

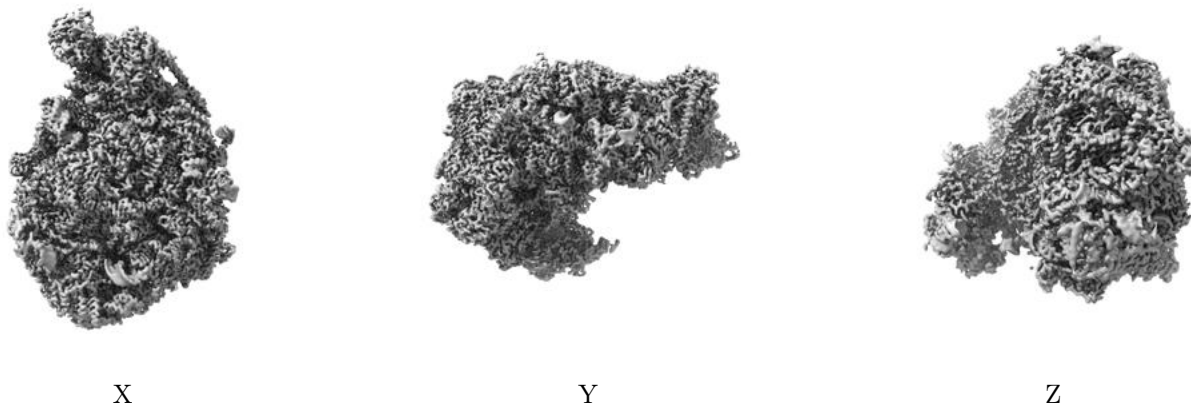


Z

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

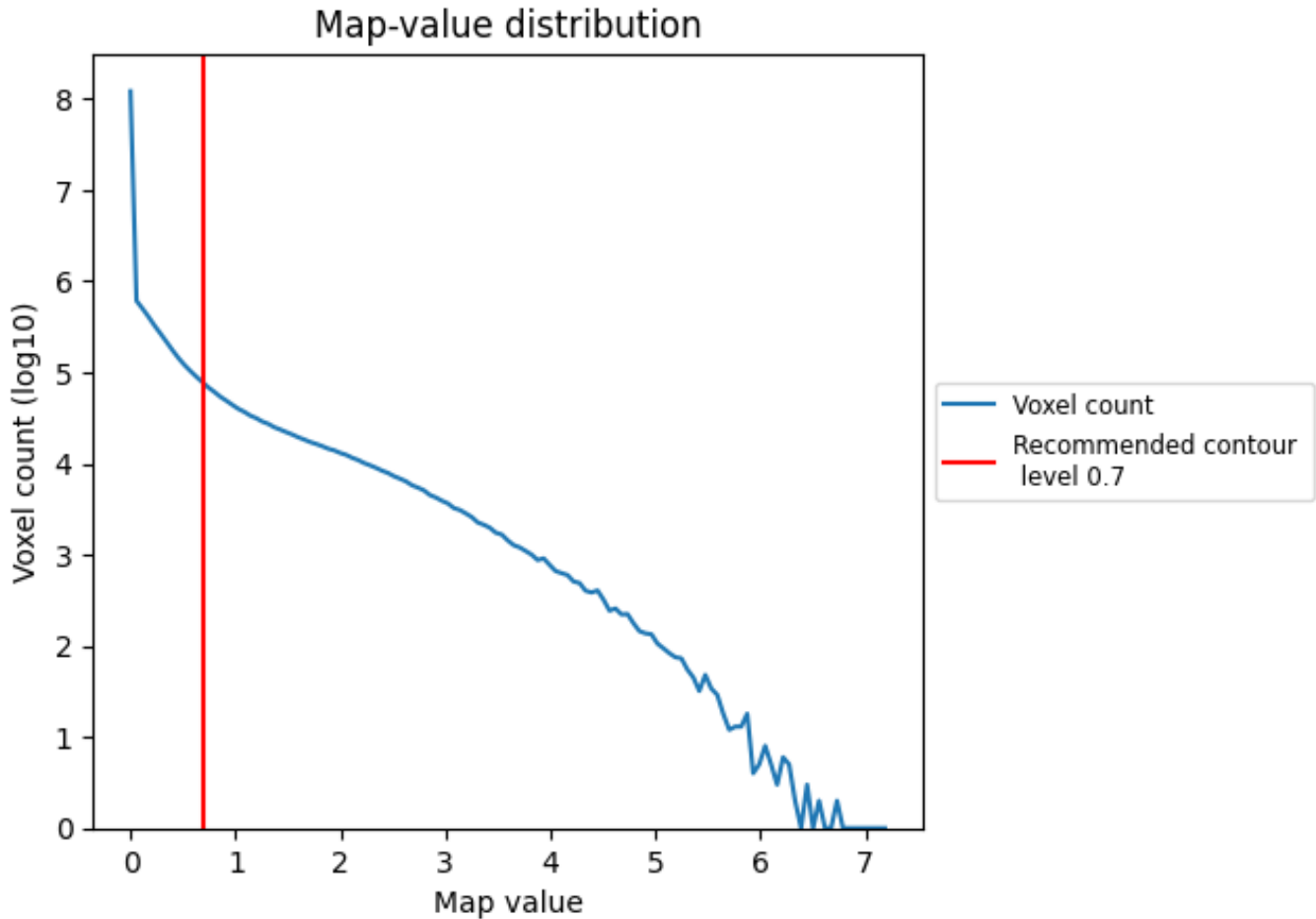
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

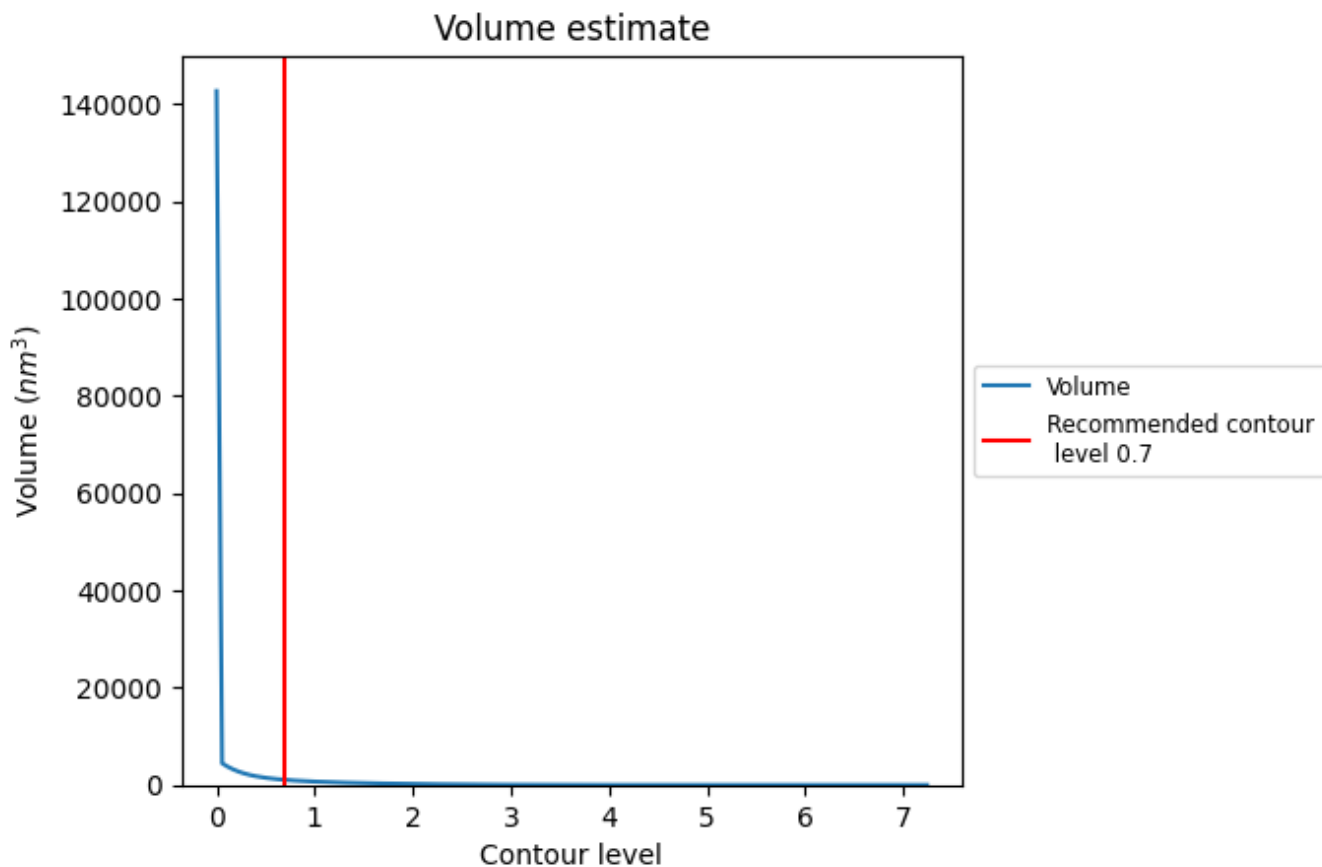
This section contains the results of statistical analysis of the map.

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.

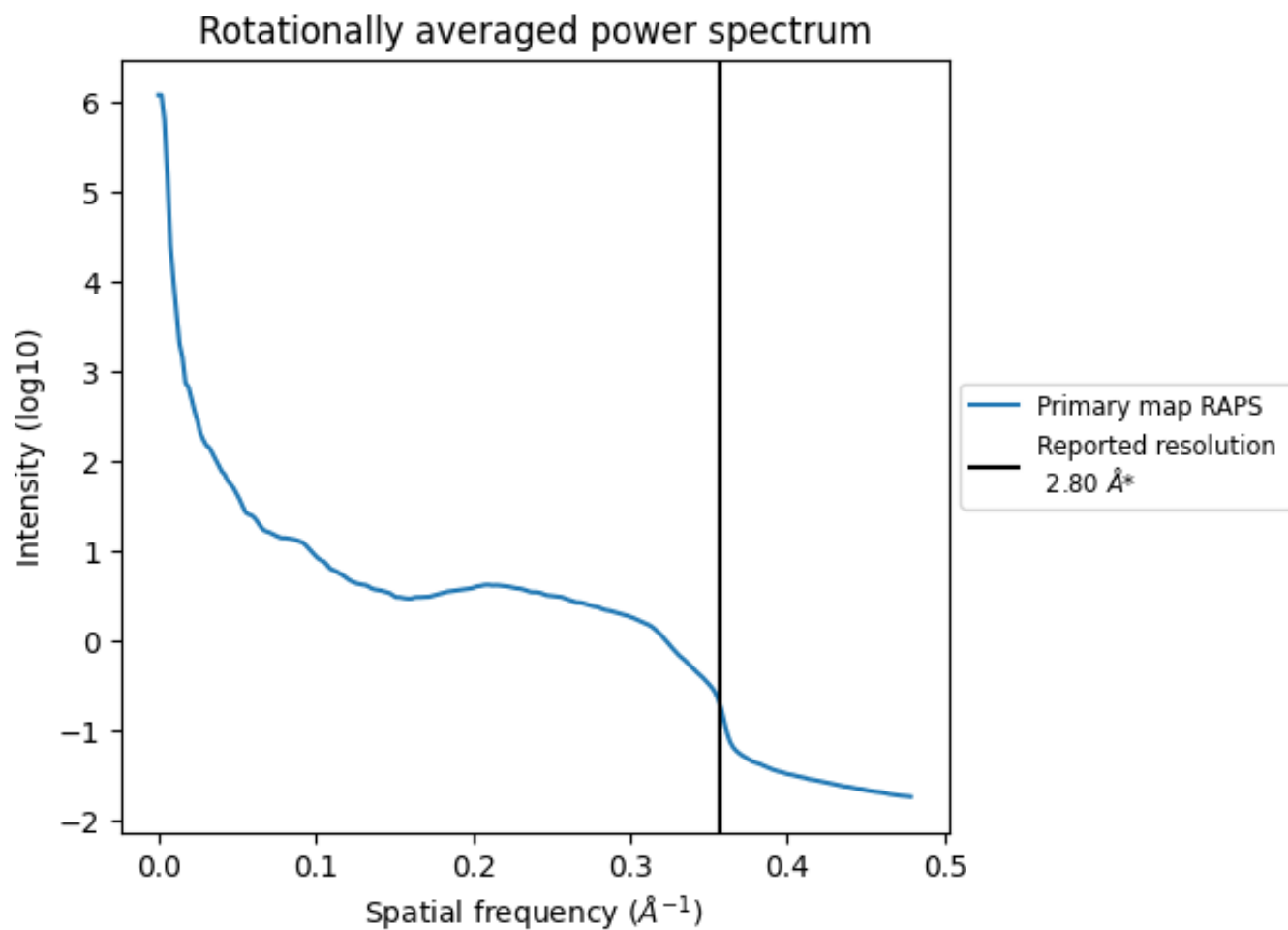
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1050 nm³; this corresponds to an approximate mass of 949 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 0.357 Å⁻¹

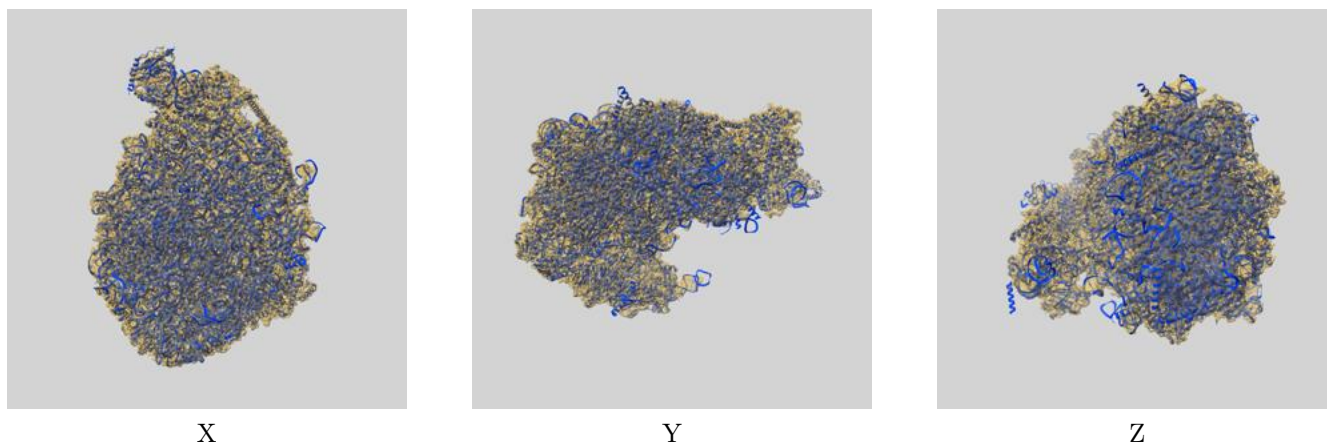
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

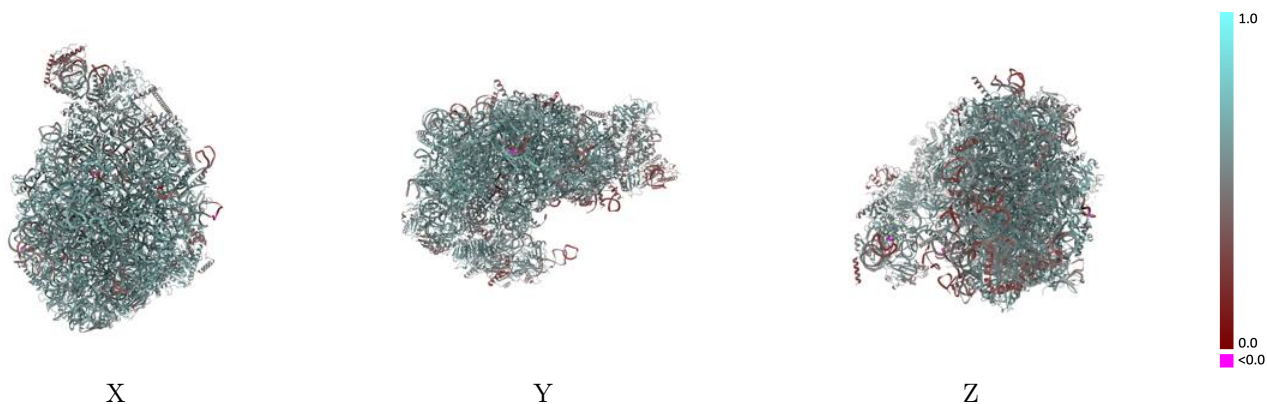
This section contains information regarding the fit between EMDB map EMD-17952 and PDB model 8PV3. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



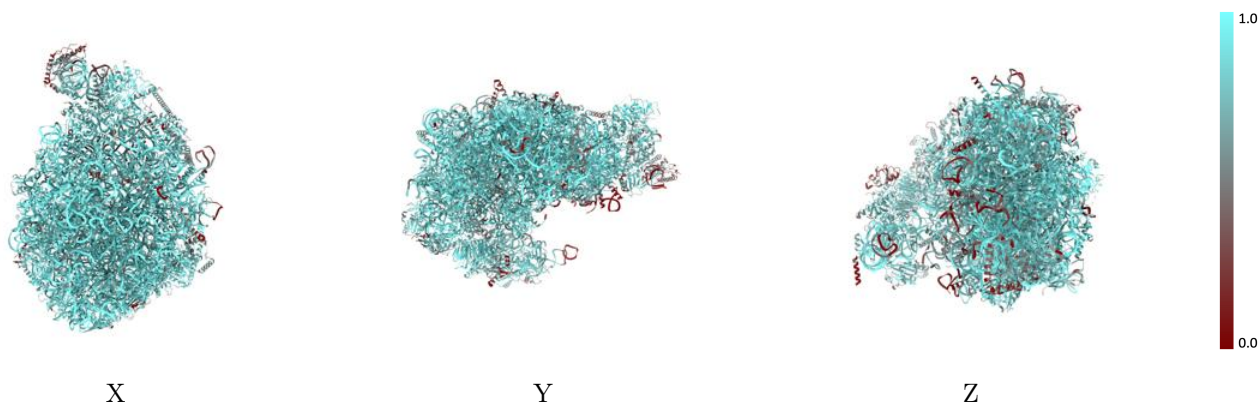
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



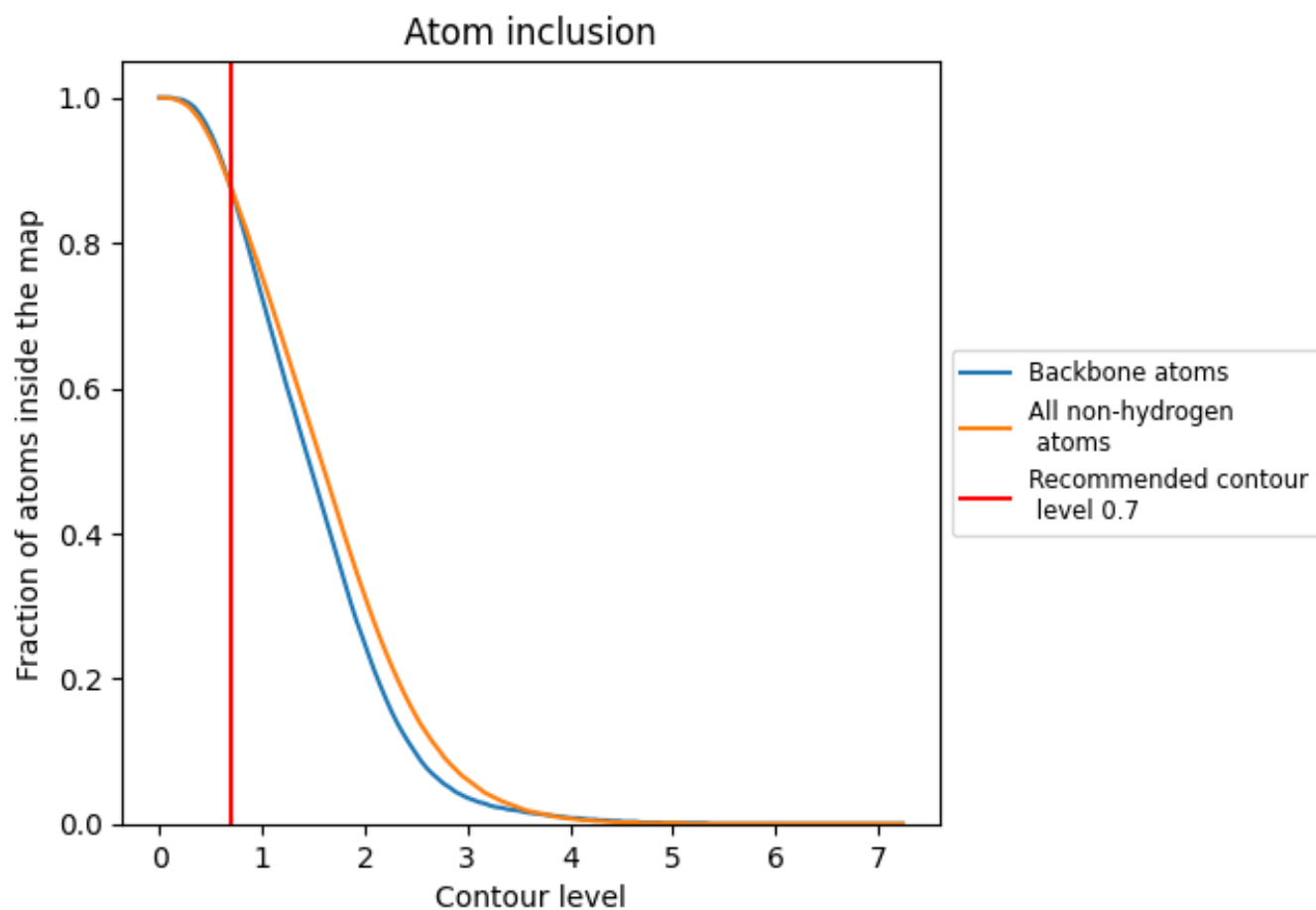
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 88% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.5730
C1	 0.9270	 0.5820
C2	 0.9590	 0.6120
C3	 0.6240	 0.4030
C4	 0.8460	 0.4860
CB	 0.5740	 0.4370
CF	 0.8050	 0.5430
CH	 0.8330	 0.5680
CI	 0.6530	 0.4580
CJ	 0.8820	 0.5720
CK	 0.9310	 0.6070
CL	 0.7820	 0.5390
CM	 0.7680	 0.5180
CN	 0.9000	 0.6070
CO	 0.8290	 0.5790
CQ	 0.8070	 0.5700
Cb	 0.7230	 0.5420
Cd	 0.8620	 0.5720
Ce	 0.6850	 0.4980
Cf	 0.8270	 0.5480
Cg	 0.7790	 0.5240
Ch	 0.7990	 0.5400
Cz	 0.6970	 0.4720
LA	 0.8420	 0.5570
LB	 0.9450	 0.6360
LC	 0.9300	 0.6260
LD	 0.8350	 0.5410
LE	 0.8160	 0.5700
LF	 0.8990	 0.6040
LG	 0.8470	 0.5670
LH	 0.9040	 0.6050
LJ	 0.7350	 0.4590
LK	 0.7190	 0.5000
LL	 0.8470	 0.5830
LM	 0.9040	 0.6040



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Chain	Atom inclusion	Q-score
LN	 0.9370	 0.6270
LO	 0.9570	 0.6400
LP	 0.9490	 0.6350
LQ	 0.8960	 0.6000
LR	 0.9140	 0.6070
LS	 0.9110	 0.6070
LT	 0.7060	 0.4770
LU	 0.8050	 0.5540
LV	 0.9560	 0.6350
LX	 0.8660	 0.5810
LY	 0.9040	 0.6040
LZ	 0.8510	 0.5560
La	 0.9120	 0.5990
Lc	 0.7910	 0.5520
Ld	 0.9010	 0.6240
Le	 0.9460	 0.6340
Lf	 0.9780	 0.6520
Lg	 0.8510	 0.5800
Lh	 0.8380	 0.5610
Li	 0.7950	 0.5330
Lj	 0.9730	 0.6510
Lk	 0.7710	 0.5510
Ll	 0.9860	 0.6570
Lp	 0.7860	 0.5470
Lq	 0.8990	 0.5900