



Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 03:45 am BST

PDB ID : 8OOP / pdb_00008oop
EMDB ID : EMD-17025
Title : CryoEM Structure INO80core Hexasome complex composite model state2
Authors : Zhang, M.; Jungblut, A.; Hoffmann, T.; Eustermann, S.
Deposited on : 2023-04-05
Resolution : 2.70 Å (reported)
Based on initial models : 7OHC, 8A5Q, 6FML

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:

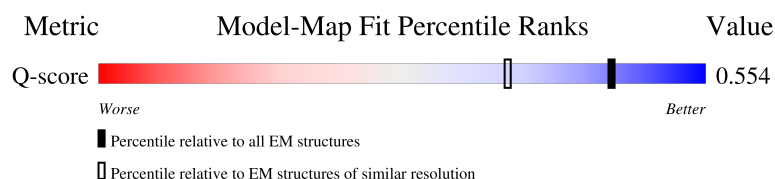
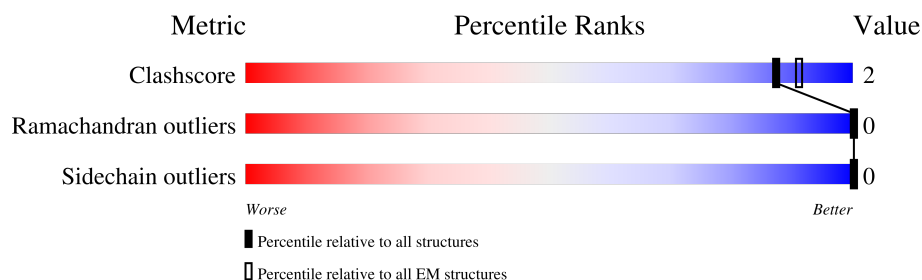
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.70 Å.

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



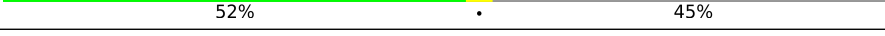
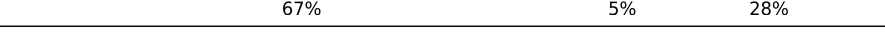
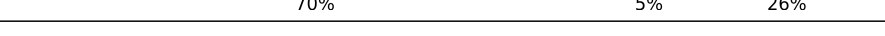
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	A	462	 95%
1	B	462	 91% 5%
1	C	462	 98%
2	D	488	 87% 10%

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Mol	Chain	Length	Quality of chain
2	E	488	
2	F	488	
3	G	1134	
4	H	492	
5	I	219	
6	J	769	
7	K	226	
8	L	226	
9	M	135	
9	Q	135	
10	N	102	
10	R	102	
11	O	129	
12	P	125	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 40747 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 protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3432	2154	610	653	15		
1	B	438	Total	C	N	O	S	0	0
			3352	2103	597	637	15		
1	C	459	Total	C	N	O	S	0	0
			3511	2199	627	670	15		

- Molecule 2 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	441	Total	C	N	O	S	0	0
			3401	2129	597	660	15		
2	E	443	Total	C	N	O	S	0	0
			3414	2136	600	663	15		
2	F	439	Total	C	N	O	S	0	0
			3394	2125	596	658	15		

- Molecule 3 is a protein called Chromatin-remodeling ATPase Ino80.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	704	Total	C	N	O	S	0	0
			5736	3657	1020	1024	35		

- Molecule 4 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	38	Total	C	N	O	S	0	0
			283	181	51	48	3		

- Molecule 5 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	109	Total	C	N	O	S	0	0
			873	546	167	156	4		

- Molecule 6 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	630	Total	C	N	O	S	0	0
			4472	2820	806	830	16		

- Molecule 7 is a DNA chain called DNA strand 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	110	Total	C	N	O	P	0	0
			2243	1063	410	660	110		

- Molecule 8 is a DNA chain called DNA Strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	107	Total	C	N	O	P	0	0
			2201	1041	411	642	107		

- Molecule 9 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	74	Total	C	N	O	S	0	0
			602	381	113	104	4		
9	Q	98	Total	C	N	O	S	0	0
			810	511	157	138	4		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	73	Total	C	N	O	S	0	0
			587	370	115	101	1		
10	R	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

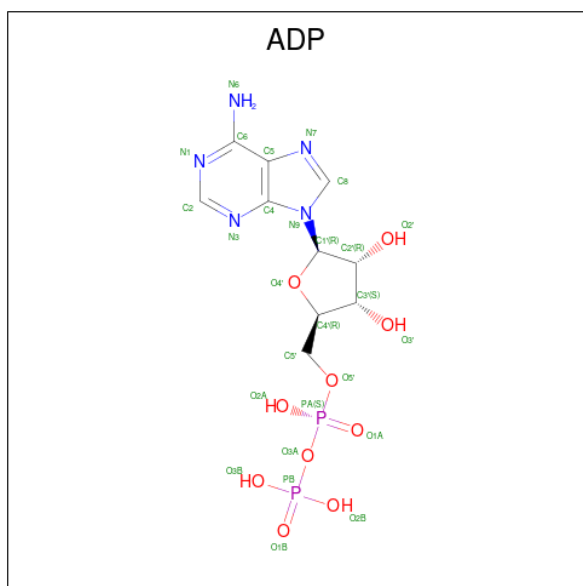
- Molecule 11 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	109	Total	C	N	O	0	0
			842	531	167	144		

- Molecule 12 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	93	Total	C	N	O	S	0	0
			729	458	131	138	2		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

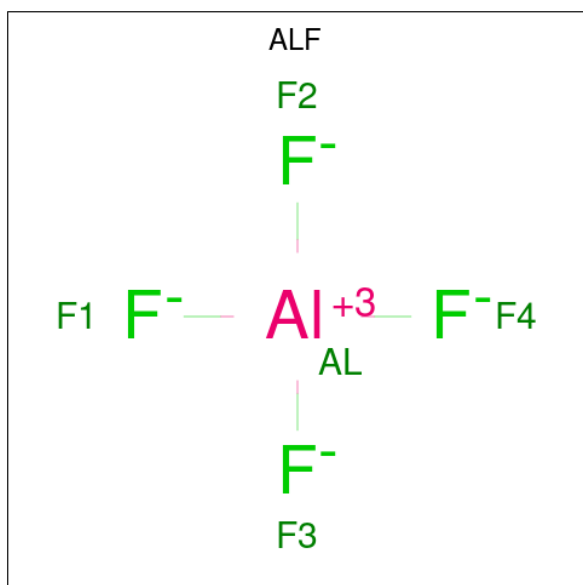


Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

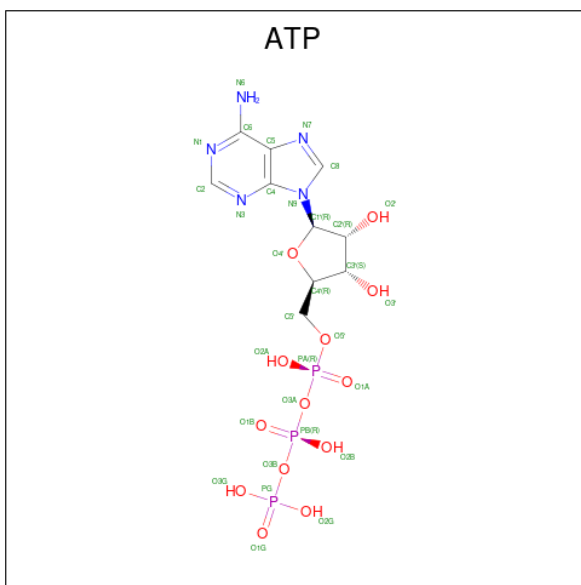
Mol	Chain	Residues	Atoms		AltConf
14	G	1	Total	Mg	0
			1	1	
14	J	1	Total	Mg	0
			1	1	

- Molecule 15 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
15	G	1	Total	Al	F	0
			5	1	4	

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

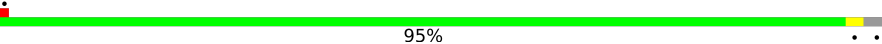


Mol	Chain	Residues	Atoms					AltConf
16	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots

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

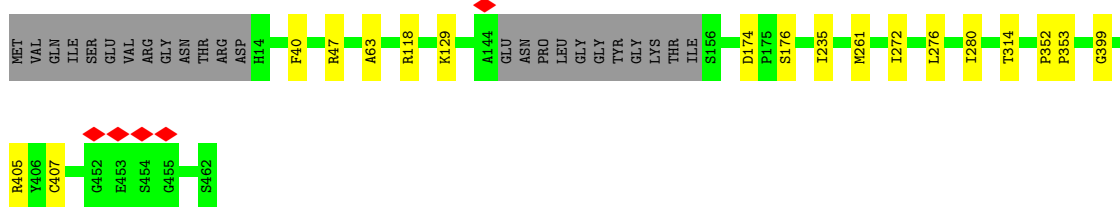
- Molecule 1: RuvB-like protein 1

Chain A: 

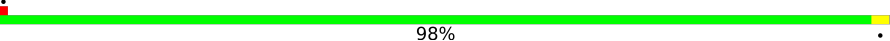


- Molecule 1: RuvB-like protein 1

Chain B: 



- Molecule 1: RuvB-like protein 1

Chain C: 



- Molecule 2: RuvB-like protein 2

Chain D: 



- Molecule 2: RuvB-like protein 2

[illegible]

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|
| GLN | GLY | ALA | ALA | GLU | ALA | ALA | ALA | PRO | THR | LEU | PRO | ALA | ASP | PRO | VAL | GLY | GLY | GLU | LYS | MET | ASP | MET | SER | | | | | | | | | | | | | |
| MET | ALA | ALA | PRO | LEU | VAL | THR | GLU | THR | THR | VAL | ARG | G17 | L20 | A55 | V59 | R90 | L103 | I108 | S114 | R124 | R149 | S150 | VAL | THR | GLY | GLY | ALA | K156 | G218 | T221 | D247 | R252 | E299 | R313 | I324 | R437 |

- [illegible]

LYS LEU LEU ASN PHE LEU ILE SER GLN THR LEU TYR SER HIS PHE ILE SER LYS LYS ILE LYS THR THR GLJ VAL GLJ ARG SER SER ASP HIS PRO ASP VAL ALA THR ASP GLJ LYS ASP LYS LYS PRO PRO GLJ THR THR LEU ASN ILE ILE ASN VAL GLJ GLY THR THR PRO ILE PRO

[illegible]

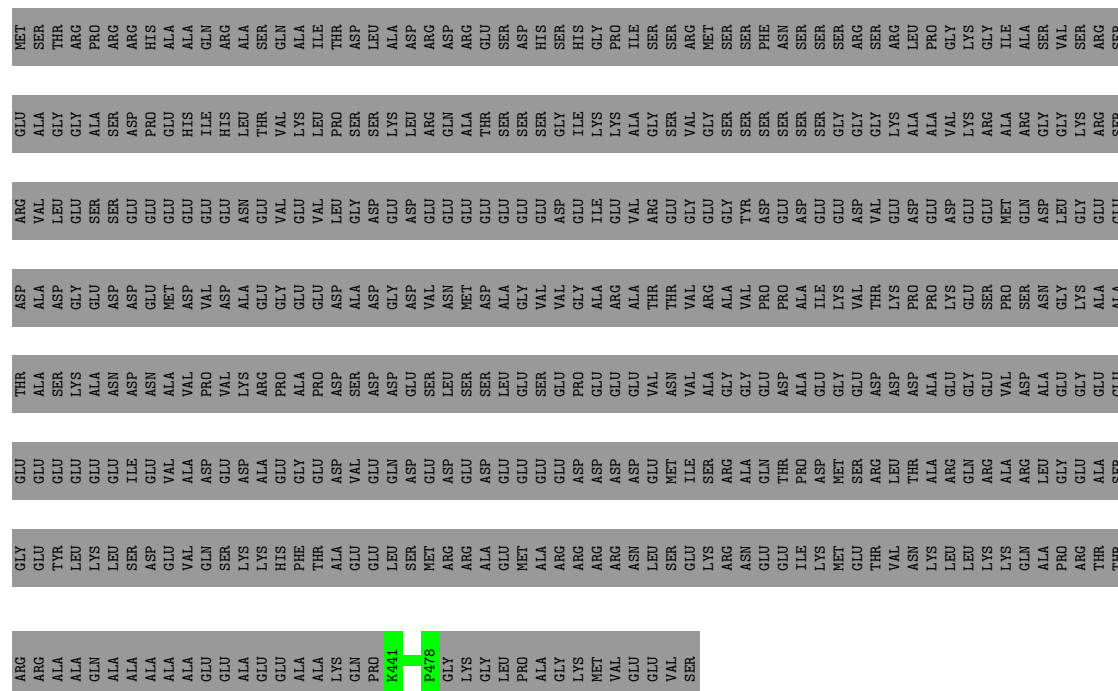
THR	GLU	PHE	GLU	VAL	ALA	K964	P965	K966	N969	E974	S1007	I1008	D1019	A1028	T1032	L1033	V1040	D1046	Q1087	D1107	I1112	W1120	R1129	L1134	S1160	HIS	ASP	GLU	PHE	SER	SER	GLU	TRP	PHE	SER	SER	LYS	ASP	ILE	GLU	SER	HIS	HIS	ALA	ALA	GLN	SER	SER	ASN
-----	-----	-----	-----	-----	-----	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

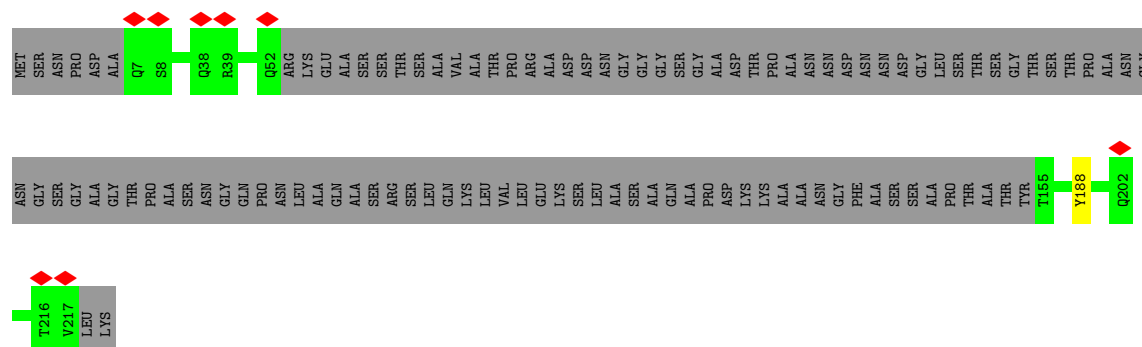
Amino Acid	Category
E1586	Amino acids in the protein
T1590	Amino acids in the protein
Y1591	Amino acids in the protein
R1592	Amino acids in the protein and in the protein-protein interface
H1593	Amino acids in the protein
Y1596	Amino acids in the protein and in the protein-protein interface
L1599	Amino acids in the protein and in the protein-protein interface
I1623	Amino acids in the protein and in the protein-protein interface
F1624	Amino acids in the protein and in the protein-protein interface
G1631	Amino acids in the protein and in the protein-protein interface
S1648	Amino acids in the protein and in the protein-protein interface
D1649	Amino acids in the protein and in the protein-protein interface
W1650	Amino acids in the protein and in the protein-protein interface
R1661	Amino acids in the protein and in the protein-protein interface
G1703	Amino acids in the protein
S1706	Amino acids in the protein and in the protein-protein interface

[illegible]

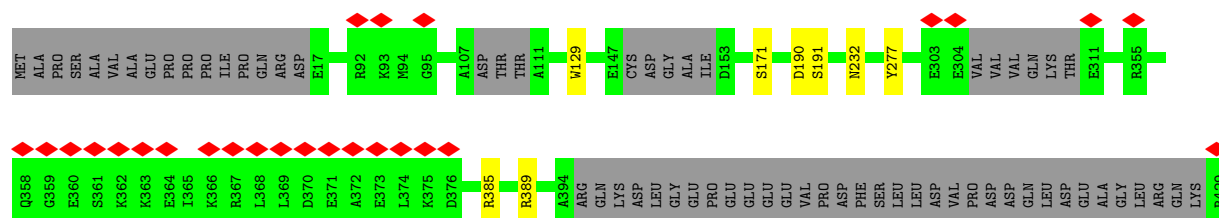
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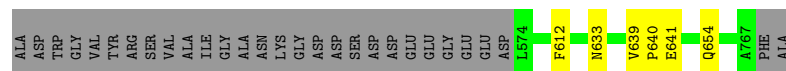


- Molecule 5: Chromatin-remodeling complex subunit IES6

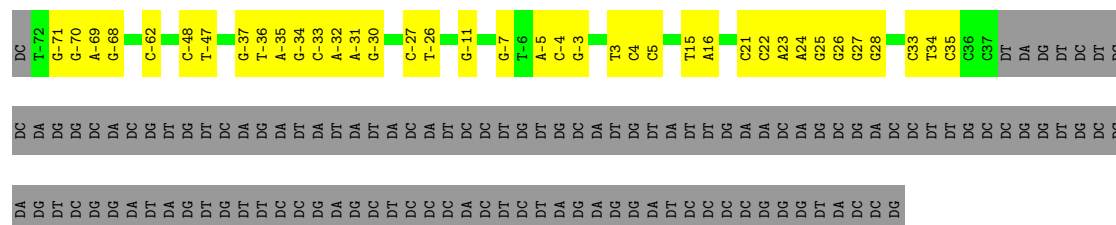
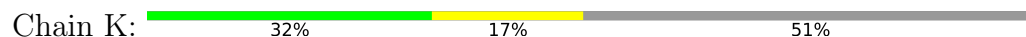


- Molecule 6: Actin-related protein 5

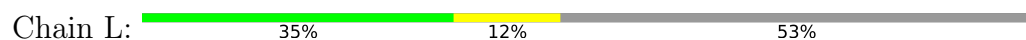




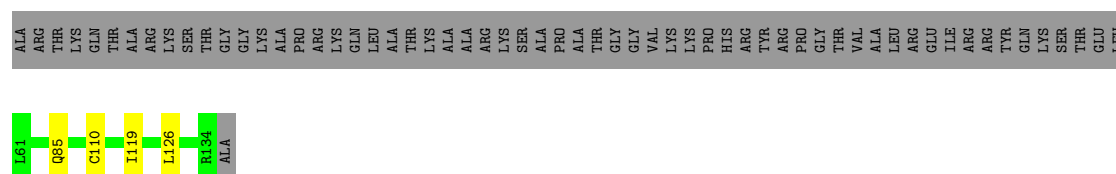
- Molecule 7: DNA strand 1



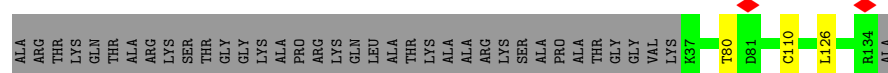
- Molecule 8: DNA Strand 2



- Molecule 9: Histone H3.1

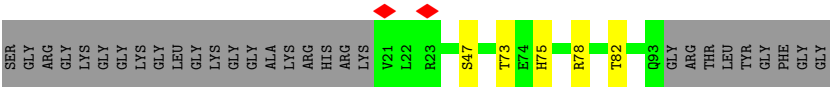


- Molecule 9: Histone H3.1

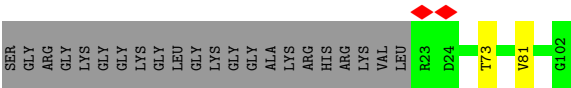
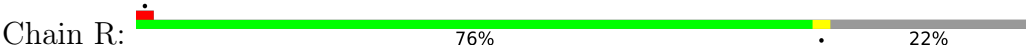


- Molecule 10: Histone H4

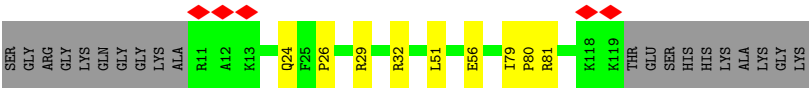
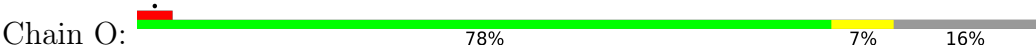




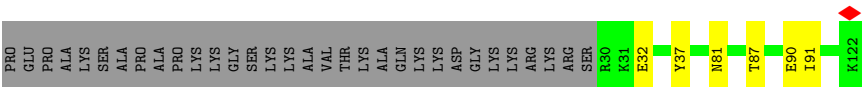
• Molecule 10: Histone H4



• Molecule 11: Histone H2A



• Molecule 12: Histone H2B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98967	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	11.515	Depositor
Minimum map value	-5.442	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.324	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	295.92, 295.92, 295.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ALF, ATP, ADP

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	A	0.21	0/3481	0.55	0/4703
1	B	0.21	0/3398	0.57	0/4589
1	C	0.19	0/3560	0.52	0/4809
2	D	0.20	0/3445	0.53	0/4640
2	E	0.20	0/3457	0.54	0/4654
2	F	0.19	0/3437	0.52	0/4627
3	G	0.22	0/5866	0.58	0/7926
4	H	0.17	0/290	0.49	0/393
5	I	0.21	0/893	0.56	0/1207
6	J	0.18	0/4564	0.49	0/6225
7	K	0.51	0/2513	0.68	0/3873
8	L	0.50	0/2470	0.67	0/3812
9	M	0.21	0/609	0.56	0/816
9	Q	0.21	0/822	0.57	0/1102
10	N	0.22	0/592	0.55	0/794
10	R	0.21	0/645	0.56	0/862
11	O	0.19	0/852	0.57	0/1147
12	P	0.19	0/740	0.53	0/993
All	All	0.26	0/41634	0.56	0/57172

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
2	D	0	1
2	F	0	2
3	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	118	ARG	Sidechain
1	B	405	ARG	Sidechain
1	C	8	ARG	Sidechain
2	D	252	ARG	Sidechain
2	F	252	ARG	Sidechain
2	F	437	ARG	Sidechain
3	G	1592	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3432	0	3518	6	0
1	B	3352	0	3438	11	0
1	C	3511	0	3595	5	0
2	D	3401	0	3472	8	0
2	E	3414	0	3482	5	0
2	F	3394	0	3464	10	0
3	G	5736	0	5776	25	0
4	H	283	0	289	0	0
5	I	873	0	868	1	0
6	J	4472	0	3904	10	0
7	K	2243	0	1233	50	0
8	L	2201	0	1200	33	0
9	M	602	0	632	3	0
9	Q	810	0	851	2	0
10	N	587	0	635	4	0
10	R	638	0	676	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	O	842	0	908	7	0
12	P	729	0	751	5	0
13	A	27	0	12	0	0
13	B	27	0	12	0	0
13	C	27	0	12	0	0
13	D	27	0	12	0	0
13	E	27	0	12	0	0
13	F	27	0	12	0	0
13	G	27	0	12	0	0
14	G	1	0	0	0	0
14	J	1	0	0	0	0
15	G	5	0	0	0	0
16	J	31	0	12	0	0
All	All	40747	0	38788	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:24:DA:H2''	7:K:25:DG:C8	2.19	0.78
7:K:-68:DG:N2	8:L:69:DT:O2	2.19	0.74
8:L:-16:DT:H2''	8:L:-15:DA:C8	2.27	0.70
7:K:-35:DA:H2''	7:K:-34:DG:C8	2.31	0.66
8:L:63:DG:H8	8:L:63:DG:OP2	1.80	0.65
8:L:-18:DG:H2''	8:L:-17:DT:C5	2.32	0.65
7:K:-71:DG:H2''	7:K:-70:DG:C8	2.32	0.64
8:L:40:DC:H2''	8:L:41:DC:H5'	1.78	0.64
3:G:1631:GLY:O	3:G:1661:ARG:NH1	2.24	0.64
8:L:3:DC:H2''	8:L:4:DG:C8	2.34	0.63
2:D:300:VAL:HG21	2:D:325:MET:HB3	1.79	0.63
3:G:1087:GLN:HG3	8:L:-28:DC:H4'	1.81	0.63
7:K:26:DG:H2''	7:K:27:DG:C8	2.34	0.62
7:K:-69:DA:C8	7:K:-69:DA:OP2	2.51	0.62
8:L:-6:DG:H2''	8:L:-5:DG:C8	2.34	0.62
7:K:21:DC:C6	7:K:21:DC:OP2	2.54	0.60
7:K:-34:DG:H1'	7:K:-33:DC:C6	2.38	0.59
3:G:1265:ARG:NH2	3:G:1648:SER:O	2.36	0.59
7:K:-62:DC:OP2	7:K:-62:DC:C6	2.56	0.58
6:J:435:LYS:O	6:J:439:GLU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:63:DG:OP2	8:L:63:DG:C8	2.56	0.58
7:K:21:DC:OP2	7:K:21:DC:H6	1.86	0.58
2:F:124:ARG:NE	2:F:247:ASP:OD2	2.37	0.58
7:K:-70:DG:H2''	7:K:-69:DA:C8	2.39	0.57
8:L:-18:DG:H2''	8:L:-17:DT:C6	2.39	0.57
7:K:-70:DG:H2''	7:K:-69:DA:N9	2.21	0.56
1:B:272:ILE:HG23	1:B:276:LEU:HD23	1.87	0.56
8:L:-11:DC:H2''	8:L:-10:DG:H5'	1.87	0.56
7:K:25:DG:H2''	7:K:26:DG:C8	2.41	0.56
3:G:1028:ALA:HB2	3:G:1107:ASP:OD2	2.06	0.55
8:L:-16:DT:H2'	8:L:-16:DT:OP2	2.07	0.55
1:A:354:ASP:OD2	2:E:328:ASN:ND2	2.39	0.55
7:K:-69:DA:OP2	7:K:-69:DA:H8	1.89	0.54
1:C:102:ILE:HG22	1:C:109:LYS:HB2	1.89	0.54
8:L:69:DT:C6	8:L:69:DT:OP2	2.60	0.54
7:K:27:DG:H2''	7:K:28:DG:C8	2.42	0.54
7:K:22:DC:H2''	7:K:23:DA:H5'	1.89	0.53
1:A:40:PHE:CG	1:A:47:ARG:HD3	2.43	0.53
7:K:-34:DG:H1'	7:K:-33:DC:C5	2.43	0.53
7:K:-7:DG:O6	8:L:6:DA:N6	2.41	0.53
7:K:15:DT:H2''	7:K:16:DA:C8	2.43	0.53
8:L:5:DT:H2''	8:L:6:DA:C8	2.44	0.53
1:A:52:VAL:HG11	2:E:407:THR:HG23	1.91	0.53
3:G:1028:ALA:HB1	3:G:1032:THR:OG1	2.09	0.53
3:G:1650:TRP:CE3	7:K:34:DT:H5''	2.46	0.51
6:J:277:TYR:CD1	6:J:641:GLU:HG3	2.45	0.51
3:G:1295:LEU:HD13	9:Q:80:THR:HG21	1.93	0.51
8:L:60:DC:OP2	8:L:60:DC:C6	2.63	0.51
2:D:124:ARG:NE	2:D:247:ASP:OD2	2.42	0.50
3:G:1325:ARG:HH12	3:G:1486:GLU:CD	2.19	0.50
8:L:60:DC:OP2	8:L:60:DC:H6	1.94	0.50
6:J:232:ASN:ND2	6:J:654:GLN:HE22	2.10	0.49
11:O:79:ILE:HG23	11:O:80:PRO:HD2	1.95	0.49
10:R:73:THR:HG21	10:R:81:VAL:HA	1.94	0.49
7:K:-36:DT:H2''	7:K:-35:DA:C5	2.48	0.49
2:D:149:ARG:HH22	2:D:182:THR:HG21	1.77	0.48
3:G:1599:LEU:HD13	3:G:1624:PHE:CZ	2.47	0.48
7:K:-62:DC:OP2	7:K:-62:DC:H6	1.96	0.48
8:L:15:DT:H2''	8:L:16:DA:C8	2.48	0.48
1:B:314:THR:HG23	2:F:299:GLU:OE1	2.13	0.48
1:C:204:VAL:HG21	3:G:1406:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:PRO:HG2	2:D:81:THR:HG21	1.94	0.48
6:J:385:ARG:O	6:J:389:ARG:N	2.37	0.48
7:K:-35:DA:H2''	7:K:-34:DG:N7	2.28	0.48
11:O:32:ARG:HH22	12:P:32:GLU:CD	2.21	0.48
3:G:1284:PHE:CZ	3:G:1307:THR:HG23	2.50	0.47
8:L:49:DC:P	11:O:29:ARG:HH22	2.37	0.47
7:K:-37:DG:H2''	7:K:-36:DT:C6	2.49	0.47
8:L:31:DT:H2''	8:L:32:DT:O5'	2.15	0.46
1:A:131:VAL:HG21	1:A:193:TYR:CE2	2.49	0.46
2:D:105:ALA:HB3	2:D:302:MET:HB2	1.96	0.46
8:L:62:DG:H2''	8:L:63:DG:C8	2.50	0.46
6:J:190:ASP:OD1	6:J:191:SER:N	2.49	0.46
3:G:1367:TRP:H	3:G:1367:TRP:CD1	2.34	0.46
11:O:26:PRO:HG3	12:P:37:TYR:CE2	2.51	0.46
3:G:1007:SER:OG	3:G:1134:LEU:HD11	2.16	0.46
7:K:33:DC:H2''	7:K:34:DT:H71	1.98	0.46
7:K:-36:DT:H2''	7:K:-35:DA:N7	2.31	0.45
8:L:59:DA:H2''	8:L:60:DC:C6	2.52	0.45
3:G:1650:TRP:CZ3	7:K:34:DT:H5''	2.52	0.45
7:K:-70:DG:C8	7:K:-70:DG:OP2	2.70	0.45
8:L:3:DC:H4'	8:L:4:DG:OP1	2.17	0.45
2:E:439:VAL:O	2:E:442:VAL:HG22	2.17	0.45
7:K:-71:DG:C2	7:K:-70:DG:C2	3.05	0.45
3:G:1284:PHE:HZ	3:G:1307:THR:HG23	1.81	0.44
1:B:40:PHE:CG	1:B:47:ARG:HD3	2.52	0.44
7:K:-70:DG:OP2	7:K:-70:DG:H8	2.00	0.44
7:K:-5:DA:N6	8:L:4:DG:C6	2.86	0.44
8:L:-11:DC:H2''	8:L:-10:DG:C5'	2.47	0.44
7:K:34:DT:H2''	7:K:35:DC:C5	2.52	0.44
8:L:-16:DT:H2''	8:L:-15:DA:N7	2.31	0.44
1:A:57:ILE:HD13	1:A:299:VAL:HG11	2.00	0.44
2:E:76:ALA:O	2:E:357:ASN:HA	2.18	0.44
7:K:34:DT:H2''	7:K:35:DC:C6	2.53	0.44
1:B:280:ILE:HG13	3:G:1349:ILE:HD11	1.99	0.44
3:G:1650:TRP:CD2	7:K:34:DT:H5''	2.53	0.44
7:K:4:DC:H2''	7:K:5:DC:C5	2.53	0.44
9:Q:110:CYS:SG	9:Q:126:LEU:HD23	2.58	0.44
1:C:104:SER:HA	2:F:114:SER:OG	2.18	0.44
9:M:85:GLN:OE1	10:N:82:THR:HG22	2.17	0.44
1:A:258:ILE:HA	1:B:261:MET:HE1	1.99	0.43
7:K:-36:DT:H2''	7:K:-35:DA:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:-18:DG:H4'	8:L:-17:DT:OP1	2.18	0.43
1:C:40:PHE:CG	1:C:47:ARG:HD3	2.53	0.43
7:K:-48:DC:H2''	7:K:-47:DT:C5	2.53	0.43
11:O:51:LEU:HB2	12:P:91:ILE:HD13	2.00	0.43
2:F:90:MET:HE1	2:F:324:ILE:HD13	2.01	0.43
6:J:277:TYR:CE1	6:J:641:GLU:HG3	2.54	0.43
1:B:352:PRO:HA	1:B:353:PRO:HD3	1.91	0.43
1:B:63:ALA:HB2	2:F:20:LEU:HB2	2.00	0.43
1:B:129:LYS:HD2	1:B:235:ILE:HD12	2.00	0.42
1:B:174:ASP:OD2	2:F:221:THR:HG21	2.18	0.42
1:B:399:GLY:N	1:B:407:CYS:SG	2.92	0.42
7:K:-48:DC:O2	7:K:-47:DT:N3	2.51	0.42
7:K:-11:DG:C2	8:L:12:DG:N2	2.87	0.42
11:O:24:GLN:N	11:O:56:GLU:OE1	2.53	0.42
7:K:-27:DC:H4'	7:K:-26:DT:H5'	2.02	0.42
7:K:22:DC:H2''	7:K:23:DA:C5'	2.49	0.42
3:G:1112:ILE:HG22	3:G:1120:TRP:HD1	1.85	0.42
6:J:441:ARG:O	6:J:445:LYS:N	2.48	0.42
6:J:612:PHE:O	6:J:633:ASN:ND2	2.52	0.42
7:K:-3:DG:C2	8:L:4:DG:N2	2.88	0.42
6:J:639:VAL:HB	6:J:640:PRO:HD3	2.01	0.42
1:B:176:SER:OG	2:F:218:GLY:HA3	2.19	0.42
7:K:3:DT:H1'	7:K:4:DC:C2	2.54	0.42
7:K:-69:DA:C5	7:K:-68:DG:C6	3.08	0.42
7:K:-5:DA:H2''	7:K:-4:DC:H6	1.85	0.41
8:L:4:DG:H2''	8:L:5:DT:C5	2.56	0.41
2:E:168:GLU:O	5:I:188:TYR:OH	2.33	0.41
7:K:-33:DC:C2	7:K:-32:DA:C8	3.09	0.41
6:J:129:TRP:CZ2	6:J:171:SER:HB2	2.56	0.41
2:F:103:LEU:HD21	2:F:108:ILE:HD11	2.03	0.41
3:G:1260:LEU:HB3	3:G:1264:PHE:CE2	2.55	0.41
7:K:-5:DA:H2''	7:K:-4:DC:C6	2.55	0.41
8:L:-27:DC:C5	8:L:-26:DC:N4	2.88	0.41
10:N:73:THR:HG23	10:N:78:ARG:HG3	2.02	0.41
3:G:1256:THR:HG22	3:G:1256:THR:O	2.21	0.41
3:G:1028:ALA:HB3	3:G:1033:LEU:HD23	2.02	0.41
3:G:1596:TYR:CB	3:G:1623:ILE:HG23	2.51	0.41
7:K:-31:DA:C6	7:K:-30:DG:C6	3.09	0.41
10:N:75:HIS:CD2	12:P:81:ASN:HD21	2.38	0.41
11:O:79:ILE:HG22	11:O:81:ARG:H	1.85	0.41
2:D:256:PHE:CD2	3:G:1531:ASP:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:-62:DC:O2	8:L:63:DG:N2	2.54	0.40
1:C:98:THR:HG23	2:F:313:ARG:HD3	2.03	0.40
7:K:-70:DG:C2'	7:K:-69:DA:C8	3.05	0.40
9:M:119:ILE:O	10:N:47:SER:OG	2.36	0.40
12:P:87:THR:H	12:P:90:GLU:HG2	1.87	0.40
2:D:341:SER:OG	2:D:342:PRO:HD2	2.21	0.40
3:G:1008:ILE:HD11	3:G:1040:VAL:HG22	2.03	0.40
3:G:1087:GLN:CG	8:L:-28:DC:H4'	2.50	0.40
2:D:333:ARG:HA	2:D:340:LYS:HA	2.03	0.40
2:F:55:ALA:O	2:F:59:VAL:HG23	2.21	0.40
9:M:110:CYS:SG	9:M:126:LEU:HD23	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/462 (97%)	433 (97%)	14 (3%)	0	100	100
1	B	434/462 (94%)	420 (97%)	14 (3%)	0	100	100
1	C	457/462 (99%)	449 (98%)	8 (2%)	0	100	100
2	D	439/488 (90%)	436 (99%)	3 (1%)	0	100	100
2	E	439/488 (90%)	430 (98%)	9 (2%)	0	100	100
2	F	435/488 (89%)	430 (99%)	5 (1%)	0	100	100
3	G	698/1134 (62%)	671 (96%)	27 (4%)	0	100	100
4	H	36/492 (7%)	35 (97%)	1 (3%)	0	100	100
5	I	105/219 (48%)	103 (98%)	2 (2%)	0	100	100
6	J	618/769 (80%)	598 (97%)	20 (3%)	0	100	100
9	M	72/135 (53%)	71 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Q	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
10	N	71/102 (70%)	70 (99%)	1 (1%)	0	100	100
10	R	78/102 (76%)	75 (96%)	3 (4%)	0	100	100
11	O	107/129 (83%)	105 (98%)	2 (2%)	0	100	100
12	P	91/125 (73%)	90 (99%)	1 (1%)	0	100	100
All	All	4623/6192 (75%)	4511 (98%)	112 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/377 (97%)	365 (100%)	0	100	100
1	B	357/377 (95%)	357 (100%)	0	100	100
1	C	374/377 (99%)	374 (100%)	0	100	100
2	D	369/402 (92%)	369 (100%)	0	100	100
2	E	370/402 (92%)	370 (100%)	0	100	100
2	F	369/402 (92%)	369 (100%)	0	100	100
3	G	625/989 (63%)	625 (100%)	0	100	100
4	H	30/398 (8%)	30 (100%)	0	100	100
5	I	93/171 (54%)	93 (100%)	0	100	100
6	J	371/644 (58%)	371 (100%)	0	100	100
9	M	64/110 (58%)	64 (100%)	0	100	100
9	Q	86/110 (78%)	86 (100%)	0	100	100
10	N	62/78 (80%)	62 (100%)	0	100	100
10	R	65/78 (83%)	65 (100%)	0	100	100
11	O	85/98 (87%)	85 (100%)	0	100	100
12	P	80/105 (76%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3765/5118 (74%)	3765 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	146	ASN
1	A	168	GLN
1	A	248	ASN
1	A	458	HIS
1	B	19	HIS
1	B	182	GLN
1	B	409	GLN
1	B	458	HIS
1	C	263	GLN
1	C	285	GLN
1	C	306	HIS
1	C	365	HIS
1	C	421	ASN
1	C	458	HIS
2	D	239	HIS
2	D	394	GLN
2	E	24	HIS
2	E	232	GLN
2	E	394	GLN
2	F	19	ASN
2	F	244	HIS
2	F	359	HIS
3	G	1006	GLN
3	G	1345	HIS
3	G	1447	ASN
3	G	1657	GLN
5	I	168	HIS
6	J	633	ASN
6	J	654	GLN
6	J	697	ASN
11	O	94	ASN
12	P	81	ASN
12	P	92	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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$
13	ADP	A	501	-	27,29,29	1.38	4 (14%)	42,45,45	1.95	10 (23%)
16	ATP	J	801	14	29,33,33	0.33	0	44,52,52	0.49	1 (2%)
13	ADP	G	2001	15,14	27,29,29	1.38	4 (14%)	42,45,45	2.03	10 (23%)
13	ADP	E	501	-	27,29,29	1.36	4 (14%)	42,45,45	1.95	10 (23%)
13	ADP	D	501	-	27,29,29	1.35	4 (14%)	42,45,45	1.96	11 (26%)
13	ADP	C	501	-	27,29,29	1.37	4 (14%)	42,45,45	1.90	9 (21%)
15	ALF	G	2003	13	0,4,4	-	-	-	-	-
13	ADP	B	501	-	27,29,29	1.34	4 (14%)	42,45,45	1.96	10 (23%)
13	ADP	F	501	-	27,29,29	1.37	4 (14%)	42,45,45	1.89	8 (19%)

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
13	ADP	A	501	-	-	2/16/32/32	0/3/3/3
16	ATP	J	801	14	-	9/22/38/38	0/3/3/3
13	ADP	G	2001	15,14	-	3/16/32/32	0/3/3/3
13	ADP	E	501	-	-	1/16/32/32	0/3/3/3
13	ADP	D	501	-	-	6/16/32/32	0/3/3/3
13	ADP	C	501	-	-	3/16/32/32	0/3/3/3
13	ADP	B	501	-	-	4/16/32/32	0/3/3/3
13	ADP	F	501	-	-	0/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	ADP	C5-C4	4.48	1.47	1.39
13	G	2001	ADP	C5-C4	4.46	1.47	1.39
13	A	501	ADP	C5-C4	4.44	1.47	1.39
13	F	501	ADP	C5-C4	4.43	1.47	1.39
13	E	501	ADP	C5-C4	4.36	1.47	1.39
13	B	501	ADP	C5-C4	4.33	1.47	1.39
13	D	501	ADP	C5-C4	4.31	1.47	1.39
13	G	2001	ADP	C5-C6	2.69	1.48	1.41
13	A	501	ADP	C5-C6	2.69	1.48	1.41
13	C	501	ADP	C5-C6	2.67	1.48	1.41
13	F	501	ADP	C5-C6	2.66	1.48	1.41
13	D	501	ADP	C5-C6	2.63	1.48	1.41
13	E	501	ADP	C5-C6	2.57	1.48	1.41
13	B	501	ADP	C5-C6	2.53	1.48	1.41
13	E	501	ADP	C5-N7	-2.41	1.34	1.39
13	F	501	ADP	C5-N7	-2.40	1.34	1.39
13	B	501	ADP	C5-N7	-2.39	1.34	1.39
13	G	2001	ADP	C8-N7	2.34	1.36	1.31
13	A	501	ADP	C8-N7	2.33	1.36	1.31
13	A	501	ADP	C5-N7	-2.32	1.34	1.39
13	C	501	ADP	C5-N7	-2.31	1.34	1.39
13	D	501	ADP	C8-N7	2.24	1.35	1.31
13	D	501	ADP	C5-N7	-2.24	1.34	1.39
13	C	501	ADP	C8-N7	2.21	1.35	1.31
13	G	2001	ADP	C5-N7	-2.15	1.35	1.39
13	F	501	ADP	C8-N7	2.13	1.35	1.31
13	E	501	ADP	C8-N7	2.12	1.35	1.31
13	B	501	ADP	C8-N7	2.04	1.35	1.31

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	501	ADP	C5-C4-N3	-6.46	118.32	126.75
13	C	501	ADP	C5-C4-N3	-6.42	118.37	126.75
13	B	501	ADP	C5-C4-N3	-6.42	118.38	126.75
13	A	501	ADP	C5-C4-N3	-6.31	118.52	126.75
13	F	501	ADP	C5-C4-N3	-6.28	118.55	126.75
13	D	501	ADP	C5-C4-N3	-6.21	118.65	126.75
13	G	2001	ADP	C5-C4-N3	-6.04	118.86	126.75
13	B	501	ADP	N3-C4-N9	5.24	135.71	127.08
13	E	501	ADP	N3-C4-N9	5.12	135.51	127.08
13	F	501	ADP	N3-C4-N9	5.08	135.45	127.08
13	C	501	ADP	N3-C4-N9	5.07	135.43	127.08
13	D	501	ADP	N3-C4-N9	4.91	135.18	127.08
13	G	2001	ADP	PA-O3A-PB	-4.90	116.00	132.83
13	G	2001	ADP	N3-C4-N9	4.89	135.15	127.08
13	A	501	ADP	N3-C4-N9	4.84	135.06	127.08
13	E	501	ADP	C2-N3-C4	4.10	121.44	111.75
13	A	501	ADP	C2-N3-C4	4.06	121.34	111.75
13	B	501	ADP	C2-N3-C4	4.05	121.32	111.75
13	C	501	ADP	C2-N3-C4	4.05	121.31	111.75
13	F	501	ADP	C2-N3-C4	4.04	121.28	111.75
13	D	501	ADP	C2-N3-C4	4.02	121.25	111.75
13	G	2001	ADP	C2-N3-C4	3.96	121.11	111.75
13	E	501	ADP	N3-C2-N1	-3.56	123.03	128.60
13	B	501	ADP	N3-C2-N1	-3.55	123.04	128.60
13	A	501	ADP	N3-C2-N1	-3.52	123.09	128.60
13	F	501	ADP	N3-C2-N1	-3.49	123.14	128.60
13	A	501	ADP	C4-C5-N7	-3.48	106.38	110.62
13	D	501	ADP	N3-C2-N1	-3.46	123.20	128.60
13	C	501	ADP	N3-C2-N1	-3.41	123.27	128.60
13	G	2001	ADP	N3-C2-N1	-3.37	123.33	128.60
13	E	501	ADP	C4-C5-N7	-3.31	106.59	110.62
13	D	501	ADP	C4-C5-N7	-3.27	106.64	110.62
13	C	501	ADP	C4-C5-N7	-3.20	106.72	110.62
13	B	501	ADP	C4-C5-N7	-3.17	106.76	110.62
13	F	501	ADP	C4-C5-N7	-3.09	106.86	110.62
13	G	2001	ADP	C4-C5-N7	-3.08	106.86	110.62
13	A	501	ADP	C5-N7-C8	2.99	107.76	103.51
13	B	501	ADP	C5-N7-C8	2.95	107.70	103.51
13	E	501	ADP	C5-N7-C8	2.94	107.68	103.51
13	A	501	ADP	PA-O3A-PB	-2.93	122.77	132.83
13	D	501	ADP	C5-N7-C8	2.93	107.67	103.51
13	G	2001	ADP	C4-N9-C8	2.87	108.84	105.73
13	D	501	ADP	C4-N9-C8	2.76	108.72	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501	ADP	C5-N7-C8	2.76	107.43	103.51
13	B	501	ADP	C4-N9-C8	2.72	108.67	105.73
13	F	501	ADP	C5-N7-C8	2.69	107.33	103.51
13	G	2001	ADP	C5-N7-C8	2.67	107.30	103.51
13	E	501	ADP	C4-N9-C8	2.54	108.48	105.73
13	F	501	ADP	C4-N9-C8	2.53	108.47	105.73
13	A	501	ADP	C4-N9-C8	2.43	108.37	105.73
13	C	501	ADP	C4-N9-C8	2.40	108.32	105.73
13	D	501	ADP	N9-C8-N7	-2.27	110.80	113.91
13	A	501	ADP	C6-C5-N7	2.26	136.24	132.02
13	D	501	ADP	PA-O3A-PB	-2.22	125.22	132.83
13	G	2001	ADP	C6-C5-N7	2.18	136.08	132.02
13	B	501	ADP	N9-C8-N7	-2.17	110.95	113.91
13	C	501	ADP	PA-O3A-PB	-2.15	125.44	132.83
13	D	501	ADP	C6-C5-N7	2.15	136.03	132.02
13	G	2001	ADP	N9-C8-N7	-2.13	111.00	113.91
13	B	501	ADP	PA-O3A-PB	-2.09	125.64	132.83
13	A	501	ADP	N9-C8-N7	-2.07	111.08	113.91
13	E	501	ADP	N9-C8-N7	-2.06	111.09	113.91
16	J	801	ATP	PB-O3B-PG	2.04	139.84	132.83
13	E	501	ADP	C6-C5-N7	2.04	135.82	132.02
13	B	501	ADP	C2-N1-C6	2.03	122.26	118.77
13	E	501	ADP	C2-N1-C6	2.03	122.25	118.77
13	D	501	ADP	O3B-PB-O2B	2.03	115.40	107.64
13	C	501	ADP	C6-C5-N7	2.02	135.79	132.02
13	F	501	ADP	C6-C5-N7	2.01	135.77	132.02

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	501	ADP	PA-O3A-PB-O2B
13	B	501	ADP	PA-O3A-PB-O2B
13	B	501	ADP	PA-O3A-PB-O3B
13	C	501	ADP	PA-O3A-PB-O2B
13	D	501	ADP	PA-O3A-PB-O3B
13	D	501	ADP	C5'-O5'-PA-O1A
16	J	801	ATP	C5'-O5'-PA-O1A
16	J	801	ATP	C5'-O5'-PA-O2A
16	J	801	ATP	C3'-C4'-C5'-O5'
16	J	801	ATP	O4'-C4'-C5'-O5'
13	G	2001	ADP	PA-O3A-PB-O1B

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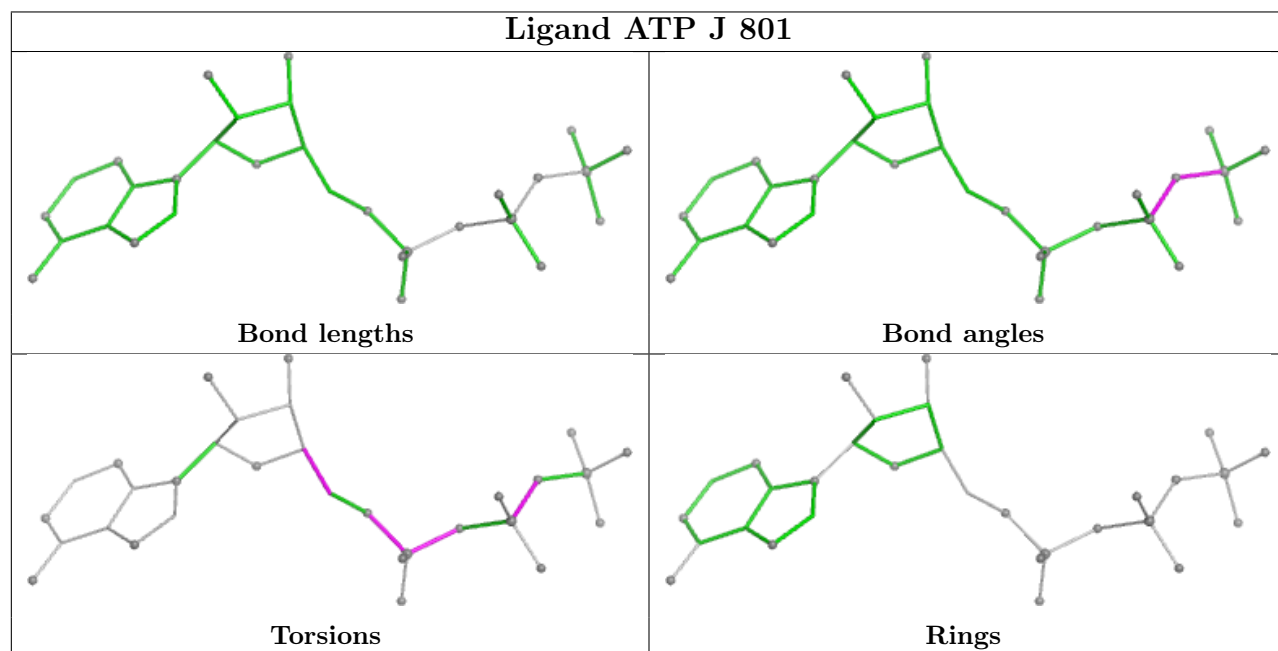
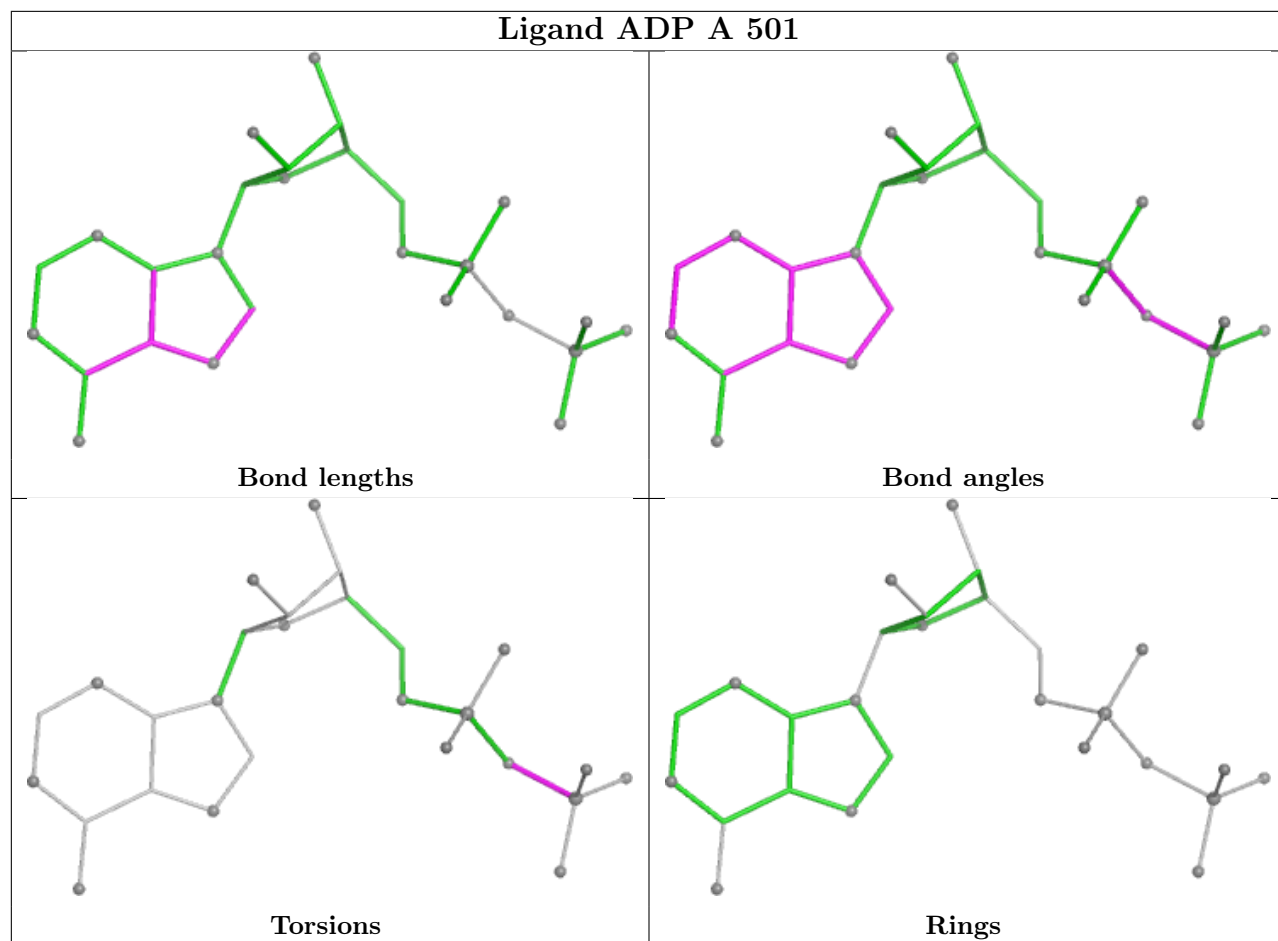
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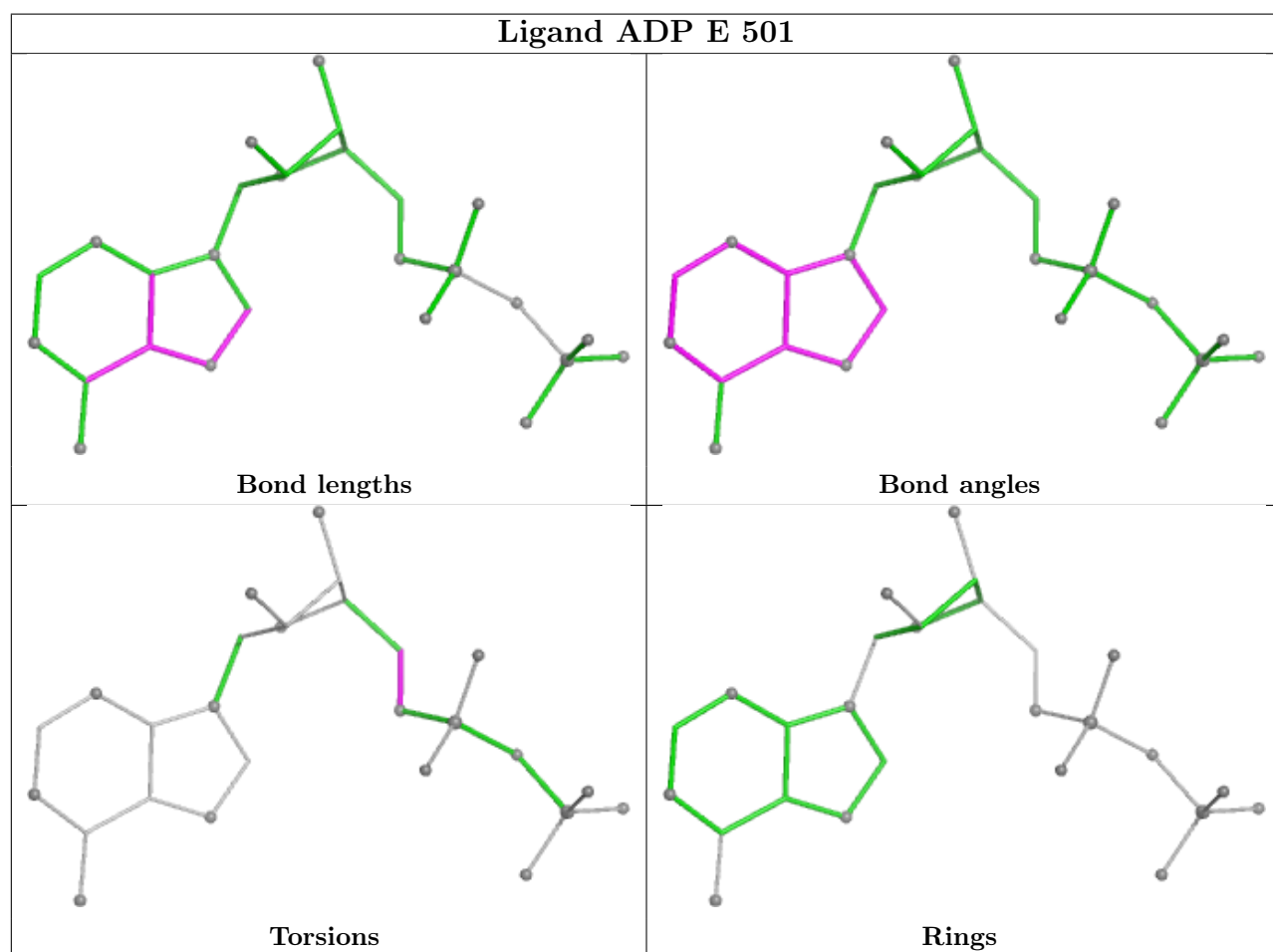
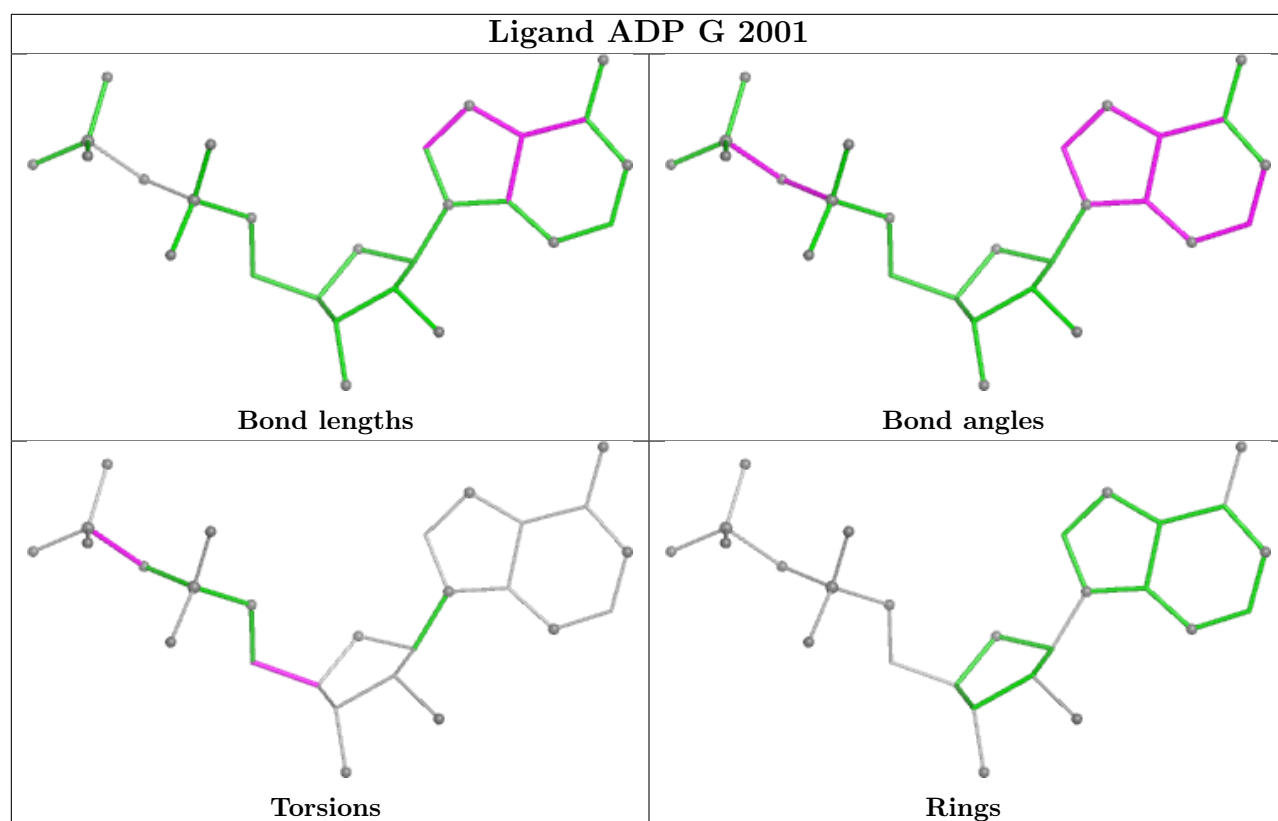
Mol	Chain	Res	Type	Atoms
13	E	501	ADP	C4'-C5'-O5'-PA
13	G	2001	ADP	PA-O3A-PB-O2B
13	D	501	ADP	C5'-O5'-PA-O3A
16	J	801	ATP	PG-O3B-PB-O1B
13	D	501	ADP	C5'-O5'-PA-O2A
13	C	501	ADP	PA-O3A-PB-O1B
13	B	501	ADP	C4'-C5'-O5'-PA
13	D	501	ADP	C4'-C5'-O5'-PA
13	B	501	ADP	PA-O3A-PB-O1B
13	D	501	ADP	PA-O3A-PB-O1B
13	A	501	ADP	PA-O3A-PB-O3B
16	J	801	ATP	C5'-O5'-PA-O3A
13	G	2001	ADP	O4'-C4'-C5'-O5'
16	J	801	ATP	PG-O3B-PB-O2B
16	J	801	ATP	PB-O3A-PA-O1A
16	J	801	ATP	PB-O3A-PA-O2A
13	C	501	ADP	C4'-C5'-O5'-PA

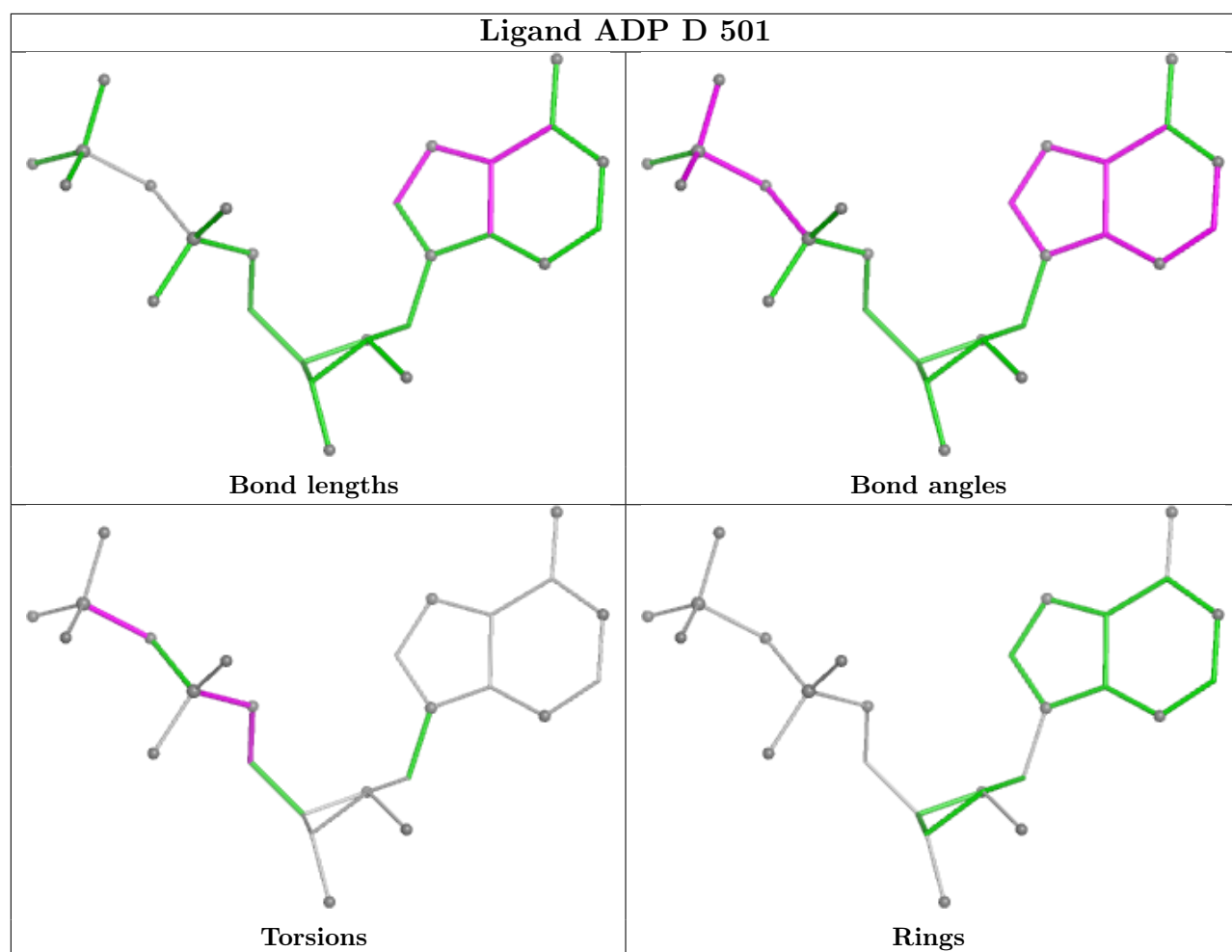
There are no ring outliers.

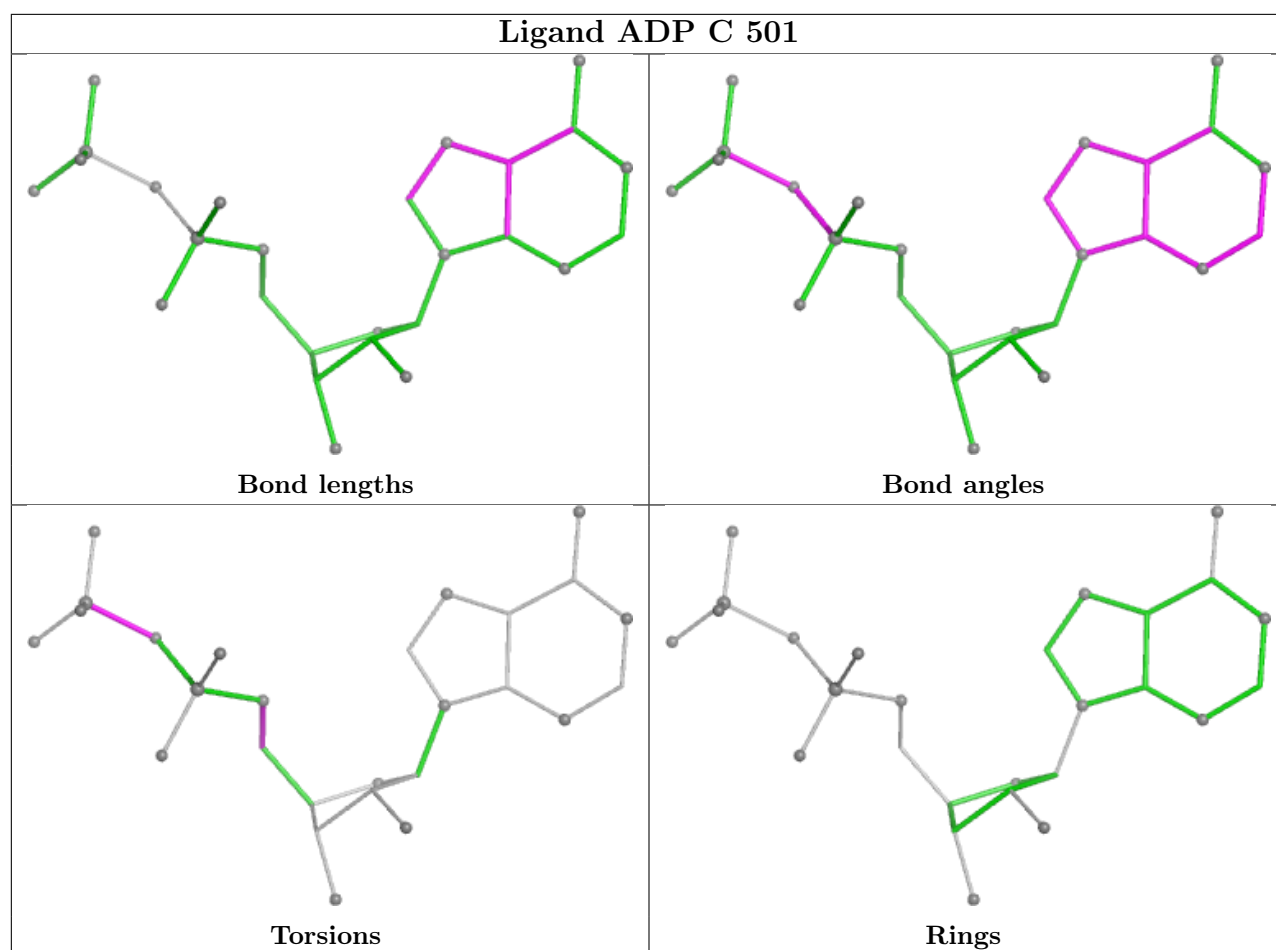
No monomer is involved in short contacts.

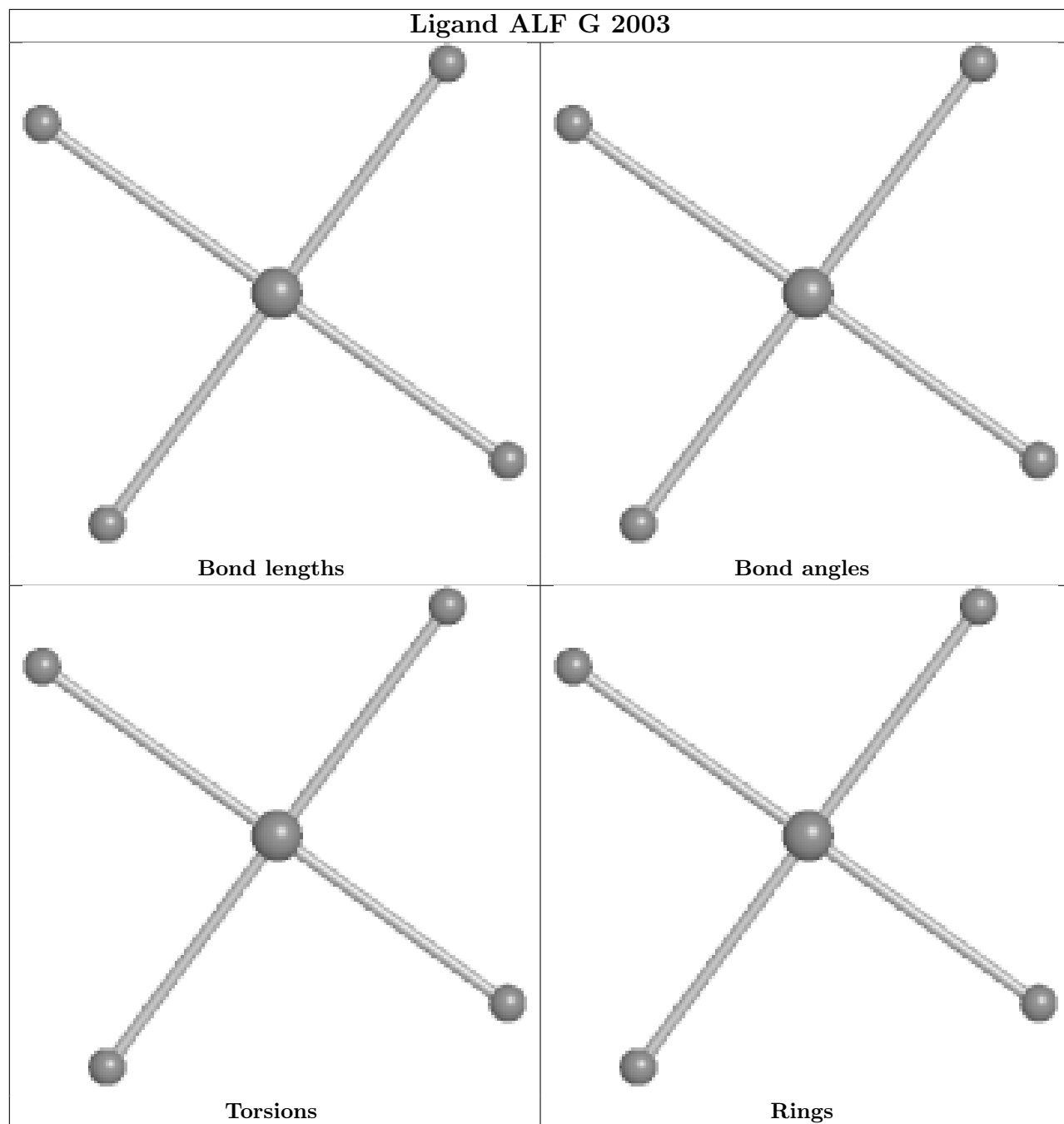
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

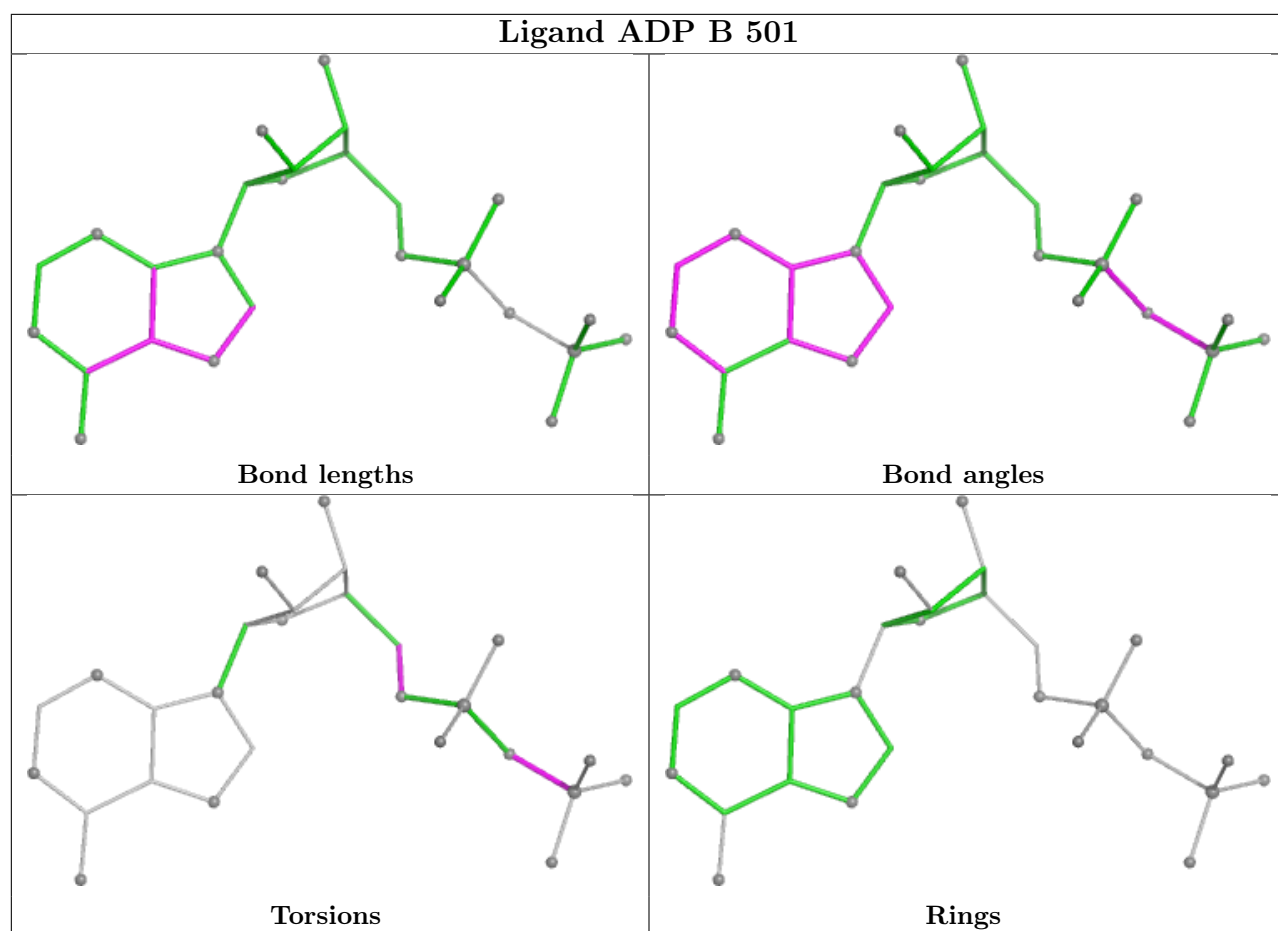


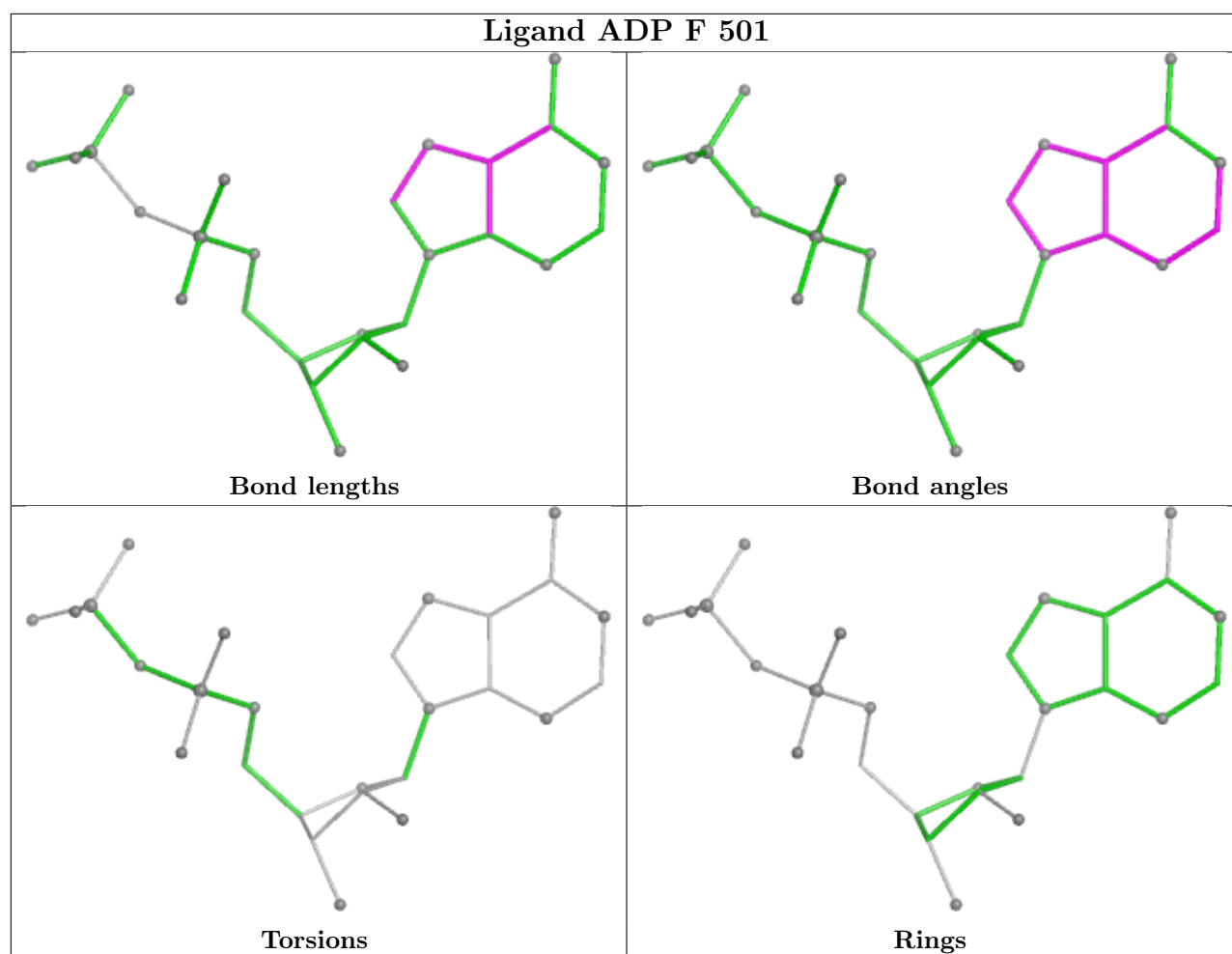












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

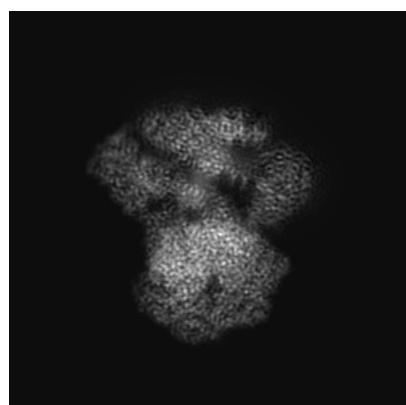
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17025. These allow visual inspection of the internal detail of the map and identification of artifacts.

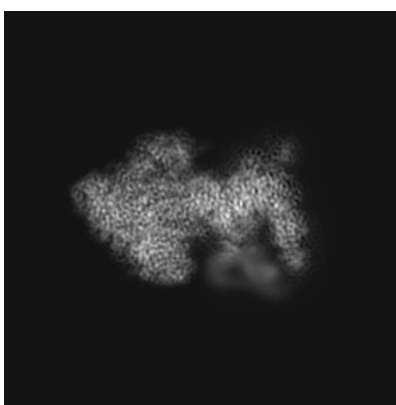
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

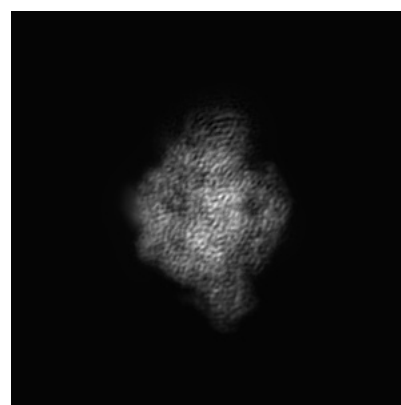
6.1.1 Primary map



X



Y

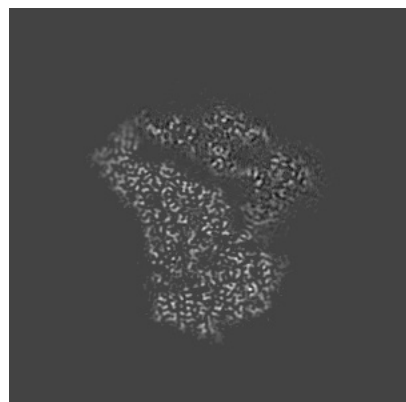


Z

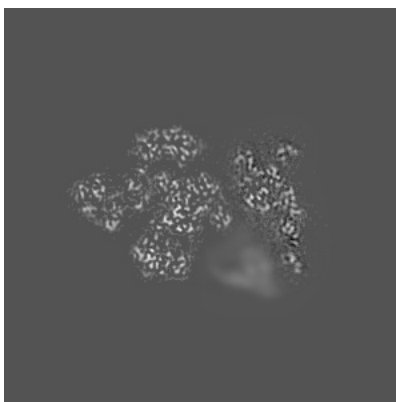
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

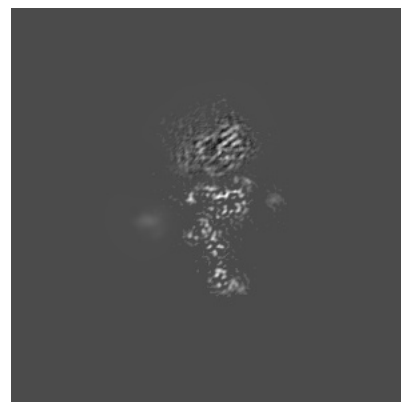
6.2.1 Primary map



X Index: 180



Y Index: 180

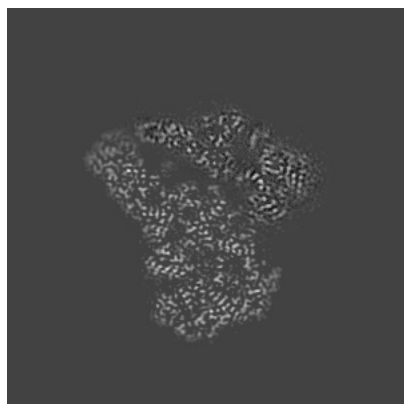


Z Index: 180

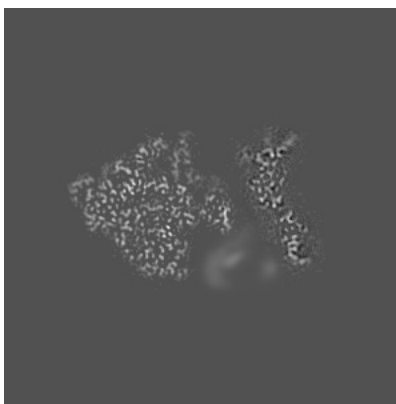
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 187



Y Index: 164

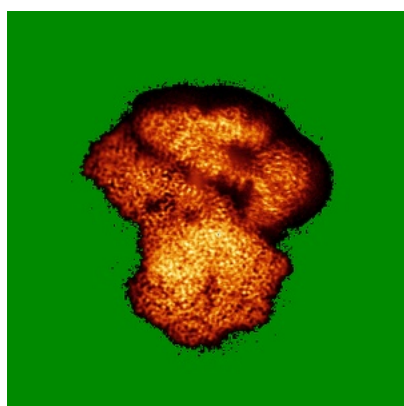


Z Index: 131

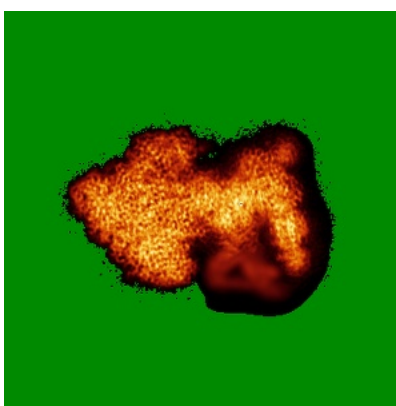
The images above show the largest variance slices of the map in three orthogonal directions.

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

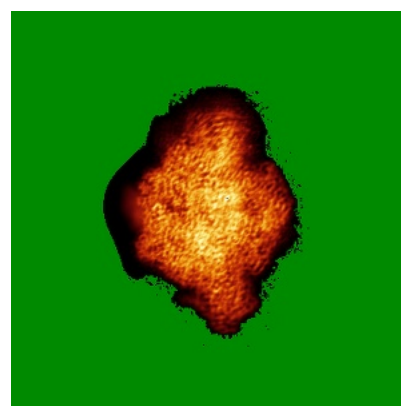
6.4.1 Primary map



X



Y

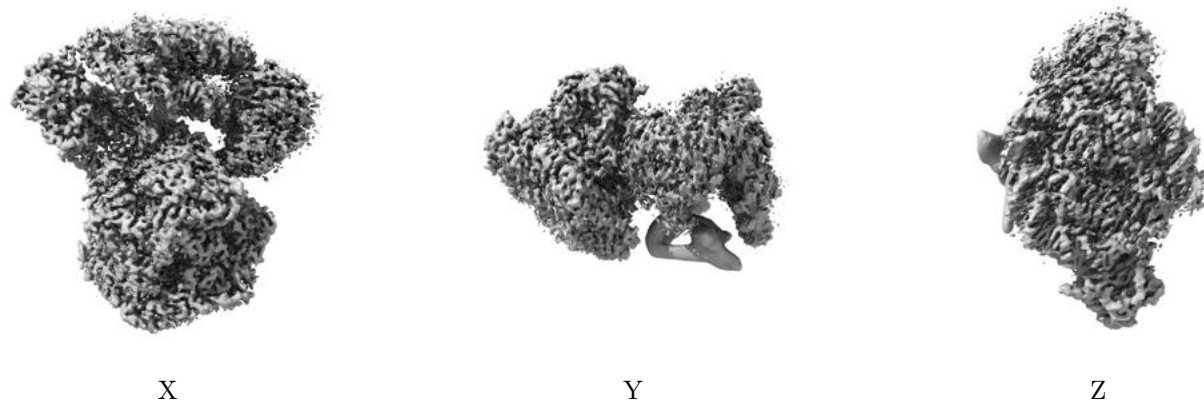


Z

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

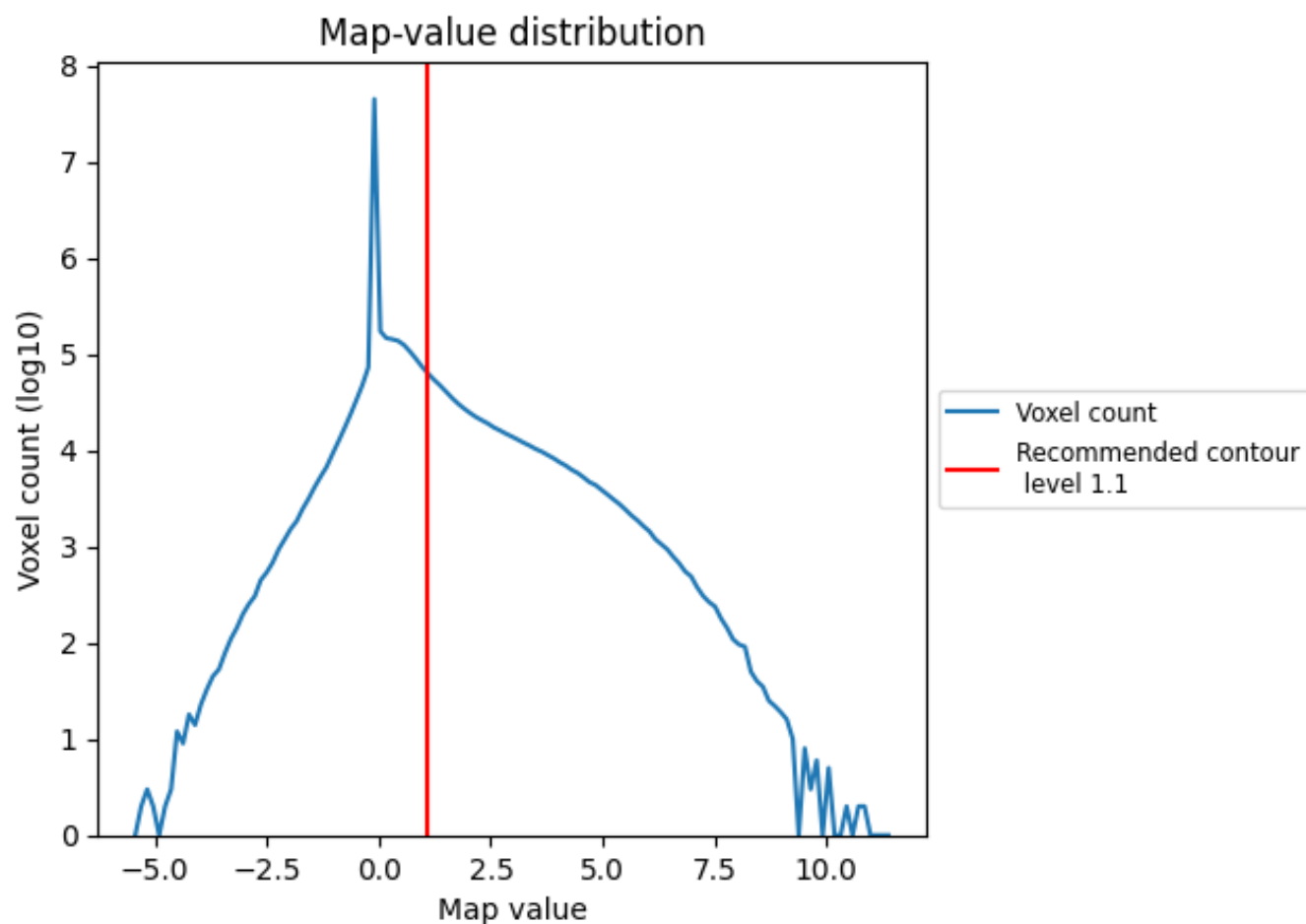
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

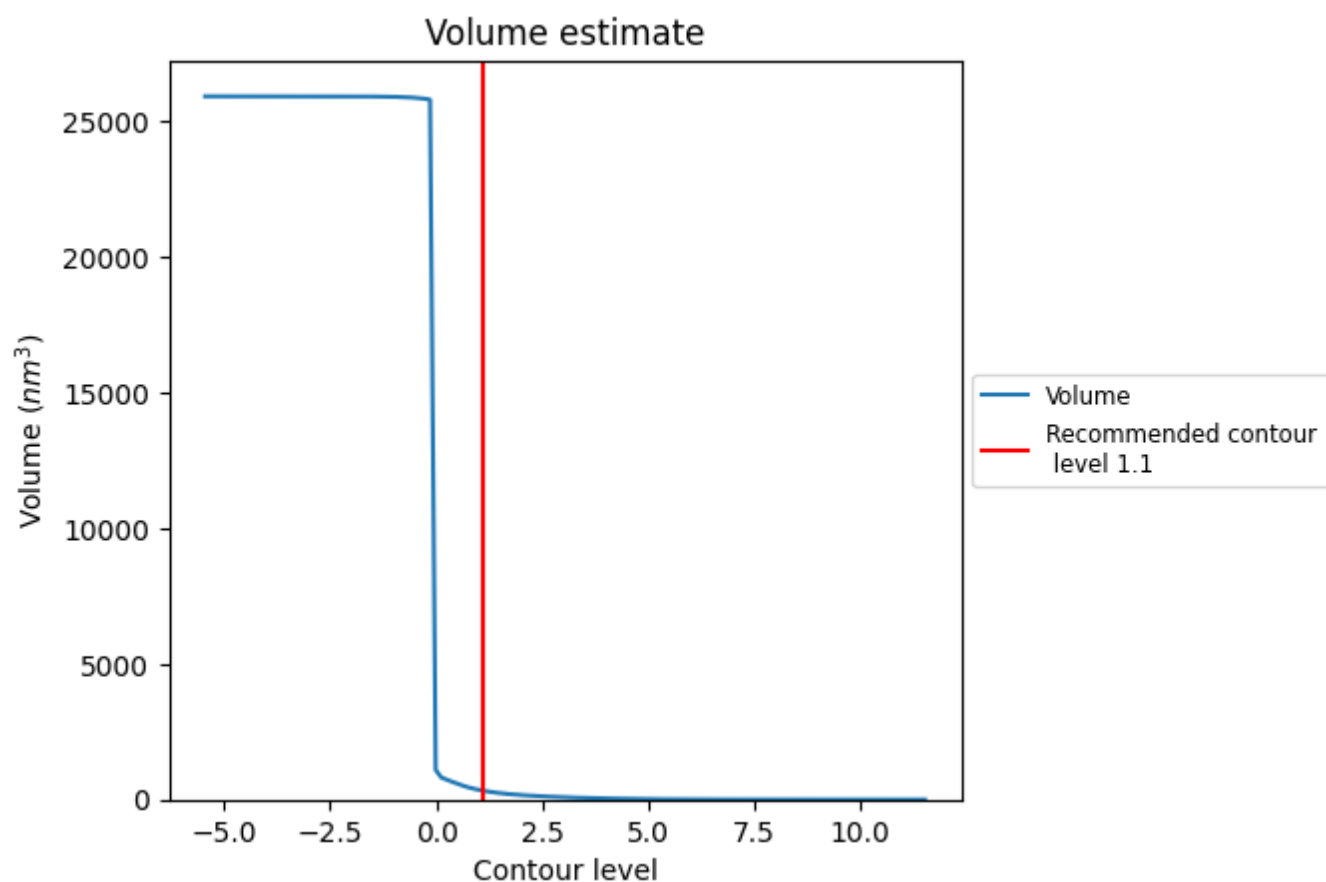
This section contains the results of statistical analysis of the map.

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.

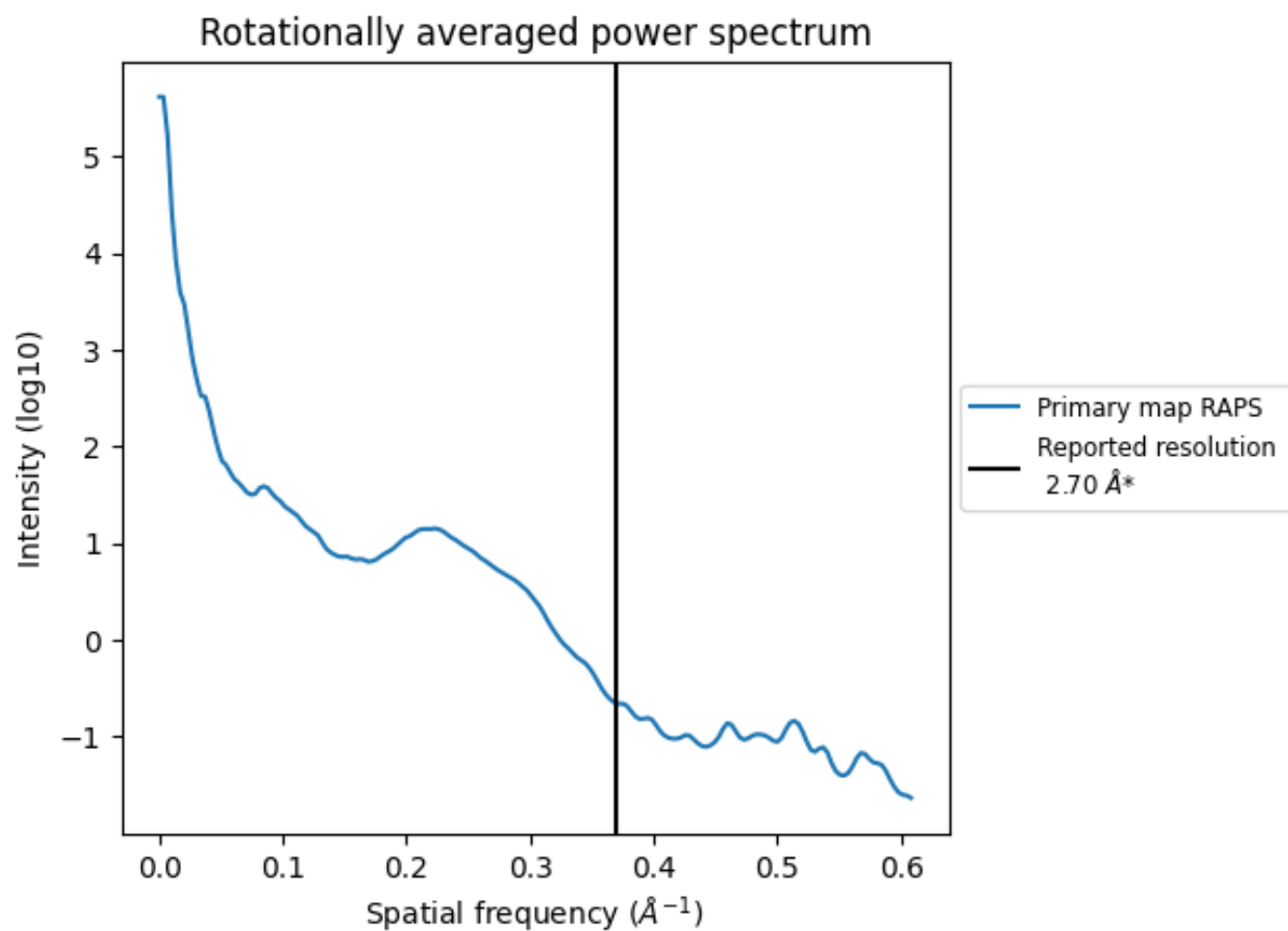
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm³; this corresponds to an approximate mass of 297 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

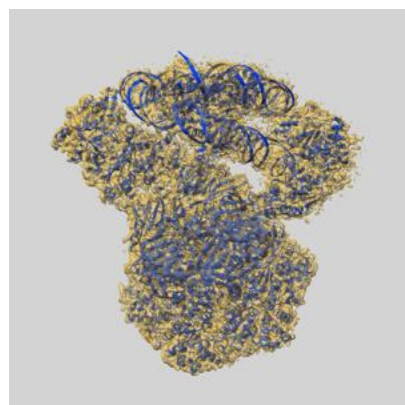
8 Fourier-Shell correlation

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

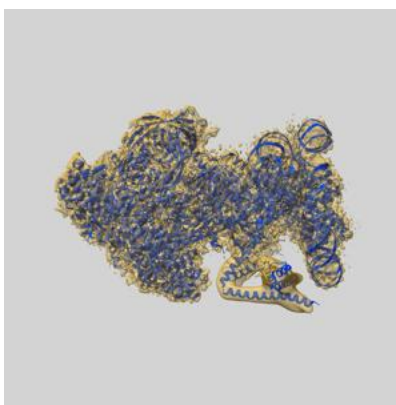
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17025 and PDB model 8OOP. Per-residue inclusion information can be found in section [3](#) on page [9](#).

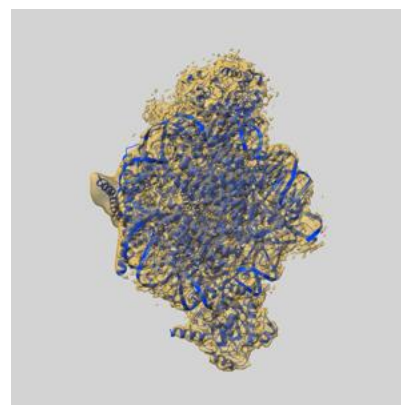
9.1 Map-model overlay [i](#)



X



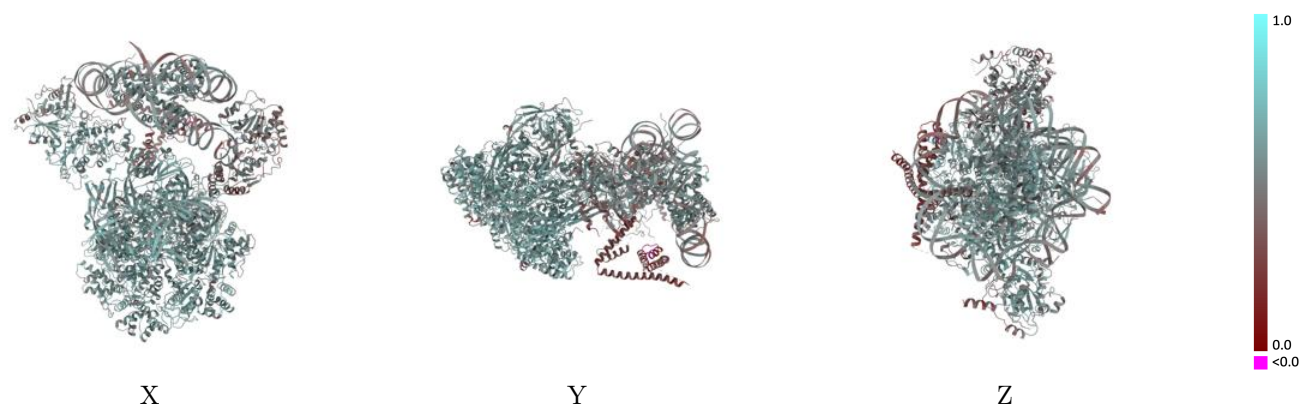
Y



Z

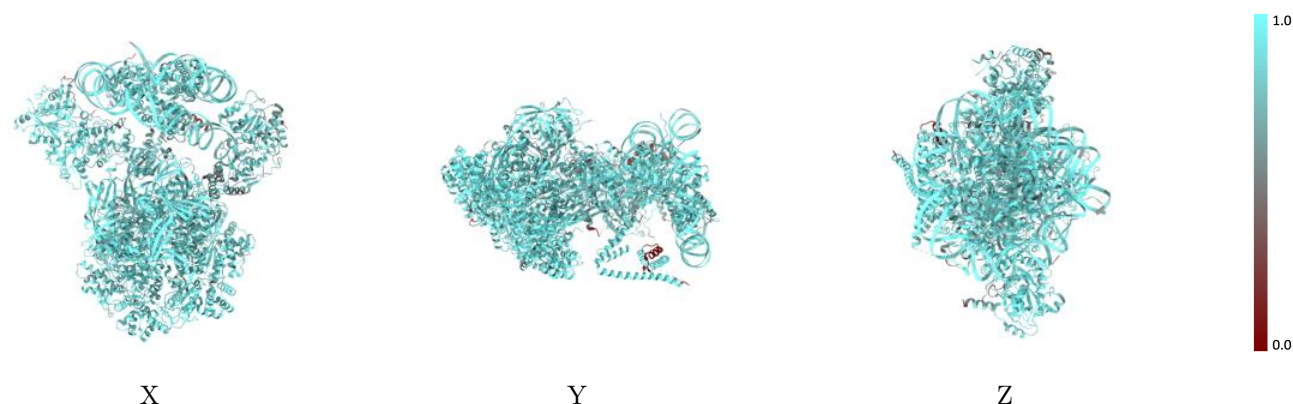
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



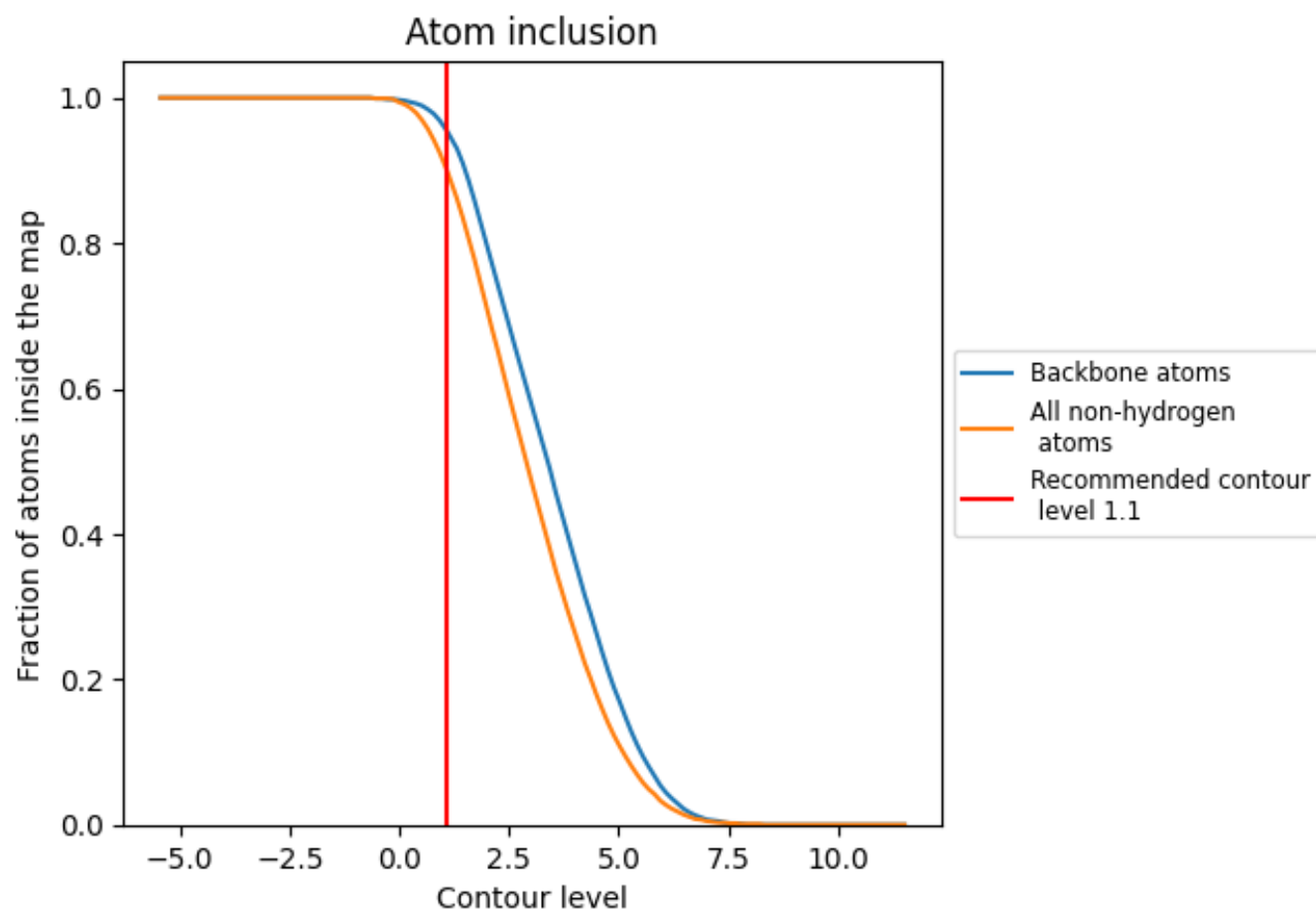
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.5540
A	 0.9260	 0.6050
B	 0.9330	 0.6020
C	 0.9190	 0.5880
D	 0.9190	 0.5840
E	 0.9300	 0.6070
F	 0.9260	 0.5990
G	 0.8450	 0.5120
H	 0.9280	 0.5690
I	 0.8150	 0.5190
J	 0.8920	 0.4970
K	 0.8700	 0.4840
L	 0.8820	 0.4890
M	 0.8970	 0.5410
N	 0.8560	 0.5240
O	 0.8710	 0.5450
P	 0.8820	 0.5420
Q	 0.8750	 0.5450
R	 0.8870	 0.5360

