



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:39 AM UTC

PDB ID : 6TU7 / pdb_00006tu7
EMDB ID : EMD-10590
Title : Structure of PfMyoA decorated Plasmodium Act1 filament
Authors : Vahokoski, J.; Calder, L.J.; Lopez, A.J.; Rosenthal, P.B.; Kursula, I.
Deposited on : 2020-01-03
Resolution : 3.10 Å(reported)
Based on initial models : 5OGW, 6I7D

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

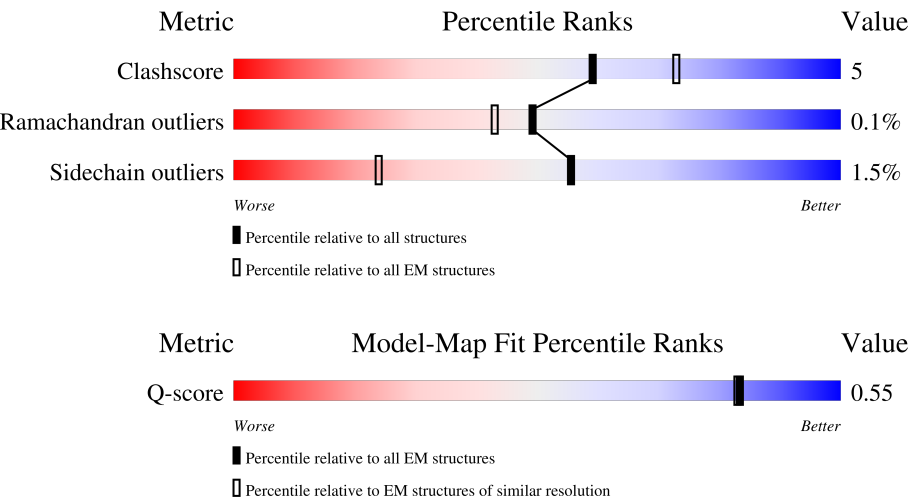
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	AP1	820	
1	GP1	820	
2	BP1	378	
2	CP1	378	

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Mol	Chain	Length	Quality of chain
2	DP1	378	90% 7% ..
2	EP1	378	90% 8% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24064 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 Myosin-A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AP1	766	Total	C	N	O	P	S	0	0
			6060	3855	1020	1153	1	31		
1	GP1	766	Total	C	N	O	P	S	0	0
			6060	3855	1020	1153	1	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP1	-1	GLY	-	expression tag	UNP Q8IDR3
AP1	0	GLN	-	expression tag	UNP Q8IDR3
AP1	1	PHE	-	expression tag	UNP Q8IDR3
GP1	-1	GLY	-	expression tag	UNP Q8IDR3
GP1	0	GLN	-	expression tag	UNP Q8IDR3
GP1	1	PHE	-	expression tag	UNP Q8IDR3

- Molecule 2 is a protein called Actin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BP1	372	Total	C	N	O	S	0	0
			2911	1842	491	562	16		
2	CP1	372	Total	C	N	O	S	0	0
			2911	1842	491	562	16		
2	DP1	372	Total	C	N	O	S	0	0
			2911	1842	491	562	16		
2	EP1	372	Total	C	N	O	S	0	0
			2911	1842	491	562	16		

There are 8 discrepancies between the modelled and reference sequences:

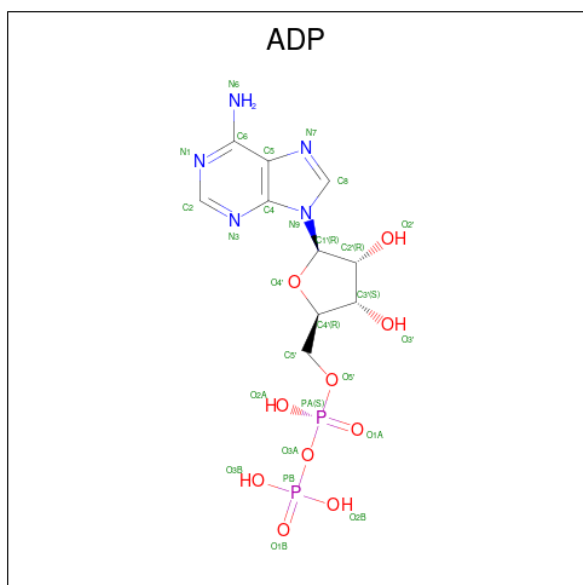
Chain	Residue	Modelled	Actual	Comment	Reference
BP1	-1	GLY	-	expression tag	UNP Q8I4X0
BP1	0	ALA	-	expression tag	UNP Q8I4X0
CP1	-1	GLY	-	expression tag	UNP Q8I4X0

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Chain	Residue	Modelled	Actual	Comment	Reference
CP1	0	ALA	-	expression tag	UNP Q8I4X0
DP1	-1	GLY	-	expression tag	UNP Q8I4X0
DP1	0	ALA	-	expression tag	UNP Q8I4X0
EP1	-1	GLY	-	expression tag	UNP Q8I4X0
EP1	0	ALA	-	expression tag	UNP Q8I4X0

- Molecule 3 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
3	BP1	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	CP1	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	DP1	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	EP1	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

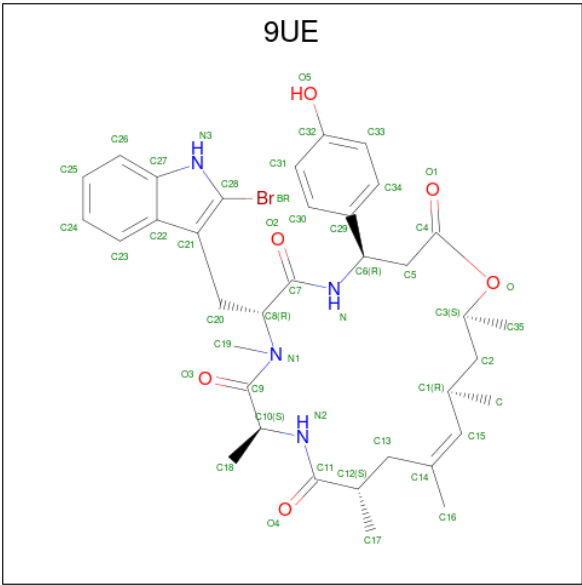
Mol	Chain	Residues	Atoms		AltConf
4	BP1	1	Total	Mg	0
			1	1	
4	CP1	1	Total	Mg	0
			1	1	

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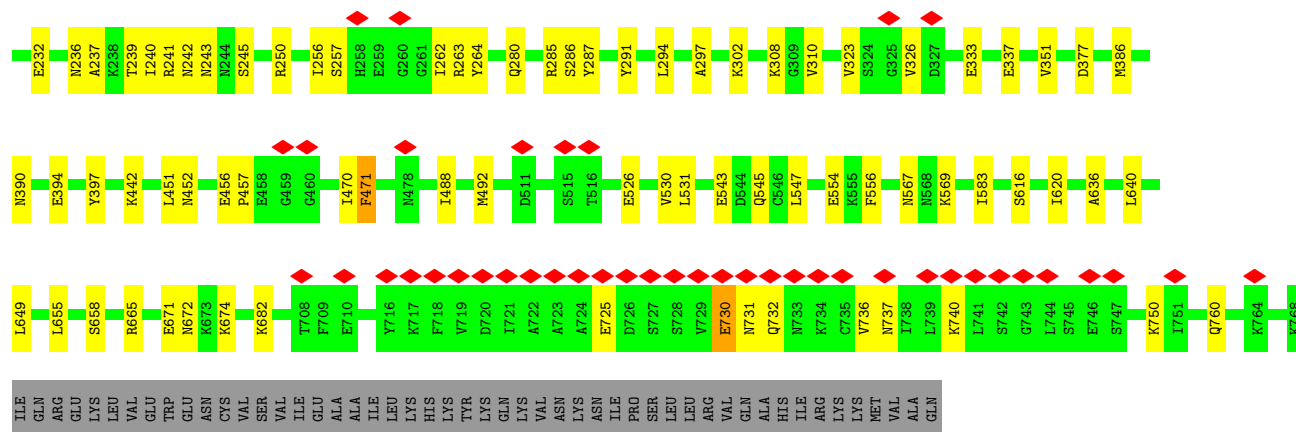
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Mol	Chain	Residues	Atoms		AltConf
4	DP1	1	Total	Mg	0
			1	1	
4	EP1	1	Total	Mg	0
			1	1	

- Molecule 5 is Jasplakinolide (CCD ID: 9UE) (formula: C₃₆H₄₅BrN₄O₆).

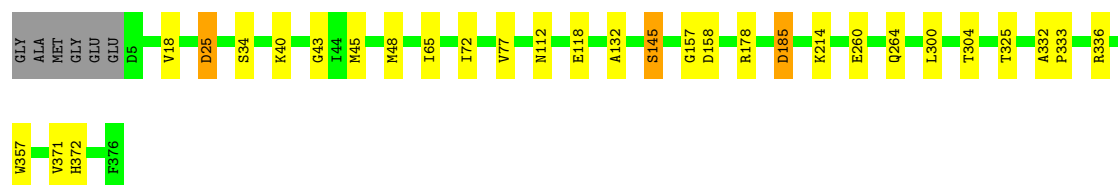


Mol	Chain	Residues	Atoms					AltConf
5	BP1	1	Total	Br	C	N	O	0
			47	1	36	4	6	
5	CP1	1	Total	Br	C	N	O	0
			47	1	36	4	6	
5	DP1	1	Total	Br	C	N	O	0
			47	1	36	4	6	
5	EP1	1	Total	Br	C	N	O	0
			47	1	36	4	6	



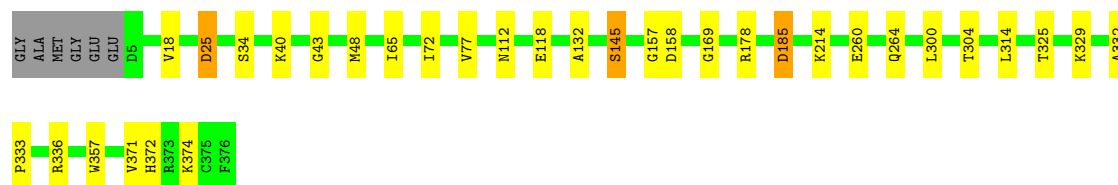
• Molecule 2: Actin-1

Chain BP1: 90% 7% ..



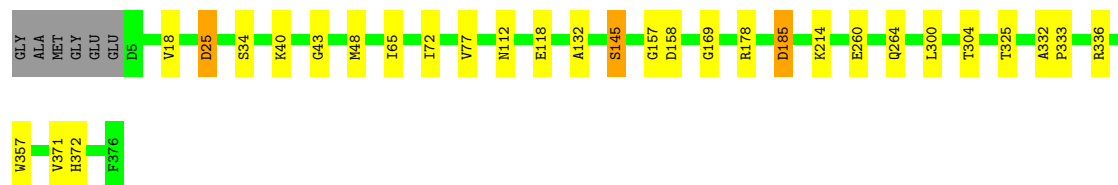
• Molecule 2: Actin-1

Chain CP1: 90% 8% ..



• Molecule 2: Actin-1

Chain DP1: 90% 7% ..



• Molecule 2: Actin-1

Chain EP1: 90% 8% ..



P333					
R336					
W357					
V371					
H372					
F376					

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.498°, rise=28.3417 Å, axial sym=C1	Depositor
Number of segments used	239021	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	49.20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.264	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	558.08, 558.08, 558.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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: MG, 9UE, SEP, 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	AP1	0.16	0/6156	0.30	0/8303
1	GP1	0.16	0/6156	0.30	0/8303
2	BP1	0.32	0/2973	0.35	0/4023
2	CP1	0.32	0/2973	0.35	0/4023
2	DP1	0.32	0/2973	0.35	0/4023
2	EP1	0.32	0/2973	0.35	0/4023
All	All	0.25	0/24204	0.33	0/32698

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	AP1	6060	0	6131	74	0
1	GP1	6060	0	6131	75	0
2	BP1	2911	0	2880	17	0
2	CP1	2911	0	2880	20	0
2	DP1	2911	0	2880	17	0
2	EP1	2911	0	2880	18	0
3	BP1	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CP1	27	0	12	2	0
3	DP1	27	0	12	2	0
3	EP1	27	0	12	2	0
4	BP1	1	0	0	0	0
4	CP1	1	0	0	0	0
4	DP1	1	0	0	0	0
4	EP1	1	0	0	0	0
5	BP1	47	0	0	0	0
5	CP1	47	0	0	0	0
5	DP1	47	0	0	0	0
5	EP1	47	0	0	0	0
All	All	24064	0	23830	218	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 5.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GP1:256:ILE:HG22	1:GP1:262:ILE:HA	1.64	0.79
1:AP1:256:ILE:HG22	1:AP1:262:ILE:HA	1.64	0.79
1:GP1:31:PHE:H	1:GP1:59:GLN:HE22	1.39	0.70
1:AP1:31:PHE:H	1:AP1:59:GLN:HE22	1.39	0.70
1:AP1:99:PHE:O	1:AP1:120:ARG:NH1	2.25	0.68
1:AP1:124:ASN:HB3	1:AP1:143:LEU:HD11	1.76	0.68
1:GP1:99:PHE:O	1:GP1:120:ARG:NH1	2.25	0.67
1:AP1:25:ASP:HB2	1:AP1:26:LYS:HD3	1.76	0.67
1:GP1:124:ASN:HB3	1:GP1:143:LEU:HD11	1.76	0.67
1:GP1:25:ASP:HB2	1:GP1:26:LYS:HD3	1.76	0.66
1:AP1:386:MET:O	1:AP1:390:ASN:ND2	2.29	0.64
1:GP1:386:MET:O	1:GP1:390:ASN:ND2	2.29	0.64
2:EP1:157:GLY:O	2:EP1:304:THR:OG1	2.15	0.64
1:AP1:205:MET:HB3	1:AP1:221:GLN:HE21	1.64	0.63
1:GP1:155:ARG:O	1:GP1:172:ARG:NH1	2.31	0.63
1:GP1:205:MET:HB3	1:GP1:221:GLN:HE21	1.64	0.63
2:CP1:157:GLY:O	2:CP1:304:THR:OG1	2.16	0.62
2:BP1:157:GLY:O	2:BP1:304:THR:OG1	2.16	0.62
2:DP1:157:GLY:O	2:DP1:304:THR:OG1	2.16	0.62
1:GP1:554:GLU:OE2	1:GP1:554:GLU:N	2.32	0.62
1:AP1:155:ARG:O	1:AP1:172:ARG:NH1	2.31	0.62
1:AP1:218:LEU:HD23	1:AP1:219:ARG:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GP1:25:ASP:OD1	1:GP1:32:LYS:NZ	2.33	0.61
1:AP1:25:ASP:OD1	1:AP1:32:LYS:NZ	2.33	0.61
1:AP1:190:SER:OG	1:AP1:665:ARG:NH1	2.33	0.61
1:GP1:218:LEU:HD23	1:GP1:219:ARG:HG3	1.82	0.61
1:AP1:554:GLU:N	1:AP1:554:GLU:OE2	2.32	0.60
1:GP1:190:SER:OG	1:GP1:665:ARG:NH1	2.33	0.60
1:AP1:242:ASN:OD1	1:AP1:243:ASN:N	2.35	0.60
1:GP1:242:ASN:OD1	1:GP1:243:ASN:N	2.35	0.59
1:GP1:297:ALA:O	1:GP1:302:LYS:NZ	2.35	0.59
1:AP1:106:ASN:O	1:AP1:760:GLN:NE2	2.36	0.59
1:GP1:106:ASN:O	1:GP1:760:GLN:NE2	2.36	0.58
1:AP1:297:ALA:O	1:AP1:302:LYS:NZ	2.35	0.58
2:CP1:112:ASN:OD1	2:CP1:178:ARG:NH1	2.29	0.58
2:BP1:72:ILE:HG12	2:BP1:77:VAL:HG22	1.86	0.57
2:DP1:72:ILE:HG12	2:DP1:77:VAL:HG22	1.86	0.57
2:DP1:43:GLY:HA3	2:DP1:48:MET:HE1	1.87	0.57
1:GP1:736:VAL:HG22	1:GP1:740:LYS:HZ2	1.70	0.57
2:BP1:43:GLY:HA3	2:BP1:48:MET:HE1	1.87	0.56
2:CP1:72:ILE:HG12	2:CP1:77:VAL:HG22	1.86	0.56
2:EP1:72:ILE:HG12	2:EP1:77:VAL:HG22	1.86	0.56
1:GP1:17:ARG:NH1	1:GP1:19:SEP:O	2.39	0.55
2:EP1:43:GLY:HA3	2:EP1:48:MET:HE1	1.87	0.55
1:AP1:17:ARG:NH1	1:AP1:19:SEP:O	2.39	0.55
2:EP1:25:ASP:N	2:EP1:25:ASP:OD1	2.40	0.55
1:AP1:232:GLU:OE1	1:AP1:250:ARG:NH2	2.40	0.55
2:CP1:25:ASP:OD1	2:CP1:25:ASP:N	2.40	0.55
2:CP1:43:GLY:HA3	2:CP1:48:MET:HE1	1.87	0.55
2:EP1:118:GLU:OE2	2:EP1:372:HIS:NE2	2.34	0.54
1:AP1:101:ASP:OD1	1:AP1:103:GLY:N	2.41	0.54
1:AP1:736:VAL:HG22	1:AP1:740:LYS:HZ2	1.72	0.54
1:GP1:232:GLU:OE1	1:GP1:250:ARG:NH2	2.40	0.54
1:GP1:101:ASP:OD1	1:GP1:103:GLY:N	2.41	0.54
1:AP1:90:CYS:SG	1:AP1:91:ASN:N	2.81	0.54
2:BP1:132:ALA:HB1	2:BP1:357:TRP:HB3	1.91	0.53
2:DP1:132:ALA:HB1	2:DP1:357:TRP:HB3	1.91	0.53
1:AP1:19:SEP:O2P	1:AP1:109:ASN:ND2	2.41	0.53
1:AP1:351:VAL:HG11	1:AP1:620:ILE:HD12	1.91	0.53
1:GP1:19:SEP:O2P	1:GP1:109:ASN:ND2	2.41	0.53
2:BP1:18:VAL:HG23	2:BP1:34:SER:HB3	1.91	0.53
2:EP1:18:VAL:HG23	2:EP1:34:SER:HB3	1.91	0.53
2:CP1:18:VAL:HG23	2:CP1:34:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DP1:18:VAL:HG23	2:DP1:34:SER:HB3	1.91	0.53
1:GP1:90:CYS:SG	1:GP1:91:ASN:N	2.81	0.52
2:DP1:25:ASP:OD1	2:DP1:25:ASP:N	2.40	0.52
2:CP1:132:ALA:HB1	2:CP1:357:TRP:HB3	1.91	0.52
2:BP1:118:GLU:OE2	2:BP1:372:HIS:NE2	2.34	0.52
2:EP1:132:ALA:HB1	2:EP1:357:TRP:HB3	1.91	0.52
2:BP1:25:ASP:N	2:BP1:25:ASP:OD1	2.40	0.52
1:AP1:54:LYS:HB3	1:AP1:72:ASP:HB2	1.92	0.51
1:GP1:351:VAL:HG11	1:GP1:620:ILE:HD12	1.91	0.51
1:GP1:54:LYS:HB3	1:GP1:72:ASP:HB2	1.91	0.51
2:CP1:214:LYS:NZ	3:CP1:401:ADP:O2'	2.39	0.50
2:EP1:214:LYS:NZ	3:EP1:401:ADP:O2'	2.39	0.50
1:AP1:31:PHE:HD2	1:AP1:59:GLN:HA	1.76	0.50
2:CP1:118:GLU:OE2	2:CP1:372:HIS:NE2	2.34	0.50
2:DP1:118:GLU:OE2	2:DP1:372:HIS:NE2	2.34	0.50
1:AP1:57:VAL:HA	1:AP1:68:VAL:HG12	1.94	0.50
2:DP1:214:LYS:NZ	3:DP1:401:ADP:O2'	2.39	0.50
1:GP1:57:VAL:HA	1:GP1:68:VAL:HG12	1.94	0.50
1:GP1:671:GLU:HB3	1:GP1:682:LYS:HZ2	1.76	0.50
2:BP1:45:MET:HG3	2:DP1:169:GLY:HA2	1.94	0.50
1:GP1:31:PHE:HD2	1:GP1:59:GLN:HA	1.76	0.50
1:GP1:333:GLU:O	1:GP1:337:GLU:HG2	2.12	0.49
2:DP1:112:ASN:OD1	2:DP1:178:ARG:NH1	2.29	0.49
2:CP1:333:PRO:HG2	2:CP1:336:ARG:HB3	1.94	0.49
2:EP1:333:PRO:HG2	2:EP1:336:ARG:HB3	1.94	0.49
2:DP1:333:PRO:HG2	2:DP1:336:ARG:HB3	1.94	0.48
1:AP1:333:GLU:O	1:AP1:337:GLU:HG2	2.12	0.48
1:GP1:232:GLU:OE2	1:GP1:236:ASN:ND2	2.45	0.48
1:GP1:655:LEU:O	1:GP1:658:SER:OG	2.31	0.48
1:AP1:232:GLU:OE2	1:AP1:236:ASN:ND2	2.45	0.48
2:CP1:158:ASP:N	3:CP1:401:ADP:O3B	2.46	0.48
1:AP1:470:ILE:HG13	1:AP1:471:PHE:H	1.78	0.48
1:AP1:545:GLN:HG3	1:AP1:556:PHE:HB2	1.95	0.48
2:BP1:333:PRO:HG2	2:BP1:336:ARG:HB3	1.94	0.48
2:EP1:112:ASN:OD1	2:EP1:178:ARG:NH1	2.29	0.48
2:BP1:112:ASN:OD1	2:BP1:178:ARG:NH1	2.29	0.48
1:AP1:294:LEU:HD21	1:AP1:308:LYS:O	2.14	0.48
2:BP1:158:ASP:N	3:BP1:401:ADP:O3B	2.47	0.48
2:BP1:214:LYS:NZ	3:BP1:401:ADP:O2'	2.39	0.48
2:EP1:158:ASP:N	3:EP1:401:ADP:O3B	2.46	0.48
1:GP1:545:GLN:HG3	1:GP1:556:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GP1:470:ILE:HG13	1:GP1:471:PHE:H	1.78	0.48
1:AP1:488:ILE:HG12	1:AP1:531:LEU:HD13	1.96	0.47
1:GP1:390:ASN:O	1:GP1:394:GLU:HG2	2.15	0.47
1:AP1:240:ILE:HG13	1:AP1:241:ARG:HG3	1.97	0.47
2:DP1:158:ASP:N	3:DP1:401:ADP:O3B	2.47	0.47
1:GP1:294:LEU:HD21	1:GP1:308:LYS:O	2.14	0.47
2:DP1:185:ASP:N	2:DP1:185:ASP:OD1	2.48	0.47
2:EP1:185:ASP:OD1	2:EP1:185:ASP:N	2.48	0.47
2:CP1:145:SER:O	2:CP1:145:SER:OG	2.32	0.47
1:GP1:240:ILE:HG13	1:GP1:241:ARG:HG3	1.97	0.47
1:AP1:390:ASN:O	1:AP1:394:GLU:HG2	2.15	0.46
2:DP1:145:SER:O	2:DP1:145:SER:OG	2.32	0.46
1:GP1:488:ILE:HG12	1:GP1:531:LEU:HD13	1.96	0.46
1:AP1:671:GLU:OE1	1:AP1:672:ASN:ND2	2.49	0.46
2:CP1:169:GLY:HA2	2:EP1:45:MET:HG3	1.96	0.46
1:GP1:55:CYS:HA	1:GP1:70:GLN:HA	1.97	0.46
1:GP1:671:GLU:OE1	1:GP1:672:ASN:ND2	2.48	0.46
1:AP1:55:CYS:HA	1:AP1:70:GLN:HA	1.96	0.46
1:AP1:526:GLU:OE1	1:AP1:567:ASN:ND2	2.31	0.46
1:GP1:39:ASP:OD1	1:GP1:39:ASP:N	2.49	0.46
1:GP1:442:LYS:HD3	1:GP1:442:LYS:HA	1.76	0.46
2:CP1:185:ASP:OD1	2:CP1:185:ASP:N	2.48	0.45
2:EP1:260:GLU:OE2	2:EP1:264:GLN:NE2	2.49	0.45
1:GP1:10:THR:O	1:GP1:14:ILE:HG13	2.17	0.45
2:CP1:260:GLU:OE2	2:CP1:264:GLN:NE2	2.49	0.45
1:AP1:671:GLU:HB3	1:AP1:682:LYS:HZ2	1.82	0.45
2:BP1:185:ASP:OD1	2:BP1:185:ASP:N	2.48	0.45
1:AP1:257:SER:HB3	1:AP1:263:ARG:HD3	1.99	0.45
2:BP1:40:LYS:HG2	2:BP1:65:ILE:O	2.17	0.45
1:AP1:39:ASP:OD1	1:AP1:39:ASP:N	2.49	0.44
1:GP1:257:SER:HB3	1:GP1:263:ARG:HD3	1.99	0.44
2:DP1:40:LYS:HG2	2:DP1:65:ILE:O	2.17	0.44
1:GP1:526:GLU:OE1	1:GP1:567:ASN:ND2	2.31	0.44
2:EP1:40:LYS:HG2	2:EP1:65:ILE:O	2.17	0.44
1:AP1:10:THR:O	1:AP1:14:ILE:HG13	2.17	0.44
1:AP1:323:VAL:HG13	1:AP1:326:VAL:HB	2.00	0.44
1:AP1:192:GLU:OE1	1:AP1:193:SER:N	2.51	0.44
1:GP1:192:GLU:OE1	1:GP1:193:SER:N	2.51	0.44
1:AP1:655:LEU:O	1:AP1:658:SER:OG	2.31	0.44
1:GP1:264:TYR:HB2	1:GP1:457:PRO:HG3	1.99	0.44
1:AP1:264:TYR:HB2	1:AP1:457:PRO:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:280:GLN:NE2	1:AP1:286:SER:HB2	2.33	0.43
1:AP1:442:LYS:HA	1:AP1:442:LYS:HD3	1.76	0.43
1:GP1:323:VAL:HG13	1:GP1:326:VAL:HB	2.00	0.43
2:CP1:40:LYS:HG2	2:CP1:65:ILE:O	2.17	0.43
1:AP1:221:GLN:HE22	1:AP1:262:ILE:HD12	1.83	0.43
1:AP1:237:ALA:O	1:AP1:245:SER:OG	2.36	0.43
1:GP1:221:GLN:HE22	1:GP1:262:ILE:HD12	1.83	0.43
1:GP1:285:ARG:HB3	1:GP1:291:TYR:CE2	2.54	0.43
1:AP1:97:MET:SD	1:AP1:123:LYS:HD2	2.58	0.43
1:AP1:286:SER:OG	1:AP1:287:TYR:N	2.52	0.43
1:AP1:530:VAL:HG21	1:AP1:569:LYS:HB2	2.01	0.43
1:AP1:730:GLU:OE2	1:AP1:731:ASN:N	2.52	0.43
1:AP1:285:ARG:HB3	1:AP1:291:TYR:CE2	2.54	0.43
1:AP1:534:LYS:HE2	1:AP1:534:LYS:HB3	1.90	0.43
1:AP1:173:GLU:O	1:AP1:177:ASN:ND2	2.35	0.43
1:GP1:97:MET:SD	1:GP1:123:LYS:HD2	2.58	0.43
1:GP1:452:ASN:HB3	1:GP1:456:GLU:OE2	2.20	0.42
1:GP1:294:LEU:HD22	1:GP1:310:VAL:HG22	2.01	0.42
1:GP1:530:VAL:HG21	1:GP1:569:LYS:HB2	2.01	0.42
1:AP1:18:VAL:HG23	1:AP1:19:SEP:H	1.84	0.42
1:AP1:452:ASN:HB3	1:AP1:456:GLU:OE2	2.20	0.42
1:GP1:25:ASP:OD1	1:GP1:25:ASP:N	2.52	0.42
1:GP1:280:GLN:NE2	1:GP1:286:SER:HB2	2.33	0.42
1:GP1:730:GLU:OE2	1:GP1:731:ASN:N	2.52	0.42
1:AP1:294:LEU:HD22	1:AP1:310:VAL:HG22	2.01	0.42
1:GP1:160:HIS:HA	1:GP1:163:LEU:HD23	2.01	0.42
1:AP1:25:ASP:OD1	1:AP1:25:ASP:N	2.52	0.42
1:GP1:18:VAL:HG23	1:GP1:19:SEP:H	1.84	0.42
1:GP1:286:SER:OG	1:GP1:287:TYR:N	2.52	0.42
2:BP1:300:LEU:HD12	2:BP1:332:ALA:HB2	2.02	0.42
1:AP1:160:HIS:HA	1:AP1:163:LEU:HD23	2.01	0.42
1:AP1:492:MET:HG3	1:AP1:649:LEU:HD21	2.02	0.42
1:GP1:397:TYR:O	1:GP1:616:SER:OG	2.33	0.42
1:AP1:531:LEU:HD21	1:AP1:583:ILE:HD13	2.01	0.42
1:AP1:725:GLU:N	1:AP1:725:GLU:OE2	2.53	0.42
1:GP1:173:GLU:O	1:GP1:177:ASN:ND2	2.35	0.42
1:GP1:725:GLU:N	1:GP1:725:GLU:OE2	2.53	0.42
2:CP1:300:LEU:HD12	2:CP1:332:ALA:HB2	2.02	0.42
2:DP1:300:LEU:HD12	2:DP1:332:ALA:HB2	2.02	0.42
2:EP1:300:LEU:HD12	2:EP1:332:ALA:HB2	2.02	0.41
1:GP1:218:LEU:HD13	1:GP1:262:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:547:LEU:HD21	1:AP1:636:ALA:O	2.20	0.41
1:GP1:531:LEU:HD21	1:GP1:583:ILE:HD13	2.01	0.41
1:GP1:737:ASN:HA	1:GP1:740:LYS:HZ3	1.85	0.41
1:GP1:237:ALA:O	1:GP1:245:SER:OG	2.36	0.41
2:BP1:145:SER:O	2:BP1:145:SER:OG	2.32	0.41
1:GP1:750:LYS:HD3	1:GP1:750:LYS:HA	1.86	0.41
1:AP1:62:LYS:HG2	1:AP1:65:LYS:O	2.21	0.41
1:GP1:543:GLU:HG3	1:GP1:640:LEU:HD12	2.03	0.41
1:AP1:218:LEU:HD13	1:AP1:262:ILE:HB	2.02	0.41
2:EP1:145:SER:O	2:EP1:145:SER:OG	2.32	0.41
1:AP1:32:LYS:HE2	1:AP1:32:LYS:HB2	1.86	0.41
1:AP1:174:ALA:HB1	1:AP1:465:MET:HE1	2.03	0.41
1:AP1:543:GLU:HG3	1:AP1:640:LEU:HD12	2.03	0.41
2:BP1:260:GLU:OE2	2:BP1:264:GLN:NE2	2.49	0.41
2:CP1:314:LEU:HD12	2:CP1:314:LEU:HA	1.92	0.41
2:DP1:260:GLU:OE2	2:DP1:264:GLN:NE2	2.49	0.41
1:GP1:32:LYS:HE2	1:GP1:32:LYS:HB2	1.86	0.41
1:GP1:65:LYS:HB3	1:GP1:81:ASP:OD1	2.21	0.41
1:GP1:492:MET:HG3	1:GP1:649:LEU:HD21	2.02	0.41
1:GP1:547:LEU:HD21	1:GP1:636:ALA:O	2.20	0.40
1:AP1:65:LYS:HB3	1:AP1:81:ASP:OD1	2.21	0.40
1:AP1:730:GLU:OE2	1:AP1:732:GLN:N	2.30	0.40
1:GP1:62:LYS:HG2	1:GP1:65:LYS:O	2.21	0.40
1:GP1:192:GLU:OE1	1:GP1:194:GLY:N	2.55	0.40
1:GP1:730:GLU:OE2	1:GP1:732:GLN:N	2.30	0.40
1:AP1:371:GLN:CD	2:CP1:329:LYS:HE2	2.46	0.40
1:GP1:63:LYS:HE2	1:GP1:63:LYS:HB2	1.91	0.40
1:AP1:192:GLU:OE1	1:AP1:194:GLY:N	2.55	0.40
2:CP1:374:LYS:HE3	2:CP1:374:LYS:HB3	1.91	0.40
1:AP1:93:GLN:OE1	1:AP1:93:GLN:N	2.55	0.40
2:EP1:107:THR:CG2	2:EP1:138:GLN:HG2	2.52	0.40
1:GP1:76:THR:OG1	1:GP1:77:GLY:N	2.55	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	AP1	763/820 (93%)	738 (97%)	24 (3%)	1 (0%)	48	78
1	GP1	763/820 (93%)	735 (96%)	27 (4%)	1 (0%)	48	78
2	BP1	370/378 (98%)	361 (98%)	9 (2%)	0	100	100
2	CP1	370/378 (98%)	361 (98%)	9 (2%)	0	100	100
2	DP1	370/378 (98%)	361 (98%)	9 (2%)	0	100	100
2	EP1	370/378 (98%)	361 (98%)	9 (2%)	0	100	100
All	All	3006/3152 (95%)	2917 (97%)	87 (3%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AP1	18	VAL
1	GP1	18	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AP1	678/726 (93%)	668 (98%)	10 (2%)	57	75
1	GP1	678/726 (93%)	668 (98%)	10 (2%)	57	75
2	BP1	319/322 (99%)	314 (98%)	5 (2%)	55	75
2	CP1	319/322 (99%)	314 (98%)	5 (2%)	55	75
2	DP1	319/322 (99%)	314 (98%)	5 (2%)	55	75
2	EP1	319/322 (99%)	314 (98%)	5 (2%)	55	75
All	All	2632/2740 (96%)	2592 (98%)	40 (2%)	55	75

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AP1	18	VAL
1	AP1	141	LYS
1	AP1	162	LYS
1	AP1	218	LEU
1	AP1	239	THR
1	AP1	377	ASP
1	AP1	451	LEU
1	AP1	471	PHE
1	AP1	674	LYS
1	AP1	730	GLU
2	BP1	25	ASP
2	BP1	145	SER
2	BP1	185	ASP
2	BP1	325	THR
2	BP1	371	VAL
2	CP1	25	ASP
2	CP1	145	SER
2	CP1	185	ASP
2	CP1	325	THR
2	CP1	371	VAL
2	DP1	25	ASP
2	DP1	145	SER
2	DP1	185	ASP
2	DP1	325	THR
2	DP1	371	VAL
2	EP1	25	ASP
2	EP1	145	SER
2	EP1	185	ASP
2	EP1	325	THR
2	EP1	371	VAL
1	GP1	18	VAL
1	GP1	141	LYS
1	GP1	162	LYS
1	GP1	218	LEU
1	GP1	239	THR
1	GP1	377	ASP
1	GP1	451	LEU
1	GP1	471	PHE
1	GP1	674	LYS
1	GP1	730	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	SEP	AP1	19	1	8,9,10	1.59	1 (12%)	7,12,14	1.33	1 (14%)
1	SEP	GP1	19	1	8,9,10	1.59	1 (12%)	7,12,14	1.33	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	AP1	19	1	-	3/6/8/10	-
1	SEP	GP1	19	1	-	3/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AP1	19	SEP	P-O1P	3.50	1.61	1.50
1	GP1	19	SEP	P-O1P	3.49	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GP1	19	SEP	OG-CB-CA	3.00	111.06	108.14
1	AP1	19	SEP	OG-CB-CA	2.98	111.05	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AP1	19	SEP	C-CA-CB-OG
1	GP1	19	SEP	C-CA-CB-OG
1	AP1	19	SEP	CA-CB-OG-P
1	GP1	19	SEP	CA-CB-OG-P
1	AP1	19	SEP	N-CA-CB-OG
1	GP1	19	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AP1	19	SEP	3	0
1	GP1	19	SEP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
3	ADP	CP1	401	4	28,29,29	1.39	5 (17%)	43,45,45	1.81	9 (20%)
3	ADP	DP1	401	4	28,29,29	1.39	5 (17%)	43,45,45	1.81	9 (20%)
5	9UE	BP1	403	-	48,50,50	1.02	5 (10%)	60,71,71	1.11	4 (6%)
3	ADP	EP1	401	4	28,29,29	1.39	5 (17%)	43,45,45	1.82	9 (20%)
5	9UE	CP1	403	-	48,50,50	1.02	5 (10%)	60,71,71	1.12	4 (6%)
5	9UE	DP1	403	-	48,50,50	1.02	5 (10%)	60,71,71	1.12	4 (6%)
5	9UE	EP1	403	-	48,50,50	1.03	5 (10%)	60,71,71	1.11	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	BP1	401	4	28,29,29	1.38	5 (17%)	43,45,45	1.81	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	CP1	401	4	-	7/16/32/32	0/3/3/3
3	ADP	DP1	401	4	-	7/16/32/32	0/3/3/3
5	9UE	BP1	403	-	-	6/56/56/56	0/3/4/4
3	ADP	EP1	401	4	-	7/16/32/32	0/3/3/3
5	9UE	CP1	403	-	-	6/56/56/56	0/3/4/4
5	9UE	DP1	403	-	-	6/56/56/56	0/3/4/4
5	9UE	EP1	403	-	-	6/56/56/56	0/3/4/4
3	ADP	BP1	401	4	-	7/16/32/32	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	EP1	401	ADP	C5-C4	4.26	1.46	1.39
3	BP1	401	ADP	C5-C4	4.22	1.46	1.39
3	CP1	401	ADP	C5-C4	4.21	1.46	1.39
3	DP1	401	ADP	C5-C4	4.21	1.46	1.39
5	BP1	403	9UE	O-C3	-2.99	1.42	1.47
5	EP1	403	9UE	O-C3	-2.97	1.42	1.47
5	DP1	403	9UE	O-C3	-2.95	1.42	1.47
5	CP1	403	9UE	O-C3	-2.93	1.42	1.47
5	CP1	403	9UE	C11-N2	2.82	1.40	1.34
5	DP1	403	9UE	C11-N2	2.82	1.40	1.34
5	EP1	403	9UE	C11-N2	2.82	1.40	1.34
5	BP1	403	9UE	C20-C21	-2.81	1.47	1.50
5	EP1	403	9UE	C20-C21	-2.81	1.47	1.50
5	CP1	403	9UE	C20-C21	-2.79	1.47	1.50
5	BP1	403	9UE	C11-N2	2.79	1.40	1.34
5	DP1	403	9UE	C20-C21	-2.77	1.47	1.50
3	EP1	401	ADP	C5-N7	-2.64	1.34	1.39
3	DP1	401	ADP	C5-N7	-2.64	1.34	1.39
3	CP1	401	ADP	C5-N7	-2.63	1.34	1.39
3	BP1	401	ADP	C5-N7	-2.60	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	EP1	403	9UE	C7-N	2.51	1.39	1.34
5	DP1	403	9UE	C7-N	2.50	1.39	1.34
3	DP1	401	ADP	C5-C6	2.49	1.47	1.41
3	CP1	401	ADP	C5-C6	2.49	1.47	1.41
5	CP1	403	9UE	C7-N	2.49	1.39	1.34
3	BP1	401	ADP	C5-C6	2.48	1.47	1.41
3	EP1	401	ADP	C5-C6	2.47	1.47	1.41
5	BP1	403	9UE	C7-N	2.47	1.39	1.34
5	BP1	403	9UE	C9-N1	2.26	1.40	1.35
5	CP1	403	9UE	C9-N1	2.26	1.40	1.35
5	DP1	403	9UE	C9-N1	2.25	1.40	1.35
5	EP1	403	9UE	C9-N1	2.24	1.40	1.35
3	EP1	401	ADP	C4-N9	-2.15	1.33	1.37
3	DP1	401	ADP	C8-N7	2.13	1.35	1.31
3	DP1	401	ADP	C4-N9	-2.12	1.33	1.37
3	BP1	401	ADP	C8-N7	2.12	1.35	1.31
3	CP1	401	ADP	C4-N9	-2.12	1.33	1.37
3	CP1	401	ADP	C8-N7	2.10	1.35	1.31
3	EP1	401	ADP	C8-N7	2.09	1.35	1.31
3	BP1	401	ADP	C4-N9	-2.08	1.33	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EP1	401	ADP	C5-C4-N3	-5.95	118.52	126.72
3	CP1	401	ADP	C5-C4-N3	-5.92	118.56	126.72
3	BP1	401	ADP	C5-C4-N3	-5.92	118.56	126.72
3	DP1	401	ADP	C5-C4-N3	-5.92	118.57	126.72
3	EP1	401	ADP	N3-C4-N9	4.61	135.01	127.17
3	CP1	401	ADP	N3-C4-N9	4.60	135.00	127.17
3	DP1	401	ADP	N3-C4-N9	4.60	135.00	127.17
3	BP1	401	ADP	N3-C4-N9	4.60	134.99	127.17
3	BP1	401	ADP	C2-N3-C4	3.76	121.02	111.83
3	EP1	401	ADP	C2-N3-C4	3.76	121.02	111.83
3	CP1	401	ADP	C2-N3-C4	3.76	121.01	111.83
3	DP1	401	ADP	C2-N3-C4	3.76	121.01	111.83
3	EP1	401	ADP	C4-C5-N7	-3.58	106.49	110.58
3	CP1	401	ADP	C4-C5-N7	-3.55	106.52	110.58
3	BP1	401	ADP	C4-C5-N7	-3.52	106.56	110.58
3	DP1	401	ADP	C4-C5-N7	-3.51	106.57	110.58
3	BP1	401	ADP	N3-C2-N1	-3.28	123.62	128.58
3	CP1	401	ADP	N3-C2-N1	-3.26	123.65	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EP1	401	ADP	N3-C2-N1	-3.25	123.67	128.58
3	DP1	401	ADP	N3-C2-N1	-3.25	123.67	128.58
5	DP1	403	9UE	C29-C6-N	-2.73	107.42	112.07
5	EP1	403	9UE	C29-C6-N	-2.72	107.43	112.07
5	BP1	403	9UE	C29-C6-N	-2.72	107.44	112.07
5	CP1	403	9UE	C29-C6-N	-2.71	107.44	112.07
5	DP1	403	9UE	C8-C20-C21	-2.62	108.33	113.98
5	CP1	403	9UE	C8-C20-C21	-2.61	108.35	113.98
5	BP1	403	9UE	C8-C20-C21	-2.61	108.35	113.98
3	CP1	401	ADP	C4-N9-C8	2.60	108.47	105.74
3	DP1	401	ADP	C4-N9-C8	2.60	108.47	105.74
5	EP1	403	9UE	C8-C20-C21	-2.59	108.38	113.98
3	EP1	401	ADP	C4-N9-C8	2.59	108.46	105.74
3	EP1	401	ADP	C5-N7-C8	2.58	107.50	103.45
3	BP1	401	ADP	C4-N9-C8	2.57	108.43	105.74
3	CP1	401	ADP	C5-N7-C8	2.56	107.47	103.45
3	BP1	401	ADP	C5-N7-C8	2.54	107.45	103.45
3	DP1	401	ADP	C5-N7-C8	2.54	107.44	103.45
3	EP1	401	ADP	C6-C5-N7	2.12	136.18	132.09
5	BP1	403	9UE	C1-C2-C3	-2.11	110.87	115.01
5	CP1	403	9UE	C1-C2-C3	-2.10	110.88	115.01
3	CP1	401	ADP	C6-C5-N7	2.10	136.14	132.09
5	DP1	403	9UE	C1-C2-C3	-2.10	110.89	115.01
5	EP1	403	9UE	C1-C2-C3	-2.09	110.92	115.01
3	BP1	401	ADP	C6-C5-N7	2.07	136.09	132.09
3	DP1	401	ADP	C6-C5-N7	2.07	136.07	132.09
5	CP1	403	9UE	O3-C9-N1	-2.05	118.39	121.76
5	DP1	403	9UE	O3-C9-N1	-2.04	118.41	121.76
5	EP1	403	9UE	O3-C9-N1	-2.03	118.43	121.76
5	BP1	403	9UE	O3-C9-N1	-2.02	118.45	121.76
3	EP1	401	ADP	N9-C8-N7	-2.01	111.08	113.94
3	DP1	401	ADP	N9-C8-N7	-2.01	111.09	113.94
3	CP1	401	ADP	N9-C8-N7	-2.00	111.09	113.94

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	BP1	403	9UE	C4-C5-C6-N
5	CP1	403	9UE	C4-C5-C6-N
5	DP1	403	9UE	C4-C5-C6-N
5	EP1	403	9UE	C4-C5-C6-N

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Mol	Chain	Res	Type	Atoms
3	BP1	401	ADP	C3'-C4'-C5'-O5'
3	CP1	401	ADP	C3'-C4'-C5'-O5'
3	DP1	401	ADP	C3'-C4'-C5'-O5'
3	EP1	401	ADP	C3'-C4'-C5'-O5'
5	BP1	403	9UE	C34-C29-C6-C5
5	BP1	403	9UE	C30-C29-C6-C5
5	CP1	403	9UE	C34-C29-C6-C5
5	CP1	403	9UE	C30-C29-C6-C5
5	DP1	403	9UE	C34-C29-C6-C5
5	DP1	403	9UE	C30-C29-C6-C5
5	EP1	403	9UE	C34-C29-C6-C5
5	EP1	403	9UE	C30-C29-C6-C5
5	CP1	403	9UE	C4-C5-C6-C29
3	BP1	401	ADP	O4'-C4'-C5'-O5'
3	CP1	401	ADP	O4'-C4'-C5'-O5'
3	DP1	401	ADP	O4'-C4'-C5'-O5'
3	EP1	401	ADP	O4'-C4'-C5'-O5'
3	BP1	401	ADP	C5'-O5'-PA-O1A
3	BP1	401	ADP	C5'-O5'-PA-O2A
3	BP1	401	ADP	C5'-O5'-PA-O3A
3	CP1	401	ADP	C5'-O5'-PA-O1A
3	CP1	401	ADP	C5'-O5'-PA-O2A
3	CP1	401	ADP	C5'-O5'-PA-O3A
3	DP1	401	ADP	C5'-O5'-PA-O1A
3	DP1	401	ADP	C5'-O5'-PA-O2A
3	DP1	401	ADP	C5'-O5'-PA-O3A
3	EP1	401	ADP	C5'-O5'-PA-O1A
3	EP1	401	ADP	C5'-O5'-PA-O2A
3	EP1	401	ADP	C5'-O5'-PA-O3A
3	BP1	401	ADP	PB-O3A-PA-O1A
3	BP1	401	ADP	PB-O3A-PA-O2A
3	CP1	401	ADP	PB-O3A-PA-O1A
3	CP1	401	ADP	PB-O3A-PA-O2A
3	DP1	401	ADP	PB-O3A-PA-O1A
3	DP1	401	ADP	PB-O3A-PA-O2A
3	EP1	401	ADP	PB-O3A-PA-O1A
3	EP1	401	ADP	PB-O3A-PA-O2A
5	BP1	403	9UE	C4-C5-C6-C29
5	DP1	403	9UE	C4-C5-C6-C29
5	EP1	403	9UE	C4-C5-C6-C29
5	BP1	403	9UE	C9-C10-N2-C11
5	CP1	403	9UE	C9-C10-N2-C11

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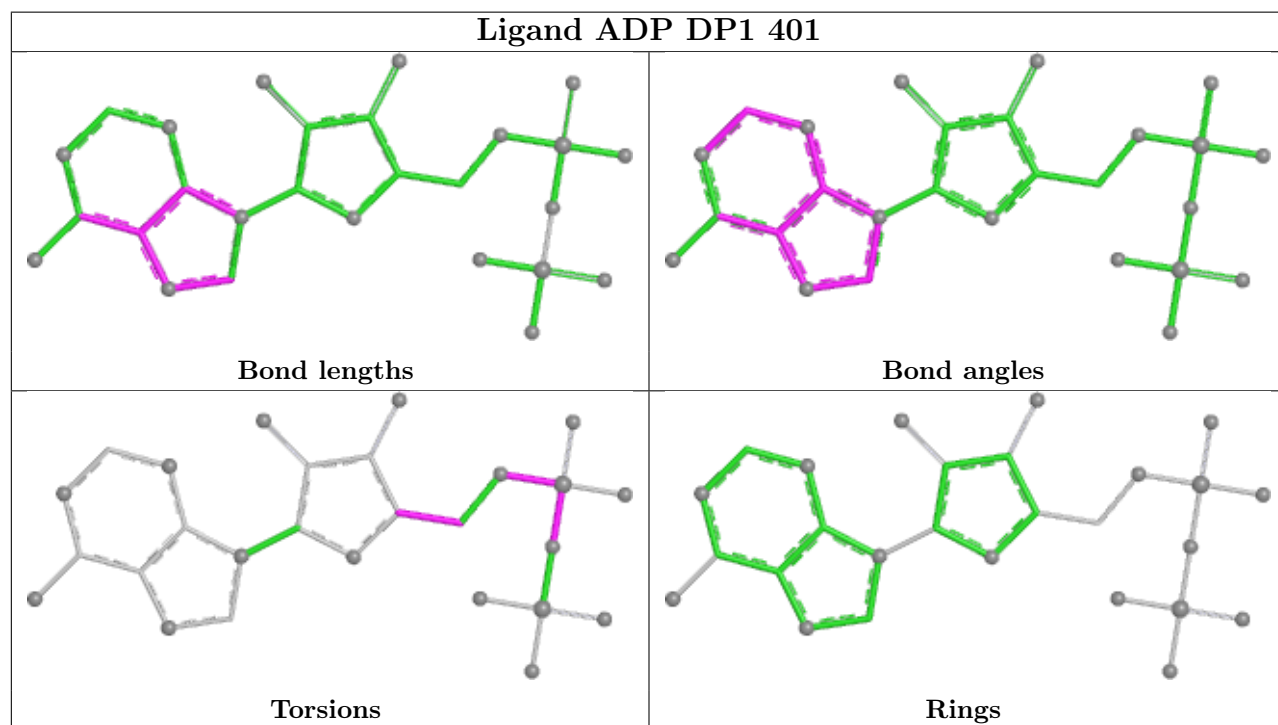
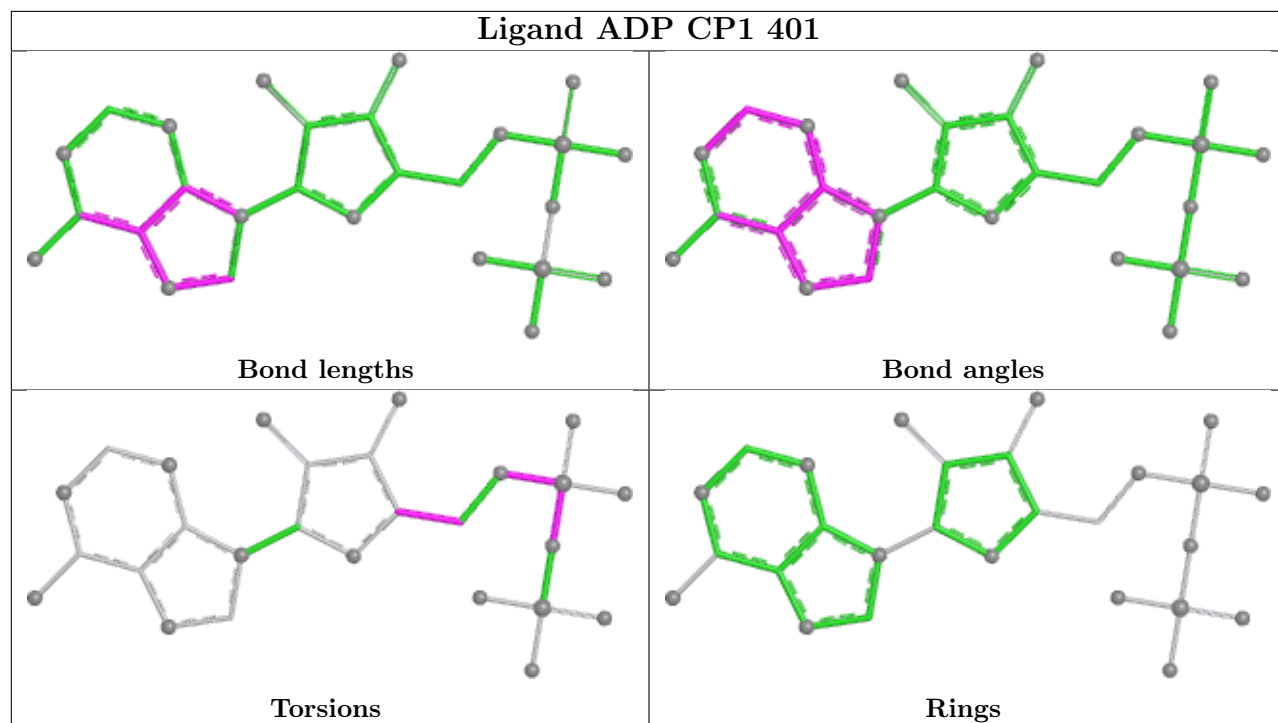
Mol	Chain	Res	Type	Atoms
5	DP1	403	9UE	C9-C10-N2-C11
5	EP1	403	9UE	C9-C10-N2-C11
5	BP1	403	9UE	C-C1-C2-C3
5	CP1	403	9UE	C-C1-C2-C3
5	DP1	403	9UE	C-C1-C2-C3
5	EP1	403	9UE	C-C1-C2-C3

There are no ring outliers.

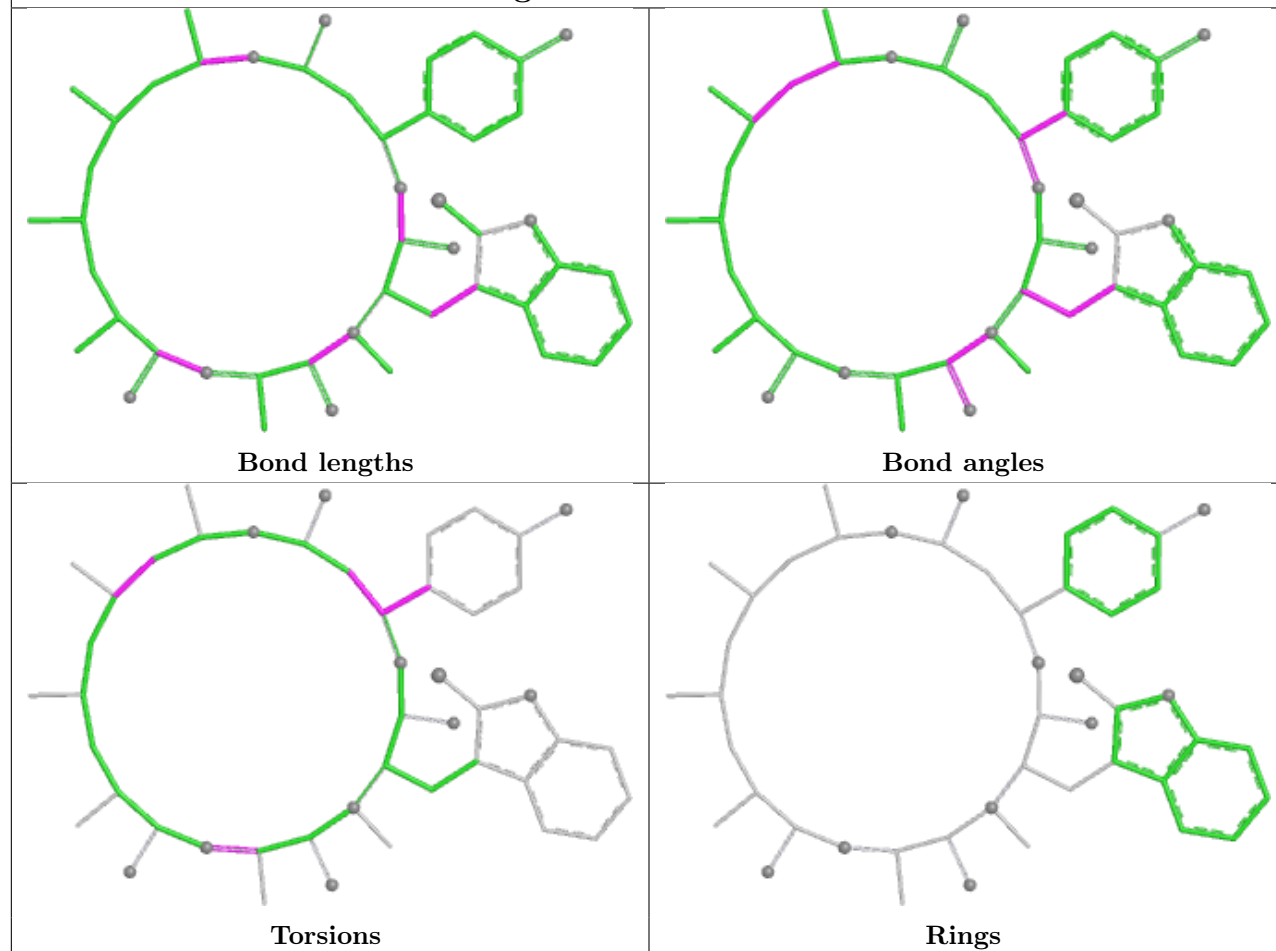
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CP1	401	ADP	2	0
3	DP1	401	ADP	2	0
3	EP1	401	ADP	2	0
3	BP1	401	ADP	2	0

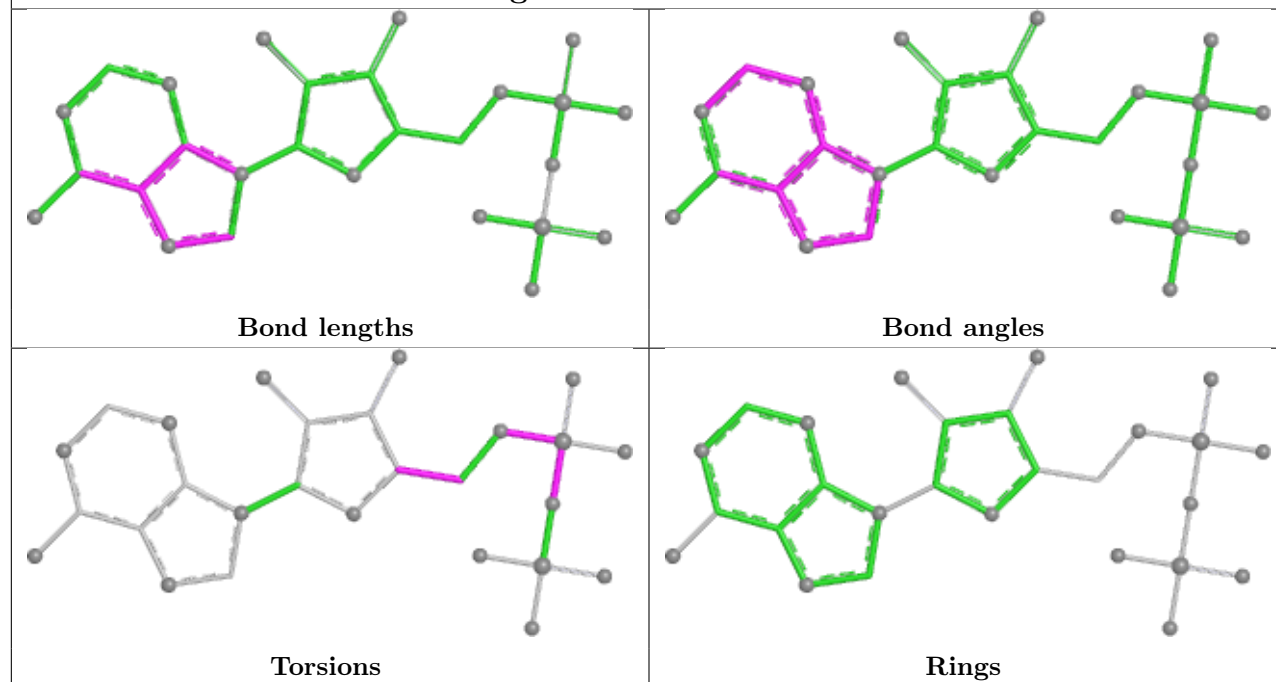
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



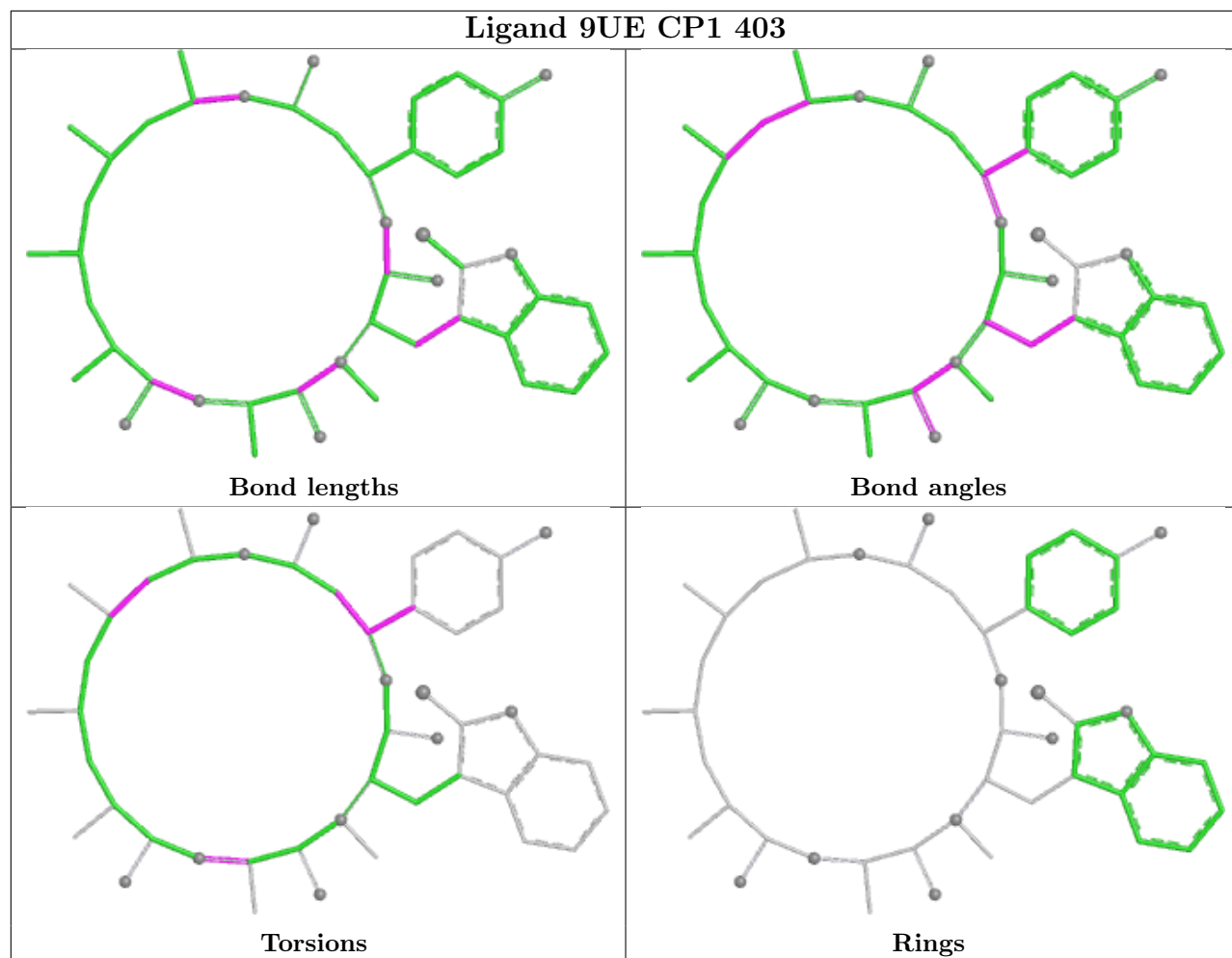
Ligand 9UE BP1 403



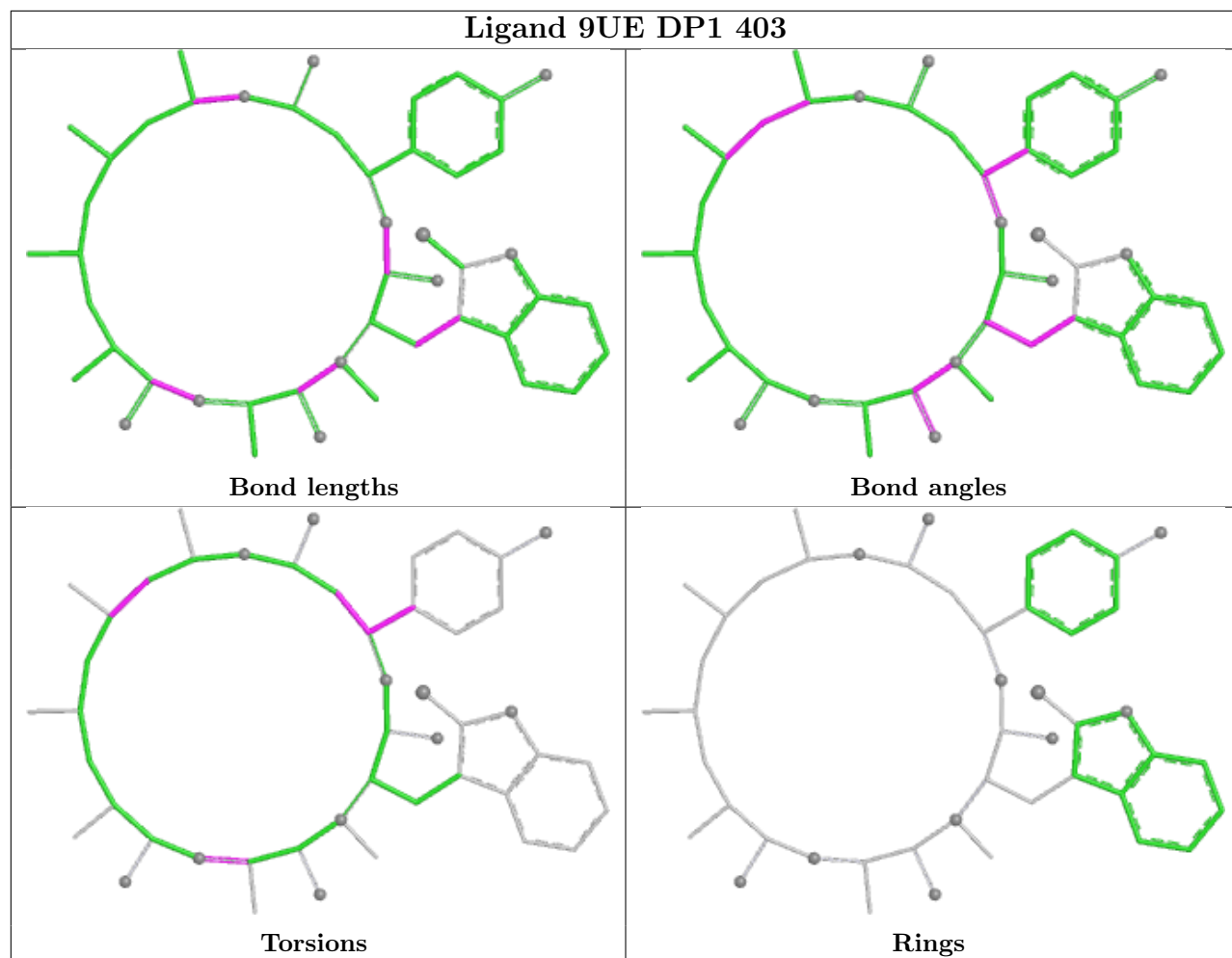
Ligand ADP EP1 401



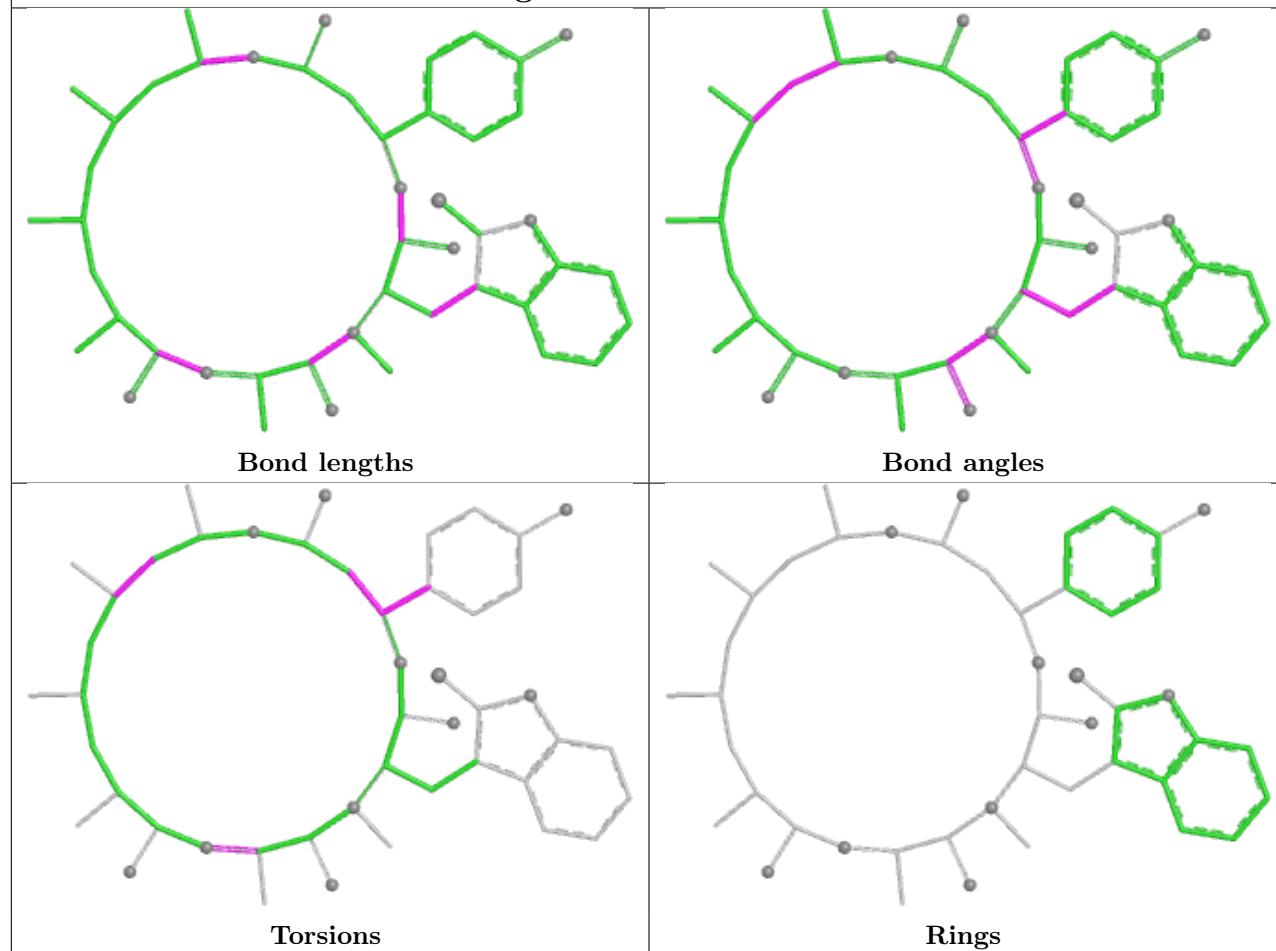
Ligand 9UE CP1 403



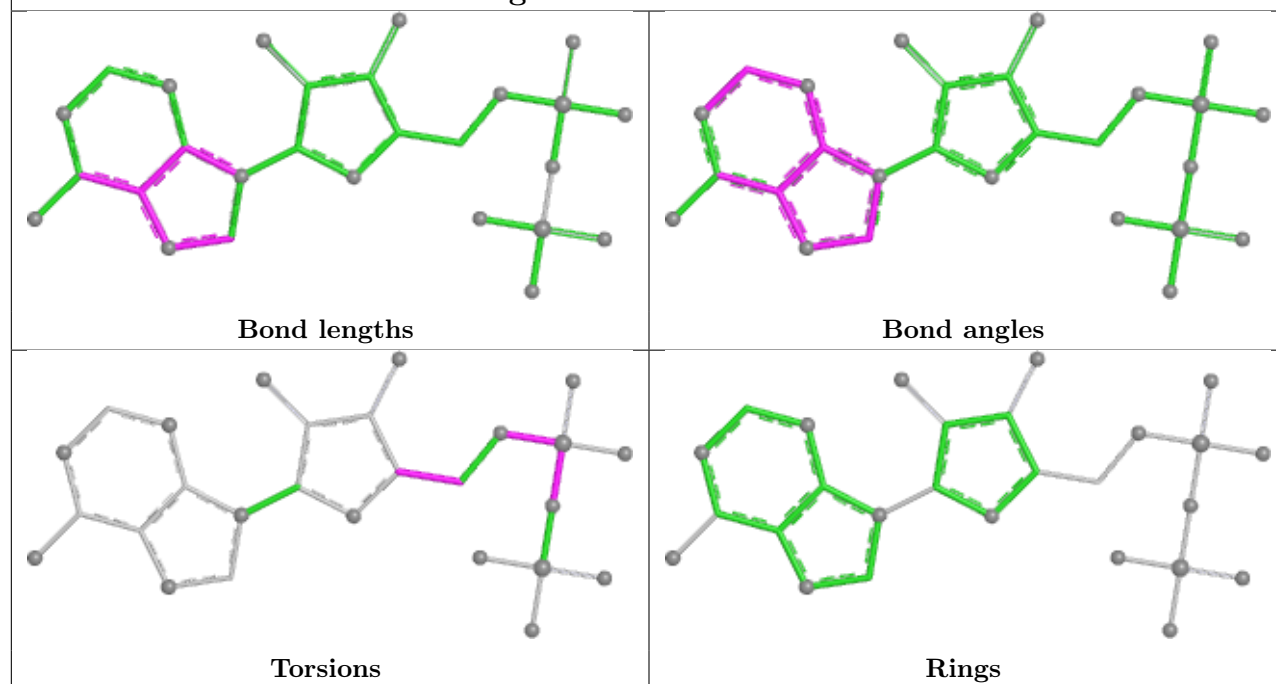
Ligand 9UE DP1 403



Ligand 9UE EP1 403



Ligand ADP BP1 401



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.

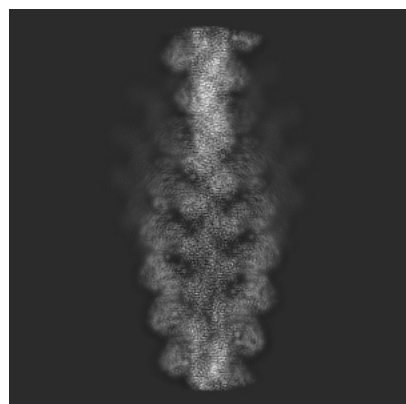
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10590. These allow visual inspection of the internal detail of the map and identification of artifacts.

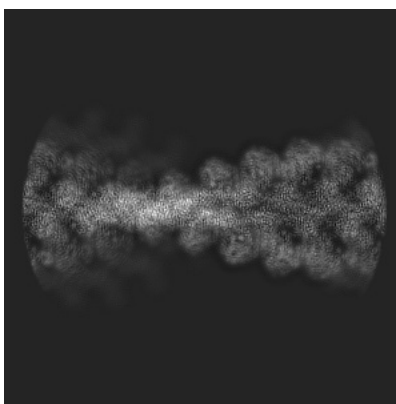
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

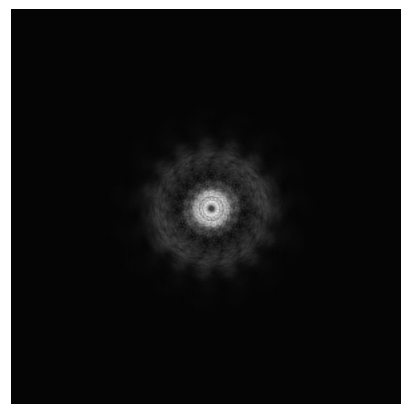
6.1.1 Primary map



X

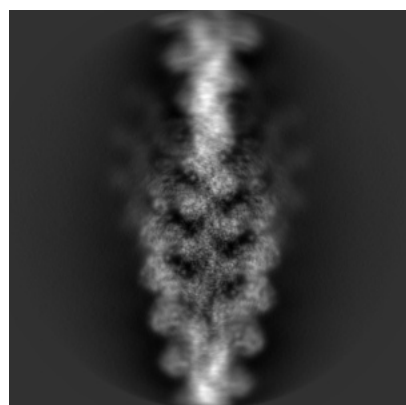


Y

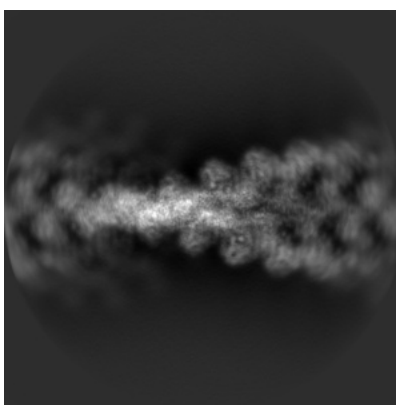


Z

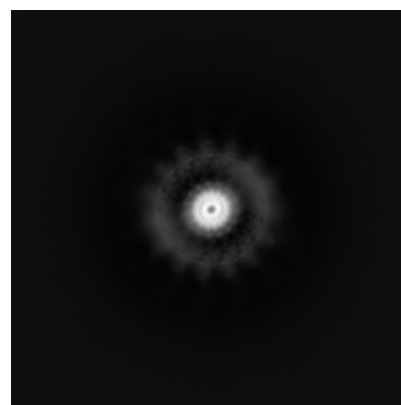
6.1.2 Raw map



X



Y

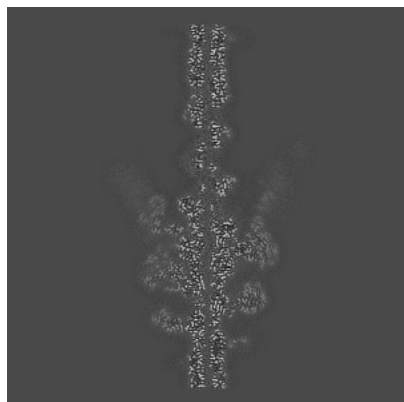


Z

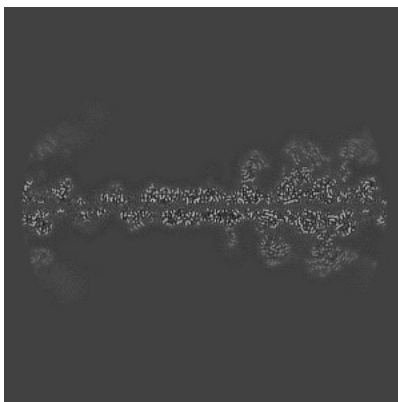
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

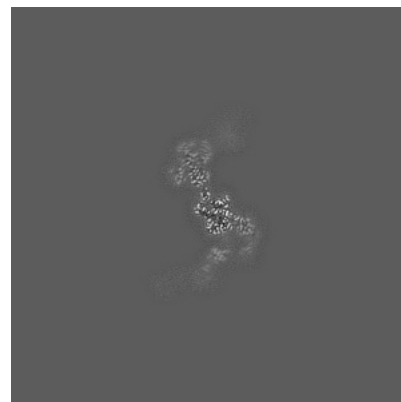
6.2.1 Primary map



X Index: 256

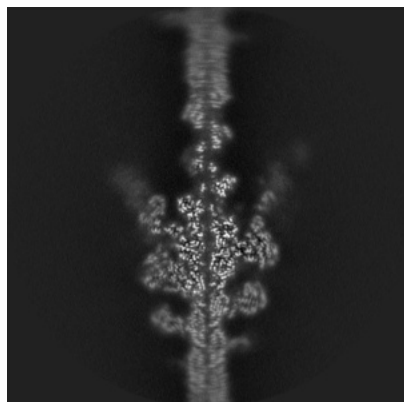


Y Index: 256

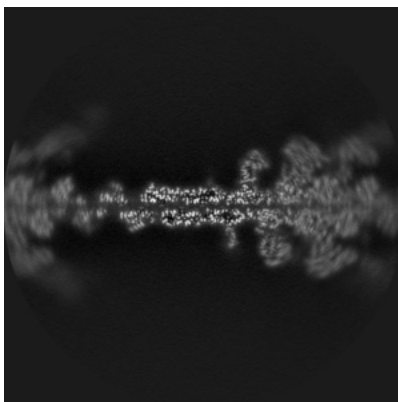


Z Index: 256

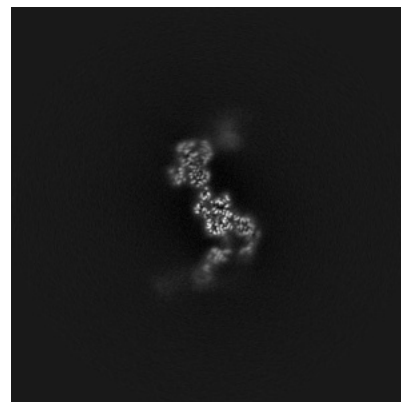
6.2.2 Raw map



X Index: 256



Y Index: 256

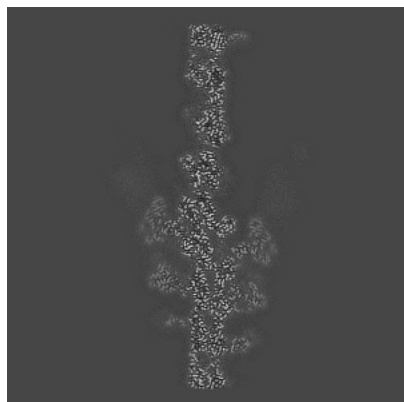


Z Index: 256

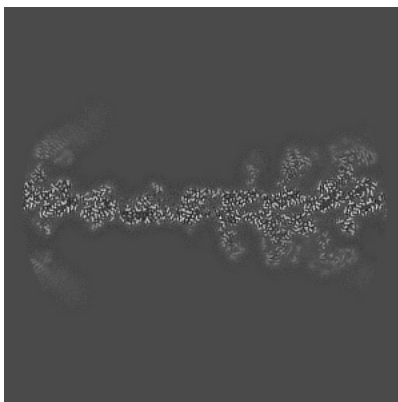
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

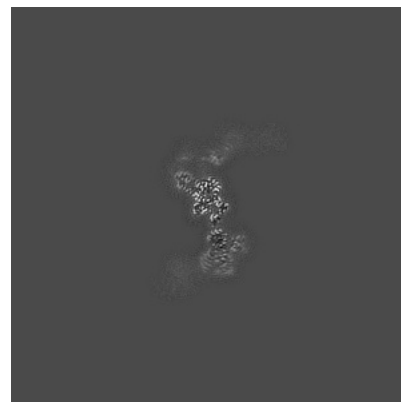
6.3.1 Primary map



X Index: 263

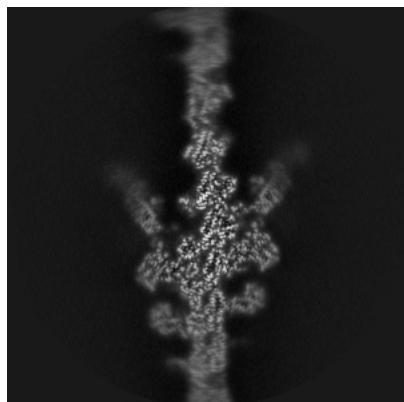


Y Index: 264

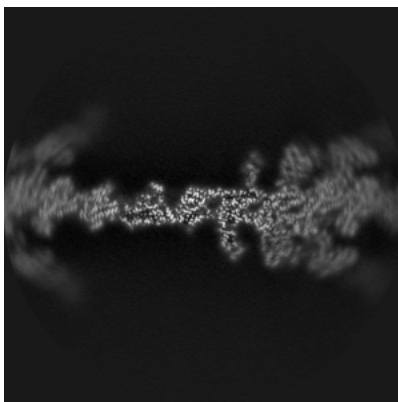


Z Index: 229

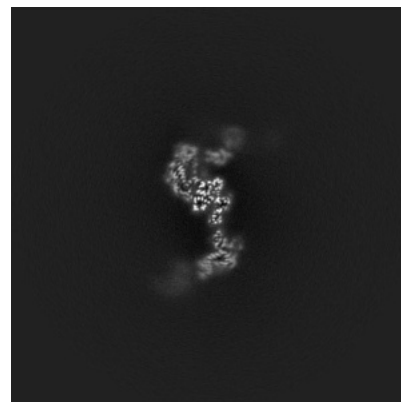
6.3.2 Raw map



X Index: 249



Y Index: 263

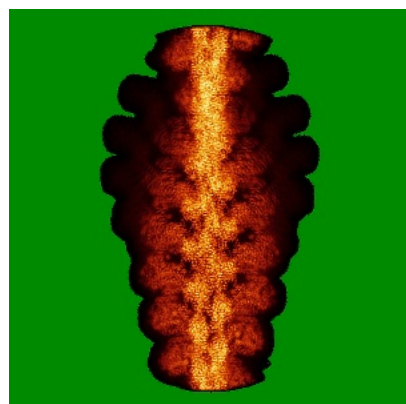


Z Index: 237

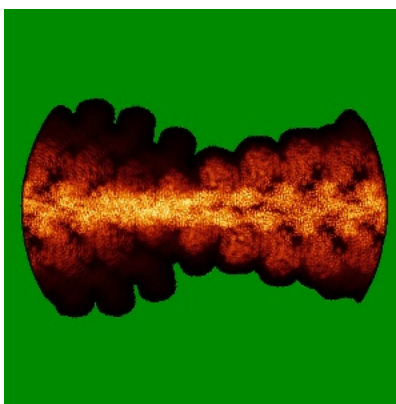
The images above show the largest variance slices of the map in three orthogonal directions.

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

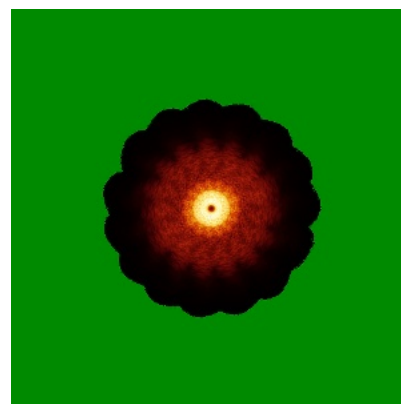
6.4.1 Primary map



X

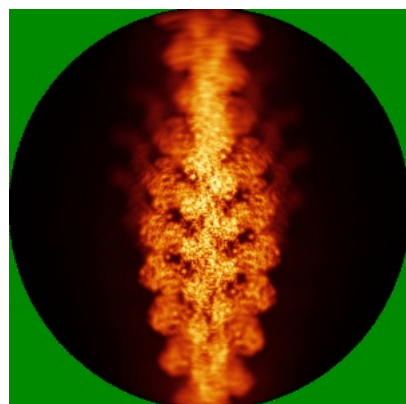


Y

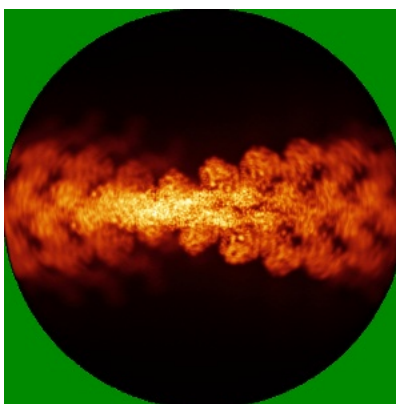


Z

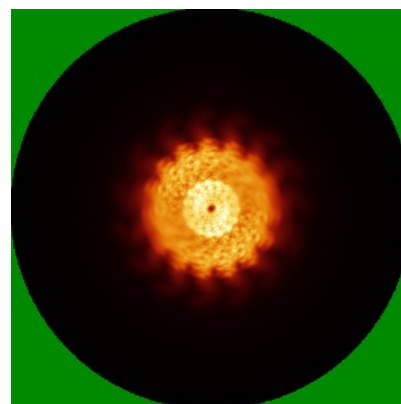
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

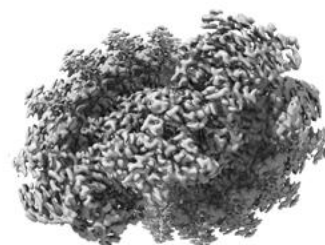
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

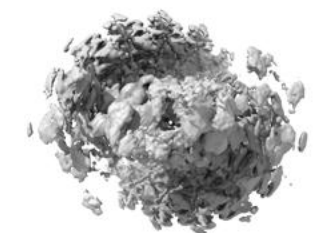
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

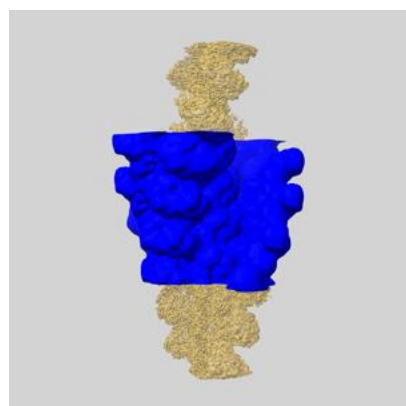
6.6 Mask visualisation [i](#)

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

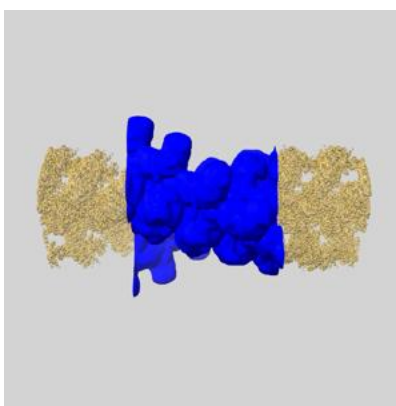
A mask typically either:

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

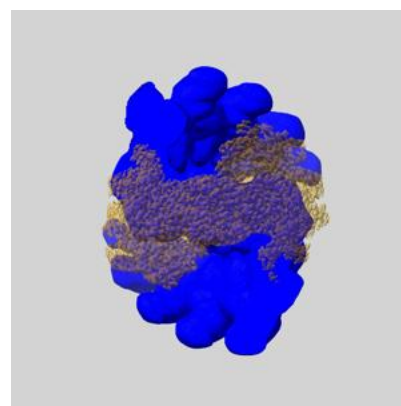
6.6.1 emd_10590_msk_1.map [i](#)



X



Y

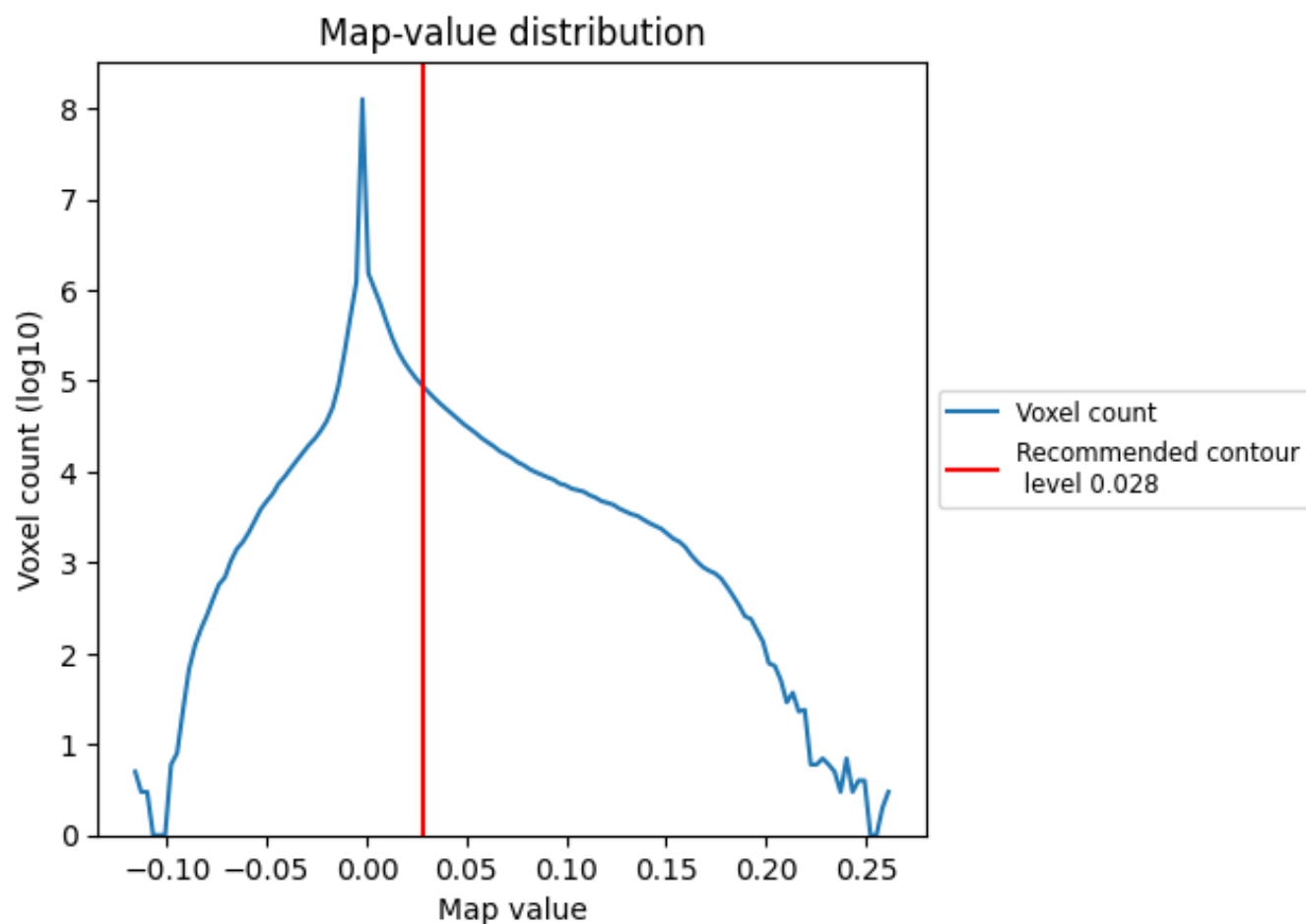


Z

7 Map analysis [i](#)

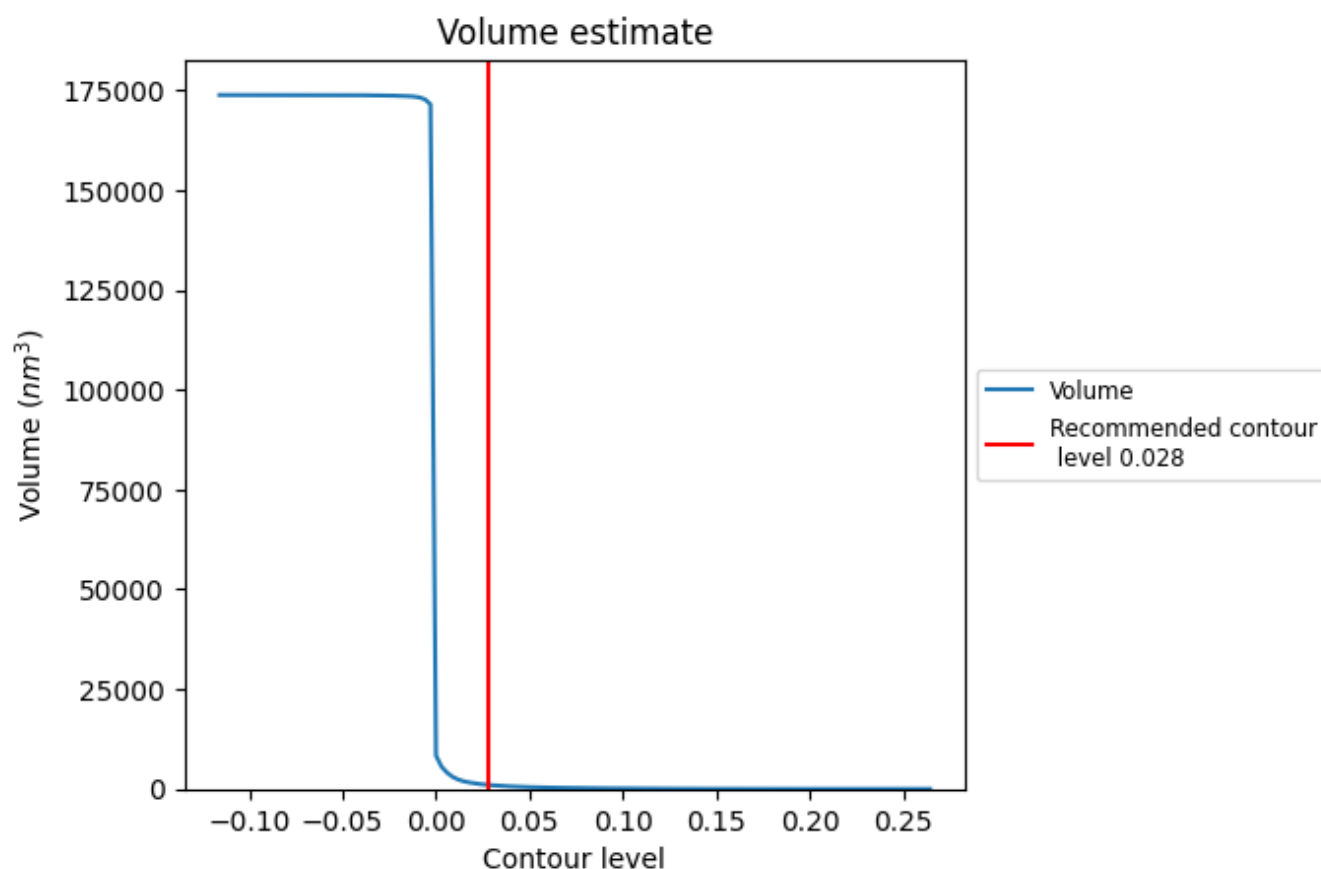
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

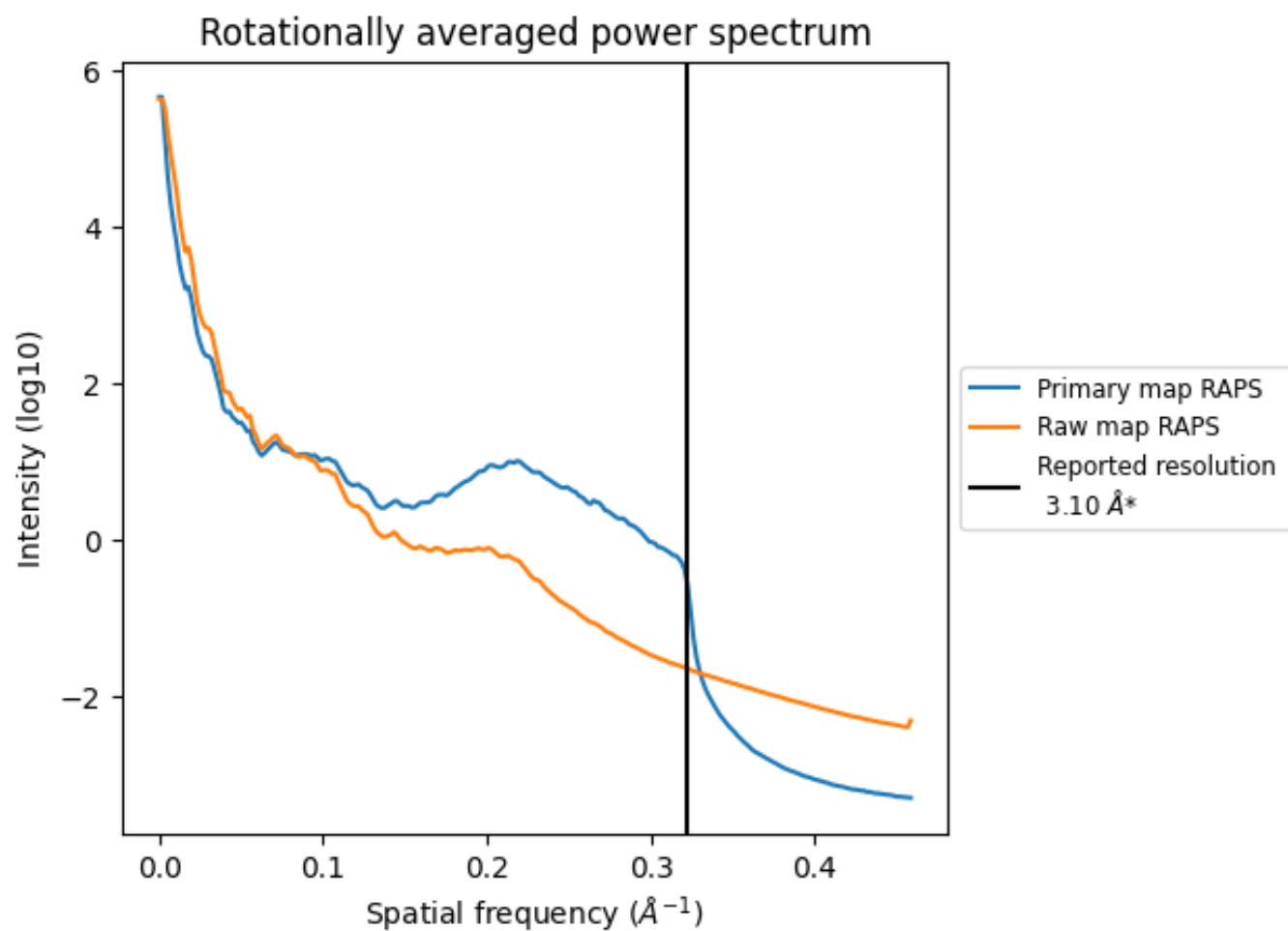
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1015 nm^3 ; this corresponds to an approximate mass of 917 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 ⓘ

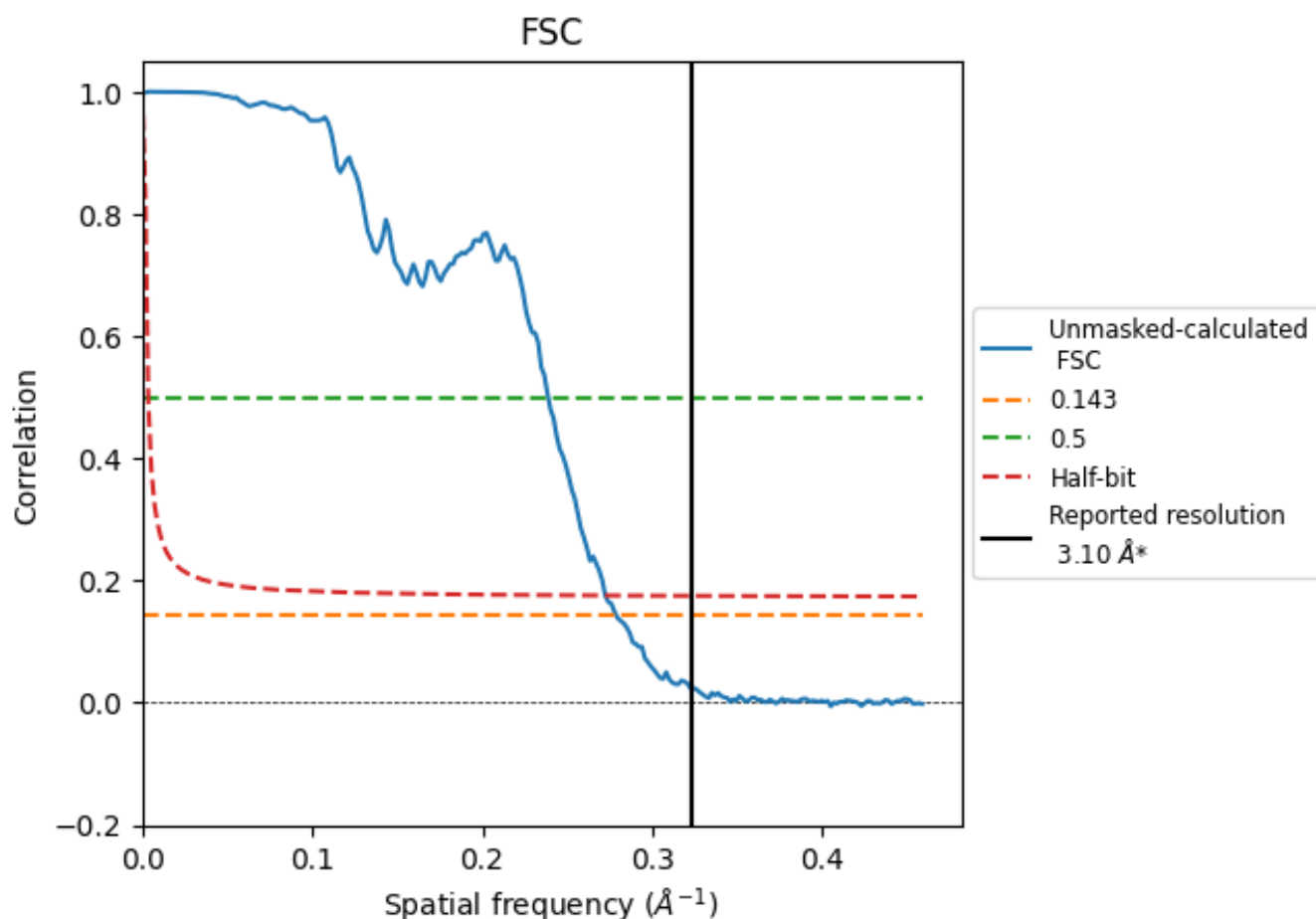


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

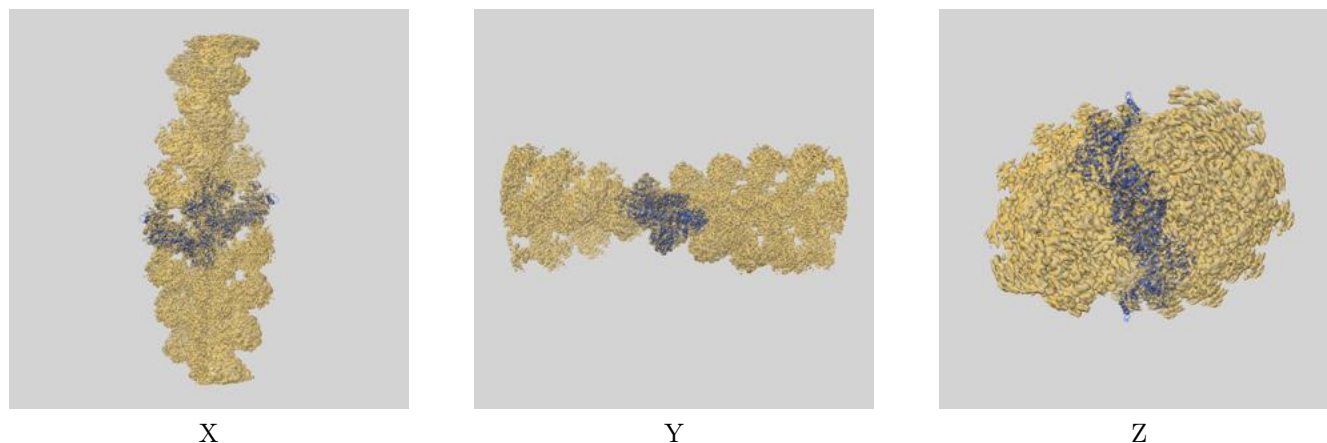
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	4.19	3.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

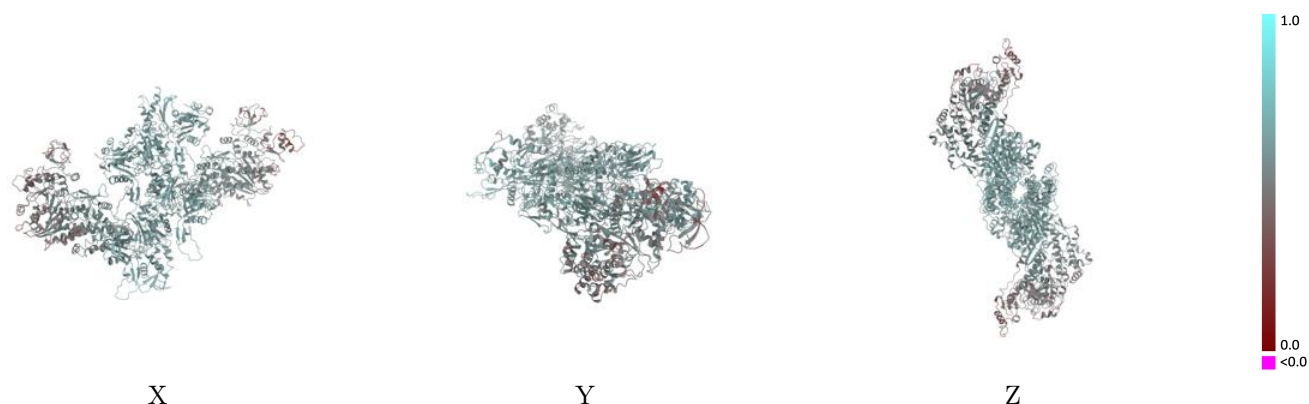
This section contains information regarding the fit between EMDB map EMD-10590 and PDB model 6TU7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



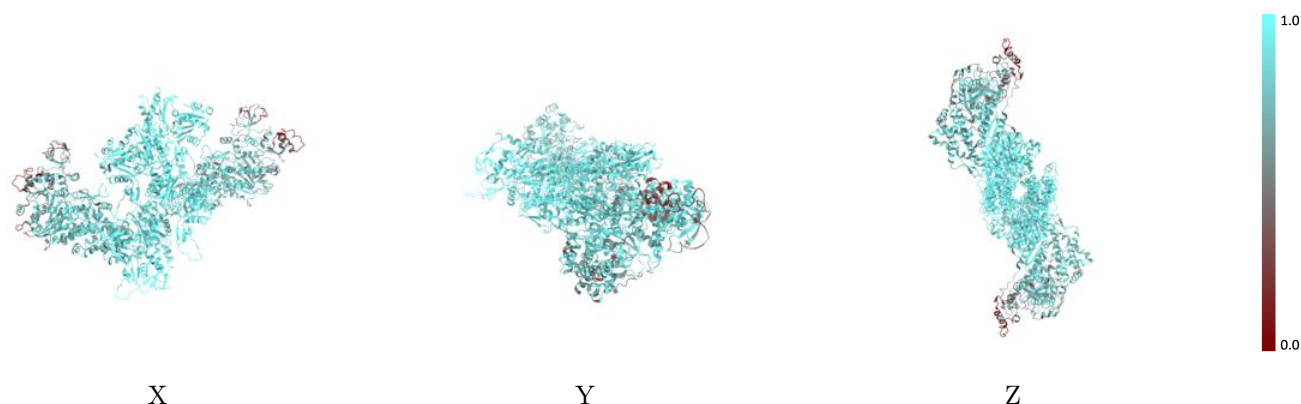
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



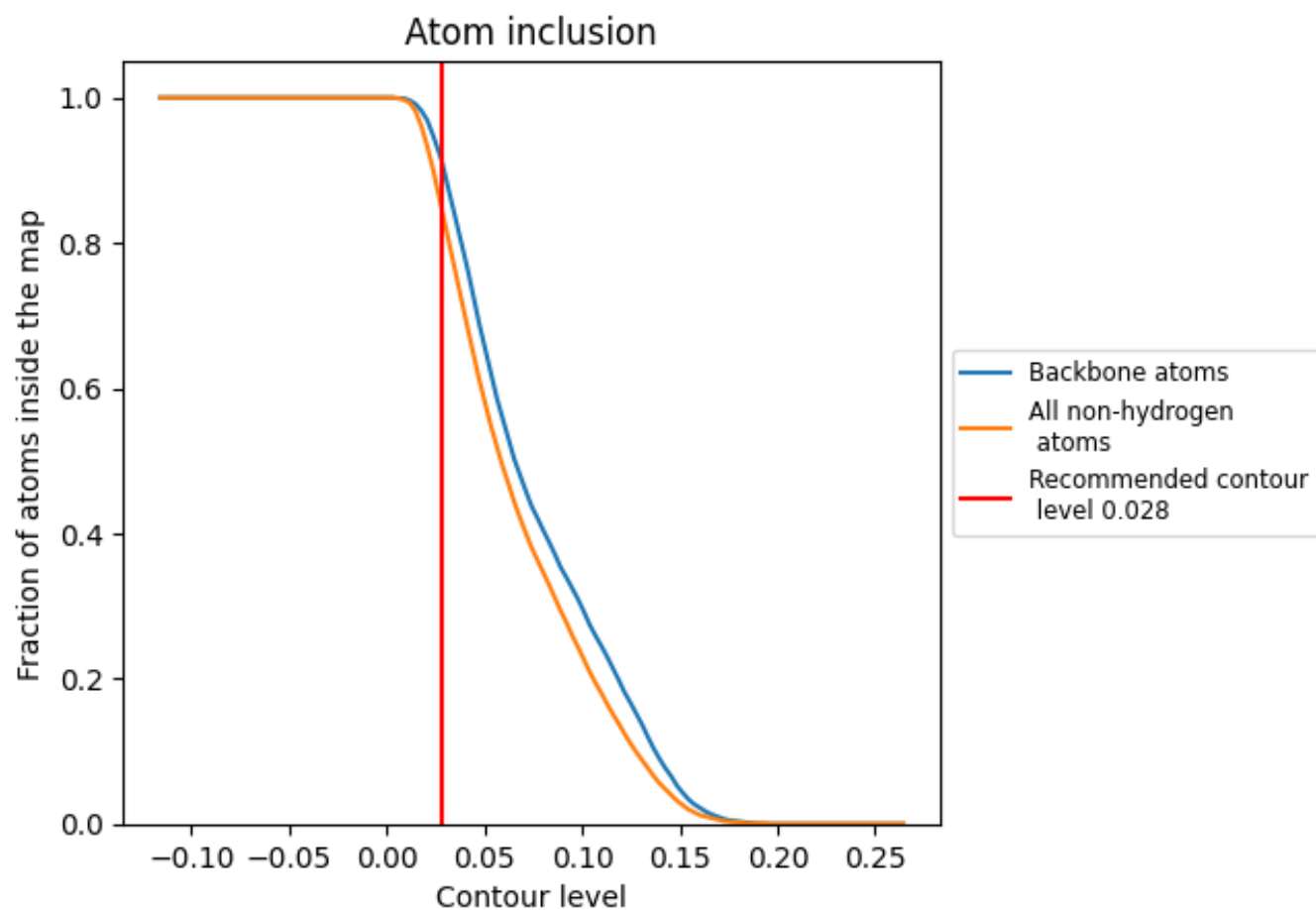
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.5500
AP1	0.7400	0.4980
BP1	0.9630	0.6030
CP1	0.9640	0.6050
DP1	0.9630	0.6020
EP1	0.9640	0.6050
GP1	0.7390	0.4980

1.0

0.0

<0.0