



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 08:32 PM UTC

PDB ID : 7BTI / pdb_00007bti
EMDB ID : EMD-30179
Title : Phalloidin bound F-actin complex
Authors : Kumari, A.; Ragunath, V.K.; Sirajuddin, M.
Deposited on : 2020-04-01
Resolution : 3.60 Å(reported)
Based on initial model : 5ONV

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

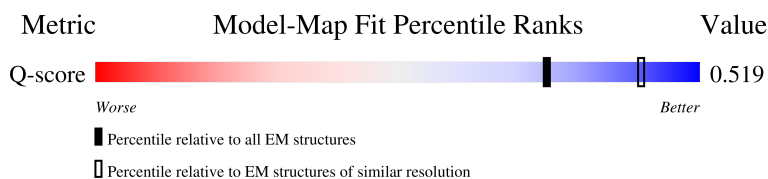
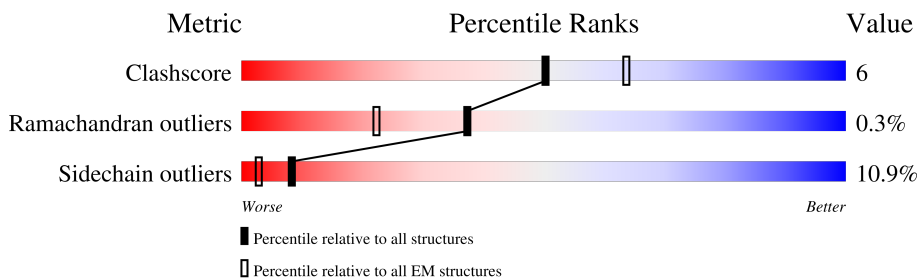
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	377	 79% 16% . .
1	B	377	 77% 19% . .
1	C	377	 75% 21% . .
1	D	377	 75% 19% . .

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Mol	Chain	Length	Quality of chain
1	E	377	77% 17%
2	X	7	71% 29%
2	Y	7	57% 43%
2	Z	7	57% 43%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14650 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	366	Total	C	N	O	S	0	0
			2855	1808	483	543	21		
1	B	369	Total	C	N	O	S	0	0
			2880	1823	487	549	21		
1	C	369	Total	C	N	O	S	0	0
			2868	1816	485	546	21		
1	D	369	Total	C	N	O	S	0	0
			2880	1823	487	549	21		
1	E	366	Total	C	N	O	S	0	0
			2862	1814	484	543	21		

- Molecule 2 is a protein called Phalloidin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
2	Y	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
2	Z	7	Total	C	N	O	S	0	0
			55	35	8	11	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

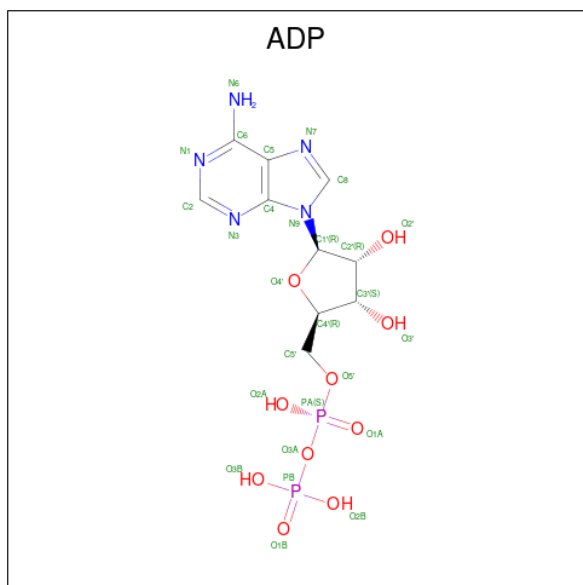
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
3	E	1	Total	Mg	0
			1	1	

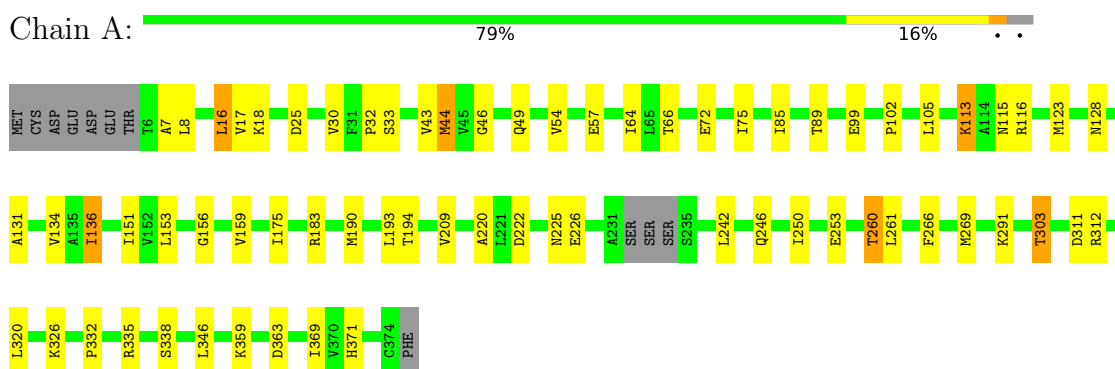
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



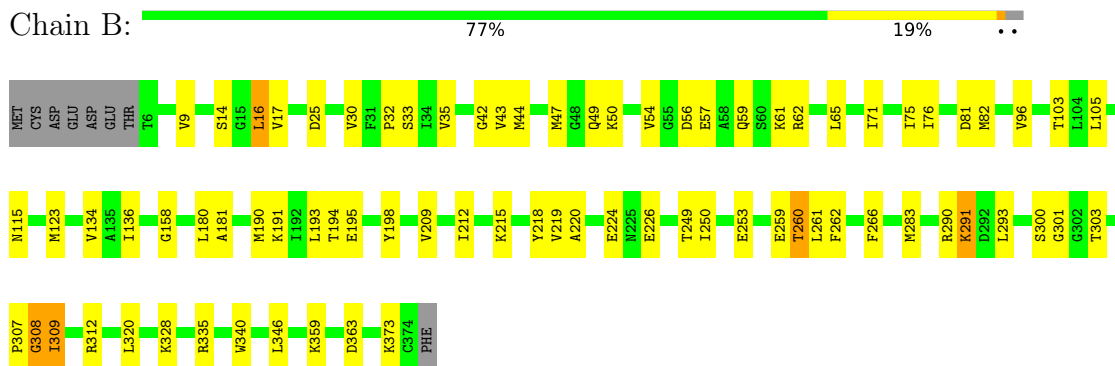
3 Residue-property plots

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.

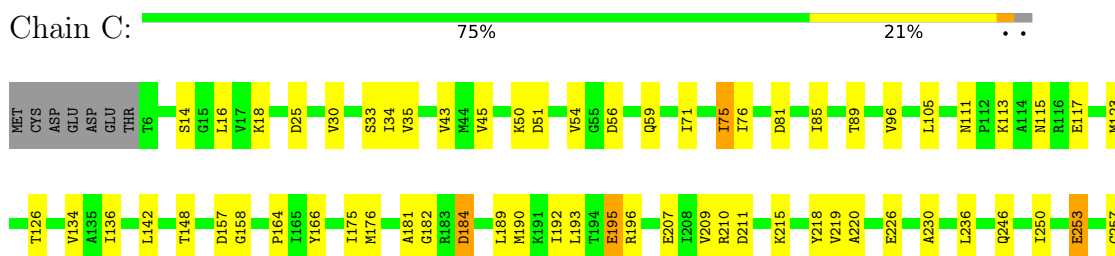
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



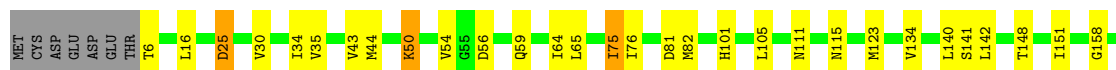
- Molecule 1: Actin, alpha skeletal muscle





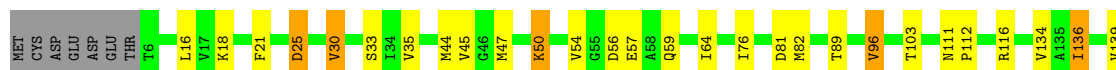
- Molecule 1: Actin, alpha skeletal muscle

Chain D: 75% 19%



- Molecule 1: Actin, alpha skeletal muscle

Chain E: 77% 17%



- Molecule 2: Phalloidin

Chain X: 71% 29%



- Molecule 2: Phalloidin

Chain Y: 57% 43%



- Molecule 2: Phalloidin

Chain Z: 57% 43%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-167°, rise=27.89 Å, axial sym=C1	Depositor
Number of segments used	91245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; GCTF for CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.536	Depositor
Minimum map value	-0.204	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.095	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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: ALO, G5G, HYP, MG, 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	0.19	0/2916	0.42	0/3951
1	B	0.22	0/2942	0.43	2/3986 (0.1%)
1	C	0.23	0/2930	0.46	2/3972 (0.1%)
1	D	0.23	0/2942	0.43	0/3986
1	E	0.23	0/2923	0.46	2/3959 (0.1%)
2	X	0.39	0/29	0.38	0/36
2	Y	0.33	0/29	0.40	0/36
2	Z	0.37	0/29	0.33	0/36
All	All	0.22	0/14740	0.44	6/19962 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	GLY	CA-C-N	5.19	131.32	121.97
1	C	308	GLY	C-N-CA	5.19	131.32	121.97
1	E	308	GLY	CA-C-N	5.10	131.14	121.97
1	E	308	GLY	C-N-CA	5.10	131.14	121.97
1	B	308	GLY	CA-C-N	5.08	131.11	121.97
1	B	308	GLY	C-N-CA	5.08	131.11	121.97

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	A	2855	0	2819	27	0
1	B	2880	0	2855	32	0
1	C	2868	0	2834	39	0
1	D	2880	0	2855	38	0
1	E	2862	0	2839	34	0
2	X	55	0	39	0	0
2	Y	55	0	39	0	0
2	Z	55	0	39	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
All	All	14650	0	14379	163	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 6.

All (163) 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:B:158:GLY:H	1:B:181:ALA:HB3	1.55	0.72
1:E:158:GLY:H	1:E:181:ALA:HB3	1.55	0.71
1:C:219:VAL:HB	1:C:308:GLY:HA3	1.78	0.66
1:E:219:VAL:HB	1:E:308:GLY:HA3	1.78	0.65
1:A:75:ILE:HA	1:A:115:ASN:HD21	1.62	0.64
1:A:105:LEU:HD11	1:A:123:MET:HG3	1.80	0.64
1:E:35:VAL:HG21	1:E:81:ASP:HB2	1.81	0.62
1:C:105:LEU:HD11	1:C:123:MET:HG3	1.85	0.59
1:C:71:ILE:HG12	1:C:76:ILE:HG12	1.83	0.59
1:D:158:GLY:H	1:D:181:ALA:HB3	1.68	0.58
1:B:219:VAL:HB	1:B:308:GLY:HA3	1.86	0.57
1:D:25:ASP:N	1:D:25:ASP:OD1	2.37	0.57
1:E:163:VAL:HA	1:E:175:ILE:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:MET:HG2	1:D:148:THR:HG22	1.87	0.56
1:C:196:ARG:NE	1:C:253:GLU:OE2	2.37	0.56
1:E:350:SER:O	1:E:353:GLN:NE2	2.39	0.56
1:A:222:ASP:OD2	1:A:225:ASN:ND2	2.39	0.56
1:B:57:GLU:OE2	1:B:61:LYS:NZ	2.40	0.55
1:D:369:ILE:O	1:D:373:LYS:HB2	2.07	0.55
1:C:207:GLU:OE1	1:C:210:ARG:NH2	2.39	0.55
1:C:105:LEU:HD21	1:C:123:MET:HE3	1.89	0.55
1:C:176:MET:SD	1:C:284:LYS:NZ	2.79	0.55
1:E:260:THR:HG23	1:E:266:PHE:HB2	1.89	0.55
1:C:211:ASP:OD1	1:C:215:LYS:NZ	2.39	0.55
1:C:184:ASP:N	1:C:184:ASP:OD1	2.41	0.54
1:D:350:SER:O	1:D:353:GLN:NE2	2.41	0.54
1:D:35:VAL:HG21	1:D:81:ASP:HB2	1.89	0.54
1:C:350:SER:O	1:C:353:GLN:NE2	2.40	0.54
1:D:75:ILE:HA	1:D:115:ASN:HD21	1.73	0.53
1:D:359:LYS:NZ	1:D:363:ASP:OD1	2.41	0.53
1:E:200:PHE:HB3	1:E:205:GLU:HB3	1.90	0.53
1:E:359:LYS:NZ	1:E:363:ASP:OD1	2.42	0.53
1:D:286:ASP:N	1:D:286:ASP:OD1	2.42	0.53
1:A:16:LEU:O	1:A:18:LYS:NZ	2.42	0.53
1:E:190:MET:HB3	1:E:209:VAL:HG11	1.90	0.53
1:B:75:ILE:HA	1:B:115:ASN:HD21	1.75	0.52
1:E:25:ASP:N	1:E:25:ASP:OD1	2.39	0.52
1:A:46:GLY:O	1:A:49:GLN:NE2	2.43	0.52
1:C:35:VAL:HG21	1:C:81:ASP:HB2	1.92	0.52
1:D:196:ARG:NH1	1:D:253:GLU:OE2	2.43	0.52
1:A:260:THR:HG23	1:A:266:PHE:HB2	1.92	0.52
1:B:190:MET:HB3	1:B:209:VAL:HG11	1.92	0.51
1:E:116:ARG:NH1	1:E:374:CYS:SG	2.83	0.51
1:B:359:LYS:NZ	1:B:363:ASP:OD2	2.44	0.51
1:D:163:VAL:HA	1:D:175:ILE:HG22	1.92	0.51
1:E:76:ILE:HD13	1:E:82:MET:HG2	1.93	0.51
1:B:16:LEU:HA	1:B:32:PRO:HA	1.93	0.51
1:C:25:ASP:N	1:C:25:ASP:OD1	2.41	0.51
1:C:230:ALA:HB2	1:C:236:LEU:HD22	1.93	0.51
1:E:56:ASP:N	1:E:56:ASP:OD1	2.44	0.50
1:B:198:TYR:HD1	2:Z:5:ALA:HB2	1.75	0.50
1:D:176:MET:SD	1:D:284:LYS:NZ	2.83	0.50
1:C:158:GLY:H	1:C:181:ALA:HB3	1.76	0.50
1:A:220:ALA:HB1	1:A:226:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ASP:H	1:C:182:GLY:H	1.60	0.50
1:D:300:SER:OG	1:D:301:GLY:N	2.44	0.50
1:B:42:GLY:HA2	1:D:169:TYR:HA	1.93	0.49
1:B:283:MET:SD	1:B:290:ARG:NH1	2.85	0.49
1:B:25:ASP:N	1:B:25:ASP:OD1	2.44	0.49
1:A:116:ARG:HH21	1:A:136:ILE:HD11	1.77	0.49
1:C:117:GLU:OE2	1:C:371:HIS:NE2	2.44	0.49
1:D:180:LEU:HD13	1:D:269:MET:HE2	1.95	0.49
1:A:190:MET:HB3	1:A:209:VAL:HG11	1.94	0.49
1:B:105:LEU:HD21	1:B:123:MET:HE3	1.95	0.49
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.93	0.48
1:B:71:ILE:HG12	1:B:76:ILE:HG12	1.94	0.48
1:A:16:LEU:HA	1:A:32:PRO:HA	1.96	0.48
1:C:16:LEU:O	1:C:18:LYS:NZ	2.47	0.48
1:D:197:GLY:HA2	1:E:112:PRO:HG3	1.96	0.48
1:E:219:VAL:HG22	1:E:258:PRO:HB2	1.95	0.48
1:C:56:ASP:OD1	1:C:56:ASP:N	2.47	0.47
1:C:81:ASP:N	1:C:81:ASP:OD1	2.41	0.47
1:A:99:GLU:HG3	1:A:128:ASN:HB2	1.95	0.47
1:C:359:LYS:NZ	1:C:359:LYS:O	2.46	0.47
1:D:105:LEU:HD21	1:D:123:MET:HE3	1.95	0.47
1:D:324:THR:O	1:D:324:THR:OG1	2.31	0.47
1:A:156:GLY:O	1:A:303:THR:OG1	2.32	0.47
1:B:218:TYR:HA	1:B:307:PRO:HD2	1.97	0.47
1:D:76:ILE:HD13	1:D:82:MET:HG2	1.97	0.46
1:E:184:ASP:N	1:E:184:ASP:OD1	2.47	0.46
1:B:260:THR:HG23	1:B:266:PHE:HB2	1.97	0.46
1:C:305:MET:HE2	1:C:305:MET:HB3	1.87	0.46
1:E:136:ILE:HG22	1:E:139:VAL:H	1.80	0.46
1:D:105:LEU:HD11	1:D:123:MET:HG3	1.98	0.46
1:C:189:LEU:HD13	1:C:257:CYS:HB2	1.97	0.46
1:D:220:ALA:HB1	1:D:226:GLU:HG3	1.98	0.46
1:A:85:ILE:O	1:A:89:THR:OG1	2.29	0.45
1:D:304:THR:O	1:D:335:ARG:NH2	2.50	0.45
1:E:47:MET:HE2	1:E:47:MET:HB3	1.86	0.45
1:B:259:GLU:OE2	1:B:312:ARG:NH1	2.49	0.45
1:C:219:VAL:HG22	1:C:258:PRO:HB2	1.98	0.45
1:B:209:VAL:HA	1:B:212:ILE:HD12	1.99	0.45
1:C:300:SER:OG	1:C:301:GLY:N	2.50	0.45
1:C:218:TYR:HA	1:C:307:PRO:HD2	1.99	0.45
1:D:215:LYS:HB3	1:D:215:LYS:HE2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:LEU:HD13	1:E:269:MET:HE2	1.98	0.44
1:B:44:MET:HE1	1:D:142:LEU:HB3	1.99	0.44
1:C:195:GLU:H	1:C:195:GLU:HG3	1.58	0.44
1:D:218:TYR:HA	1:D:307:PRO:HD2	1.99	0.44
1:E:142:LEU:HD13	1:E:298:VAL:HG21	2.00	0.44
1:A:113:LYS:HB2	1:A:371:HIS:CE1	2.52	0.44
1:C:85:ILE:O	1:C:89:THR:OG1	2.32	0.44
1:A:17:VAL:HG23	1:A:33:SER:HB2	1.99	0.44
1:A:359:LYS:NZ	1:A:363:ASP:OD1	2.50	0.44
1:A:25:ASP:OD1	1:A:25:ASP:N	2.49	0.44
1:B:76:ILE:HD13	1:B:82:MET:HG2	1.99	0.44
1:B:300:SER:OG	1:B:301:GLY:N	2.51	0.44
1:D:269:MET:HE3	1:D:269:MET:HB3	1.87	0.44
1:D:304:THR:HA	1:D:309:ILE:HD13	1.99	0.44
1:E:18:LYS:HG2	1:E:30:VAL:HG12	2.00	0.44
1:E:369:ILE:HG12	1:E:372:ARG:HH11	1.83	0.44
1:B:35:VAL:HG21	1:B:81:ASP:HB2	2.00	0.44
1:A:7:ALA:HA	1:A:102:PRO:HD2	2.00	0.44
1:D:257:CYS:O	1:D:260:THR:OG1	2.35	0.44
1:E:192:ILE:HD12	1:E:192:ILE:HA	1.85	0.43
1:B:291:LYS:HB3	1:B:291:LYS:HE3	1.82	0.43
1:D:292:ASP:OD1	1:D:292:ASP:N	2.47	0.43
1:E:141:SER:HB2	1:E:152:VAL:HG11	1.99	0.43
1:B:56:ASP:N	1:B:56:ASP:OD1	2.52	0.43
1:A:332:PRO:O	1:A:335:ARG:NH1	2.43	0.43
1:E:21:PHE:HZ	1:E:96:VAL:HG11	1.84	0.43
1:E:355:MET:HE2	1:E:355:MET:HB2	1.90	0.43
1:D:184:ASP:OD1	1:D:184:ASP:N	2.52	0.43
1:A:44:MET:HE2	1:C:148:THR:HG22	1.99	0.42
1:C:189:LEU:HA	1:C:192:ILE:HG22	2.01	0.42
1:D:216:LEU:HD11	1:D:240:TYR:HB2	2.00	0.42
1:C:314:GLN:O	1:C:318:THR:OG1	2.32	0.42
1:C:300:SER:O	1:C:304:THR:OG1	2.35	0.42
1:A:242:LEU:N	1:A:246:GLN:O	2.48	0.42
1:E:369:ILE:HG12	1:E:372:ARG:HD2	2.01	0.42
1:B:195:GLU:HG3	1:C:113:LYS:HB3	2.01	0.42
1:C:190:MET:HB3	1:C:209:VAL:HG11	2.02	0.42
1:D:190:MET:HB3	1:D:209:VAL:HG11	2.01	0.42
1:D:330:ILE:HD12	1:D:332:PRO:HD3	2.01	0.41
1:A:269:MET:HE3	1:A:269:MET:HB3	1.96	0.41
1:B:220:ALA:HB1	1:B:226:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ILE:HD12	1:C:192:ILE:HA	1.89	0.41
1:D:50:LYS:HE2	1:D:50:LYS:HB3	1.91	0.41
1:B:191:LYS:HE3	1:B:191:LYS:HB3	1.91	0.41
1:D:6:THR:O	1:D:101:HIS:ND1	2.46	0.41
1:D:317:ILE:HG22	1:D:327:ILE:HD13	2.02	0.41
1:E:33:SER:O	1:E:33:SER:OG	2.36	0.41
1:D:287:ILE:H	1:D:287:ILE:HG12	1.66	0.41
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.94	0.41
1:E:191:LYS:HE3	1:E:191:LYS:HB3	1.85	0.41
1:A:335:ARG:HA	1:A:338:SER:HB3	2.02	0.41
1:B:9:VAL:O	1:B:340:TRP:NE1	2.45	0.41
1:E:50:LYS:NZ	1:E:57:GLU:OE2	2.52	0.41
1:E:176:MET:SD	1:E:284:LYS:NZ	2.79	0.41
1:C:75:ILE:HA	1:C:115:ASN:HD21	1.86	0.41
1:C:287:ILE:H	1:C:287:ILE:HG12	1.72	0.40
1:D:353:GLN:OE1	1:D:354:GLN:NE2	2.54	0.40
1:A:64:ILE:HD11	1:C:166:TYR:HB3	2.04	0.40
1:A:72:GLU:OE2	1:A:183:ARG:NH1	2.55	0.40
1:B:215:LYS:HE2	1:B:215:LYS:HB3	1.93	0.40
1:B:262:PHE:HZ	1:B:309:ILE:HG13	1.86	0.40
1:C:164:PRO:HD2	1:C:175:ILE:HG22	2.02	0.40
1:C:220:ALA:HB1	1:C:226:GLU:HG3	2.03	0.40
1:E:215:LYS:HB3	1:E:215:LYS:HE2	1.81	0.40
1:E:220:ALA:HB1	1:E:226:GLU:HG3	2.03	0.40
1:A:105:LEU:HD21	1:A:123:MET:HE3	2.03	0.40
1:B:17:VAL:HG23	1:B:33:SER:HB3	2.03	0.40
1:E:50:LYS:H	1:E:50:LYS:HG3	1.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	362/377 (96%)	343 (95%)	19 (5%)	0	100	100
1	B	367/377 (97%)	349 (95%)	17 (5%)	1 (0%)	36	65
1	C	367/377 (97%)	346 (94%)	19 (5%)	2 (0%)	24	57
1	D	367/377 (97%)	341 (93%)	26 (7%)	0	100	100
1	E	362/377 (96%)	338 (93%)	23 (6%)	1 (0%)	36	65
2	X	3/7 (43%)	1 (33%)	2 (67%)	0	100	100
2	Y	3/7 (43%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	Z	3/7 (43%)	0	3 (100%)	0	100	100
All	All	1834/1906 (96%)	1719 (94%)	110 (6%)	5 (0%)	37	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	3	TRP
1	C	50	LYS
1	E	50	LYS
1	B	309	ILE
1	C	309	ILE

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	307/320 (96%)	278 (91%)	29 (9%)	8	32
1	B	312/320 (98%)	281 (90%)	31 (10%)	7	31
1	C	309/320 (97%)	278 (90%)	31 (10%)	7	30
1	D	312/320 (98%)	269 (86%)	43 (14%)	3	20
1	E	309/320 (97%)	273 (88%)	36 (12%)	5	25
2	X	2/2 (100%)	2 (100%)	0	100	100
2	Y	2/2 (100%)	2 (100%)	0	100	100
2	Z	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1555/1606 (97%)	1385 (89%)	170 (11%)	8 27

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	16	LEU
1	A	30	VAL
1	A	43	VAL
1	A	44	MET
1	A	54	VAL
1	A	57	GLU
1	A	66	THR
1	A	113	LYS
1	A	134	VAL
1	A	136	ILE
1	A	151	ILE
1	A	153	LEU
1	A	159	VAL
1	A	175	ILE
1	A	193	LEU
1	A	194	THR
1	A	250	ILE
1	A	253	GLU
1	A	260	THR
1	A	261	LEU
1	A	291	LYS
1	A	303	THR
1	A	311	ASP
1	A	312	ARG
1	A	320	LEU
1	A	326	LYS
1	A	346	LEU
1	A	369	ILE
1	B	14	SER
1	B	16	LEU
1	B	30	VAL
1	B	43	VAL
1	B	47	MET
1	B	49	GLN
1	B	50	LYS
1	B	54	VAL

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Mol	Chain	Res	Type
1	B	59	GLN
1	B	62	ARG
1	B	65	LEU
1	B	96	VAL
1	B	103	THR
1	B	134	VAL
1	B	136	ILE
1	B	180	LEU
1	B	193	LEU
1	B	194	THR
1	B	224	GLU
1	B	249	THR
1	B	250	ILE
1	B	253	GLU
1	B	260	THR
1	B	261	LEU
1	B	291	LYS
1	B	303	THR
1	B	320	LEU
1	B	328	LYS
1	B	335	ARG
1	B	346	LEU
1	B	373	LYS
1	C	14	SER
1	C	30	VAL
1	C	33	SER
1	C	34	ILE
1	C	43	VAL
1	C	45	VAL
1	C	51	ASP
1	C	54	VAL
1	C	59	GLN
1	C	75	ILE
1	C	96	VAL
1	C	111	ASN
1	C	126	THR
1	C	134	VAL
1	C	136	ILE
1	C	142	LEU
1	C	184	ASP
1	C	193	LEU
1	C	195	GLU

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Mol	Chain	Res	Type
1	C	246	GLN
1	C	250	ILE
1	C	253	GLU
1	C	267	ILE
1	C	318	THR
1	C	320	LEU
1	C	339	VAL
1	C	346	LEU
1	C	351	THR
1	C	353	GLN
1	C	358	THR
1	C	370	VAL
1	D	16	LEU
1	D	25	ASP
1	D	30	VAL
1	D	34	ILE
1	D	43	VAL
1	D	44	MET
1	D	50	LYS
1	D	54	VAL
1	D	56	ASP
1	D	59	GLN
1	D	64	ILE
1	D	65	LEU
1	D	75	ILE
1	D	111	ASN
1	D	134	VAL
1	D	140	LEU
1	D	141	SER
1	D	151	ILE
1	D	162	ASN
1	D	184	ASP
1	D	193	LEU
1	D	194	THR
1	D	236	LEU
1	D	246	GLN
1	D	250	ILE
1	D	253	GLU
1	D	260	THR
1	D	261	LEU
1	D	267	ILE
1	D	276	GLU

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Mol	Chain	Res	Type
1	D	286	ASP
1	D	292	ASP
1	D	303	THR
1	D	311	ASP
1	D	312	ARG
1	D	328	LYS
1	D	330	ILE
1	D	335	ARG
1	D	346	LEU
1	D	353	GLN
1	D	354	GLN
1	D	369	ILE
1	D	373	LYS
1	E	16	LEU
1	E	25	ASP
1	E	30	VAL
1	E	44	MET
1	E	45	VAL
1	E	54	VAL
1	E	59	GLN
1	E	64	ILE
1	E	89	THR
1	E	96	VAL
1	E	103	THR
1	E	111	ASN
1	E	134	VAL
1	E	136	ILE
1	E	152	VAL
1	E	165	ILE
1	E	184	ASP
1	E	193	LEU
1	E	194	THR
1	E	202	THR
1	E	253	GLU
1	E	260	THR
1	E	261	LEU
1	E	267	ILE
1	E	269	MET
1	E	286	ASP
1	E	298	VAL
1	E	303	THR
1	E	346	LEU

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Mol	Chain	Res	Type
1	E	351	THR
1	E	353	GLN
1	E	354	GLN
1	E	358	THR
1	E	364	GLU
1	E	369	ILE
1	E	374	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	41	GLN
1	A	92	ASN
1	A	115	ASN
1	A	252	ASN
1	B	40	HIS
1	B	49	GLN
1	B	111	ASN
1	B	115	ASN
1	B	246	GLN
1	C	88	HIS
1	C	92	ASN
1	C	111	ASN
1	C	115	ASN
1	C	246	GLN
1	C	252	ASN
1	C	314	GLN
1	D	41	GLN
1	D	88	HIS
1	D	92	ASN
1	D	115	ASN
1	D	161	HIS
1	D	246	GLN
1	D	314	GLN
1	D	354	GLN
1	D	371	HIS
1	E	59	GLN
1	E	128	ASN
1	E	137	GLN
1	E	161	HIS
1	E	162	ASN

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Mol	Chain	Res	Type
1	E	314	GLN
1	E	354	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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
2	HYP	Z	1	2	7,8,9	0.90	0	5,10,12	1.83	2 (40%)
2	HYP	Y	1	2	7,8,9	0.84	0	5,10,12	1.67	1 (20%)
2	ALO	X	6	2	5,6,7	0.72	0	5,7,9	1.03	0
2	HYP	X	1	2	7,8,9	0.85	0	5,10,12	1.87	3 (60%)
2	G5G	Y	4	2	7,9,10	3.19	2 (28%)	3,12,14	0.69	0
2	G5G	Z	4	2	7,9,10	3.17	2 (28%)	3,12,14	0.48	0
2	ALO	Y	6	2	5,6,7	0.79	0	5,7,9	0.75	0
2	G5G	X	4	2	7,9,10	3.20	2 (28%)	3,12,14	0.49	0
2	ALO	Z	6	2	5,6,7	0.76	0	5,7,9	0.79	0

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
2	HYP	Z	1	2	-	0/0/11/13	0/1/1/1
2	HYP	Y	1	2	-	0/0/11/13	0/1/1/1
2	ALO	X	6	2	-	3/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	X	1	2	-	0/0/11/13	0/1/1/1
2	G5G	Y	4	2	-	8/9/10/12	-
2	G5G	Z	4	2	-	7/9/10/12	-
2	ALO	Y	6	2	-	1/5/6/8	-
2	G5G	X	4	2	-	8/9/10/12	-
2	ALO	Z	6	2	-	1/5/6/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	4	G5G	CA-N	-7.23	1.27	1.48
2	X	4	G5G	CA-N	-7.16	1.28	1.48
2	Z	4	G5G	CA-N	-7.05	1.28	1.48
2	Z	4	G5G	CD2-CG	-3.73	1.48	1.52
2	X	4	G5G	CD2-CG	-3.68	1.48	1.52
2	Y	4	G5G	CD2-CG	-3.60	1.48	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	1	HYP	OD1-CG-CB	2.31	115.70	110.10
2	X	1	HYP	OD1-CG-CB	2.26	115.58	110.10
2	Y	1	HYP	OD1-CG-CB	2.26	115.58	110.10
2	Z	1	HYP	O-C-CA	-2.23	119.02	124.77
2	X	1	HYP	CB-CG-CD	-2.20	100.71	103.16
2	X	1	HYP	O-C-CA	-2.06	119.48	124.77

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	4	G5G	CA-CB-CG-CD1
2	X	4	G5G	O2-CD1-CG-CB
2	X	4	G5G	O2-CD1-CG-O1
2	X	4	G5G	O2-CD1-CG-CD2
2	X	4	G5G	N-CA-CB-CG
2	Y	4	G5G	CA-CB-CG-CD1
2	Y	4	G5G	O2-CD1-CG-CB
2	Y	4	G5G	O2-CD1-CG-O1
2	Y	4	G5G	O2-CD1-CG-CD2

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Mol	Chain	Res	Type	Atoms
2	Y	4	G5G	N-CA-CB-CG
2	Y	4	G5G	C-CA-CB-CG
2	Z	4	G5G	O2-CD1-CG-CB
2	Z	4	G5G	N-CA-CB-CG
2	X	4	G5G	CA-CB-CG-CD2
2	Y	4	G5G	CA-CB-CG-CD2
2	Z	4	G5G	CA-CB-CG-CD2
2	X	6	ALO	N-CA-CB-CG2
2	X	4	G5G	CA-CB-CG-O1
2	Z	4	G5G	CA-CB-CG-O1
2	X	6	ALO	C-CA-CB-CG2
2	Z	4	G5G	CA-CB-CG-CD1
2	Z	4	G5G	O2-CD1-CG-O1
2	X	4	G5G	C-CA-CB-CG
2	Y	4	G5G	CA-CB-CG-O1
2	X	6	ALO	O-C-CA-CB
2	Y	6	ALO	O-C-CA-CB
2	Z	6	ALO	O-C-CA-CB
2	Z	4	G5G	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z > 2$
4	ADP	A	402	3	28,29,29	3.33	12 (42%)	43,45,45	1.87	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	B	402	3	28,29,29	3.32	11 (39%)	43,45,45	1.82	10 (23%)
4	ADP	C	402	3	28,29,29	3.32	12 (42%)	43,45,45	1.81	10 (23%)
4	ADP	D	402	3	28,29,29	3.33	11 (39%)	43,45,45	1.82	11 (25%)
4	ADP	E	402	3	28,29,29	3.30	11 (39%)	43,45,45	1.83	10 (23%)

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
4	ADP	A	402	3	-	5/16/32/32	0/3/3/3
4	ADP	B	402	3	-	5/16/32/32	0/3/3/3
4	ADP	C	402	3	-	5/16/32/32	0/3/3/3
4	ADP	D	402	3	-	3/16/32/32	0/3/3/3
4	ADP	E	402	3	-	3/16/32/32	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	ADP	O4'-C1'	8.52	1.61	1.42
4	E	402	ADP	O4'-C1'	8.48	1.61	1.42
4	A	402	ADP	O4'-C1'	8.47	1.61	1.42
4	C	402	ADP	O4'-C1'	8.46	1.61	1.42
4	B	402	ADP	O4'-C1'	8.39	1.61	1.42
4	B	402	ADP	PA-O3A	8.08	1.68	1.59
4	A	402	ADP	PA-O3A	8.08	1.68	1.59
4	D	402	ADP	PA-O3A	8.06	1.68	1.59
4	C	402	ADP	PA-O3A	7.98	1.68	1.59
4	E	402	ADP	PA-O3A	7.72	1.67	1.59
4	D	402	ADP	C2'-C1'	-7.50	1.29	1.53
4	E	402	ADP	C2'-C1'	-7.50	1.29	1.53
4	C	402	ADP	C2'-C1'	-7.45	1.30	1.53
4	A	402	ADP	C2'-C1'	-7.40	1.30	1.53
4	B	402	ADP	C2'-C1'	-7.38	1.30	1.53
4	B	402	ADP	O4'-C4'	-5.82	1.32	1.45
4	D	402	ADP	O4'-C4'	-5.76	1.32	1.45
4	E	402	ADP	O4'-C4'	-5.75	1.32	1.45
4	C	402	ADP	O4'-C4'	-5.72	1.32	1.45
4	A	402	ADP	O4'-C4'	-5.68	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	ADP	C6-N6	4.67	1.46	1.34
4	B	402	ADP	C6-N6	4.64	1.46	1.34
4	C	402	ADP	C6-N6	4.64	1.46	1.34
4	A	402	ADP	C6-N6	4.61	1.46	1.34
4	E	402	ADP	C6-N6	4.59	1.45	1.34
4	A	402	ADP	O2'-C2'	3.37	1.51	1.43
4	C	402	ADP	O2'-C2'	3.28	1.51	1.43
4	B	402	ADP	O2'-C2'	3.26	1.51	1.43
4	E	402	ADP	O2'-C2'	3.20	1.50	1.43
4	D	402	ADP	O2'-C2'	3.20	1.50	1.43
4	E	402	ADP	C5-C4	-3.14	1.33	1.39
4	D	402	ADP	C5-C4	-3.09	1.33	1.39
4	B	402	ADP	C5-C4	-3.08	1.33	1.39
4	A	402	ADP	C5-C4	-3.05	1.33	1.39
4	C	402	ADP	C5-C4	-3.01	1.33	1.39
4	C	402	ADP	PB-O2B	-2.67	1.44	1.54
4	C	402	ADP	C5-N7	-2.66	1.34	1.39
4	B	402	ADP	C5-N7	-2.63	1.34	1.39
4	E	402	ADP	C5-N7	-2.62	1.34	1.39
4	A	402	ADP	C5-N7	-2.61	1.34	1.39
4	A	402	ADP	PB-O2B	-2.61	1.45	1.54
4	D	402	ADP	C5-N7	-2.59	1.34	1.39
4	A	402	ADP	PA-O5'	2.41	1.68	1.59
4	E	402	ADP	O3'-C3'	-2.37	1.37	1.43
4	D	402	ADP	PA-O5'	2.35	1.68	1.59
4	C	402	ADP	O3'-C3'	-2.34	1.37	1.43
4	B	402	ADP	PA-O5'	2.31	1.68	1.59
4	D	402	ADP	O3'-C3'	-2.28	1.37	1.43
4	B	402	ADP	O3'-C3'	-2.28	1.37	1.43
4	C	402	ADP	PA-O5'	2.28	1.68	1.59
4	A	402	ADP	O3'-C3'	-2.28	1.37	1.43
4	E	402	ADP	PA-O5'	2.26	1.68	1.59
4	B	402	ADP	C8-N9	-2.24	1.33	1.37
4	C	402	ADP	C8-N9	-2.22	1.33	1.37
4	E	402	ADP	C8-N9	-2.20	1.33	1.37
4	D	402	ADP	C8-N9	-2.18	1.33	1.37
4	A	402	ADP	C8-N9	-2.16	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	402	ADP	N3-C2-N1	-5.71	119.94	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	ADP	N3-C2-N1	-5.66	120.01	128.58
4	B	402	ADP	N3-C2-N1	-5.62	120.08	128.58
4	D	402	ADP	N3-C2-N1	-5.59	120.12	128.58
4	C	402	ADP	N3-C2-N1	-5.54	120.20	128.58
4	A	402	ADP	C5-C4-N3	-4.79	120.13	126.72
4	D	402	ADP	C5-C4-N3	-4.73	120.21	126.72
4	C	402	ADP	C5-C4-N3	-4.59	120.39	126.72
4	E	402	ADP	C5-C4-N3	-4.58	120.41	126.72
4	B	402	ADP	C5-C4-N3	-4.55	120.44	126.72
4	B	402	ADP	N9-C8-N7	-4.06	108.17	113.94
4	E	402	ADP	N9-C8-N7	-4.05	108.19	113.94
4	C	402	ADP	N9-C8-N7	-4.02	108.24	113.94
4	A	402	ADP	N9-C8-N7	-4.01	108.25	113.94
4	D	402	ADP	N9-C8-N7	-3.97	108.30	113.94
4	A	402	ADP	C2-N3-C4	3.35	120.00	111.83
4	E	402	ADP	C2-N3-C4	3.33	119.97	111.83
4	D	402	ADP	C2-N3-C4	3.31	119.91	111.83
4	B	402	ADP	C2-N3-C4	3.23	119.73	111.83
4	C	402	ADP	C2-N3-C4	3.23	119.73	111.83
4	A	402	ADP	C3'-C2'-C1'	3.15	107.41	101.46
4	B	402	ADP	C3'-C2'-C1'	2.89	106.93	101.46
4	C	402	ADP	C3'-C2'-C1'	2.88	106.91	101.46
4	A	402	ADP	N3-C4-N9	2.86	132.03	127.17
4	C	402	ADP	C5-N7-C8	2.83	107.90	103.45
4	E	402	ADP	C5-N7-C8	2.80	107.85	103.45
4	A	402	ADP	C5-N7-C8	2.80	107.84	103.45
4	B	402	ADP	C5-N7-C8	2.79	107.83	103.45
4	D	402	ADP	C5-N7-C8	2.78	107.81	103.45
4	D	402	ADP	N3-C4-N9	2.72	131.80	127.17
4	D	402	ADP	C3'-C2'-C1'	2.71	106.59	101.46
4	C	402	ADP	N3-C4-N9	2.62	131.63	127.17
4	B	402	ADP	N3-C4-N9	2.61	131.61	127.17
4	E	402	ADP	C3'-C2'-C1'	2.53	106.25	101.46
4	E	402	ADP	N3-C4-N9	2.47	131.37	127.17
4	E	402	ADP	N6-C6-N1	-2.33	113.19	118.38
4	D	402	ADP	N6-C6-N1	-2.22	113.42	118.38
4	C	402	ADP	N6-C6-N1	-2.22	113.43	118.38
4	A	402	ADP	N6-C6-N1	-2.20	113.47	118.38
4	E	402	ADP	C5-C4-N9	2.20	108.21	105.81
4	E	402	ADP	C4-C5-N7	-2.17	108.10	110.58
4	B	402	ADP	N6-C6-N1	-2.12	113.66	118.38
4	A	402	ADP	C6-C5-C4	2.11	120.06	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	ADP	C4-C5-N7	-2.09	108.19	110.58
4	B	402	ADP	C6-C5-C4	2.05	119.98	117.18
4	B	402	ADP	C4-C5-N7	-2.04	108.25	110.58
4	D	402	ADP	C6-C5-C4	2.04	119.96	117.18
4	D	402	ADP	C4-C5-N7	-2.04	108.25	110.58
4	C	402	ADP	C6-C5-C4	2.02	119.93	117.18
4	D	402	ADP	C5-C4-N9	2.00	108.00	105.81

There are no chirality outliers.

All (21) torsion outliers are listed below:

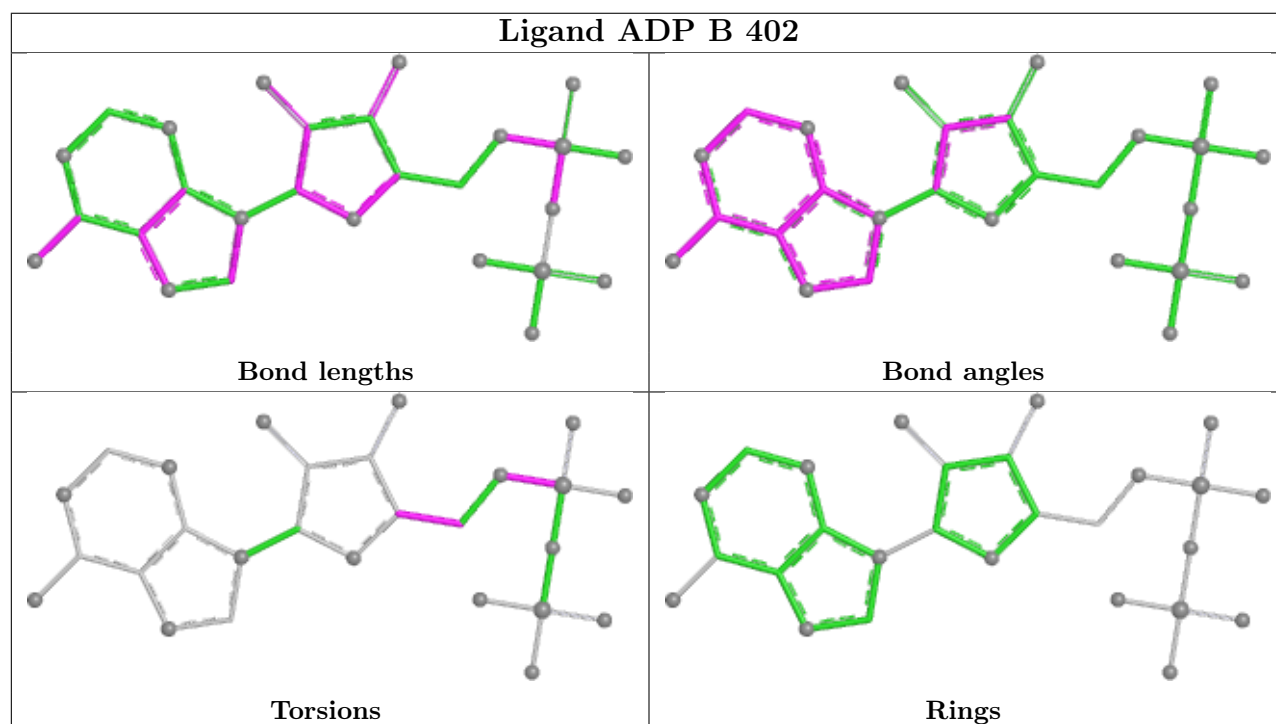
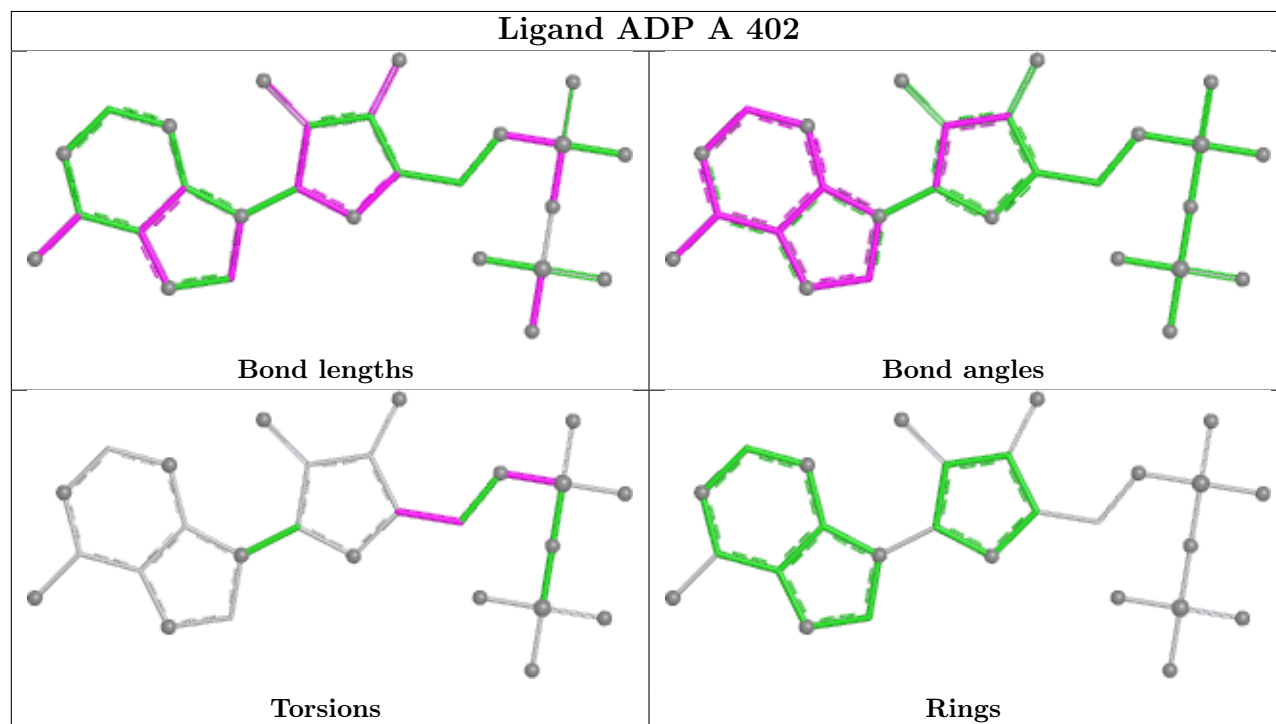
Mol	Chain	Res	Type	Atoms
4	D	402	ADP	C5'-O5'-PA-O1A
4	E	402	ADP	C5'-O5'-PA-O1A
4	A	402	ADP	O4'-C4'-C5'-O5'
4	A	402	ADP	C3'-C4'-C5'-O5'
4	B	402	ADP	O4'-C4'-C5'-O5'
4	B	402	ADP	C3'-C4'-C5'-O5'
4	C	402	ADP	O4'-C4'-C5'-O5'
4	C	402	ADP	C3'-C4'-C5'-O5'
4	D	402	ADP	O4'-C4'-C5'-O5'
4	D	402	ADP	C3'-C4'-C5'-O5'
4	E	402	ADP	O4'-C4'-C5'-O5'
4	E	402	ADP	C3'-C4'-C5'-O5'
4	A	402	ADP	C5'-O5'-PA-O1A
4	A	402	ADP	C5'-O5'-PA-O2A
4	A	402	ADP	C5'-O5'-PA-O3A
4	B	402	ADP	C5'-O5'-PA-O1A
4	B	402	ADP	C5'-O5'-PA-O2A
4	B	402	ADP	C5'-O5'-PA-O3A
4	C	402	ADP	C5'-O5'-PA-O1A
4	C	402	ADP	C5'-O5'-PA-O2A
4	C	402	ADP	C5'-O5'-PA-O3A

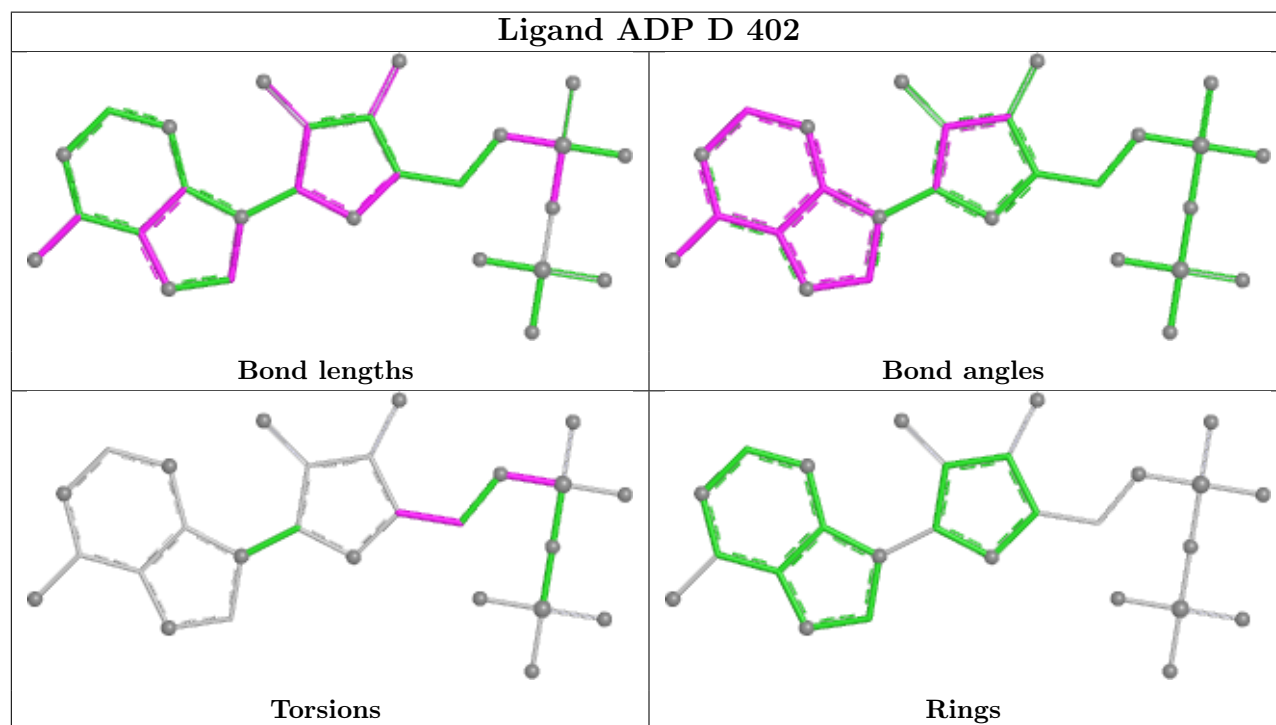
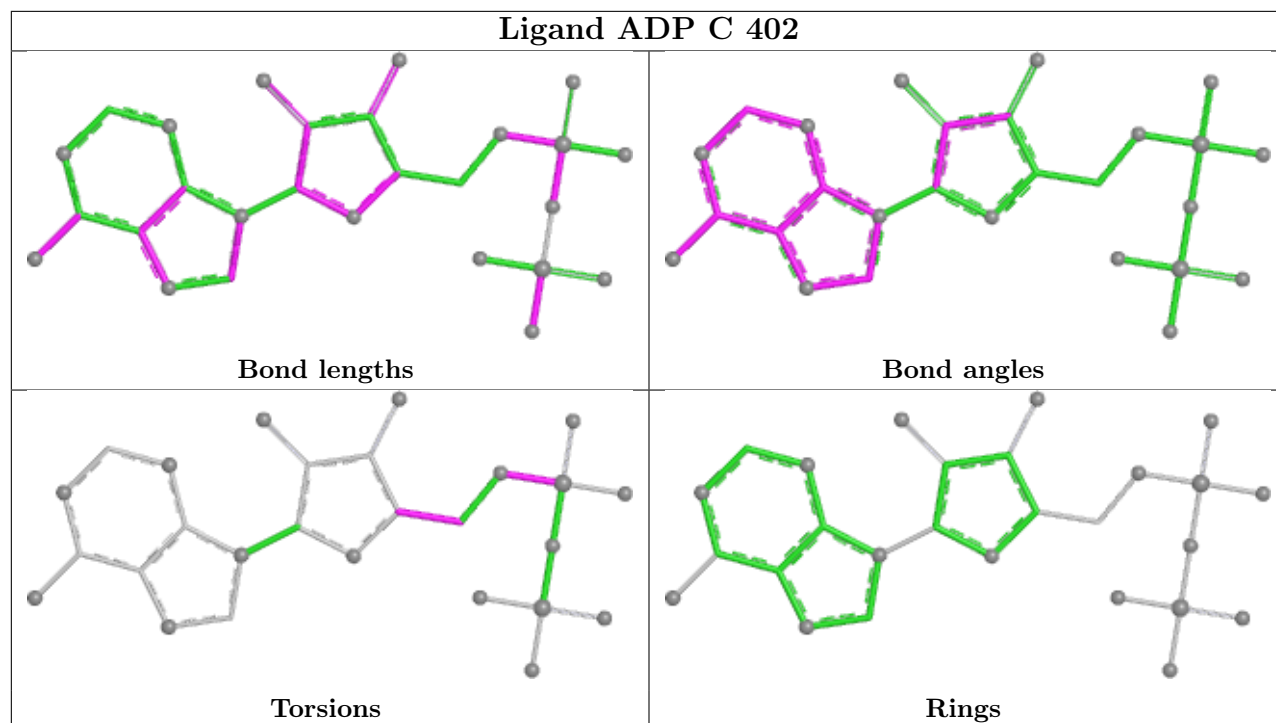
There are no ring outliers.

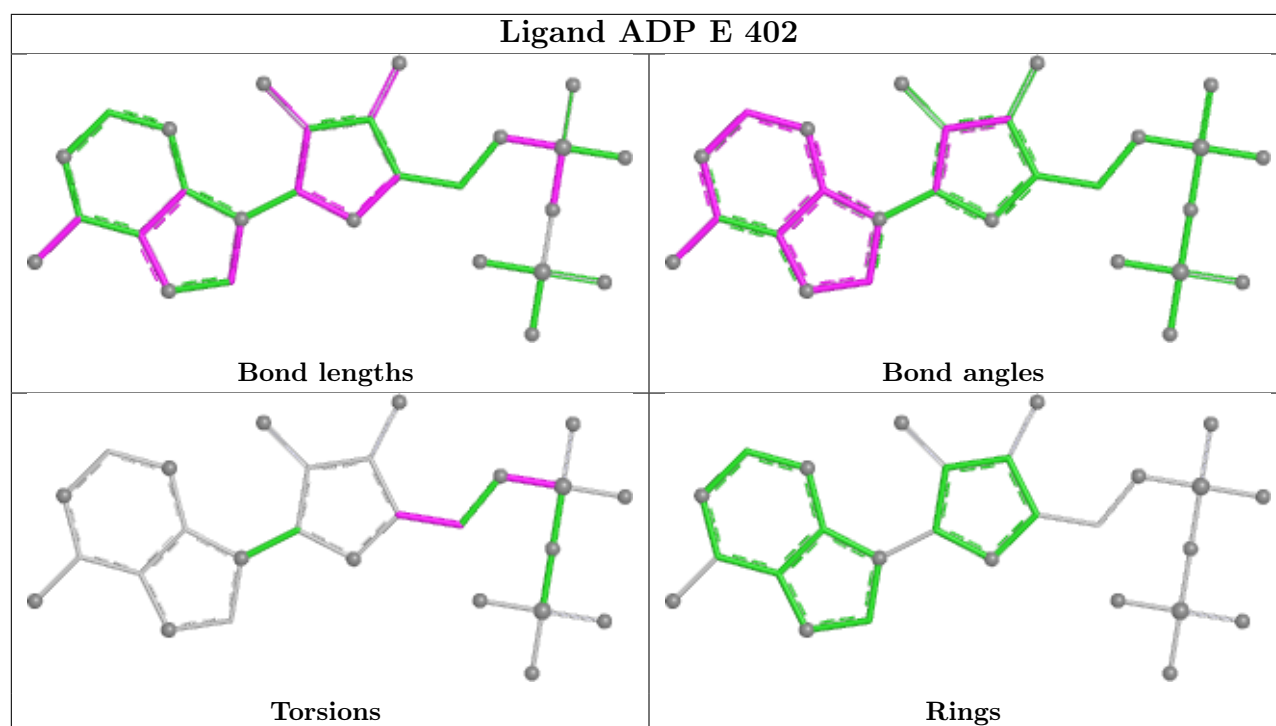
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

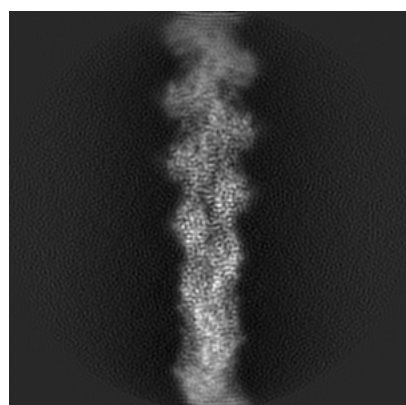
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30179. These allow visual inspection of the internal detail of the map and identification of artifacts.

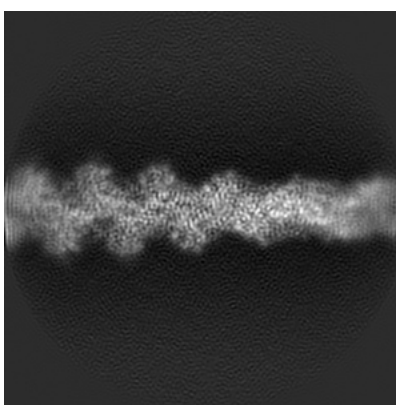
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

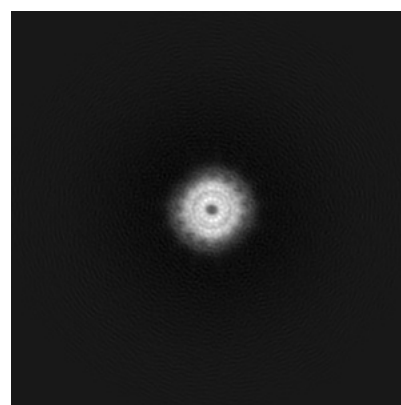
6.1.1 Primary map



X



Y

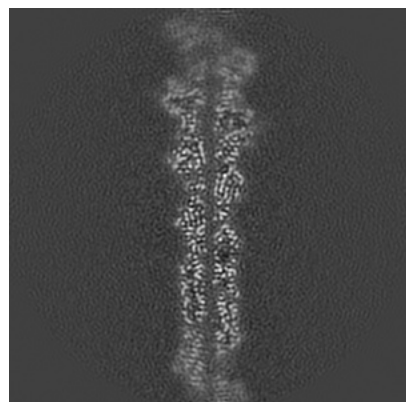


Z

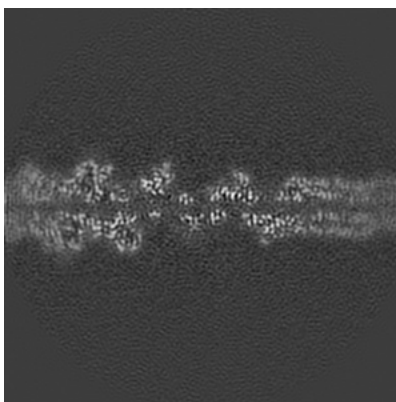
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

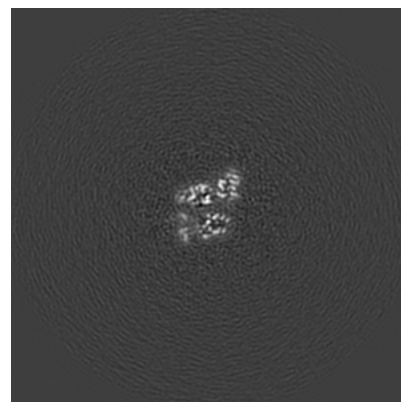
6.2.1 Primary map



X Index: 128



Y Index: 128

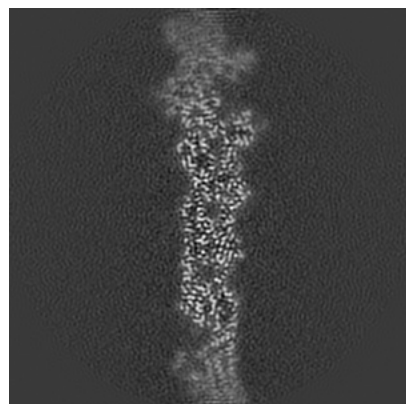


Z Index: 128

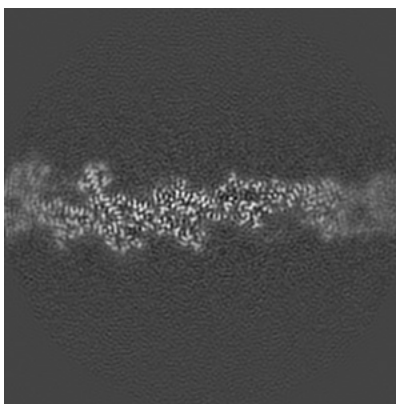
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

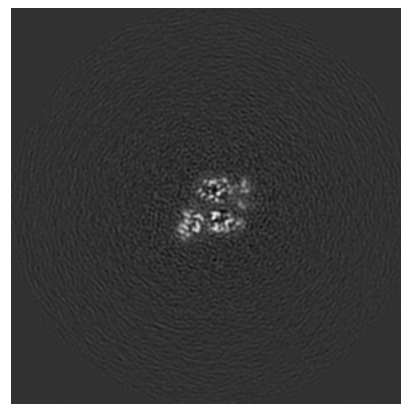
6.3.1 Primary map



X Index: 133



Y Index: 121

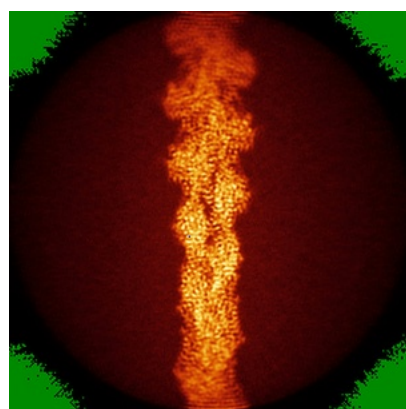


Z Index: 108

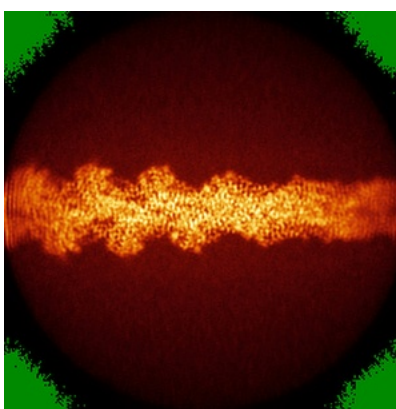
The images above show the largest variance slices of the map in three orthogonal directions.

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

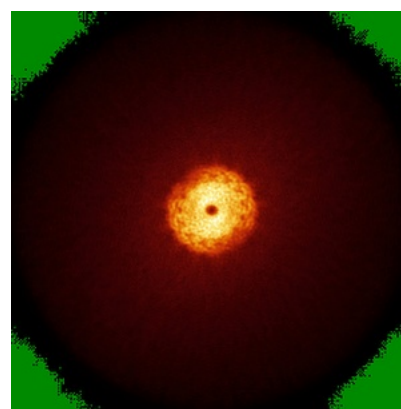
6.4.1 Primary map



X



Y

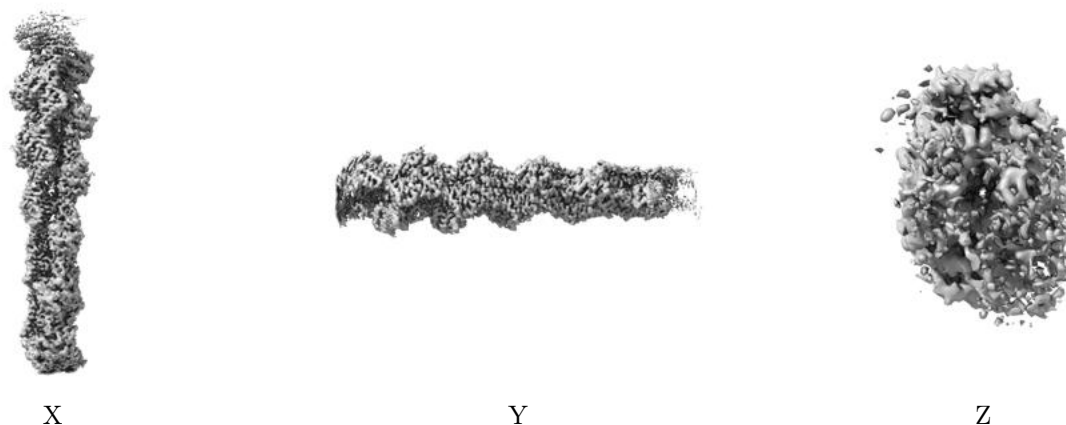


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

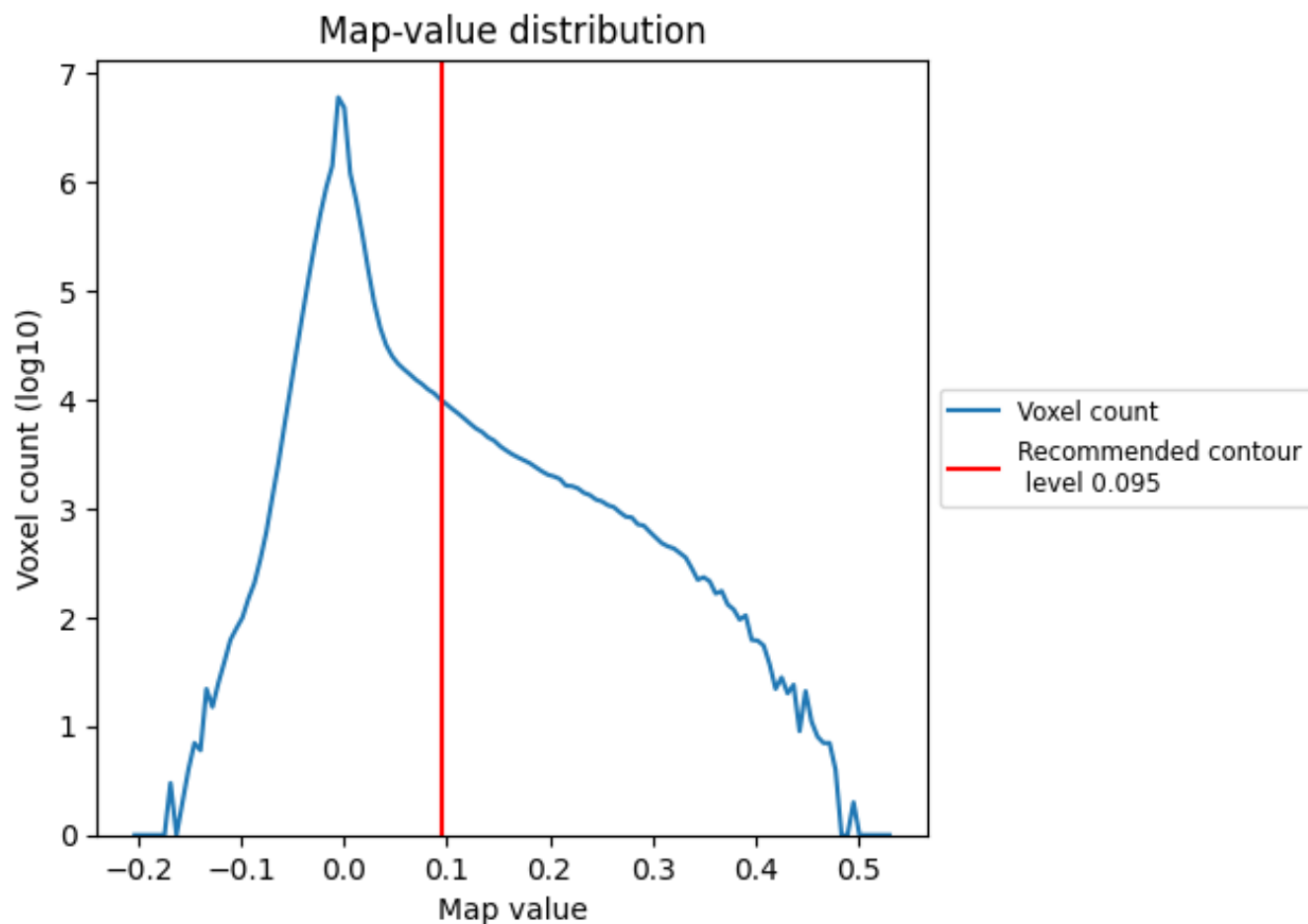
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

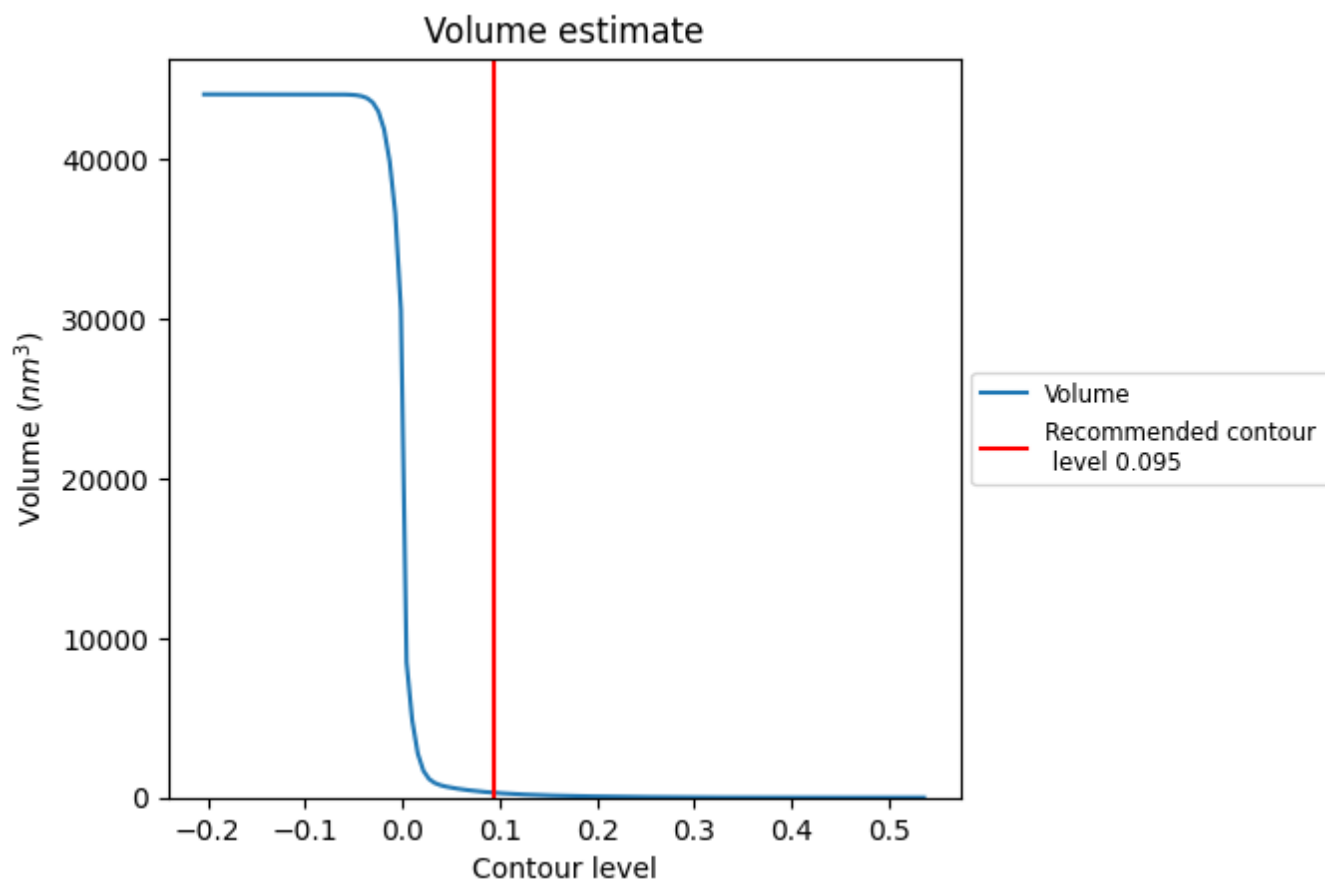
This section contains the results of statistical analysis of the map.

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.

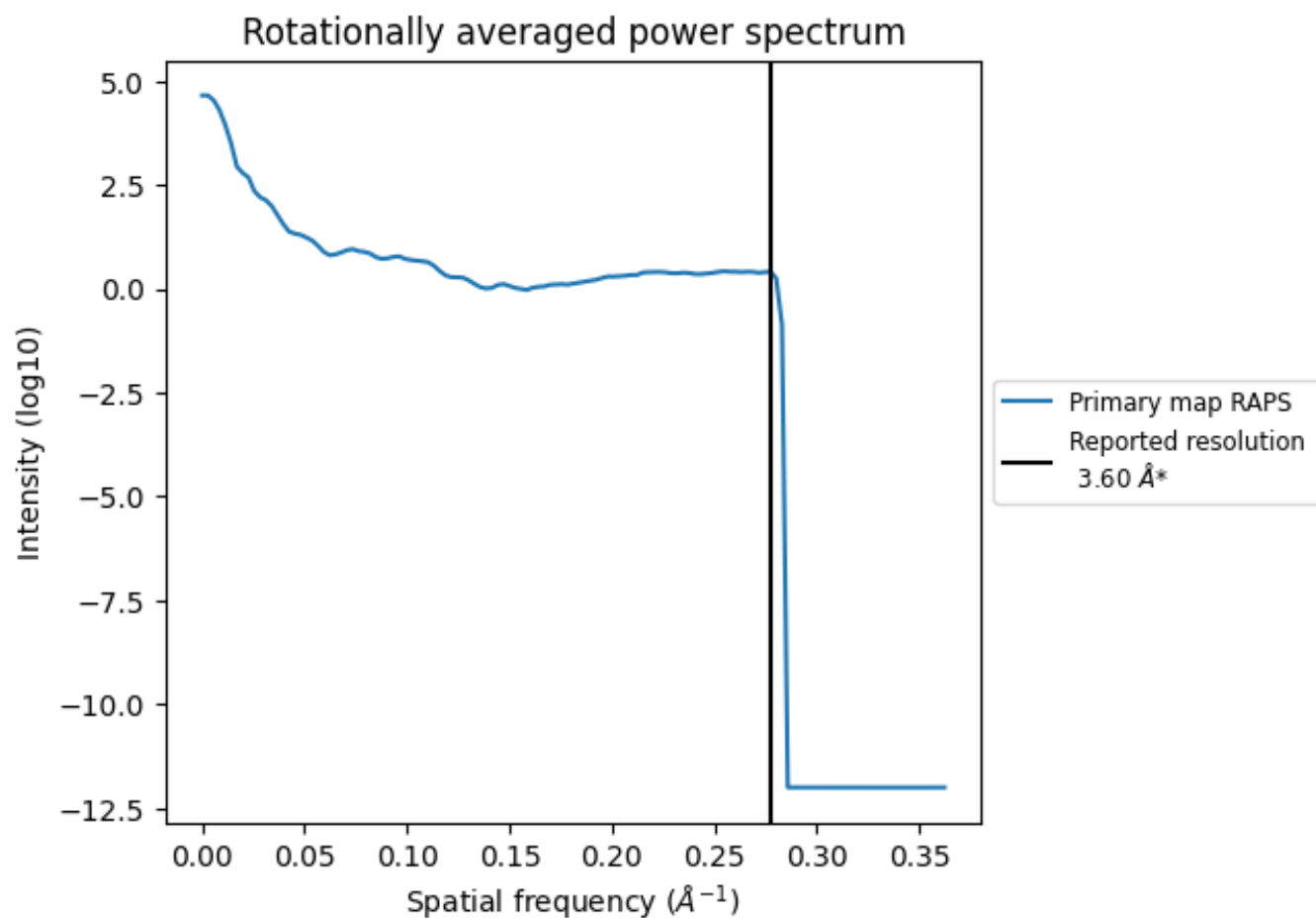
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm³; this corresponds to an approximate mass of 271 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 ⓘ

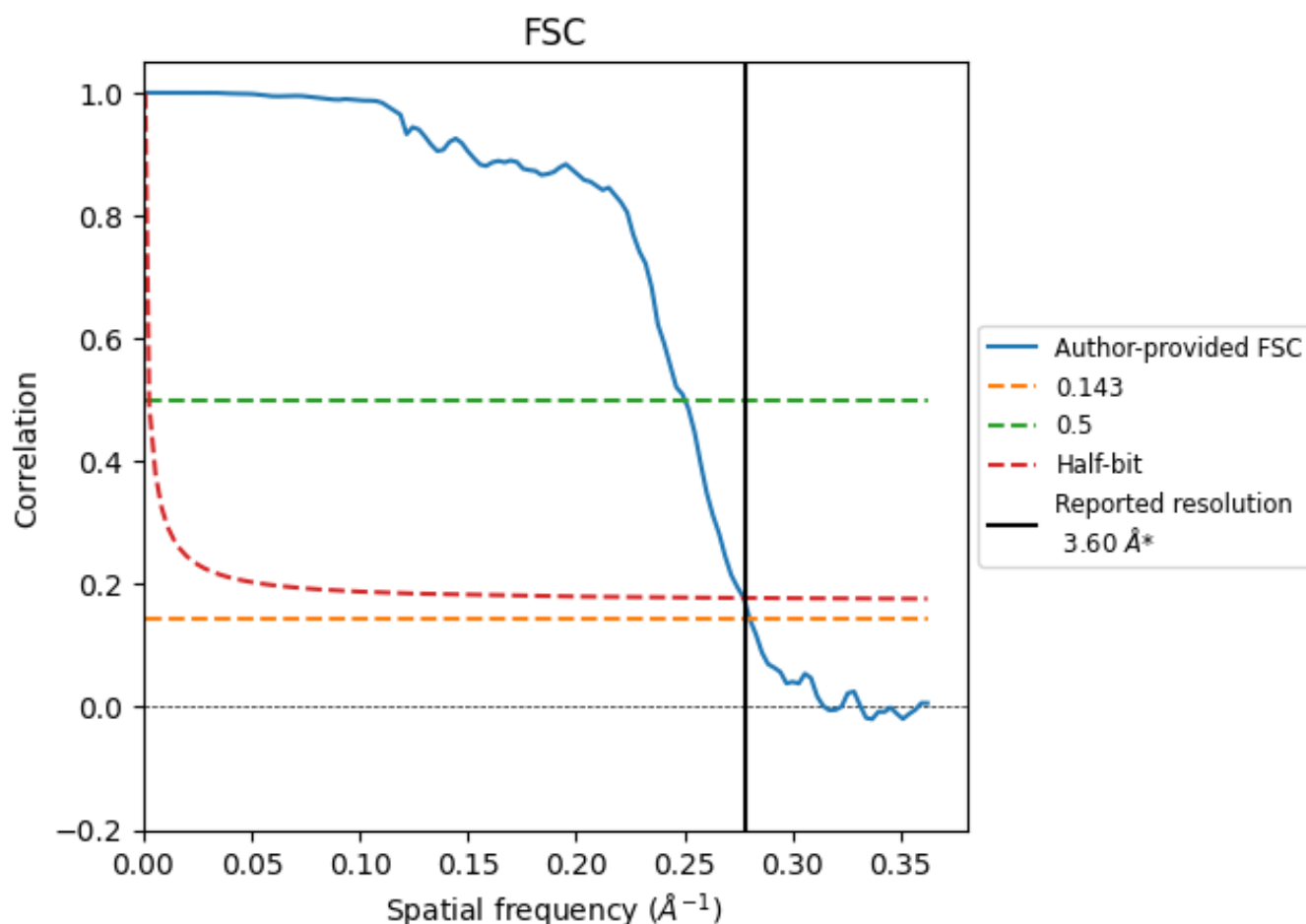


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

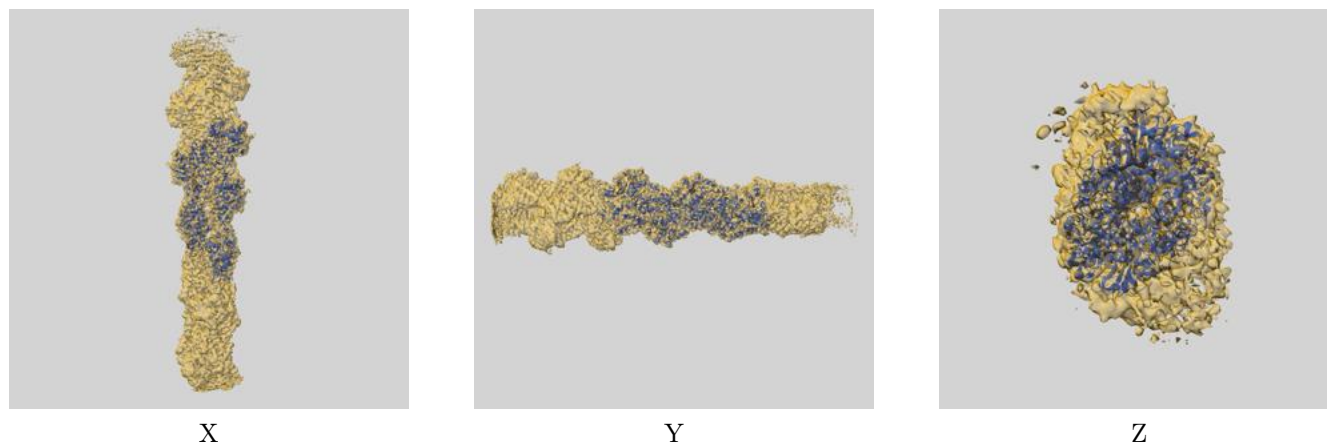
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.00	3.60
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

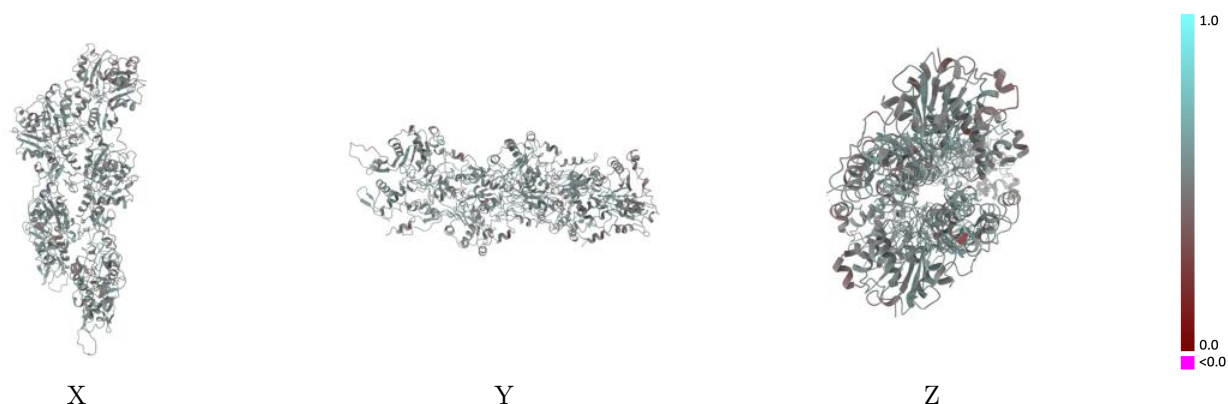
This section contains information regarding the fit between EMDB map EMD-30179 and PDB model 7BTI. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



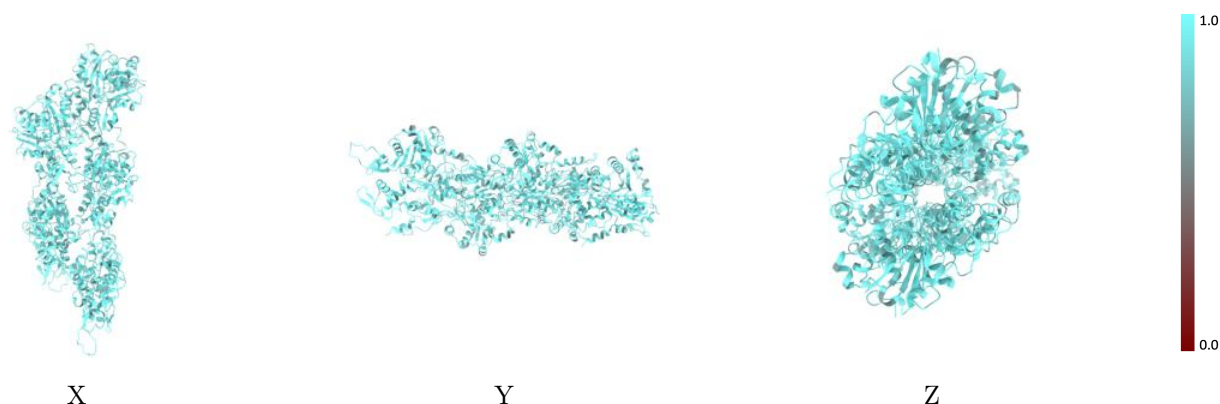
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



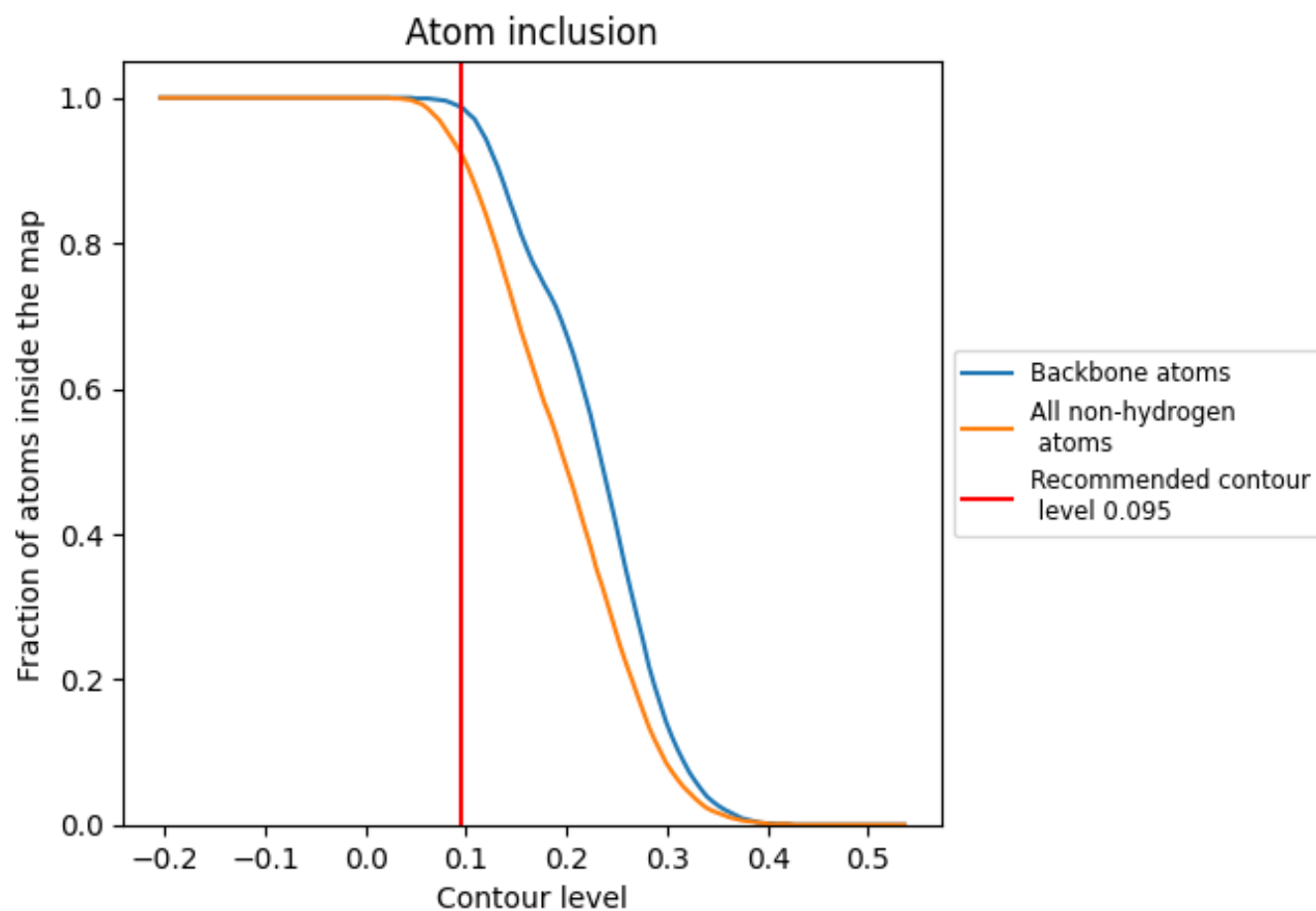
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.5190
A	0.9070	0.5050
B	0.9240	0.5220
C	0.9350	0.5260
D	0.9290	0.5250
E	0.9250	0.5200
X	0.9070	0.5120
Y	0.9440	0.5180
Z	0.9440	0.5150

1.0

0.0

<0.0