WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Mar 18, 2024 – 03:32 PM EDT

PDB ID	:	8GJ0
EMDB ID	:	EMD-40081
Title	:	E. coli clamp loader with open clamp on primed template DNA (form 1)
Authors	:	Oakley, A.J.; Xu, Z.-Q.; Dixon, N.E.
Deposited on	:	2023-03-14
Resolution	:	2.90 Å(reported)
Based on initial models	:	3GLH, 1MMI

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 (i) 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 (i)) were used in the production of this report:

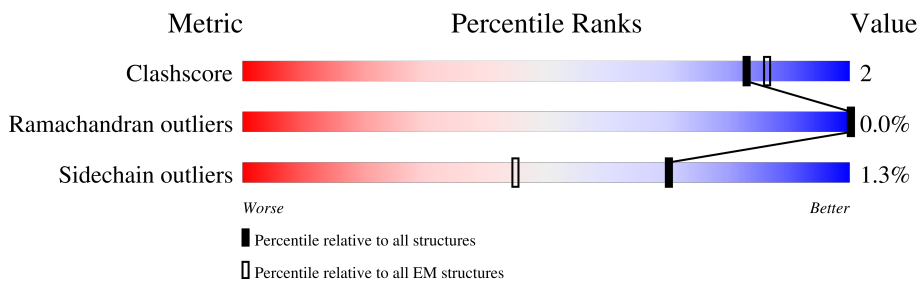|		
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.90 Å.

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

Metric	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		0.0%
Sidechain outliers		1.3%

Worse · *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	343	93% 6% ·
2	B	643	52% 5% 43%
2	C	643	53% · 43%
2	D	643	51% 5% 44%
3	E	334	95% 5%
4	F	137	18% 82%
5	H	366	92% 8%
5	I	366	93% 7%

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Mol	Chain	Length	Quality of chain
6	X	23	22% ▬▬▬ 100%
7	Y	68	6% ▬ 40% · 57%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ALF	D	701	-	-	X	-

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 41411 atoms, of which 20512 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 DNA polymerase III subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	0
			5496	1728	2770	493	495	10		

- Molecule 2 is a protein called DNA polymerase III subunit tau.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	365	Total	C	H	N	O	S	0	0
			5714	1786	2874	513	525	16		
2	C	368	Total	C	H	N	O	S	0	0
			5758	1801	2893	516	532	16		
2	D	360	Total	C	H	N	O	S	0	0
			5640	1762	2836	508	519	15		

- Molecule 3 is a protein called DNA polymerase III subunit delta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	334	Total	C	H	N	O	S	0	0
			5190	1655	2588	468	466	13		

- Molecule 4 is a protein called DNA polymerase III subunit psi.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	25	Total	C	H	N	O	0	0
			423	131	212	44	36		

- Molecule 5 is a protein called Beta sliding clamp.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	366	Total	C	H	N	O	S	0	0
			5698	1786	2854	498	541	19		
5	I	366	Total	C	H	N	O	S	0	0
			5698	1786	2854	498	541	19		

- Molecule 6 is a DNA chain called Primer.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	X	23	Total 732	C 226	H 260	N 92	O 132	P 22	0	0

- Molecule 7 is a DNA chain called Template.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Y	29	Total 923	C 285	H 335	N 90	O 184	P 29	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
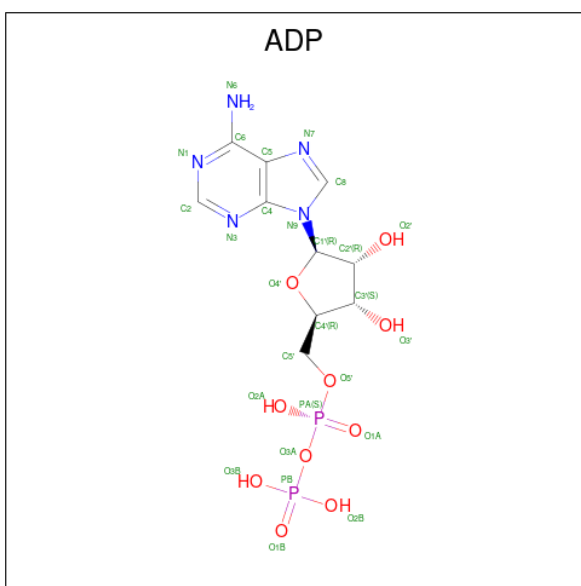
Mol	Chain	Residues	Atoms						AltConf
8	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
8	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
8	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	B	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
9	C	1	Total 1	Mg 1	0
9	D	1	Total 1	Mg 1	0

- Molecule 10 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).
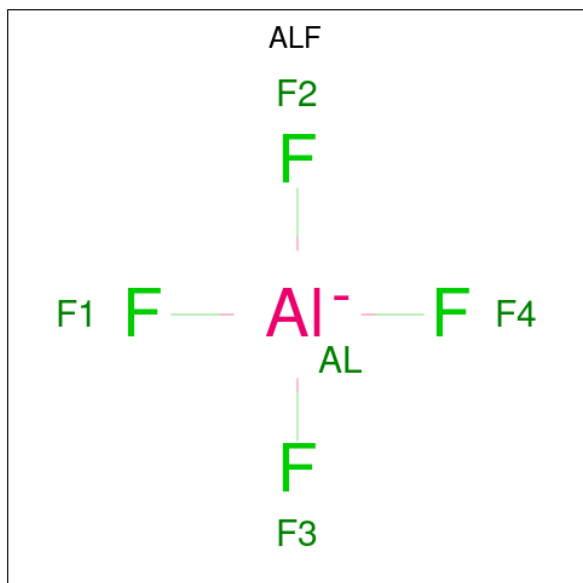
Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total 5	Al 1	F 4	0
10	D	1	Total 5	Al 1	F 4	0
10	D	1	Total 5	Al 1	F 4	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total 1	Zn 1	0
11	C	1	Total 1	Zn 1	0
11	D	1	Total 1	Zn 1	0
11	E	1	Total 1	Zn 1	0

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: DNA polymerase III subunit delta

Chain A:

93%   6% ·

M1 R18 N26 D27 E33 L81 L82 N90 A91 L97 L100 T101 V135 R154 K196 R201 L293 Q300 R307 K313 Q318 L336 A337 D338 I341 D342 G343

- Molecule 2: DNA polymerase III subunit tau

Chain B:

52%   5%   43%

MET S2 A7 H23 V24 C64 C73 G74 I82 L90 V101 R119 D126 E127 H134 P163 I166 L175 D179 V180 Q186 L214 D245 I268 R274 Q296 D305 M306 I320 P343 L353 L354 M363 P366

GLU PRO GLU VAL PRO ARG GLN SER PHE ALA ALA PRO VAL ALA PRO THR ALA VAL MET THR PRO THR PRO THR GLN VAL PRO PRO GLN PRO GLN SER ALA PRO GLN GLN ALA PRO THR VAL PRO LEU PRO GLU THR THR SER GLN VAL LEU ALA ALA ARG GLN GLN LEU GLN ARG VAL GLN GLY ALA THR

LYS ALA LYS LYS SER GLU PRO ALA ALA ALA THR ARG ALA ARG PRO ALA ALA PRO VAL ALA ASN ALA ALA ALA LEU GLU ARG LEU ALA SER VAL THR ASP ARG VAL GLN ALA ALA ARG PRO VAL PRO SER ALA LEU GLU LYS ALA PRO ALA LYS LYS GLU ALA ALA TYR ARG TRP LYS ALA THR THR PRO VAL MET GLN

GLN LYS GLU VAL VAL ALA THR PRO LYS ALA LEU LYS LYS ALA LEU GLU GLU HIS GLU LYS THR PRO GLU LEU ALA ALA LYS LEU ALA ALA GLU ILE GLU ARG ASP PRO TRP ALA ALA ALA GLN VAL SER GLN LEU SER LEU PRO LYS LEU VAL GLU GLN VAL ALA LEU ASN ALA TRP LYS GLU

GLU SER ASP ASN ALA VAL CYS LEU HIS LEU ARG SER SER GLN ARG HIS LEU ASN ASN ARG GLY ALA GLN GLN LYS LEU LEU ALA ALA GLU LEU SER MET LEU LYS GLY SER THR VAL GLU LEU THR ILE VAL GLU ASP ASN PRO ALA VAL ARG THR PRO LEU GLU TRP ARG GLN ALA ILE

TYR GLU GLU LYS LEU ALA GLN ALA ALA ARG GLU GLU SER ILE ILE ALA ASP ASN ILE GLN THR LEU ARG ARG PHE PHE ASP ALA GLU LEU ASP GLU GLU SER ILE ARG PRO ILE

- Molecule 2: DNA polymerase III subunit tau

Chain C:

53%   ·   43%

MET S2 Q13 R47 K60 V75 R80 D89 K100 L108 V111 Q112 G118 K121 K176 R215 L244 D245 Q248 I268 N269 E270 R274 W278 V283 L297 V349 L353 L354 M363 E369 VAL PRO ARG GLN SER

PHE ALA PRO VAL ALA PRO THR ALA VAL MET THR PRO THR GLN VAL PRO PRO GLN PRO GLN SER ALA PRO GLN GLN ALA PRO THR VAL PRO LEU PRO GLU THR THR SER GLN VAL LEU ALA ALA ARG GLN GLN LEU GLN ARG VAL GLN GLY ALA THR LYS ALA LYS LYS SER GLU GLU PRO ALA

ALA ALA THR ARG ALA ARG PRO VAL ASN ASN ALA ALA LEU LEU GLU ARG LEU ALA SER VAL THR ASP ARG VAL GLN ALA ARG PRO VAL PRO SER ALA LEU GLU LYS GLN ALA PRO ALA LYS LYS GLU GLN ALA ARG TRP LYS ALA THR THR PRO VAL MET GLN GLN LYS GLU VAL VAL ALA THR PRO

LYS ALA LEU LYS LYS ALA LEU GLU HIS GLU LYS THR PRO GLU LEU ALA ALA LYS LEU ALA ALA GLU ALA ILE GLU ARG ASP PRO TRP ALA ALA GLN VAL SER GLU LEU SER LEU PRO LYS LEU VAL GLU GLN VAL ALA LEU ASN ALA TRP GLU GLU ASP ASN ALA VAL CYS LEU

HIS LEU ARG SER GLN HIS LEU ASN ARG GLY ALA GLN GLN LYS LEU ALA GLU ALA LEU SER MET LEU LYS GLY SER THR VAL GLU LEU THR ILE VAL GLU ASP ASN PRO ALA VAL ARG THR PRO LEU GLU TRP ARG GLN ILE TYR GLU LYS LEU ALA GLN ALA

ARG GLU SER ILE ILE ALA ASP ASN ILE GLN THR LEU ARG ARG PHE PHE ASP GLU ALA GLU LEU ASP GLU SER ILE ARG PRO ILE

• Molecule 2: DNA polymerase III subunit tau

Chain D: 51% 5% 44%

MET SER Y3 A7 E22 H23 V24 I37 I68 V75 R80 R86 V101 R133 N137 L171 L175 A224 G228 I268 N269 E270 R274 Q296 L297 D305 M306 I309 I320 L327 D344 R345 R346 L353 F359

R362 MET PRO LEU PRO GLU PRO GLU VAL PRO ARG GLN SER PHE ALA PRO VAL ALA PRO THR ALA VAL MET THR PRO THR GLN VAL PRO PRO GLN PRO GLN SER ALA PRO GLN GLN ALA PRO THR VAL PRO LEU PRO GLU THR THR SER GLN VAL LEU ALA ALA ARG GLN GLU LEU GLN ARG

VAL GLN GLY ALA THR LYS ALA LYS LYS SER GLU PRO ALA ALA THR ARG ALA ARG PRO VAL ASN ALA ALA LEU GLU LEU ALA SER VAL THR ASP ARG VAL GLN ALA ARG PRO VAL PRO SER ALA LEU GLU LYS ALA PRO ALA LYS LYS GLU ALA TYR ARG TRP LYS ALA THR

THR PRO VAL MET GLN LYS VAL VAL ALA THR PRO LYS ALA LEU LYS LYS ALA LEU THR PRO LYS ALA LEU LYS LYS ALA LEU GLU HIS GLU LYS THR PRO GLU LEU ALA ALA LYS LEU ALA ALA GLU ALA ILE GLU ARG ASP PRO TRP ALA ALA GLN VAL SER GLU LEU SER LEU PRO LYS LEU VAL GLU GLN VAL ALA LEU

ASN ALA TRP LYS GLU GLU ASP ASN ALA VAL CYS LEU HIS LEU ARG SER GLN HIS LEU ASN ARG GLY ALA GLN GLN LYS LEU ALA GLU ALA LEU SER MET LEU LYS GLY SER THR VAL GLU LEU THR ILE VAL GLU ASP ASN PRO ALA VAL ARG THR PRO LEU GLU

TRP ARG GLN ILE TYR GLU GLU LYS LEU ALA GLN ALA ALA ARG GLU SER ILE ILE ALA ASP ASN ILE GLN THR LEU ARG ARG PHE PHE ASP GLU ALA GLU LEU ASP GLU SER ILE ARG PRO ILE

• Molecule 3: DNA polymerase III subunit delta'

Chain E: 95% 5%

M1 D38 A39 L88 H103 L120 T121 D122 N126 F142 L143 E149 R158 L176 V180 H259 G305 L334

• Molecule 4: DNA polymerase III subunit psi

Chain F: 18% 82%

MET T2 Q26 GLY GLU ILE ILE ALA ILE ILE PRO ALA HIS VAL ARG LEU VAL MET VAL ALA ASN ASP LEU PRO ALA LEU THR ASP PRO ASP LEU VAL SER ASP VAL LEU ARG ALA ALA LEU THR VAL SER PRO ASP VAL LEU GLN LEU LEU THR PRO GLU LYS ILE ALA MET LEU PRO GLN GLY

SER HIS CYS ASN SER TRP ARG LEU GLY THR ASP GLU PRO LEU SER LEU GLU GLY ALA GLN VAL ALA LEU ALA ASN ASP PRO THR ALA ARG ALA LEU TRP GLN GLN ILE CYS THR TYR GLU HIS ASP PHE PHE PRO ARG ASN ASP

• Molecule 5: Beta sliding clamp

Chain H: 92% 8%

M1 R7 L35 V70 L119 D120 Q132 K136 H148 Q149 D150 V151 L159 E165 I184 R197 E202 L203 M204 G209 K250 E257 L273 Y284 N288 E298 Q299 E300 I305 L306 T309 Y310 C333 E334 M339 L366

- Molecule 5: Beta sliding clamp

Chain I:

93%   7%

M1 R7 T26 L27 D39 H63 E64 V70 R103 L108 W122 Q123 S124 T142 D150 V151 L159 S187 L188 S192 V193 M204 L325 C333 E334 L340 Q348 I349 E350 M362 L366

- Molecule 6: Primer

22%

Chain X:

100%

G1 A2 G3 A4 T5 G23

- Molecule 7: Template

6%

Chain Y:

40%   .   57%

DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT DT T40 C50 T54 T65 C66 T67 C68

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF refinement per-particle was performed in RELION before final 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00303	Depositor
Map size (Å)	302.4, 302.4, 302.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: ALF, MG, ADP, ZN

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	0.23	0/2775	0.47	0/3769
2	B	0.23	0/2887	0.48	0/3914
2	C	0.23	0/2913	0.49	0/3950
2	D	0.23	0/2849	0.49	0/3861
3	E	0.23	0/2667	0.46	0/3639
4	F	0.22	0/215	0.57	0/290
5	H	0.24	0/2893	0.51	0/3915
5	I	0.24	0/2893	0.50	0/3915
6	X	0.53	0/531	0.95	0/818
7	Y	0.57	0/654	1.10	0/1007
All	All	0.26	0/21277	0.54	0/29078

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	A	2726	2770	2779	12	0
2	B	2840	2874	2887	19	0
2	C	2865	2893	2906	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2804	2836	2848	17	0
3	E	2602	2588	2603	9	0
4	F	211	212	212	0	0
5	H	2844	2854	2861	15	0
5	I	2844	2854	2861	14	0
6	X	472	260	260	0	0
7	Y	588	335	335	2	0
8	B	27	12	12	2	0
8	C	27	12	12	2	0
8	D	27	12	12	1	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	B	5	0	0	1	0
10	D	10	0	0	4	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
All	All	20899	20512	20588	100	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 (100) 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:A:97:LEU:O	1:A:101:THR:HG23	1.95	0.66
2:D:7:ALA:O	8:D:702:ADP:O3'	2.15	0.62
2:B:354:LEU:HD13	2:C:297:LEU:HD22	1.82	0.62
8:C:701:ADP:O2B	10:D:701:ALF:F4	2.08	0.61
5:H:257:GLU:O	5:H:309:THR:OG1	2.19	0.61
5:I:159:LEU:HD12	5:I:193:VAL:O	2.02	0.59
5:I:348:GLN:NE2	5:I:350:GLU:OE2	2.37	0.58
5:I:333:CYS:SG	5:I:334:GLU:N	2.77	0.58
5:H:288:ASN:N	5:H:310:TYR:O	2.36	0.57
3:E:122:ASP:O	3:E:126:ASN:ND2	2.37	0.57
2:B:245:ASP:O	2:B:274:ARG:NH1	2.36	0.57
2:C:354:LEU:HD21	2:D:297:LEU:HD22	1.87	0.55
1:A:300:GLN:HB3	1:A:341:ILE:HD13	1.89	0.55
2:D:133:ARG:O	2:D:137:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:701:ADP:O2B	10:B:703:ALF:F4	2.15	0.55
5:H:333:CYS:SG	5:H:334:GLU:N	2.80	0.54
5:H:165:GLU:N	5:H:165:GLU:OE1	2.41	0.54
2:D:344:ASP:OD1	2:D:345:ARG:N	2.41	0.54
2:B:268:ILE:HD11	2:B:353:LEU:HD12	1.89	0.53
2:B:296:GLN:NE2	2:B:320:ILE:O	2.40	0.53
3:E:149:GLU:N	3:E:149:GLU:OE1	2.42	0.52
5:I:362:MET:N	5:I:362:MET:SD	2.82	0.52
1:A:90:ASN:OD1	1:A:91:ALA:N	2.41	0.51
2:D:22:GLU:OE1	2:D:22:GLU:N	2.43	0.51
2:D:269:ASN:OD1	2:D:346:ARG:NH2	2.44	0.51
5:H:288:ASN:O	5:H:288:ASN:ND2	2.44	0.51
2:B:101:VAL:HG21	2:B:134:HIS:HB2	1.93	0.51
5:H:150:ASP:OD1	5:H:151:VAL:N	2.44	0.51
1:A:336:LEU:O	1:A:338:ASP:N	2.43	0.50
8:C:701:ADP:PB	10:D:701:ALF:F4	2.59	0.50
2:B:179:ASP:OD1	2:B:180:VAL:N	2.43	0.50
1:A:196:LYS:O	1:A:201:ARG:NH1	2.45	0.50
5:H:132:GLN:OE1	5:H:209:GLY:N	2.42	0.50
1:A:33:GLU:OE2	1:A:154:ARG:NH2	2.39	0.49
2:D:75:VAL:O	2:D:80:ARG:NE	2.45	0.49
2:C:13:GLN:OE1	2:C:60:LYS:NZ	2.46	0.49
5:I:159:LEU:HD11	5:I:192:SER:HB3	1.94	0.49
1:A:81:LEU:HD23	1:A:82:LEU:N	2.28	0.49
2:D:101:VAL:HG23	7:Y:50:DC:OP1	2.12	0.48
2:B:82:ILE:HG23	2:B:90:LEU:HD22	1.96	0.48
3:E:38:ASP:OD1	3:E:39:ALA:N	2.46	0.48
2:C:75:VAL:O	2:C:80:ARG:NE	2.46	0.48
2:C:369:GLU:N	2:C:369:GLU:OE1	2.46	0.48
2:B:363:MET:SD	2:B:363:MET:N	2.84	0.47
2:D:224:ALA:O	2:D:228:GLY:N	2.47	0.47
1:A:18:ARG:HG2	1:A:135:VAL:HG23	1.96	0.47
2:B:23:HIS:CD2	2:B:24:VAL:HG23	2.49	0.47
2:D:305:ASP:OD1	2:D:306:MET:N	2.48	0.46
5:I:150:ASP:OD1	5:I:151:VAL:N	2.48	0.46
2:B:7:ALA:O	8:B:701:ADP:O3'	2.34	0.46
2:C:268:ILE:HD11	2:C:353:LEU:CD1	2.46	0.46
5:H:148:HIS:O	5:H:197:ARG:NH1	2.49	0.46
5:I:64:GLU:N	5:I:64:GLU:OE1	2.49	0.46
2:B:101:VAL:HG23	7:Y:54:DT:OP1	2.16	0.45
2:C:248:GLN:OE1	2:C:274:ARG:NE	2.49	0.45

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:70:VAL:HG13	5:I:108:LEU:HD21	1.97	0.45
5:I:187:SER:C	5:I:188:LEU:HD12	2.37	0.45
2:D:270:GLU:OE2	2:D:274:ARG:NE	2.50	0.45
10:D:704:ALF:F4	3:E:158:ARG:NH2	2.39	0.45
5:H:136:LYS:NZ	5:H:204:MET:SD	2.89	0.45
2:B:24:VAL:HG21	2:B:175:LEU:HD23	1.99	0.44
2:C:89:ASP:OD2	2:C:118:GLY:N	2.45	0.44
2:B:305:ASP:OD1	2:B:306:MET:N	2.50	0.44
2:C:268:ILE:HD11	2:C:353:LEU:HD12	1.98	0.44
2:B:163:PRO:HD2	2:B:166:ILE:HD12	1.98	0.44
5:H:305:ILE:C	5:H:306:LEU:HD22	2.37	0.44
2:C:108:LEU:O	2:C:111:VAL:HG12	2.17	0.44
1:A:318:GLN:N	1:A:318:GLN:OE1	2.51	0.44
2:D:37:ILE:HD11	2:D:68:ILE:HG21	2.00	0.44
5:I:39:ASP:O	5:I:63:HIS:NE2	2.48	0.44
2:B:64:CYS:O	2:B:119:ARG:NH1	2.46	0.43
5:H:35:LEU:HD13	5:H:70:VAL:HG12	2.00	0.43
1:A:26:ASN:OD1	1:A:27:ASP:N	2.52	0.43
1:A:100:LEU:HD23	1:A:100:LEU:O	2.18	0.43
2:C:248:GLN:NE2	2:C:270:GLU:OE1	2.51	0.43
2:D:327:LEU:HD21	2:D:359:PHE:CD1	2.53	0.43
5:H:339:MET:N	5:H:339:MET:SD	2.91	0.43
5:I:142:THR:HG22	5:I:142:THR:O	2.19	0.43
2:D:268:ILE:HD11	2:D:353:LEU:CD1	2.49	0.43
2:C:278:TRP:HB3	2:C:349:VAL:HG21	2.01	0.43
2:B:126:ASP:OD1	2:B:127:GLU:N	2.52	0.42
2:D:23:HIS:CD2	2:D:24:VAL:HG23	2.54	0.42
5:I:122:TRP:HE1	5:I:124:SER:HG	1.66	0.42
3:E:88:LEU:HD23	3:E:120:LEU:HD21	2.00	0.42
3:E:88:LEU:HD23	3:E:120:LEU:CD2	2.49	0.42
5:H:119:LEU:HD23	5:H:120:ASP:N	2.34	0.42
2:C:112:GLN:OE1	2:C:112:GLN:N	2.52	0.42
2:C:215:ARG:NH2	10:D:701:ALF:F3	2.42	0.42
3:E:176:LEU:O	3:E:180:VAL:N	2.47	0.42
5:I:26:THR:HG22	5:I:26:THR:O	2.18	0.42
2:D:24:VAL:HG21	2:D:175:LEU:HD23	2.01	0.41
3:E:142:PHE:C	3:E:143:LEU:HD12	2.41	0.41
2:B:343:PRO:HB3	2:C:283:VAL:HG13	2.02	0.41
5:I:340:LEU:HD23	5:I:340:LEU:N	2.36	0.41
5:H:300:GLU:OE1	5:H:300:GLU:N	2.48	0.41
2:D:296:GLN:NE2	2:D:320:ILE:O	2.48	0.40

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:CYS:SG	2:B:74:GLY:N	2.94	0.40
2:B:186:GLN:HG2	2:B:214:LEU:HD21	2.02	0.40
1:A:313:LYS:NZ	3:E:305:GLY:O	2.54	0.40
5:H:165:GLU:O	5:H:184:ILE:N	2.47	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	341/343 (99%)	335 (98%)	5 (2%)	1 (0%)	41	71
2	B	363/643 (56%)	362 (100%)	1 (0%)	0	100	100
2	C	366/643 (57%)	357 (98%)	9 (2%)	0	100	100
2	D	358/643 (56%)	347 (97%)	11 (3%)	0	100	100
3	E	332/334 (99%)	329 (99%)	3 (1%)	0	100	100
4	F	23/137 (17%)	23 (100%)	0	0	100	100
5	H	364/366 (100%)	355 (98%)	9 (2%)	0	100	100
5	I	364/366 (100%)	353 (97%)	11 (3%)	0	100	100
All	All	2511/3475 (72%)	2461 (98%)	49 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/291 (100%)	287 (99%)	4 (1%)	67	89
2	B	302/533 (57%)	301 (100%)	1 (0%)	92	98
2	C	305/533 (57%)	298 (98%)	7 (2%)	50	80
2	D	297/533 (56%)	294 (99%)	3 (1%)	76	92
3	E	270/270 (100%)	267 (99%)	3 (1%)	73	92
4	F	22/116 (19%)	22 (100%)	0	100	100
5	H	313/313 (100%)	308 (98%)	5 (2%)	62	86
5	I	313/313 (100%)	308 (98%)	5 (2%)	62	86
All	All	2113/2902 (73%)	2085 (99%)	28 (1%)	70	90

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ARG
1	A	293	LEU
1	A	307	ARG
1	A	336	LEU
2	B	363	MET
2	C	47	ARG
2	C	100	LYS
2	C	121	LYS
2	C	176	LYS
2	C	244	LEU
2	C	245	ASP
2	C	363	MET
2	D	86	ARG
2	D	171	LEU
2	D	309	ILE
3	E	103	HIS
3	E	259	HIS
3	E	334	LEU
5	H	7	ARG

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Mol	Chain	Res	Type
5	H	159	LEU
5	H	202	GLU
5	H	250	LYS
5	H	284	TYR
5	I	7	ARG
5	I	27	LEU
5	I	204	MET
5	I	325	LEU
5	I	362	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	198	HIS

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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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
10	ALF	D	704	-	0,4,4	-	-	-		
8	ADP	B	701	9	24,29,29	0.93	1 (4%)	29,45,45	1.54	4 (13%)
10	ALF	B	703	-	0,4,4	-	-	-		
10	ALF	D	701	-	0,4,4	-	-	-		
8	ADP	C	701	9	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)
8	ADP	D	702	9	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)

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
8	ADP	C	701	9	-	2/12/32/32	0/3/3/3
8	ADP	D	702	9	-	5/12/32/32	0/3/3/3
8	ADP	B	701	9	-	2/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	701	ADP	C5-C4	2.36	1.47	1.40
8	D	702	ADP	C5-C4	2.34	1.47	1.40
8	B	701	ADP	C5-C4	2.29	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	701	ADP	N3-C2-N1	-3.69	122.91	128.68
8	B	701	ADP	PA-O3A-PB	-3.66	120.27	132.83
8	D	702	ADP	PA-O3A-PB	-3.65	120.30	132.83
8	D	702	ADP	N3-C2-N1	-3.61	123.04	128.68
8	B	701	ADP	C3'-C2'-C1'	3.61	106.41	100.98
8	C	701	ADP	N3-C2-N1	-3.59	123.06	128.68
8	C	701	ADP	PA-O3A-PB	-3.51	120.78	132.83
8	C	701	ADP	C3'-C2'-C1'	3.35	106.02	100.98
8	D	702	ADP	C3'-C2'-C1'	3.11	105.65	100.98
8	B	701	ADP	C4-C5-N7	-2.65	106.64	109.40
8	D	702	ADP	C4-C5-N7	-2.60	106.69	109.40
8	C	701	ADP	C4-C5-N7	-2.57	106.72	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	701	ADP	C5'-O5'-PA-O2A
8	C	701	ADP	C5'-O5'-PA-O3A
8	D	702	ADP	PA-O3A-PB-O3B
8	D	702	ADP	C5'-O5'-PA-O3A
8	B	701	ADP	O4'-C4'-C5'-O5'
8	B	701	ADP	C3'-C4'-C5'-O5'
8	D	702	ADP	PA-O3A-PB-O2B
8	D	702	ADP	C5'-O5'-PA-O1A
8	D	702	ADP	PA-O3A-PB-O1B

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	704	ALF	1	0
8	B	701	ADP	2	0
10	B	703	ALF	1	0
10	D	701	ALF	3	0
8	C	701	ADP	2	0
8	D	702	ADP	1	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 then 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 ADP B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 701

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 702

Bond lengths

Bond angles

Torsions

Rings
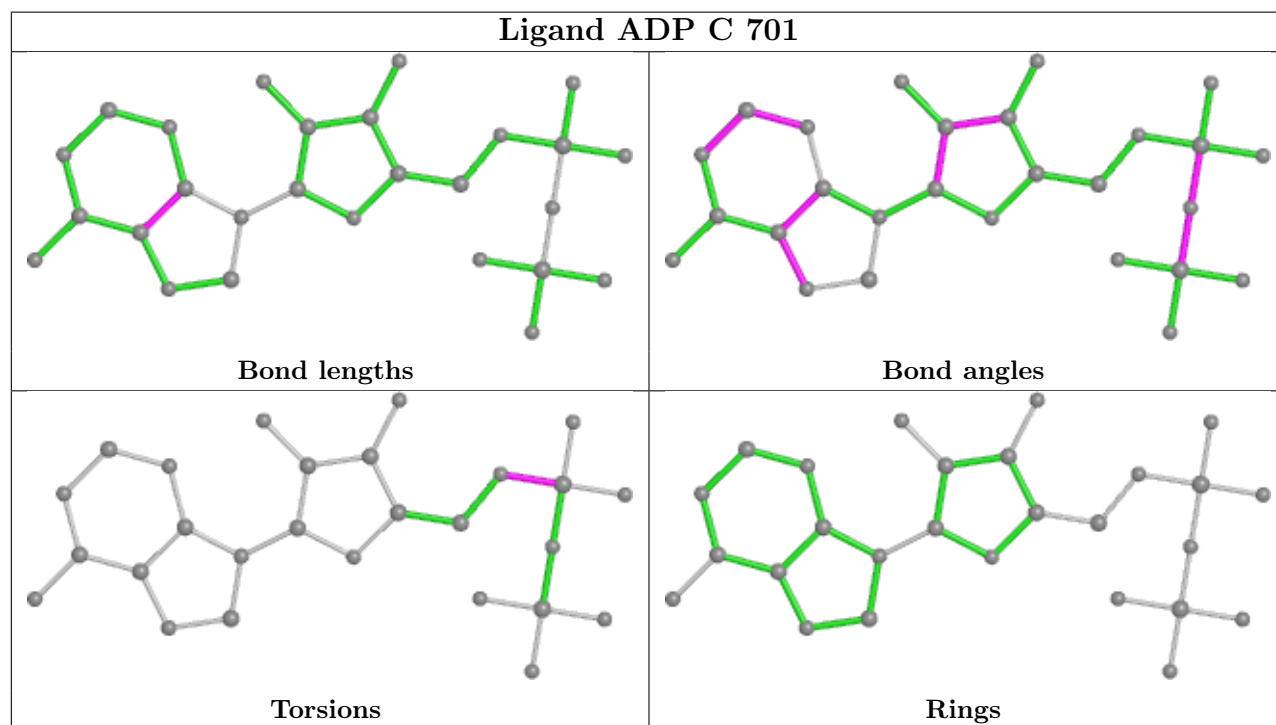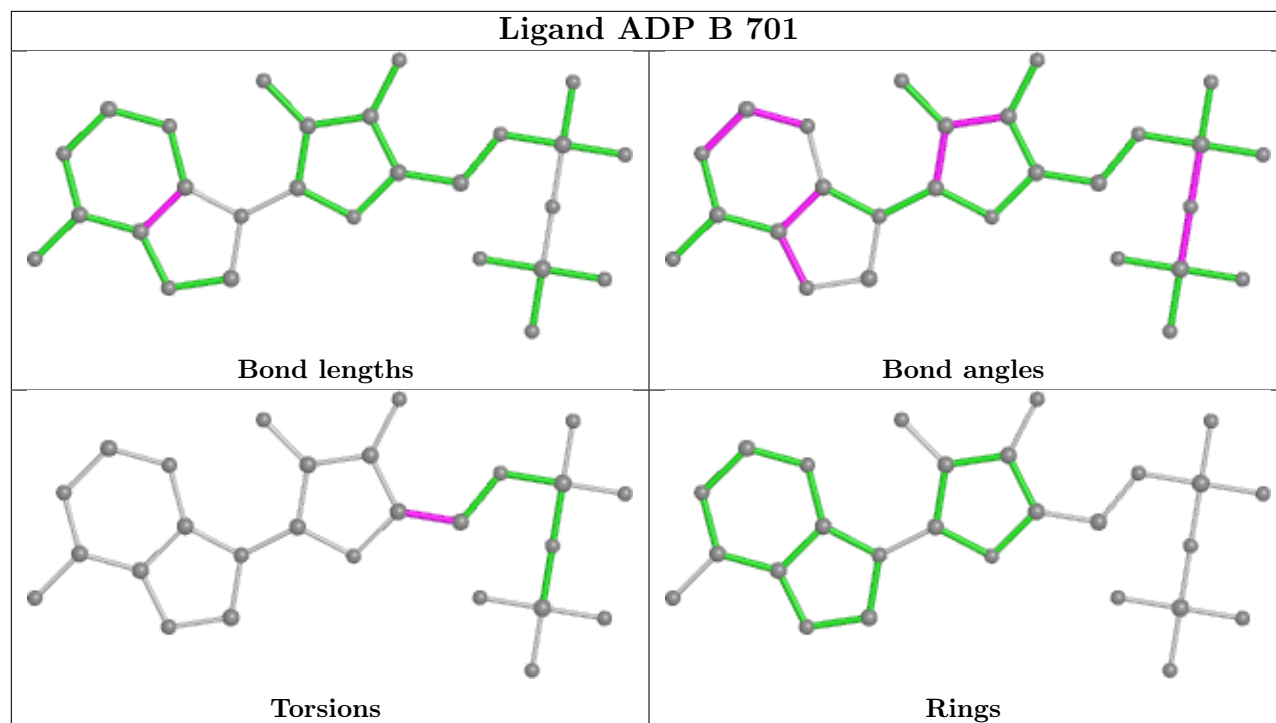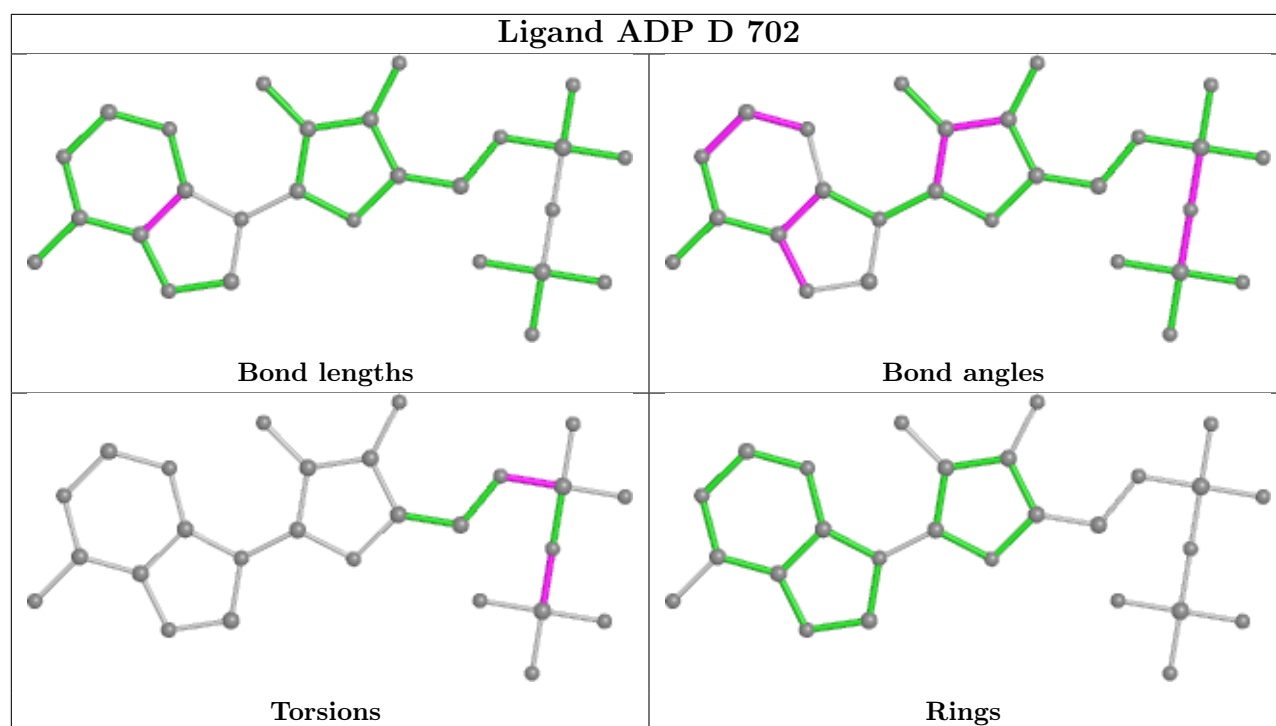
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40081. 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
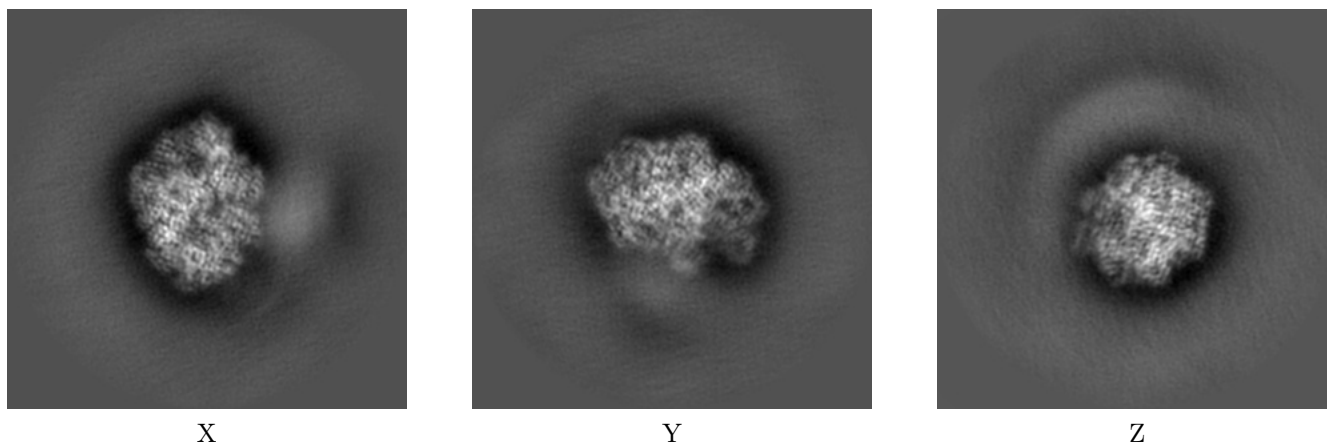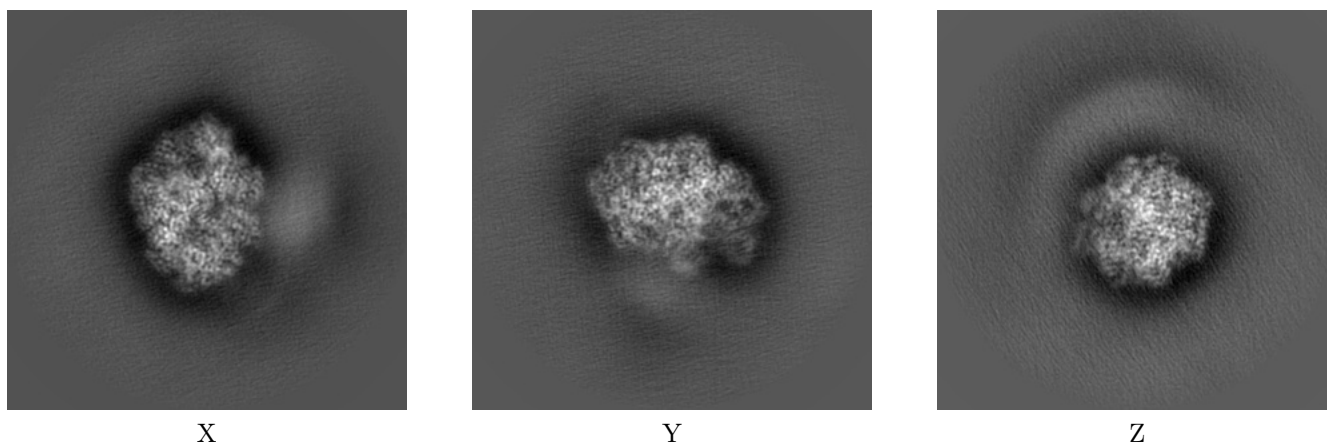
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
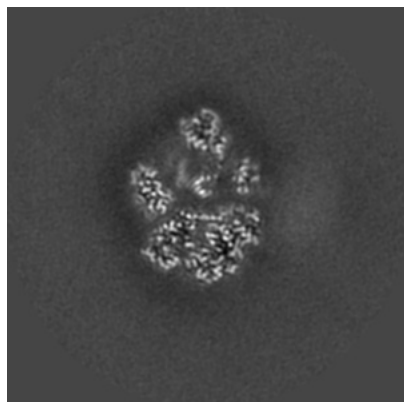
6.2.1 Primary map
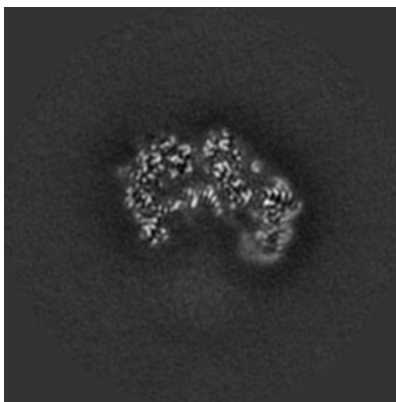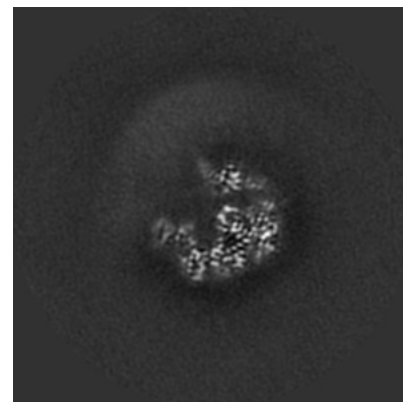
| X Index: 180 | Y Index: 180 | Z Index: 180 |

6.2.2 Raw map
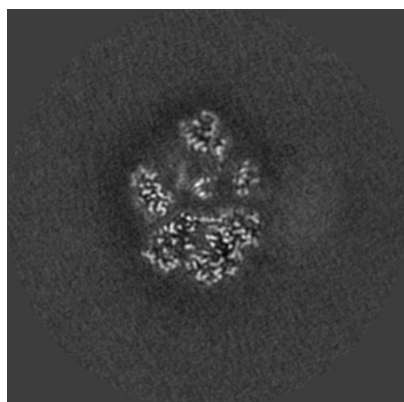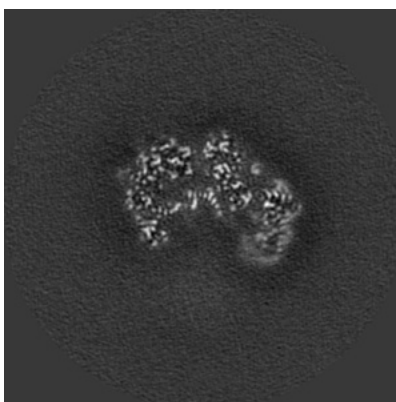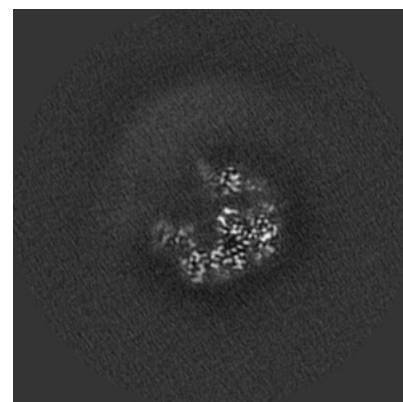
| X Index: 180 | Y Index: 180 | Z Index: 180 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
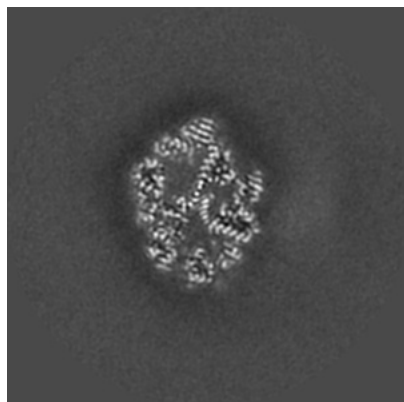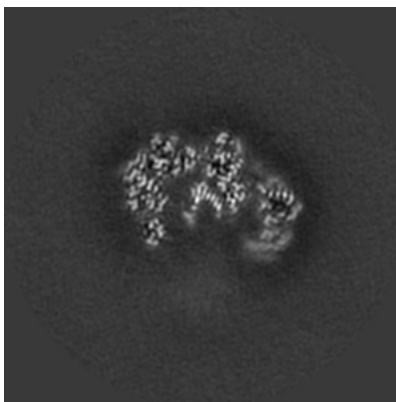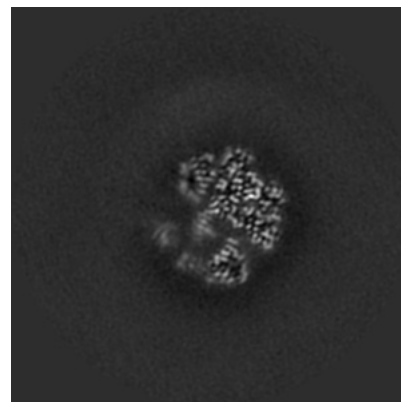
| X Index: 191 | Y Index: 176 | Z Index: 206 |

6.3.2 Raw map
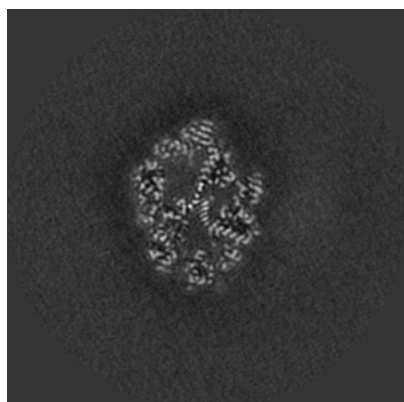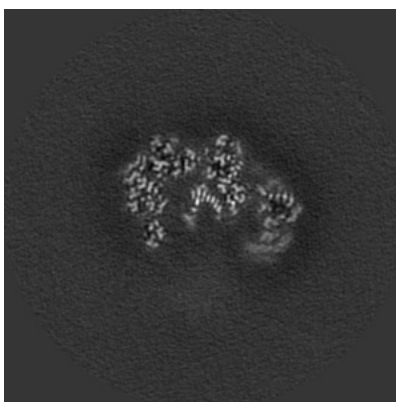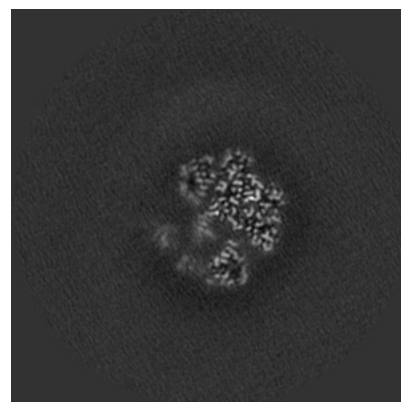
| X Index: 191 | Y Index: 176 | Z Index: 206 |

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
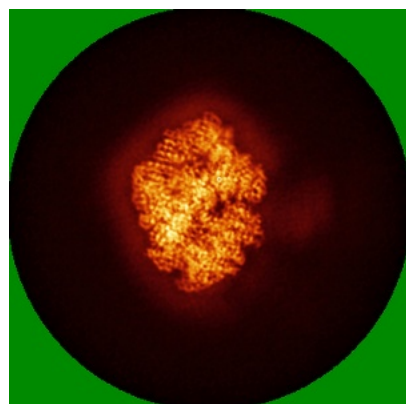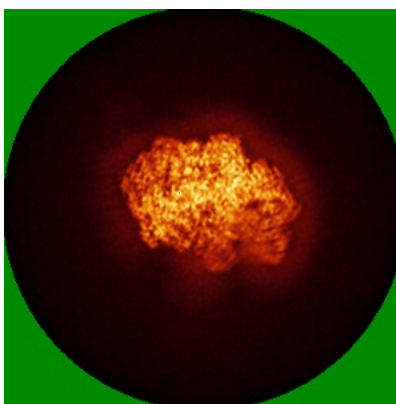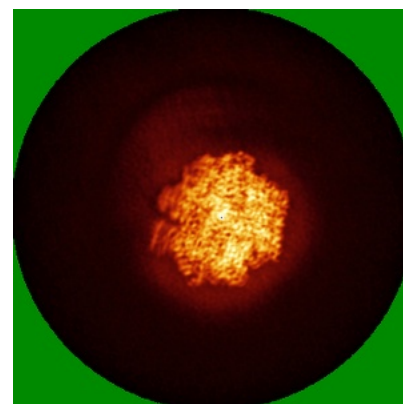
X	Y	Z

6.4.2 Raw map

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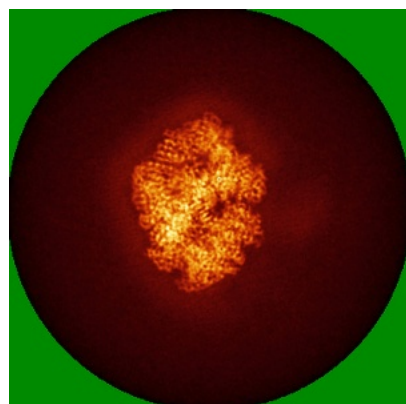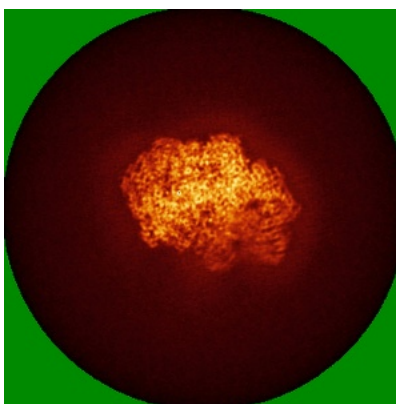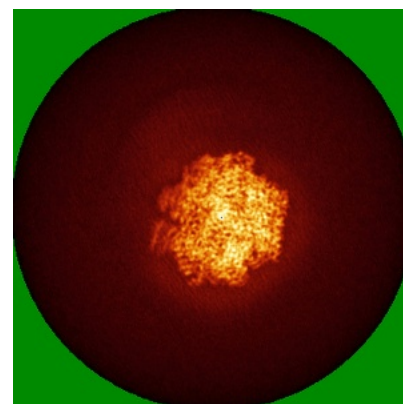
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.00303. 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
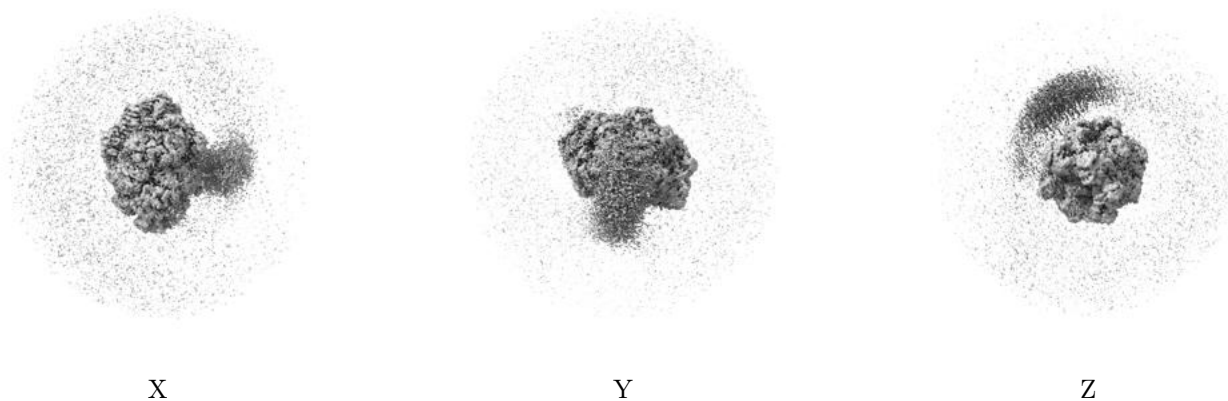
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6　Mask visualisation (i)

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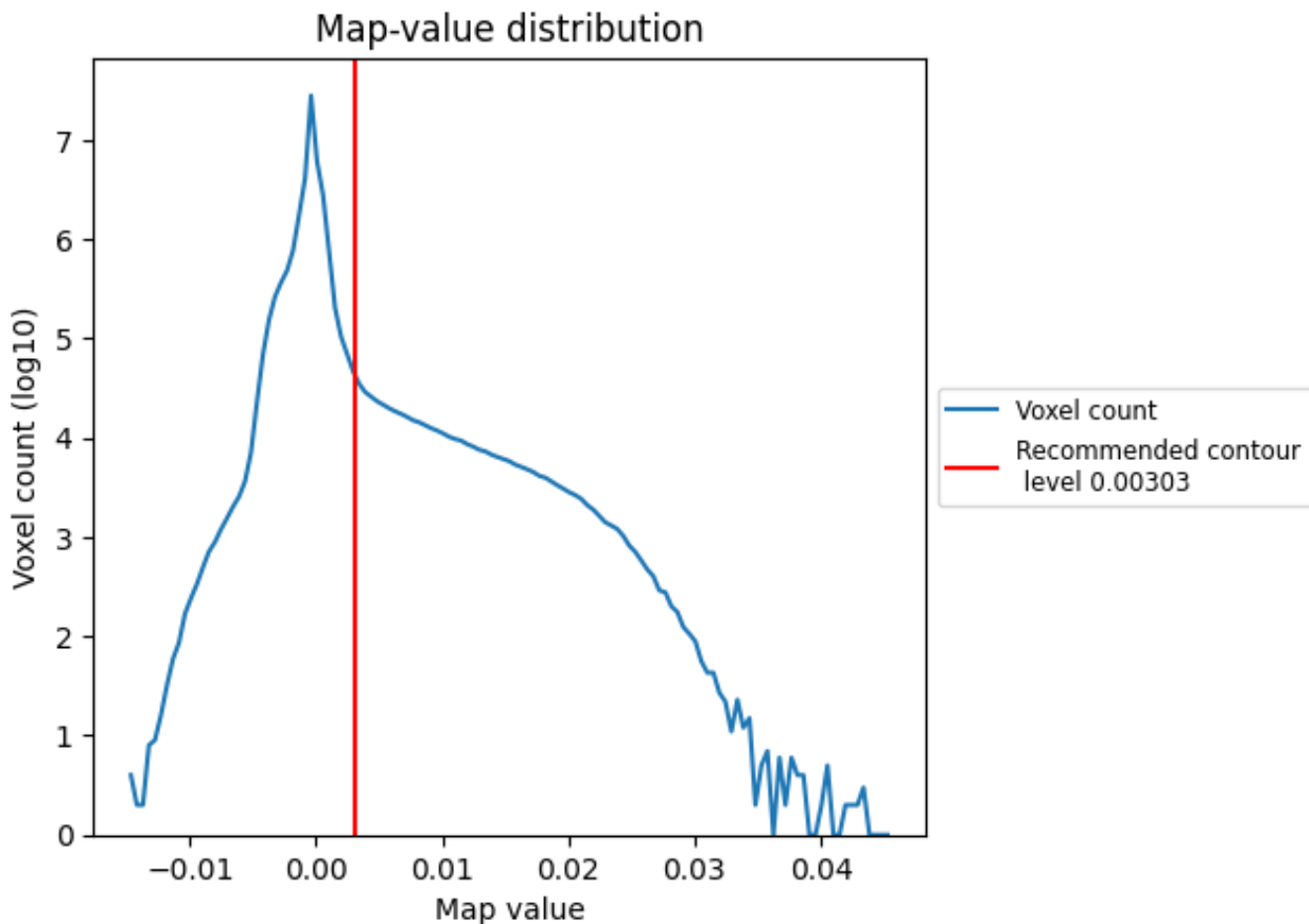
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
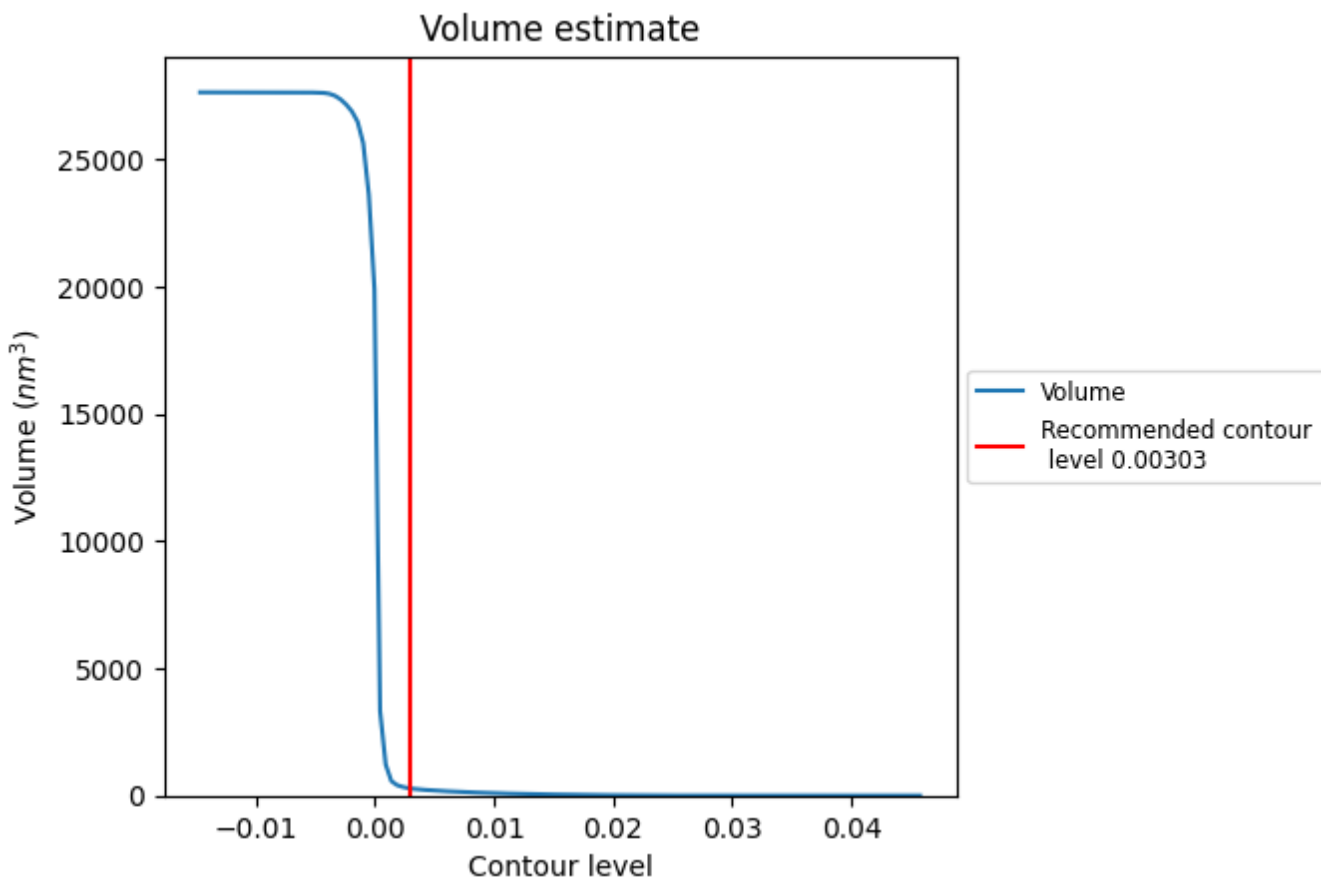
The volume at the recommended contour level is 279 nm^3; this corresponds to an approximate mass of 252 kDa.

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

7.3 Rotationally averaged power spectrum (i)
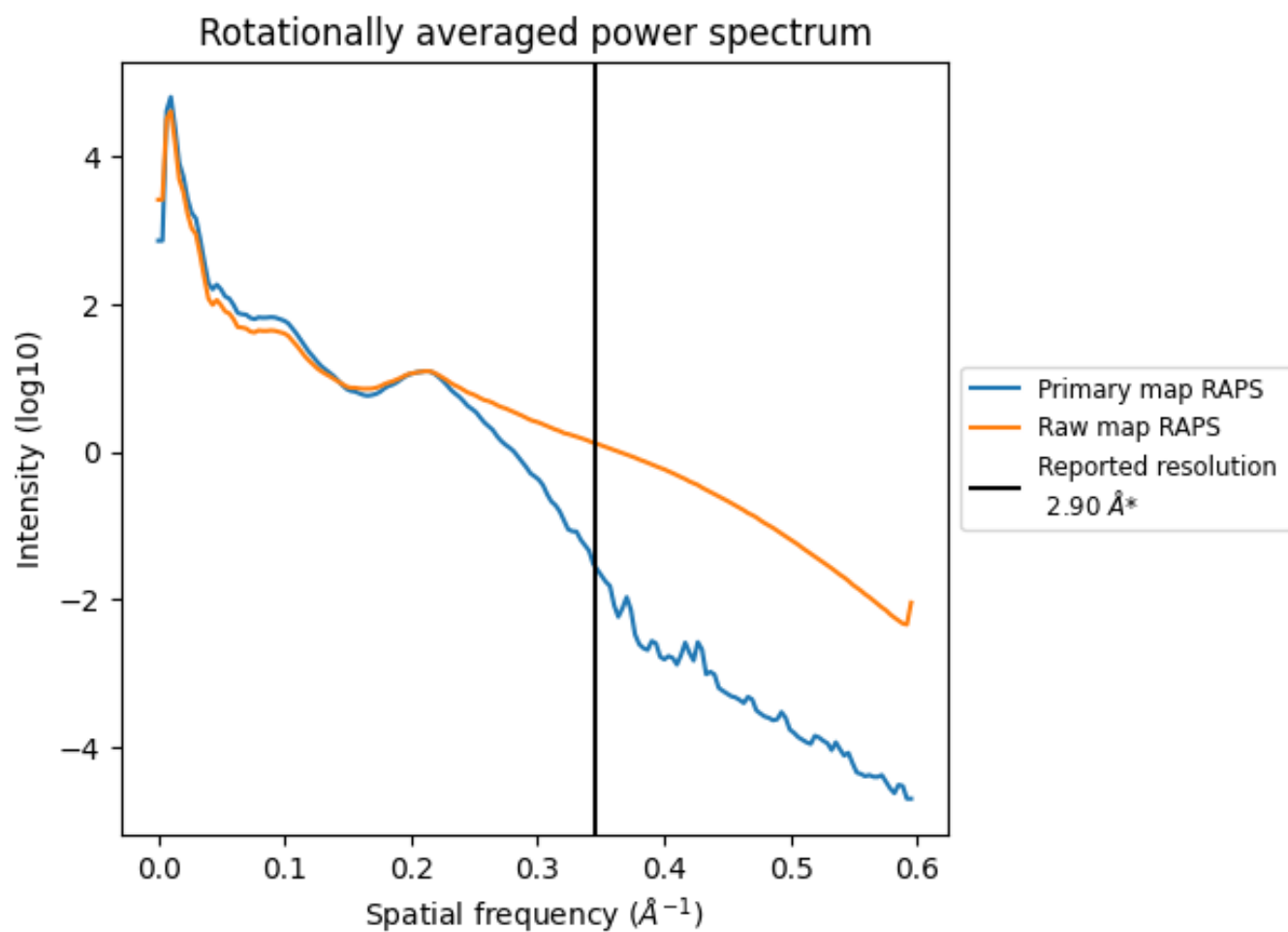
*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
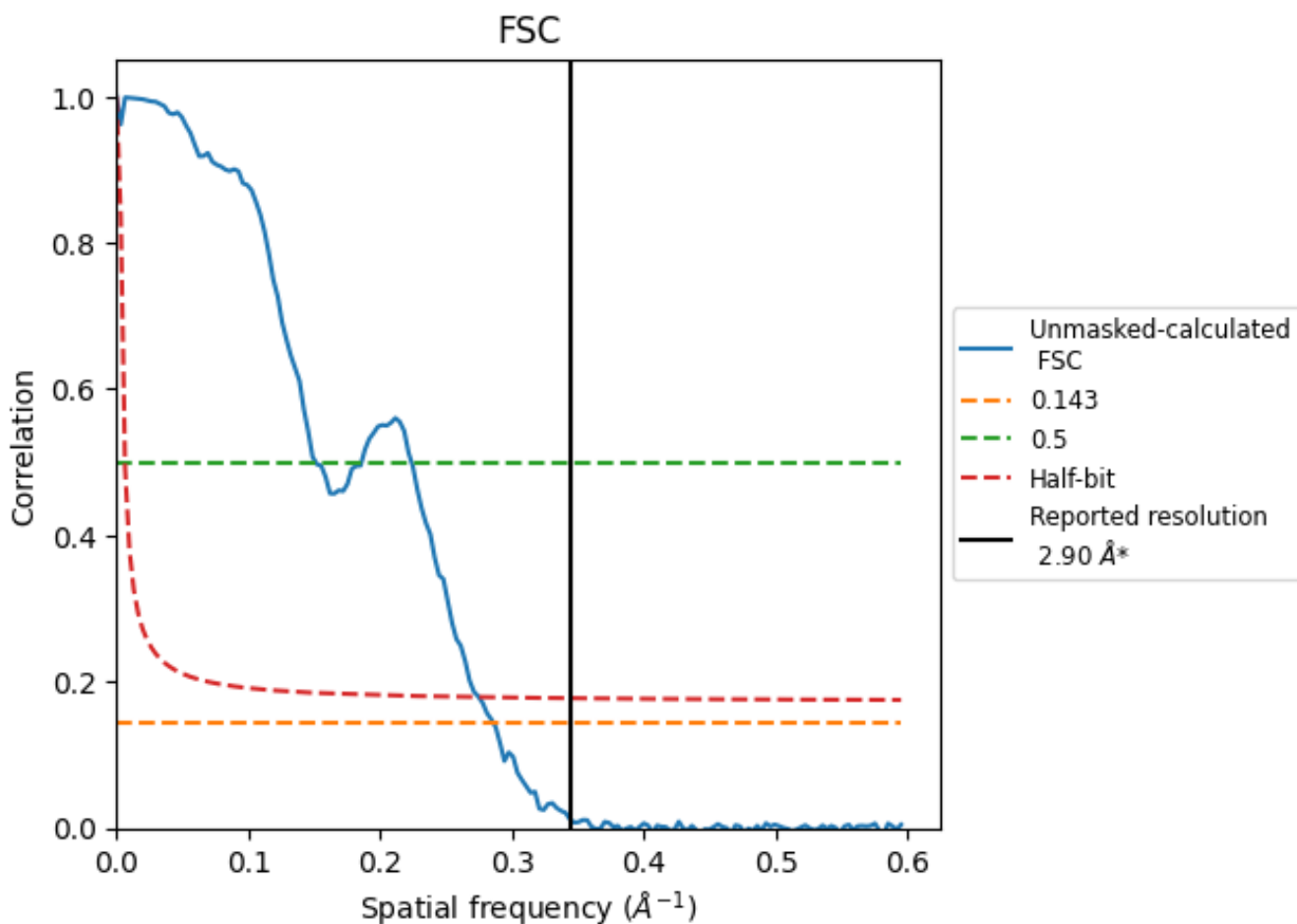
*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	6.61	3.64

*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 3.50 differs from the reported value 2.9 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-40081 and PDB model 8GJ0. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ
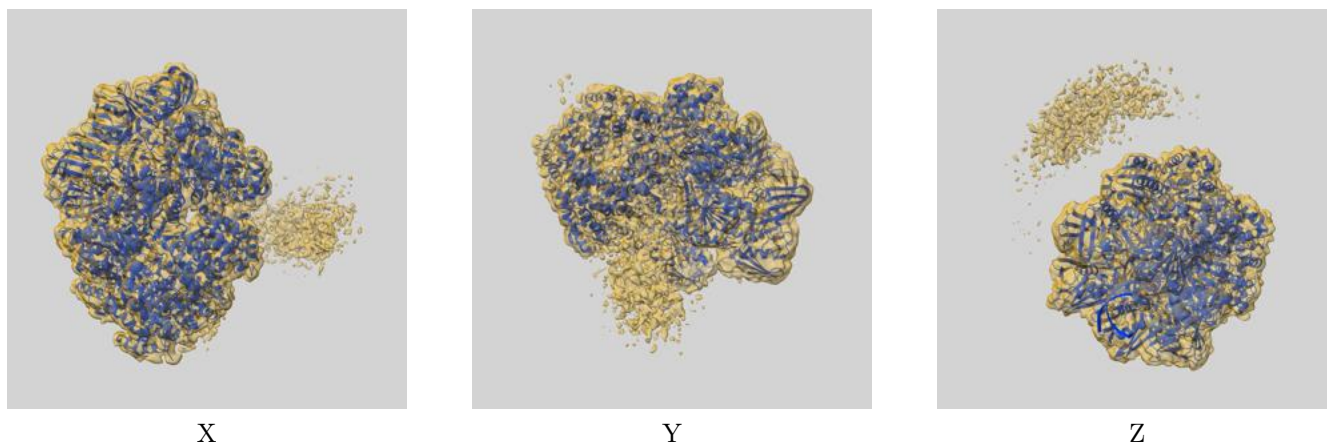
X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.00303 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 ⓘ
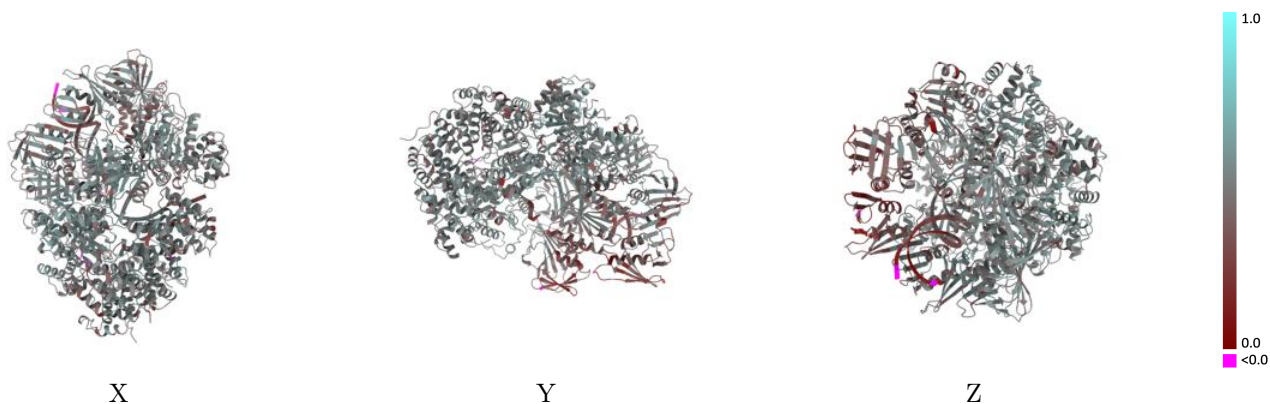
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
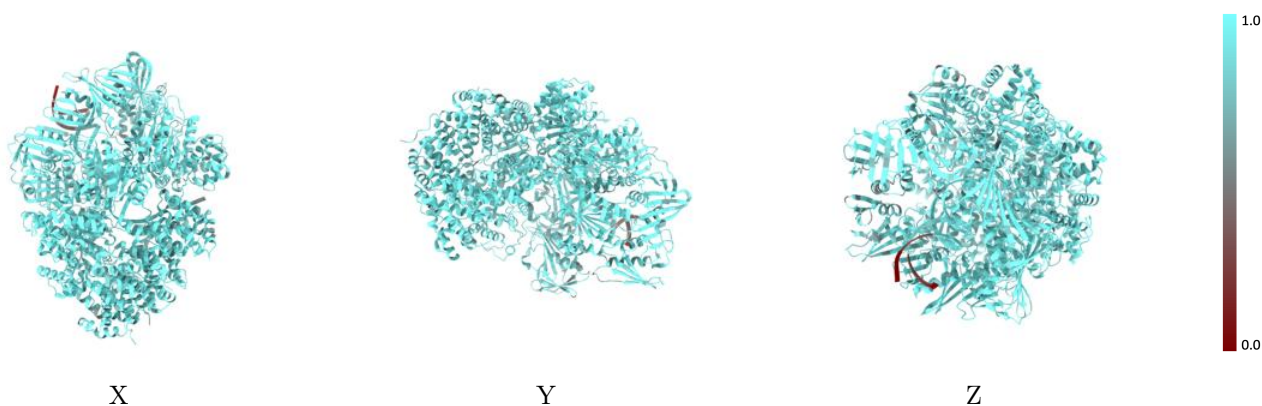
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00303).

9.4   Atom inclusion (i)
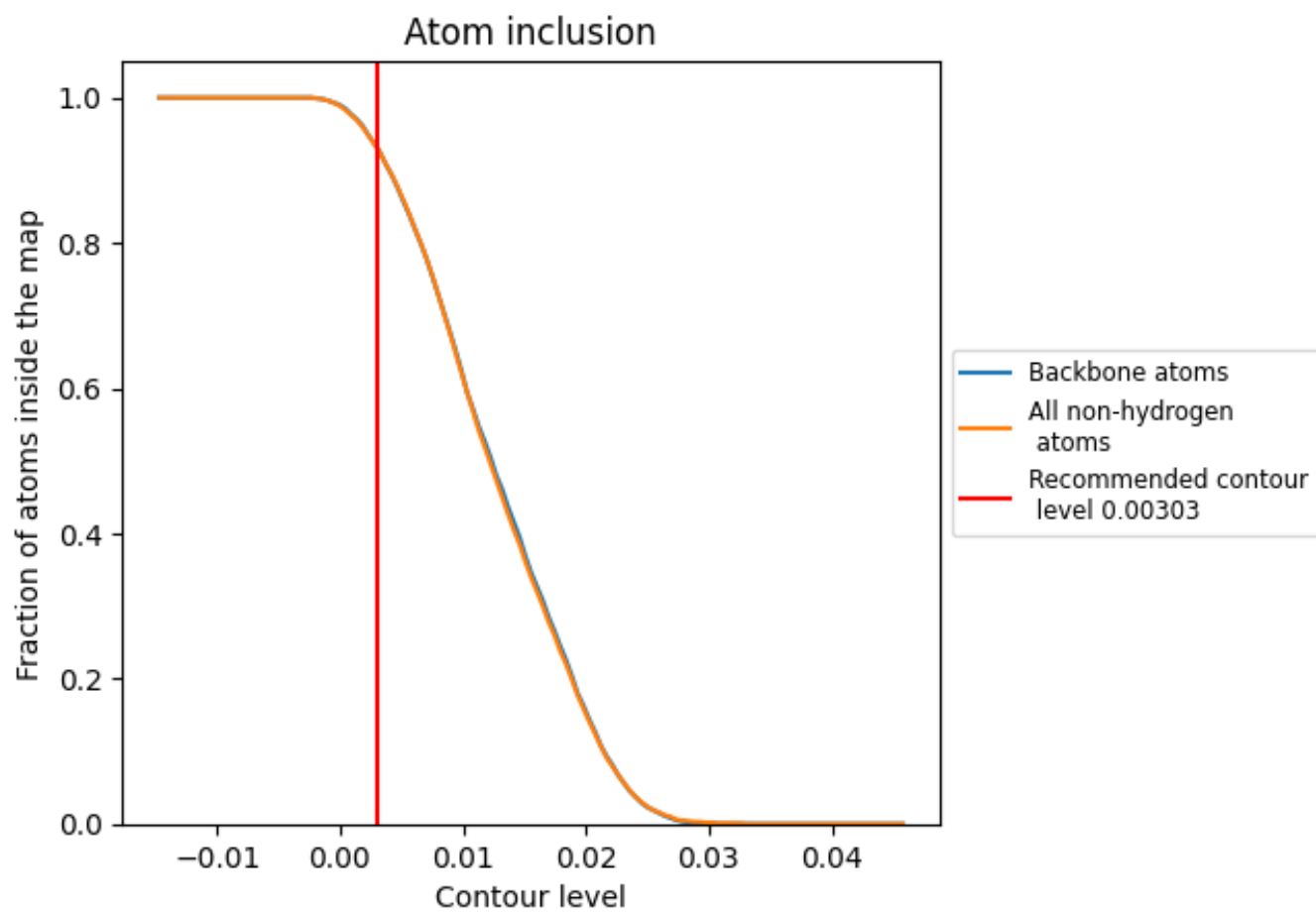
Atom inclusion

At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00303) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9300	0.4690
A	0.9320	0.4560
B	0.9470	0.4830
C	0.9580	0.5010
D	0.9600	0.5100
E	0.9690	0.5190
F	0.9600	0.4910
H	0.9210	0.4230
I	0.9100	0.4260
X	0.7860	0.3600
Y	0.8300	0.4000

1.0

0.0

<0.0