Full wwPDB EM Validation Report (i)

Feb 24, 2024 – 09:30 PM EST

PDB ID	:	7JGS
EMDB ID	:	EMD-22330
Title	:	Structure of Drosophila ORC bound to poly(dA/dT) DNA and Cdc6 (conformation 2)
Authors	:	Schmidt, J.M.; Bleichert, F.
Deposited on	:	2020-07-19
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

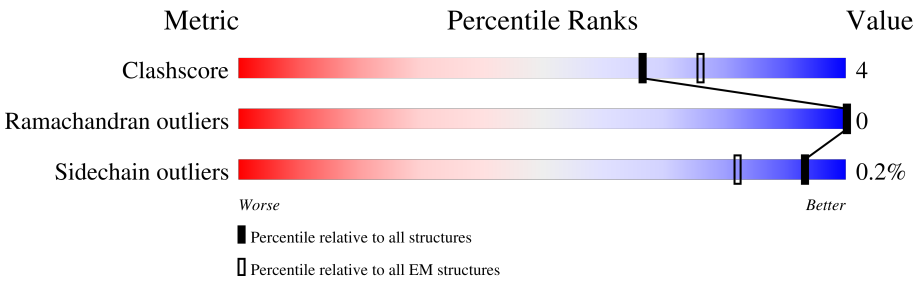
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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)
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	B	618	39% 7% 54%
2	C	721	75% 10% 15%
3	D	462	86% 9% 5%
4	E	460	78% 8% 13%
5	F	257	5% • 93%
6	A	488	74% 8% 18%
7	G	424	75% 13% 12%
8	H	60	5% 55% • 42%

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Mol	Chain	Length	Quality of chain
9	I	60	50% 7% 42%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21743 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 Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	285	2290	1471	381	425	13	0	0

- Molecule 2 is a protein called AT22044p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	614	4934	3163	863	879	29	0	0

- Molecule 3 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	441	3549	2264	626	643	16	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q9W102
D	-1	ASN	-	expression tag	UNP Q9W102
D	0	ALA	-	expression tag	UNP Q9W102

- Molecule 4 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	398	3161	2022	538	584	17	0	0

- Molecule 5 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	17	143	92	25	25	1	0	0

- Molecule 6 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	401	3129	1965	565	579	20	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	SER	-	expression tag	UNP O16810
A	438	ASN	-	expression tag	UNP O16810
A	439	ALA	-	expression tag	UNP O16810

- Molecule 7 is a protein called Cell division control protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	372	2974	1874	547	538	15	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	239	SER	-	expression tag	UNP Q9VSM9
G	240	ASN	-	expression tag	UNP Q9VSM9
G	241	ALA	-	expression tag	UNP Q9VSM9

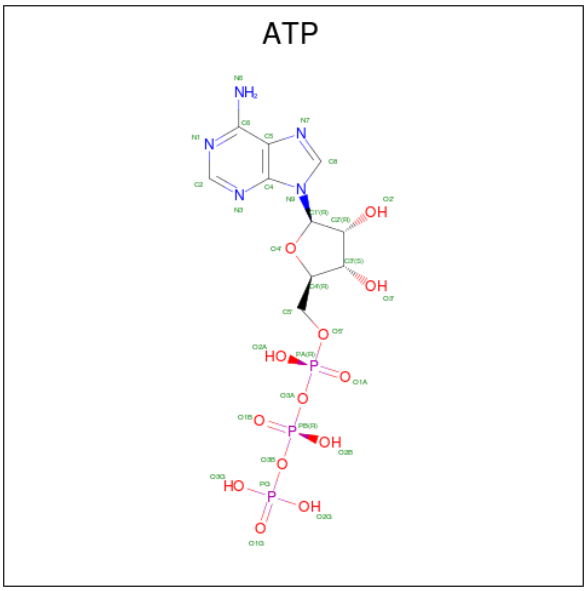
- Molecule 8 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	H	35	700	350	70	245	35	0	0

- Molecule 9 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	I	35	735	350	175	175	35	0	0

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

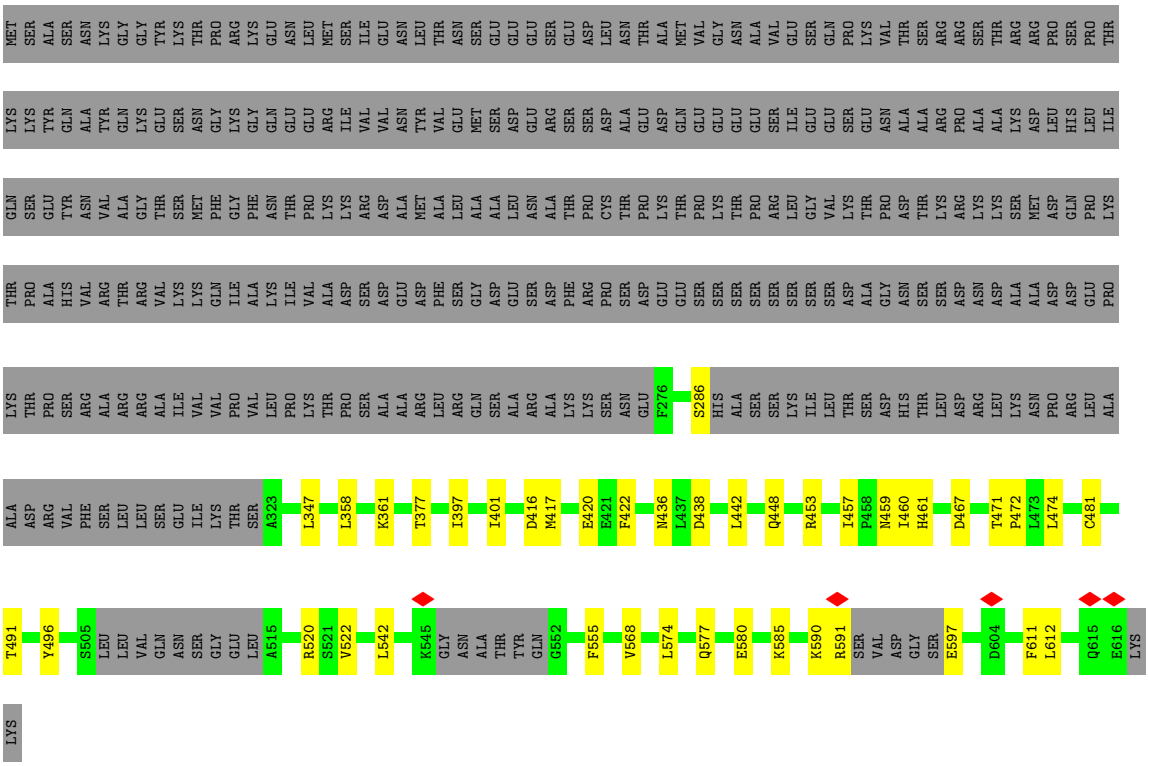
Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Mg	0
			1	1	
11	E	1	Total	Mg	0
			1	1	
11	A	1	Total	Mg	0
			1	1	
11	G	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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.

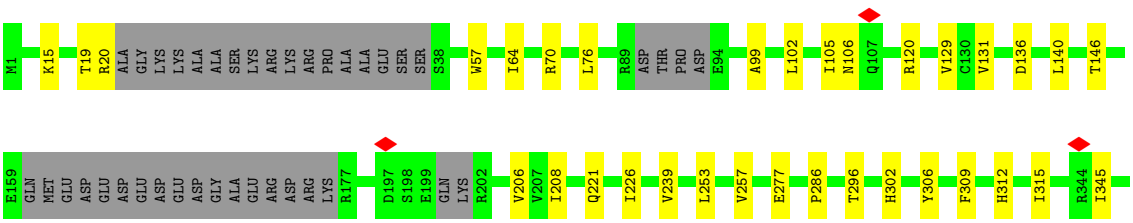
• Molecule 1: Origin recognition complex subunit 2

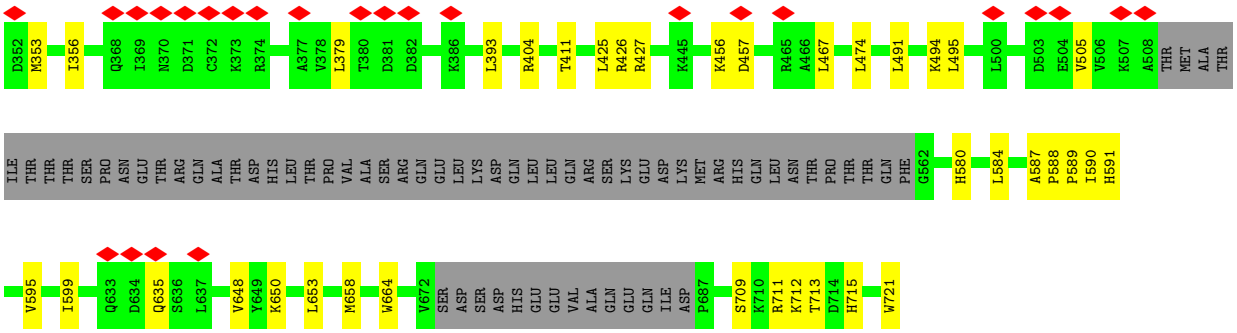
Chain B:



• Molecule 2: AT22044p1

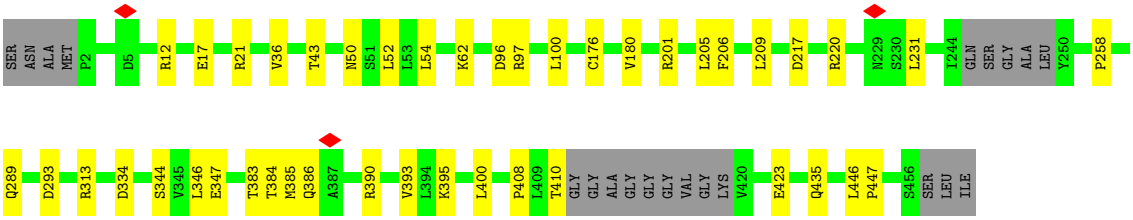
Chain C:





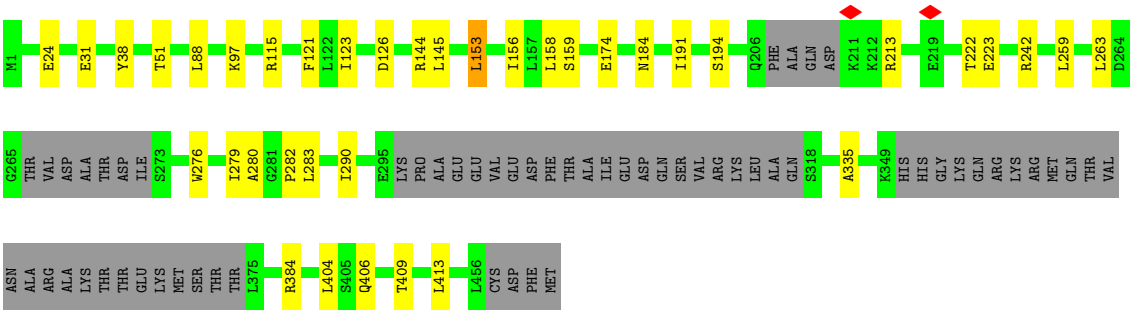
• Molecule 3: Origin recognition complex subunit 4

Chain D:



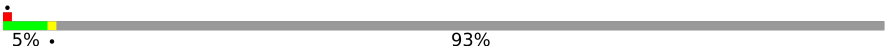
• Molecule 4: Origin recognition complex subunit 5

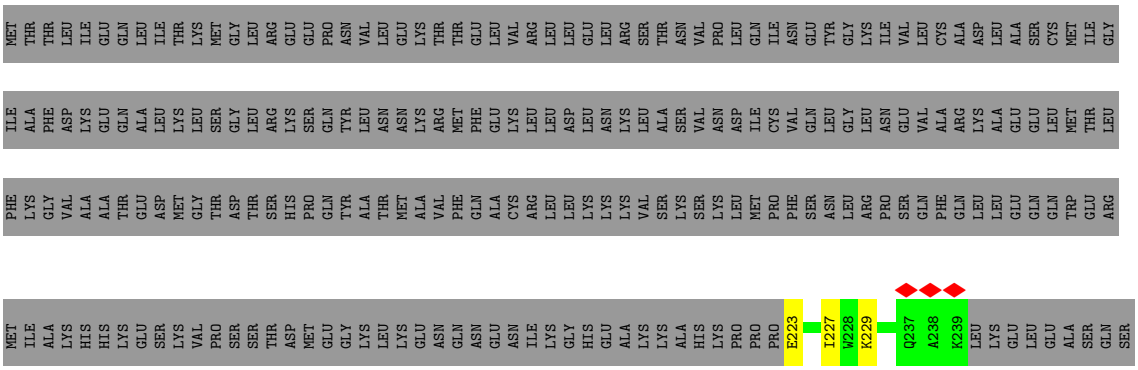
Chain E:



• Molecule 5: Origin recognition complex subunit 6

Chain F:





HIS MET ASP SER GLN LEU LEU GLU ALA

- Molecule 6: Origin recognition complex subunit 1

Chain A: 74% 8% 18%

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

SER THR THR THR LYS THR ALA THR THR PRO SER LYS GLY ILE THR THR ALA THR ALA THR PRO MET T519 D546 N577 I578 Y579 D588 G591 G592 C593 M594 Y595 V596 M618 M635 I688 R693 Q694 D695 D702 T705 V712 R725 L726 L737 T738

R739 L740 G760 A768 I789 E795 T806 M807 V810 M817 K822 N828 Q838 R880 I891 I892 L905 L906 N907 V908 L917 R918 V919 GLU GLU MET VAL ASN

- Molecule 7: Cell division control protein

Chain G: 75% 13% 12%

SER ASN ALA ASN ASN LEU PRO SER PRO SER R249 N250 K251 Y252 A255 R256 R257 V258 L259 A262 R278 L285 V295 D313 L320 Q321 R322 V323 T328 L340 E343 I360 K368 R369 I378 D379 Q380 L398 P399 L404 A409 N410 S411 L412

D413 L414 T415 D416 R417 A418 L419 L422 C426 E427 L428 K429 M433 K440 R450 L451 A452 E453 V456 L457 A470 R488 E491 R498 ASP GLY GLU LYS GLU PHE ASN MET LYS ALA LEU GLN LEU GLU GLY LYS ASP ALA VAL GLU ALA LYS GLU LYS GLN ASP

THR L526 K527 V541 Y542 GLY ALA SER GLN ASN LEU GLU GLU ASP ILE GLU ALA SER F556 Q559 R575 D578 Y588 L600 E604 V609 I620 Q634 E637 H641 D646 D656 L660 SER LYS

- Molecule 8: DNA (33-MER)

Chain H: 5% 55% 42%

T-3 T-2 T11 T27 T28 T29 T30 T31 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

- Molecule 9: DNA (33-MER)

Chain I: 50% 7% 42%

A36 A37 A38 A44 A45 A66 A67 A70 DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81248	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	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	0.097	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	260.1, 260.1, 260.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86700004, 0.86700004, 0.86700004	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: ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	B	0.29	0/2340	0.48	0/3164
2	C	0.31	0/5029	0.52	1/6798 (0.0%)
3	D	0.29	0/3616	0.50	1/4877 (0.0%)
4	E	0.30	0/3208	0.54	1/4332 (0.0%)
5	F	0.26	0/145	0.37	0/192
6	A	0.29	0/3174	0.51	0/4290
7	G	0.28	0/3012	0.51	1/4060 (0.0%)
8	H	0.67	0/769	1.30	0/1186
9	I	0.64	0/839	0.89	1/1291 (0.1%)
All	All	0.33	0/22132	0.58	5/30190 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	66	DA	P-O3'-C3'	5.59	126.41	119.70
2	C	653	LEU	CA-CB-CG	5.22	127.31	115.30
3	D	209	LEU	CA-CB-CG	5.18	127.22	115.30
7	G	404	LEU	CA-CB-CG	5.15	127.14	115.30
4	E	153	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	259	LEU	Peptide

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	B	2290	0	2261	26	0
2	C	4934	0	5021	50	0
3	D	3549	0	3586	26	0
4	E	3161	0	3226	27	0
5	F	143	0	145	2	0
6	A	3129	0	3237	22	0
7	G	2974	0	3114	30	0
8	H	700	0	421	3	0
9	I	735	0	386	7	0
10	A	31	0	12	0	0
10	D	31	0	12	1	0
10	E	31	0	12	0	0
10	G	31	0	12	2	0
11	A	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	G	1	0	0	0	0
All	All	21743	0	21445	171	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 4.

All (171) 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)
8:H:29:DT:N3	9:I:38:DA:N1	2.19	0.90
2:C:709:SER:OG	2:C:715:HIS:C	2.14	0.86
2:C:709:SER:OG	2:C:715:HIS:O	2.03	0.73
8:H:29:DT:O4	9:I:38:DA:N6	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:LEU:HD21	2:C:120:ARG:HG3	1.79	0.65
1:B:448:GLN:HG3	1:B:474:LEU:HD13	1.79	0.65
3:D:206:PHE:HB3	6:A:828:ASN:HD22	1.64	0.63
2:C:590:ILE:HG13	2:C:590:ILE:O	1.97	0.62
3:D:97:ARG:NH1	8:H:11:DT:OP1	2.34	0.60
1:B:590:LYS:HE3	9:I:44:DA:OP2	2.02	0.60
2:C:648:VAL:HG13	2:C:664:TRP:HZ2	1.69	0.57
7:G:488:ARG:HA	7:G:491:GLU:HG2	1.86	0.57
3:D:62:LYS:HG2	3:D:205:LEU:HD12	1.86	0.57
3:D:43:THR:OG1	3:D:50:ASN:ND2	2.38	0.57
2:C:474:LEU:HD11	2:C:491:LEU:HD23	1.87	0.56
7:G:323:VAL:HG13	7:G:343:GLU:HG2	1.86	0.56
2:C:713:THR:O	2:C:713:THR:HG22	2.04	0.56
4:E:213:ARG:HD2	4:E:263:LEU:HD13	1.88	0.56
4:E:126:ASP:HA	4:E:158:LEU:HB2	1.86	0.56
2:C:296:THR:HG22	2:C:599:ILE:HD13	1.88	0.56
1:B:481:CYS:SG	2:C:312:HIS:ND1	2.79	0.55
1:B:436:ASN:ND2	1:B:467:ASP:OD2	2.39	0.55
7:G:295:VAL:HG12	7:G:433:MET:HB3	1.89	0.55
7:G:259:LEU:O	7:G:450:ARG:NH1	2.40	0.55
7:G:422:LEU:HD22	7:G:428:LEU:HB3	1.89	0.55
6:A:694:GLN:NE2	6:A:726:LEU:O	2.40	0.55
2:C:136:ASP:HB3	2:C:146:THR:HG21	1.88	0.54
6:A:768:ALA:HB1	6:A:810:VAL:HG21	1.89	0.54
2:C:105:ILE:HG23	4:E:413:LEU:HD11	1.88	0.54
2:C:456:LYS:HE3	2:C:505:VAL:HG22	1.89	0.54
3:D:217:ASP:OD1	3:D:220:ARG:NH1	2.40	0.54
2:C:99:ALA:HB3	2:C:239:VAL:HG12	1.90	0.54
2:C:411:THR:HG21	2:C:426:ARG:HA	1.90	0.54
2:C:286:PRO:HG3	2:C:404:ARG:HG2	1.88	0.53
2:C:658:MET:CE	2:C:712:LYS:HD2	2.38	0.53
4:E:222:THR:OG1	4:E:223:GLU:N	2.41	0.53
3:D:17:GLU:OE2	3:D:21:ARG:NH1	2.41	0.53
6:A:635:MET:HG2	6:A:688:ILE:HG13	1.90	0.53
4:E:174:GLU:OE2	6:A:880:ARG:NH1	2.42	0.53
2:C:709:SER:OG	2:C:715:HIS:CA	2.56	0.52
7:G:262:ALA:O	10:G:901:ATP:O2'	2.27	0.52
2:C:713:THR:O	2:C:715:HIS:HD2	1.92	0.52
4:E:259:LEU:HG	4:E:263:LEU:HG	1.92	0.52
4:E:276:TRP:O	4:E:280:ALA:HB2	2.09	0.52
7:G:609:VAL:HG12	7:G:620:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:MET:HA	1:B:420:GLU:HG2	1.92	0.52
4:E:38:TYR:OH	4:E:159:SER:OG	2.29	0.52
6:A:577:ASN:HD22	6:A:740:LEU:HD13	1.75	0.51
7:G:368:LYS:HE2	7:G:369:ARG:HG3	1.92	0.51
1:B:577:GLN:NE2	1:B:580:GLU:OE1	2.43	0.51
3:D:12:ARG:NH1	4:E:31:GLU:OE2	2.43	0.51
7:G:637:GLU:O	7:G:641:HIS:ND1	2.40	0.51
3:D:334:ASP:OD2	3:D:435:GLN:NE2	2.44	0.51
3:D:344:SER:OG	3:D:347:GLU:OE1	2.22	0.51
4:E:145:LEU:HB3	4:E:153:LEU:HD11	1.92	0.51
2:C:302:HIS:O	2:C:306:TYR:HB2	2.10	0.51
1:B:520:ARG:HG2	1:B:611:PHE:HE1	1.76	0.51
2:C:106:ASN:ND2	2:C:309:PHE:O	2.44	0.51
7:G:411:SER:HB3	7:G:414:LEU:HB2	1.93	0.50
3:D:43:THR:HG21	3:D:176:CYS:HB2	1.93	0.50
3:D:383:THR:H	3:D:386:GLN:HE21	1.59	0.50
6:A:593:CYS:SG	6:A:594:MET:N	2.85	0.50
6:A:596:VAL:HG12	6:A:740:LEU:HB3	1.94	0.50
7:G:411:SER:OG	7:G:417:ARG:NH2	2.45	0.50
2:C:70:ARG:NH2	2:C:277:GLU:OE2	2.45	0.49
6:A:838:GLN:HE21	6:A:917:LEU:HD13	1.76	0.49
3:D:446:LEU:HD12	3:D:447:PRO:HD2	1.94	0.49
2:C:494:LYS:HE3	2:C:580:HIS:HE1	1.78	0.49
3:D:36:VAL:HG22	3:D:52:LEU:HD21	1.93	0.49
7:G:426:CYS:HA	7:G:429:LYS:HE2	1.93	0.49
2:C:19:THR:OG1	2:C:20:ARG:N	2.46	0.49
2:C:425:LEU:HD22	2:C:427:ARG:HE	1.78	0.49
2:C:588:PRO:HB3	2:C:589:PRO:HD2	1.93	0.49
6:A:579:TYR:OH	6:A:618:MET:SD	2.64	0.49
7:G:285:LEU:HD21	7:G:320:LEU:HD23	1.95	0.48
7:G:559:GLN:OE1	7:G:588:TYR:OH	2.29	0.48
2:C:709:SER:OG	2:C:715:HIS:N	2.46	0.48
2:C:658:MET:HE1	2:C:712:LYS:HD2	1.94	0.48
4:E:51:THR:HG21	4:E:158:LEU:HD21	1.96	0.48
1:B:377:THR:HG23	2:C:15:LYS:HA	1.96	0.48
2:C:713:THR:O	2:C:715:HIS:CD2	2.67	0.48
7:G:378:ILE:HG22	7:G:409:ALA:HB2	1.95	0.48
7:G:600:LEU:HB3	7:G:604:GLU:HB2	1.96	0.47
3:D:347:GLU:HB3	3:D:400:LEU:HD21	1.95	0.47
6:A:695:ASP:OD1	6:A:695:ASP:N	2.42	0.47
6:A:789:ILE:HG12	6:A:817:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:587:ALA:HB3	2:C:591:HIS:ND1	2.30	0.47
10:D:901:ATP:O1G	4:E:144:ARG:NH1	2.46	0.47
5:F:223:GLU:HB2	5:F:227:ILE:HD11	1.97	0.47
1:B:347:LEU:HD22	1:B:461:HIS:HB3	1.97	0.46
3:D:346:LEU:HD11	3:D:393:VAL:HG22	1.96	0.46
4:E:279:ILE:HG13	4:E:283:LEU:HG	1.96	0.46
7:G:452:ALA:HB2	7:G:457:LEU:HD21	1.98	0.46
3:D:390:ARG:NH2	3:D:423:GLU:OE2	2.42	0.46
4:E:406:GLN:HA	4:E:409:THR:HG22	1.97	0.46
4:E:279:ILE:HD12	4:E:282:PRO:HG2	1.98	0.46
6:A:822:LYS:HD3	6:A:908:VAL:HG23	1.98	0.46
2:C:379:LEU:HD13	5:F:229:LYS:HG3	1.98	0.46
3:D:408:PRO:HB2	3:D:410:THR:HG23	1.98	0.45
9:I:66:DA:C6	9:I:67:DA:C6	3.04	0.45
6:A:591:GLY:HA2	6:A:712:VAL:HG22	1.97	0.45
2:C:64:ILE:HG21	2:C:315:ILE:HD11	1.97	0.45
6:A:891:ILE:HG22	6:A:906:LEU:HD12	1.98	0.45
7:G:328:THR:HG22	7:G:380:GLN:HG3	1.99	0.45
2:C:711:ARG:NH2	9:I:44:DA:O4'	2.34	0.45
1:B:522:VAL:HG23	7:G:412:LEU:HD23	1.99	0.45
4:E:335:ALA:O	4:E:384:ARG:NH1	2.47	0.45
6:A:892:ILE:HB	6:A:905:LEU:HB2	1.98	0.45
1:B:585:LYS:HB2	1:B:585:LYS:HE2	1.79	0.45
3:D:54:LEU:HB2	3:D:180:VAL:HG22	1.98	0.45
3:D:96:ASP:O	3:D:100:LEU:HB2	2.18	0.44
3:D:384:THR:HG23	3:D:385:MET:HG2	1.99	0.44
7:G:278:ARG:NH1	7:G:313:ASP:OD2	2.50	0.44
3:D:289:GLN:NE2	3:D:293:ASP:OD1	2.49	0.44
6:A:702:ASP:O	6:A:705:THR:OG1	2.30	0.44
1:B:542:LEU:HD12	1:B:612:LEU:HD13	1.99	0.44
2:C:467:LEU:HD13	2:C:495:LEU:HD22	1.99	0.44
1:B:397:ILE:HA	1:B:401:ILE:HD13	2.00	0.44
4:E:115:ARG:HD2	4:E:115:ARG:HA	1.71	0.44
1:B:457:ILE:HD12	1:B:460:ILE:HD12	2.00	0.43
1:B:358:LEU:O	1:B:496:TYR:OH	2.35	0.43
1:B:438:ASP:HB3	1:B:471:THR:HG23	2.01	0.43
3:D:313:ARG:NH2	4:E:24:GLU:HG2	2.33	0.43
3:D:231:LEU:HD22	3:D:258:PRO:HB2	2.00	0.43
3:D:344:SER:HB3	4:E:242:ARG:HG3	2.01	0.43
6:A:806:THR:OG1	6:A:807:MET:N	2.52	0.43
2:C:131:VAL:HG22	2:C:208:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:353:MET:HA	2:C:356:ILE:HG12	2.00	0.43
9:I:66:DA:C2	9:I:67:DA:C4	3.06	0.43
1:B:472:PRO:HG2	4:E:404:LEU:HD12	1.99	0.43
2:C:494:LYS:HE3	2:C:580:HIS:CE1	2.54	0.43
1:B:422:PHE:O	1:B:459:ASN:ND2	2.51	0.43
2:C:221:GLN:HG2	2:C:257:VAL:HG21	2.01	0.43
7:G:252:TYR:OH	7:G:527:LYS:O	2.31	0.43
7:G:340:LEU:HD23	7:G:360:ILE:HD13	2.01	0.43
1:B:542:LEU:HD23	1:B:542:LEU:HA	1.89	0.42
7:G:440:LYS:HD2	7:G:470:ALA:HB2	2.02	0.42
2:C:584:LEU:HD11	2:C:595:VAL:HG21	2.01	0.42
4:E:88:LEU:HD22	4:E:121:PHE:HD2	1.84	0.42
1:B:555:PHE:HB2	1:B:597:GLU:HB3	2.00	0.42
4:E:276:TRP:O	4:E:280:ALA:CB	2.67	0.42
1:B:358:LEU:H	1:B:491:THR:HG23	1.85	0.42
2:C:345:ILE:HD11	2:C:393:LEU:HD22	2.02	0.42
2:C:456:LYS:HE2	2:C:456:LYS:HB3	1.82	0.42
7:G:255:ALA:HA	7:G:258:VAL:HG12	2.01	0.42
1:B:286:SER:OG	2:C:721:TRP:NE1	2.48	0.42
2:C:129:VAL:HG22	2:C:206:VAL:HB	2.01	0.42
2:C:457:ASP:N	2:C:457:ASP:OD1	2.53	0.42
6:A:737:LEU:HD13	7:G:541:VAL:HG11	2.01	0.41
6:A:588:ASP:OD2	7:G:256:ARG:NE	2.52	0.41
10:G:901:ATP:H8	10:G:901:ATP:H5'1	1.85	0.41
4:E:97:LYS:HE3	4:E:97:LYS:HB2	1.87	0.41
2:C:57:TRP:HH2	2:C:315:ILE:HG23	1.85	0.41
2:C:253:LEU:O	3:D:395:LYS:NZ	2.53	0.41
6:A:725:ARG:NH1	7:G:634:GLN:OE1	2.54	0.41
7:G:415:THR:HG22	7:G:419:LEU:HD12	2.03	0.41
1:B:442:LEU:O	1:B:448:GLN:NE2	2.41	0.41
2:C:635:GLN:O	2:C:650:LYS:NZ	2.53	0.41
2:C:711:ARG:HD3	9:I:45:DA:H5'	2.02	0.41
7:G:251:LYS:HD2	7:G:456:VAL:HG13	2.03	0.41
2:C:140:LEU:HD11	2:C:226:ILE:HD12	2.02	0.41
4:E:184:ASN:OD1	4:E:184:ASN:N	2.54	0.41
4:E:191:ILE:O	4:E:194:SER:OG	2.38	0.41
4:E:290:ILE:HD12	4:E:290:ILE:HA	1.91	0.41
1:B:361:LYS:HE2	1:B:361:LYS:HB2	1.92	0.41
1:B:568:VAL:HG21	1:B:574:LEU:HB2	2.03	0.40
2:C:102:LEU:HD23	2:C:102:LEU:HA	1.94	0.40
4:E:123:ILE:O	4:E:156:ILE:N	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:398:LEU:HD12	7:G:399:PRO:HD2	2.03	0.40
3:D:201:ARG:NH1	6:A:795:GLU:OE1	2.54	0.40
1:B:416:ASP:OD1	1:B:453:ARG:NH2	2.37	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	B	275/618 (44%)	269 (98%)	6 (2%)	0	100	100
2	C	600/721 (83%)	584 (97%)	16 (3%)	0	100	100
3	D	435/462 (94%)	419 (96%)	16 (4%)	0	100	100
4	E	388/460 (84%)	373 (96%)	15 (4%)	0	100	100
5	F	15/257 (6%)	15 (100%)	0	0	100	100
6	A	399/488 (82%)	391 (98%)	8 (2%)	0	100	100
7	G	366/424 (86%)	360 (98%)	6 (2%)	0	100	100
All	All	2478/3430 (72%)	2411 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	256/545 (47%)	255 (100%)	1 (0%)	91	95
2	C	541/636 (85%)	541 (100%)	0	100	100
3	D	389/400 (97%)	389 (100%)	0	100	100
4	E	347/402 (86%)	347 (100%)	0	100	100
5	F	13/227 (6%)	13 (100%)	0	100	100
6	A	341/422 (81%)	339 (99%)	2 (1%)	86	94
7	G	331/374 (88%)	330 (100%)	1 (0%)	92	96
All	All	2218/3006 (74%)	2214 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	591	ARG
6	A	693	ARG
6	A	738	THR
7	G	322	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	366	GLN
1	B	429	HIS
1	B	544	ASN
1	B	609	GLN
2	C	133	GLN
2	C	194	ASN
2	C	370	ASN
2	C	449	GLN
2	C	580	HIS
2	C	619	ASN
2	C	666	GLN
2	C	715	HIS
4	E	68	HIS
4	E	137	ASN
6	A	577	ASN
6	A	838	GLN
7	G	260	ASN
7	G	410	ASN
7	G	573	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ATP	D	901	11	26,33,33	0.93	1 (3%)	31,52,52	1.42	5 (16%)
10	ATP	G	901	11	26,33,33	0.91	1 (3%)	31,52,52	1.54	7 (22%)
10	ATP	E	901	11	26,33,33	0.91	1 (3%)	31,52,52	1.44	5 (16%)
10	ATP	A	1001	11	26,33,33	0.91	1 (3%)	31,52,52	1.58	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ATP	D	901	11	-	5/18/38/38	0/3/3/3
10	ATP	G	901	11	-	5/18/38/38	0/3/3/3
10	ATP	E	901	11	-	5/18/38/38	0/3/3/3
10	ATP	A	1001	11	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	901	ATP	C5-C4	2.37	1.47	1.40
10	E	901	ATP	C5-C4	2.31	1.47	1.40
10	A	1001	ATP	C5-C4	2.30	1.47	1.40
10	G	901	ATP	C5-C4	2.28	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1001	ATP	PA-O3A-PB	-3.95	119.26	132.83
10	D	901	ATP	PB-O3B-PG	-3.57	120.57	132.83
10	A	1001	ATP	C3'-C2'-C1'	3.50	106.24	100.98
10	G	901	ATP	N3-C2-N1	-3.45	123.28	128.68
10	A	1001	ATP	N3-C2-N1	-3.42	123.33	128.68
10	E	901	ATP	PA-O3A-PB	-3.28	121.59	132.83
10	G	901	ATP	PB-O3B-PG	-3.25	121.67	132.83
10	D	901	ATP	N3-C2-N1	-3.25	123.60	128.68
10	E	901	ATP	N3-C2-N1	-3.25	123.60	128.68
10	G	901	ATP	C3'-C2'-C1'	3.00	105.50	100.98
10	E	901	ATP	C3'-C2'-C1'	2.61	104.92	100.98
10	E	901	ATP	C4-C5-N7	-2.57	106.72	109.40
10	E	901	ATP	PB-O3B-PG	-2.46	124.37	132.83
10	D	901	ATP	C4-C5-N7	-2.38	106.92	109.40
10	G	901	ATP	C4-C5-N7	-2.37	106.93	109.40
10	A	1001	ATP	C4-C5-N7	-2.31	106.99	109.40
10	D	901	ATP	PA-O3A-PB	-2.25	125.09	132.83
10	G	901	ATP	O3G-PG-O2G	2.21	116.08	107.64
10	A	1001	ATP	PB-O3B-PG	-2.16	125.42	132.83
10	G	901	ATP	C2-N1-C6	2.11	122.36	118.75
10	G	901	ATP	PA-O3A-PB	-2.10	125.62	132.83
10	A	1001	ATP	C2-N1-C6	2.08	122.31	118.75
10	D	901	ATP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	901	ATP	C5'-O5'-PA-O1A
10	E	901	ATP	C5'-O5'-PA-O1A
10	E	901	ATP	C5'-O5'-PA-O2A
10	G	901	ATP	C5'-O5'-PA-O2A
10	D	901	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	G	901	ATP	O4'-C4'-C5'-O5'
10	D	901	ATP	C3'-C4'-C5'-O5'
10	A	1001	ATP	PB-O3B-PG-O3G
10	D	901	ATP	C5'-O5'-PA-O3A
10	G	901	ATP	C5'-O5'-PA-O3A
10	E	901	ATP	PA-O3A-PB-O2B
10	G	901	ATP	PG-O3B-PB-O2B
10	G	901	ATP	C5'-O5'-PA-O1A
10	E	901	ATP	C5'-O5'-PA-O3A
10	D	901	ATP	PB-O3A-PA-O2A
10	E	901	ATP	PA-O3A-PB-O1B
10	A	1001	ATP	O4'-C4'-C5'-O5'

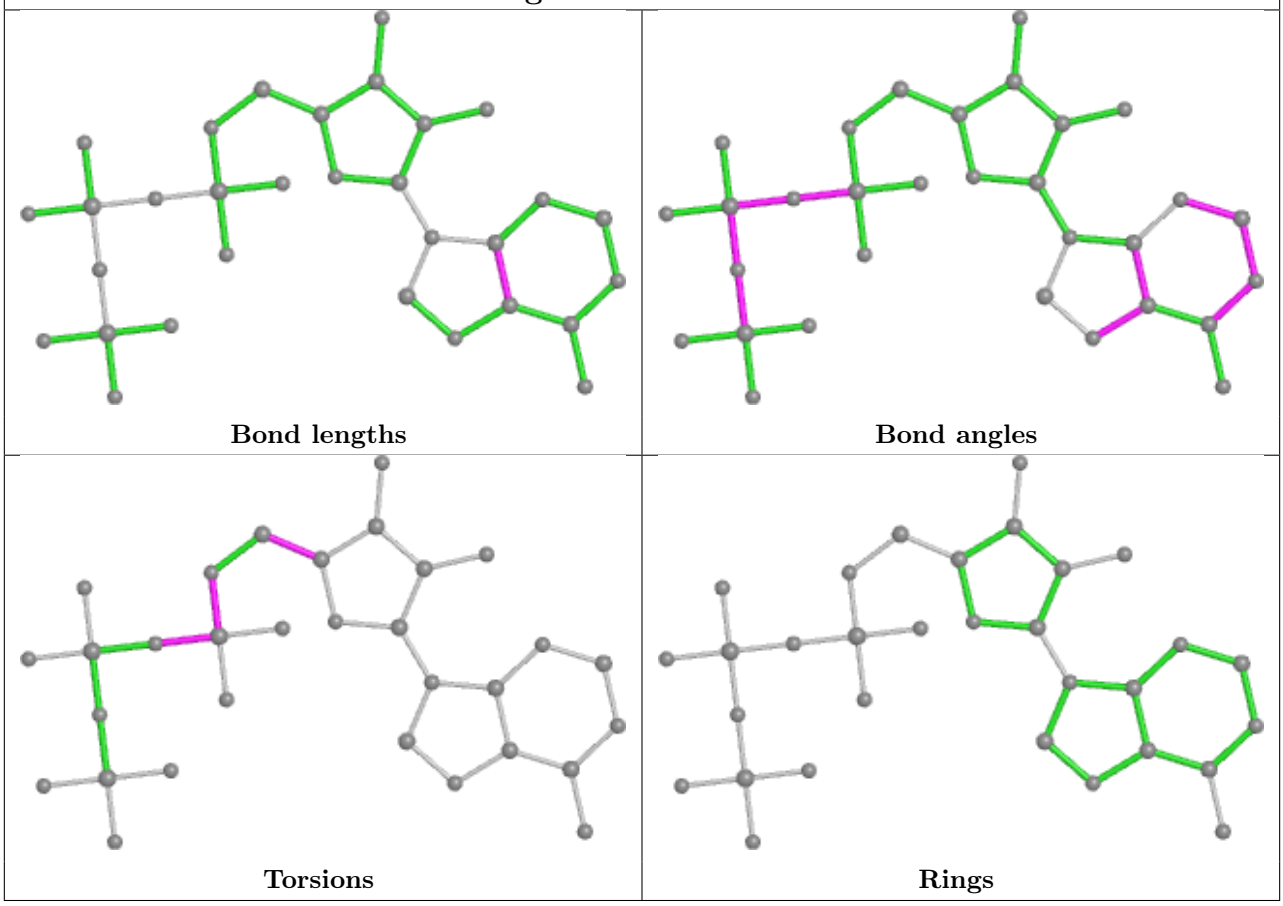
There are no ring outliers.

2 monomers are involved in 3 short contacts:

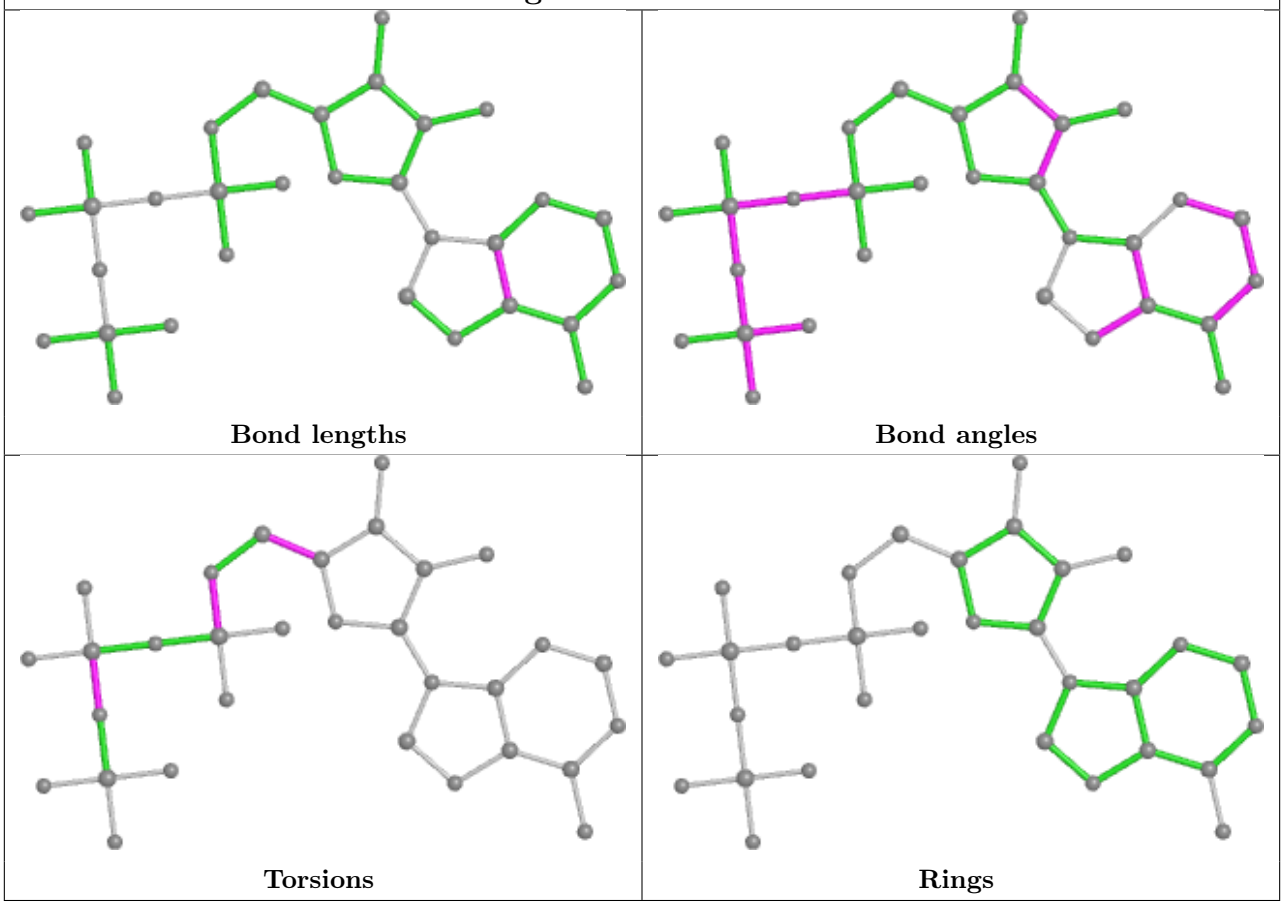
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	901	ATP	1	0
10	G	901	ATP	2	0

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 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.

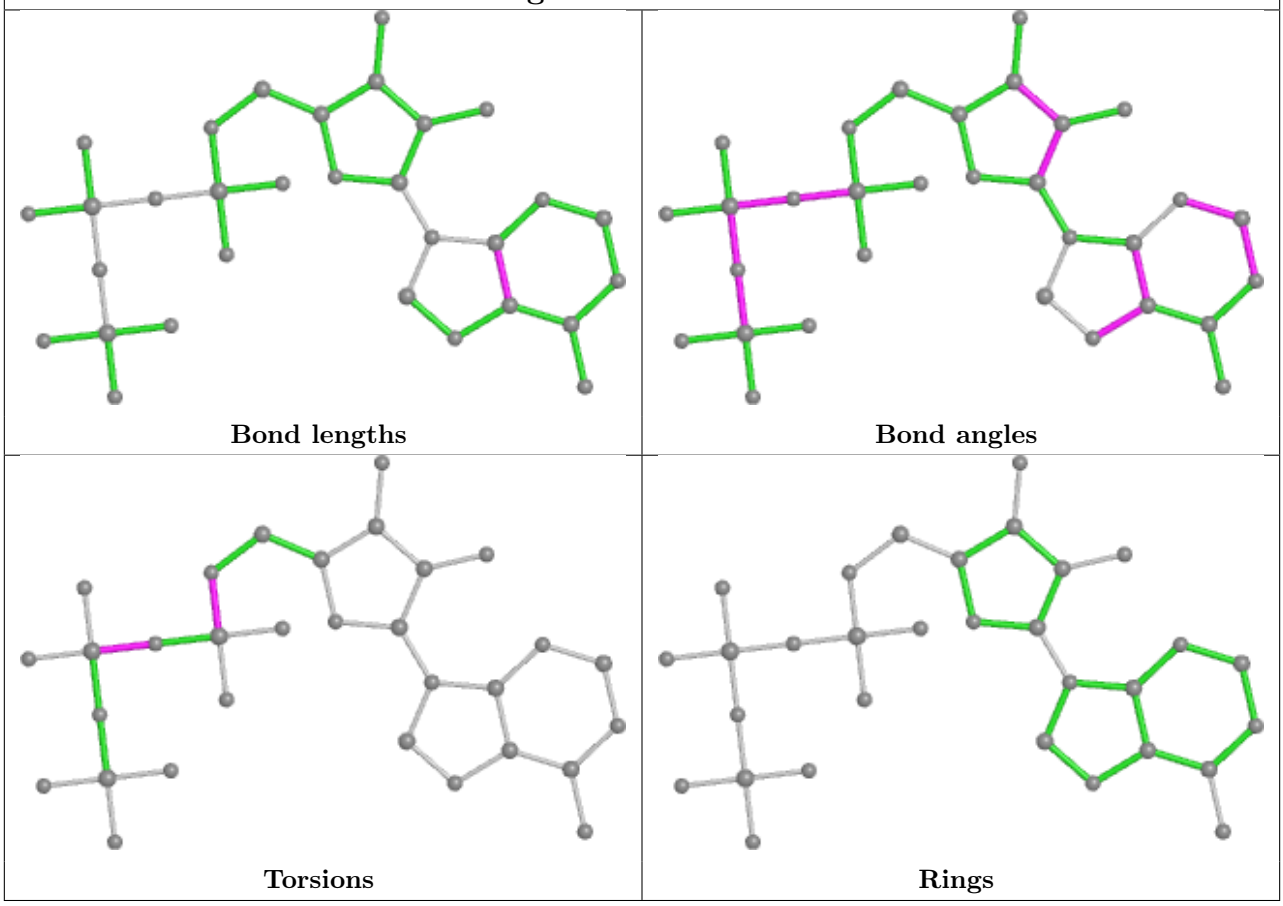
Ligand ATP D 901

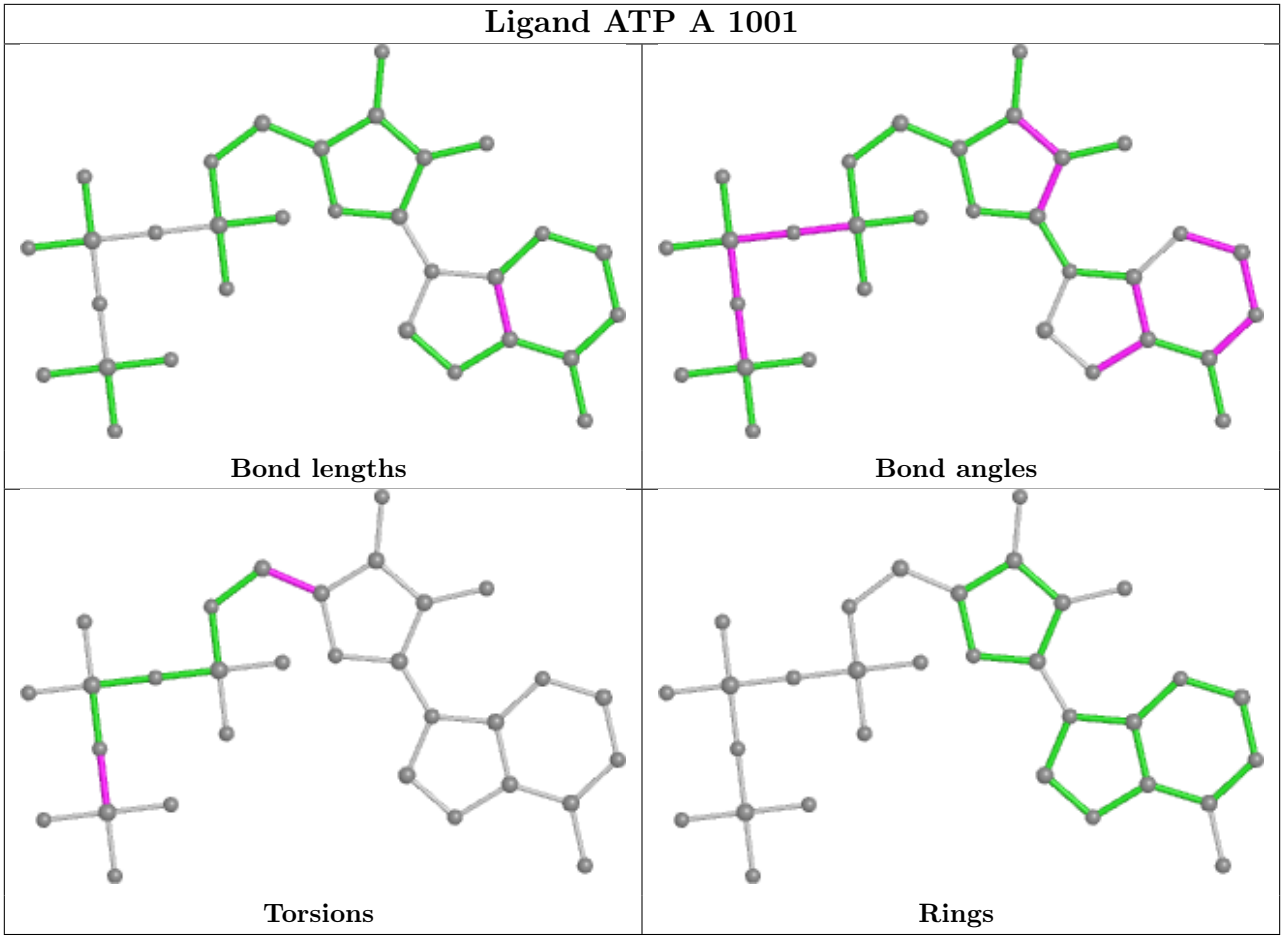


Ligand ATP G 901



Ligand ATP E 901





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.

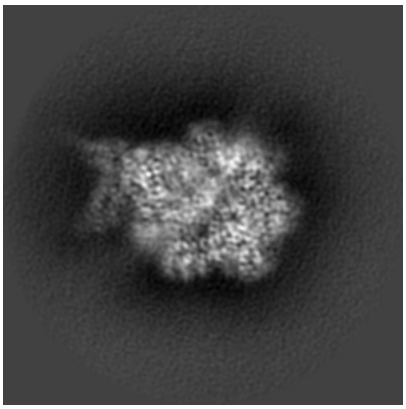
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22330. These allow visual inspection of the internal detail of the map and identification of artifacts.

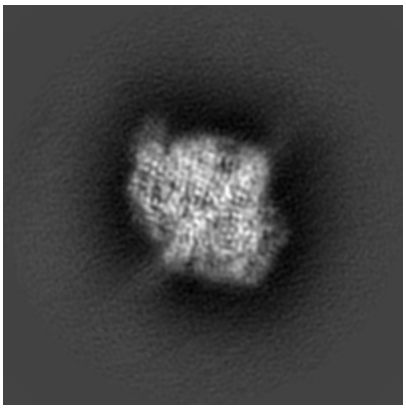
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

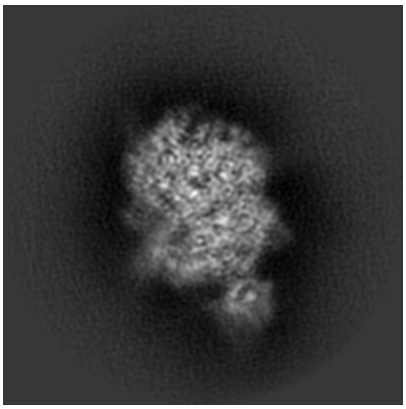
6.1.1 Primary map



X

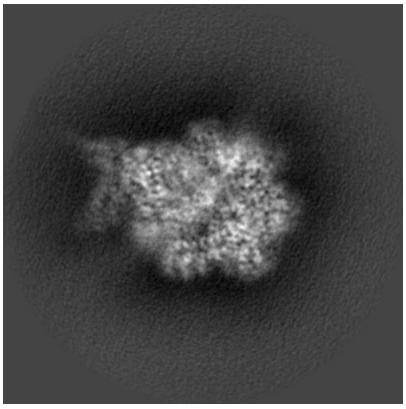


Y

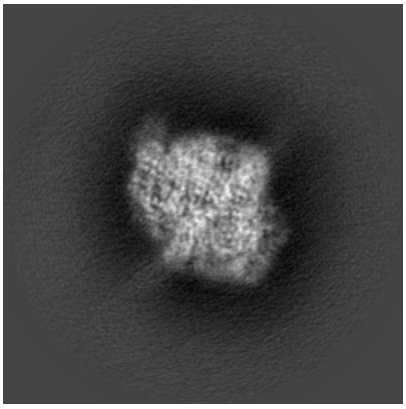


Z

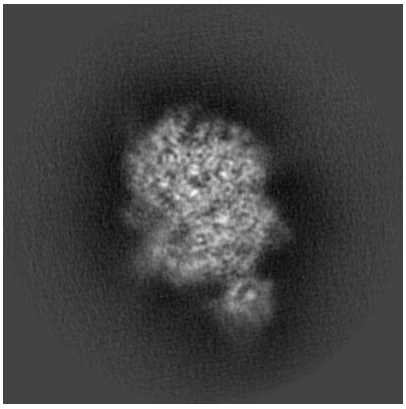
6.1.2 Raw map



X



Y

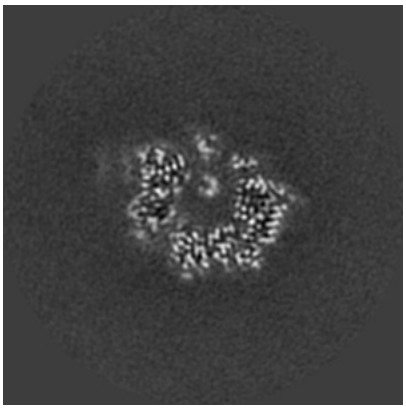


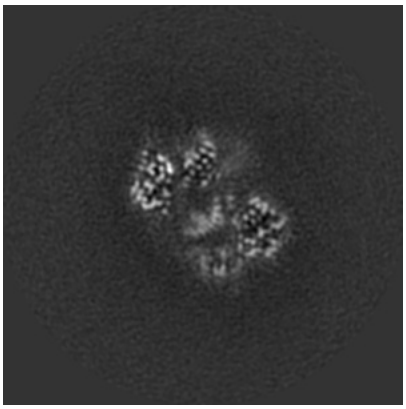
Z

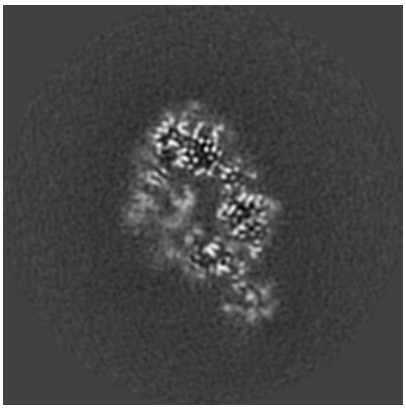
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

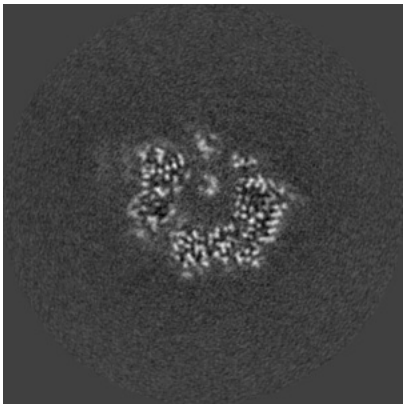
6.2.1 Primary map

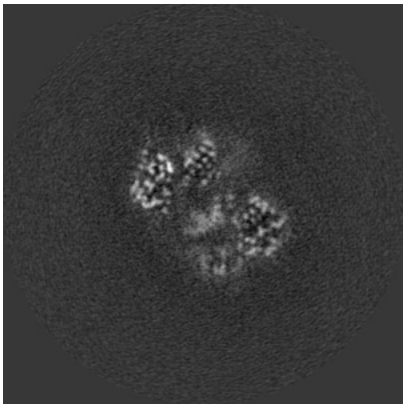

X Index: 150

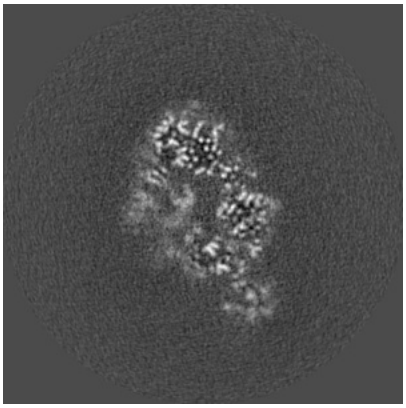

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

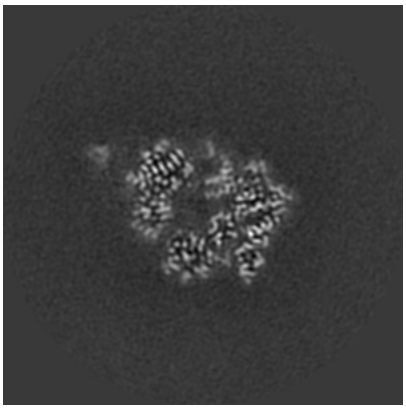

Y Index: 150

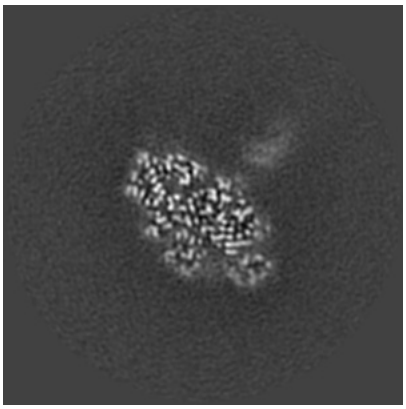

Z Index: 150

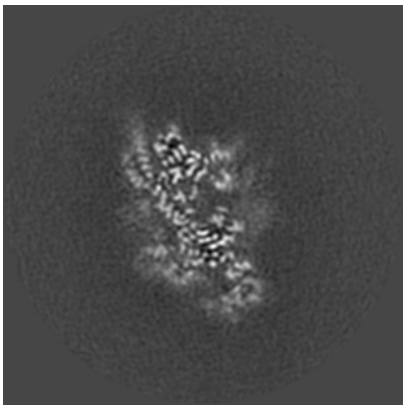
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

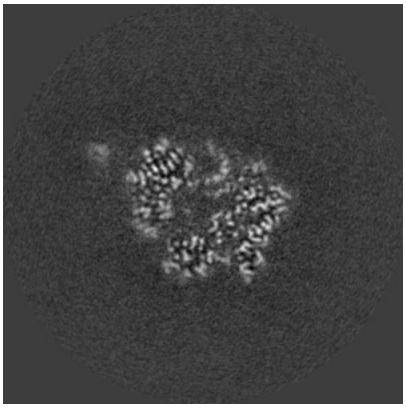
6.3.1 Primary map

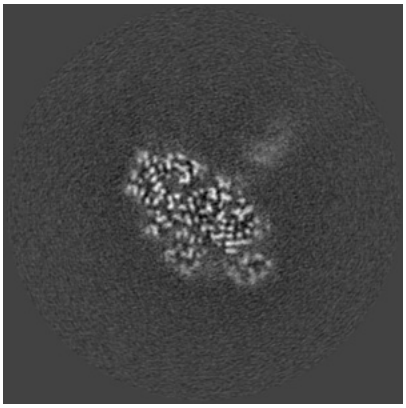

X Index: 158

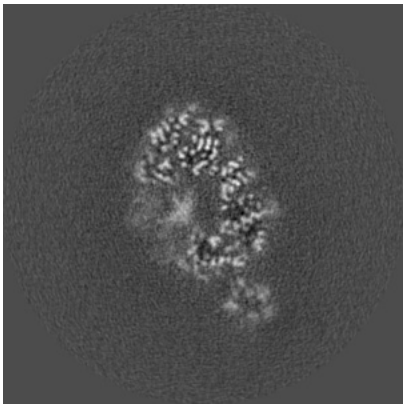

Y Index: 182


Z Index: 178

6.3.2 Raw map


X Index: 159

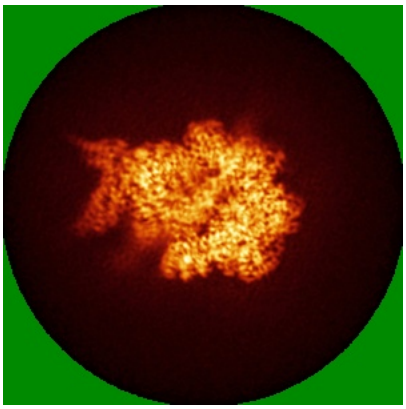

Y Index: 182

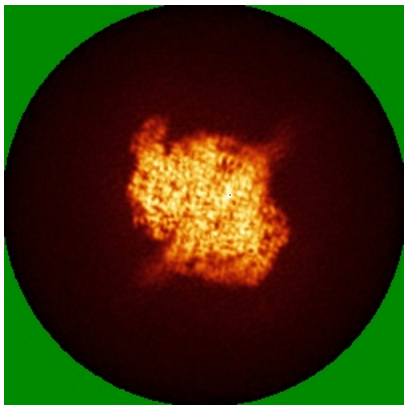

Z Index: 147

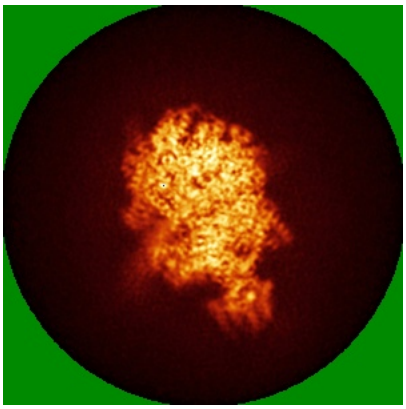
The images above show the largest variance slices of the map in three orthogonal directions.

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

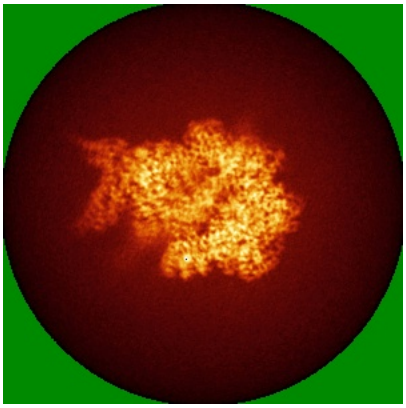
6.4.1 Primary map

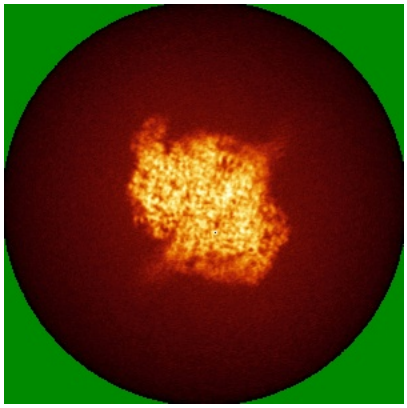

X

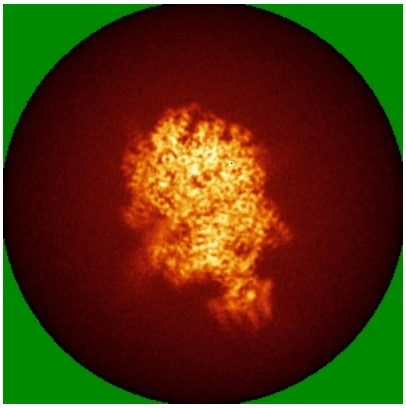

Y


Z

6.4.2 Raw map


X

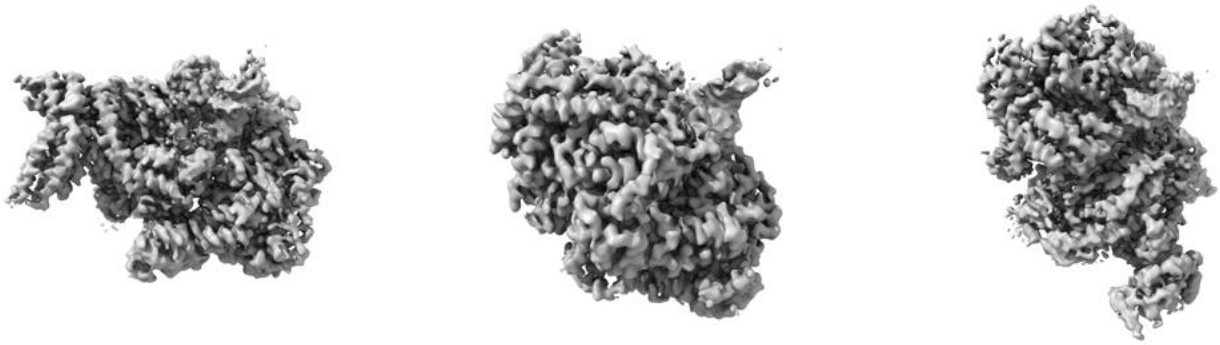

Y


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)

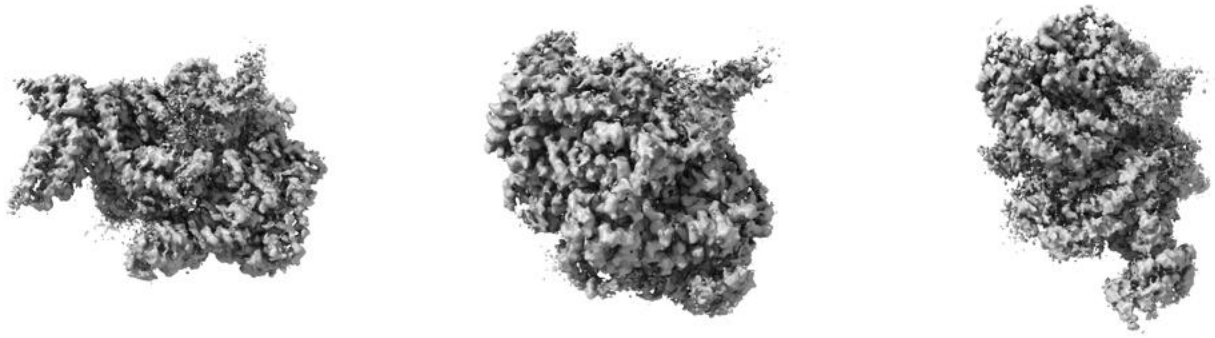
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

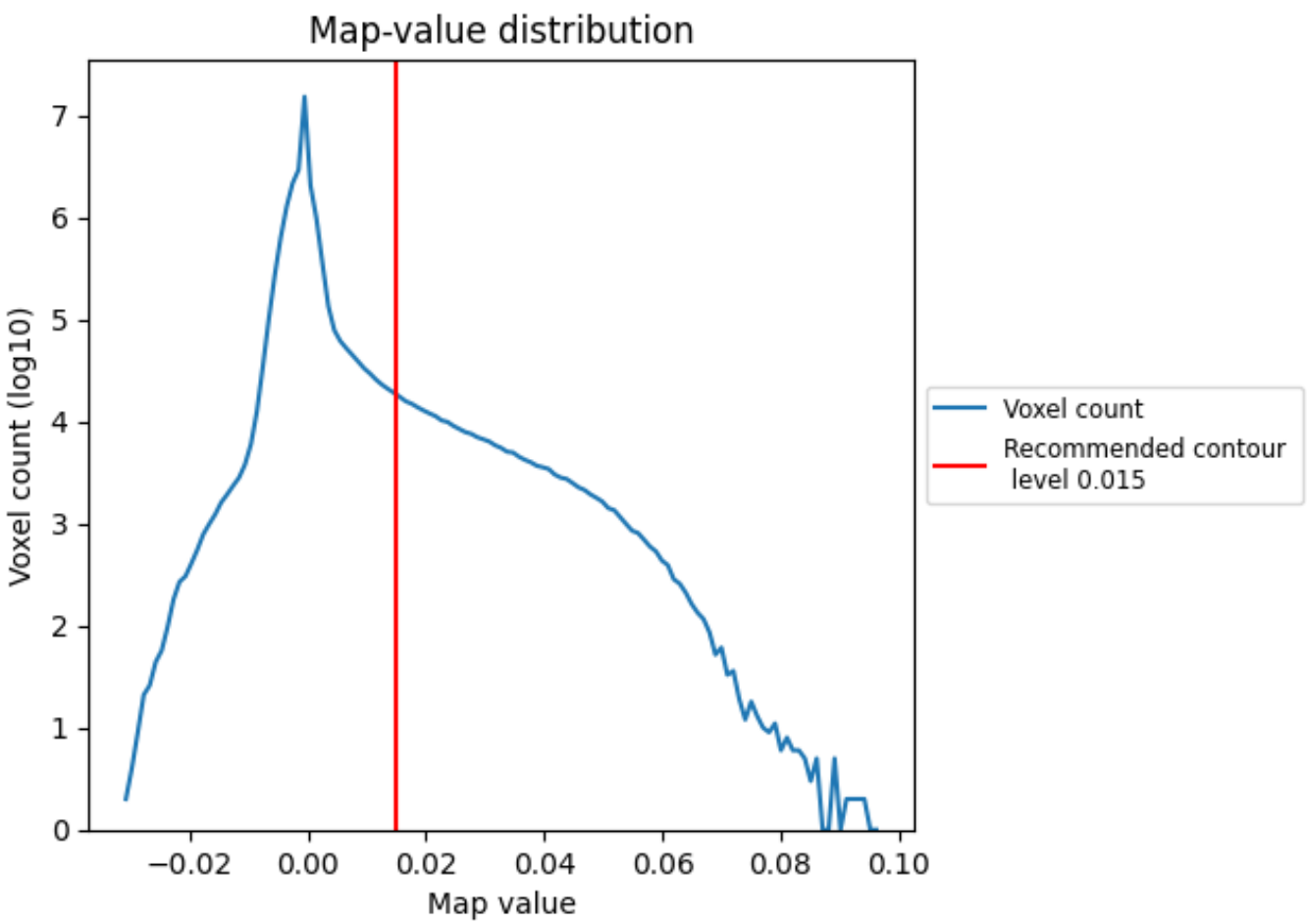
6.6 Mask visualisation (i)

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

7 Map analysis (i)

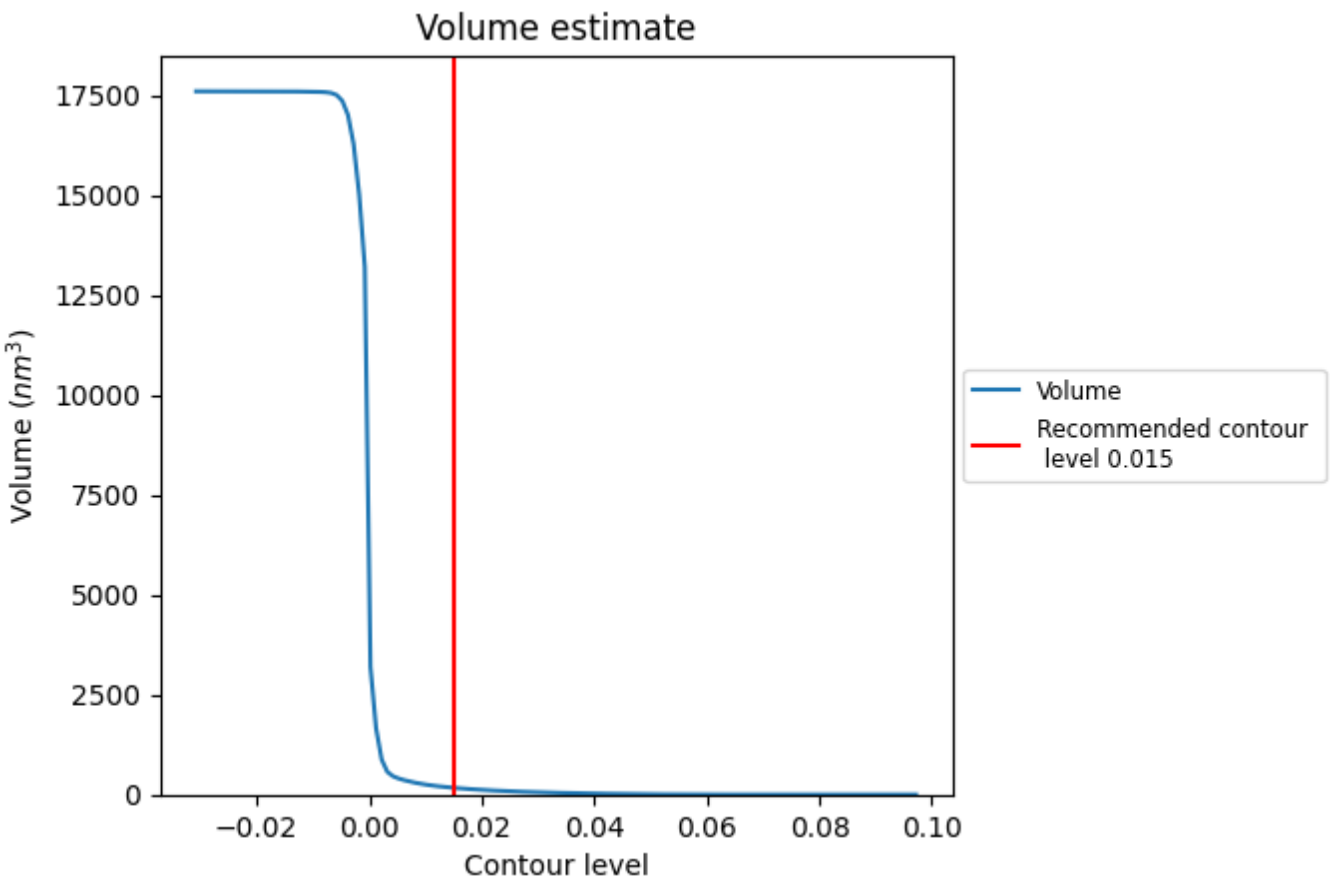
This section contains the results of statistical analysis of the map.

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.

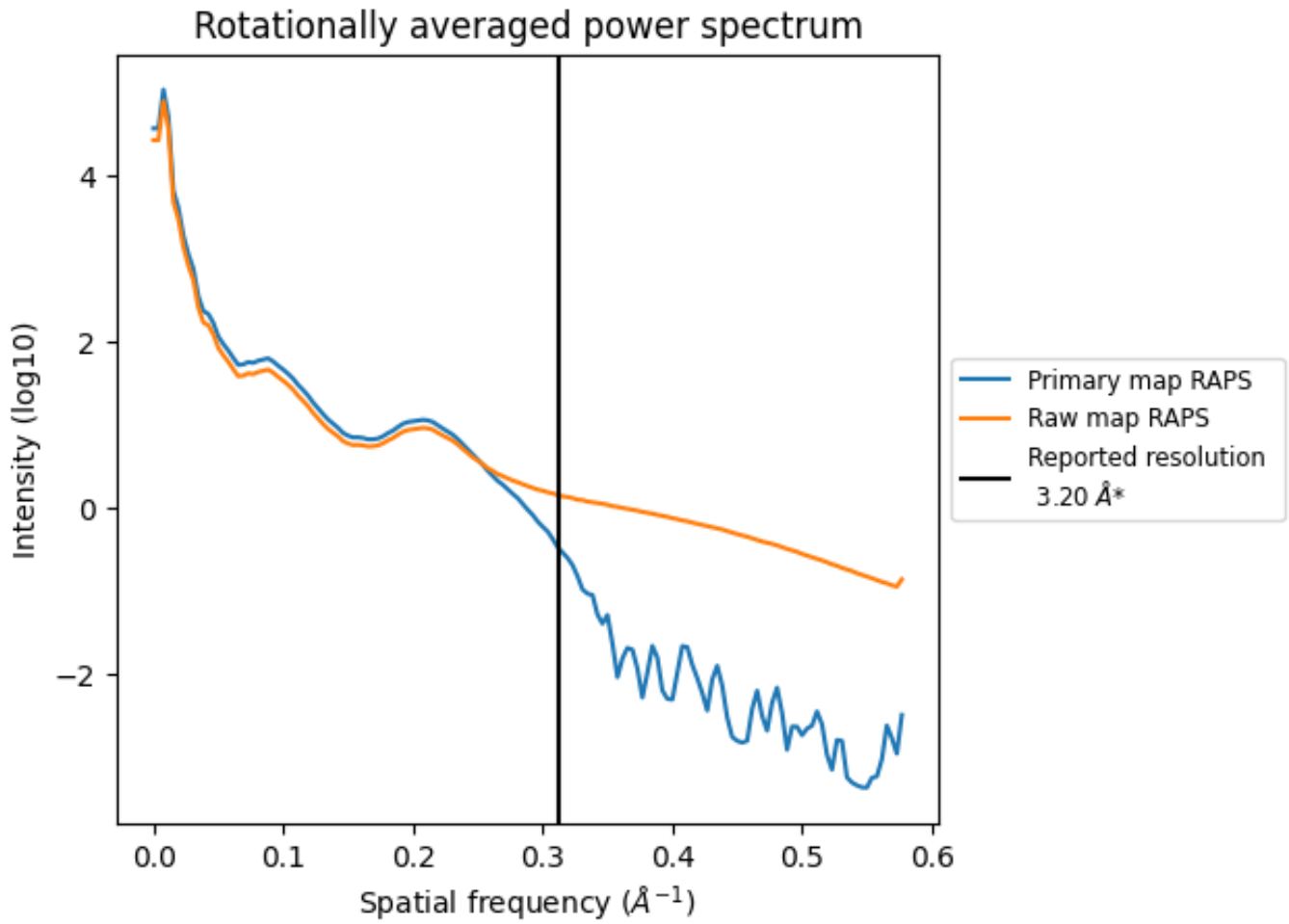
7.2 Volume estimate (i)



The volume at the recommended contour level is 169 nm^3; this corresponds to an approximate mass of 153 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)

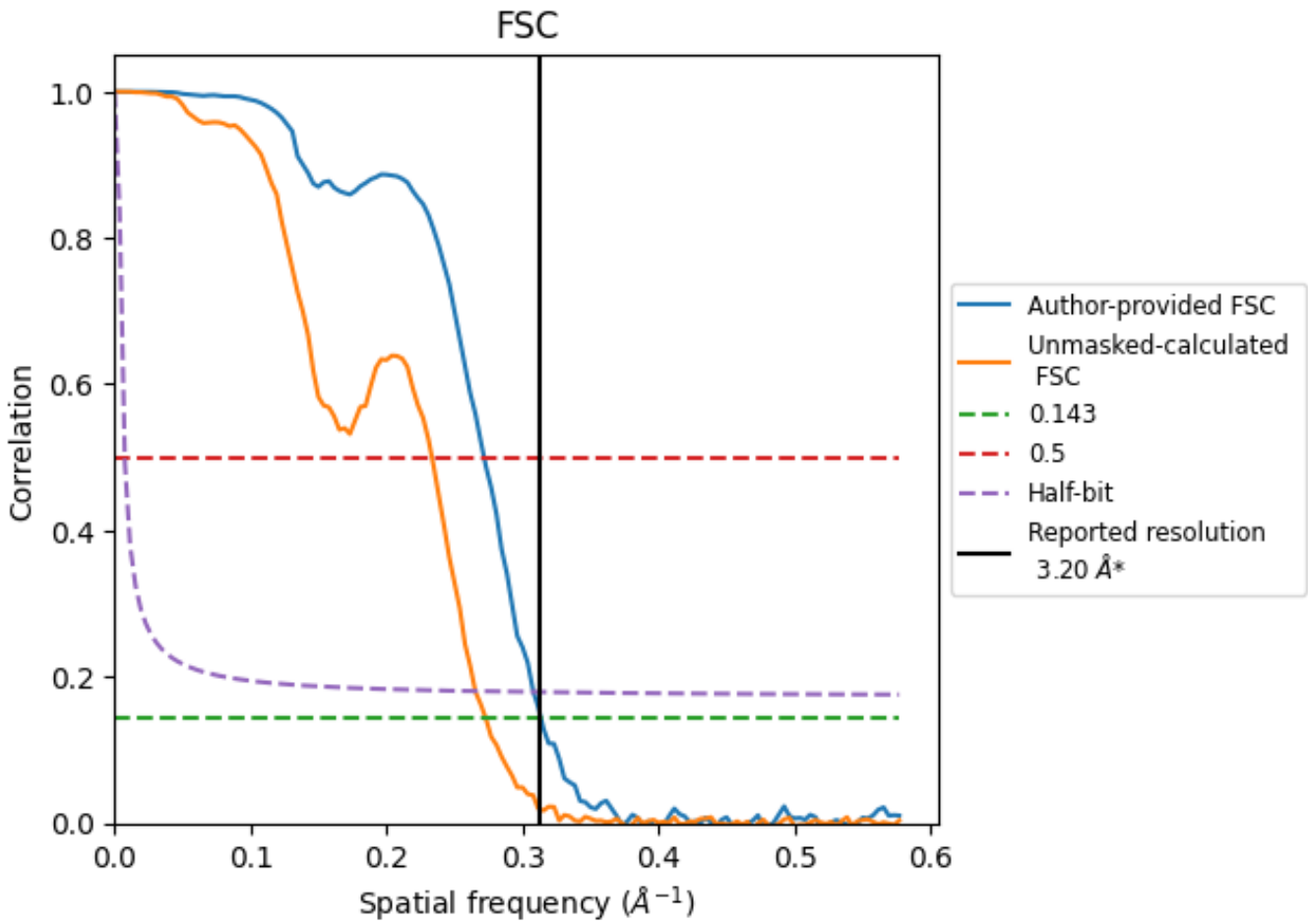


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

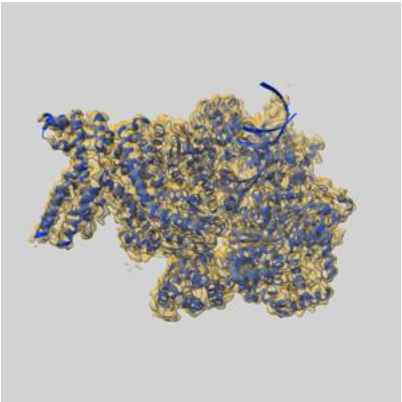
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.68	3.25
Unmasked-calculated*	3.66	4.29	3.77

*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 3.66 differs from the reported value 3.2 by more than 10 %

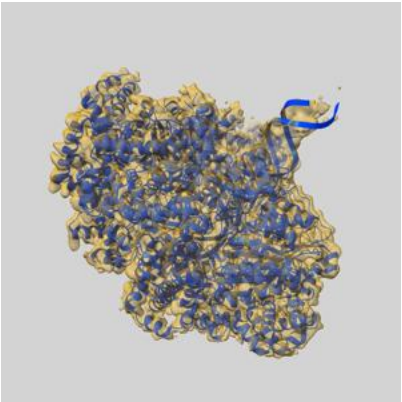
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22330 and PDB model 7JGS. Per-residue inclusion information can be found in section 3 on page 7.

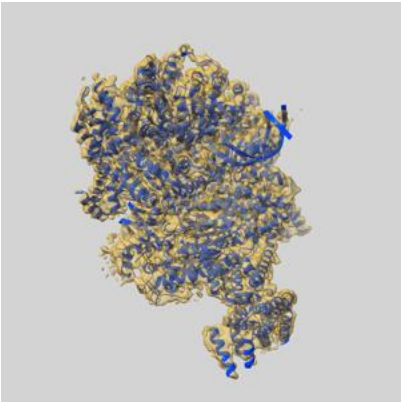
9.1 Map-model overlay (i)



X



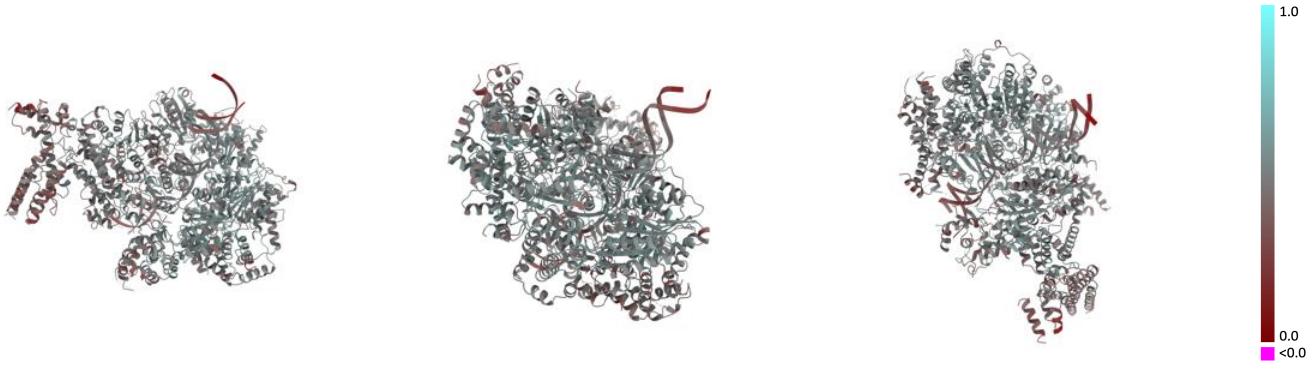
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

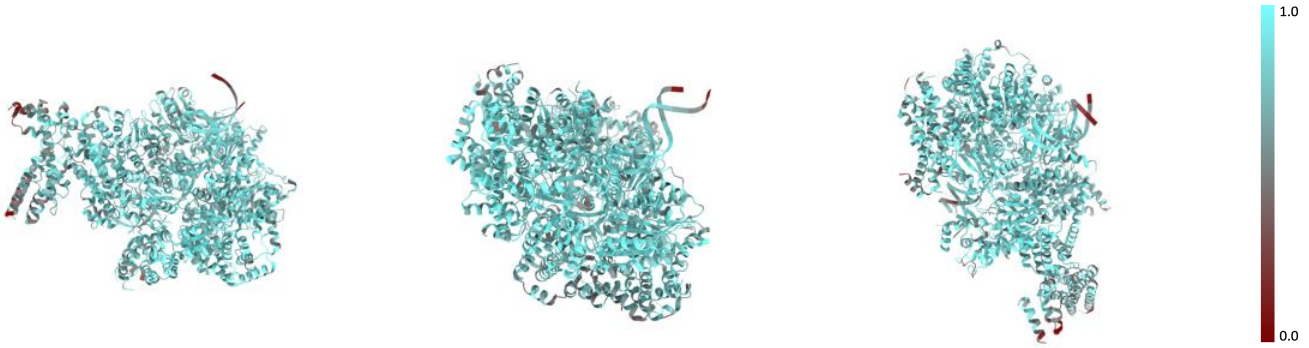
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

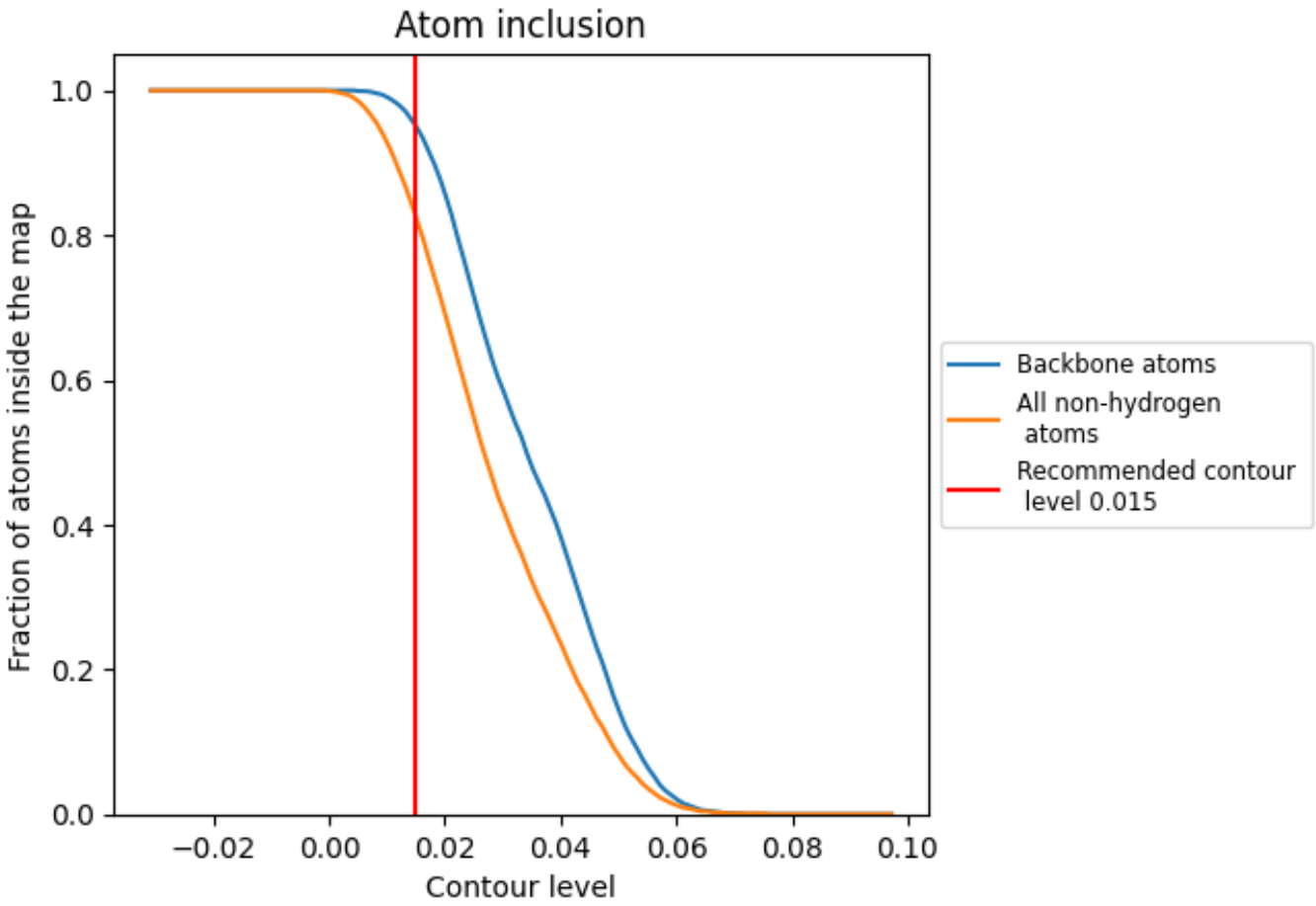
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.4800
A	0.8710	0.5130
B	0.8070	0.4780
C	0.7870	0.4560
D	0.8810	0.5160
E	0.8410	0.4940
F	0.6400	0.3460
G	0.7990	0.4830
H	0.7760	0.3740
I	0.8050	0.3760