



Full wwPDB EM Validation Report ⓘ

Oct 8, 2022 – 06:14 PM EDT

PDB ID : 7TJI
EMDB ID : EMD-25926
Title : *S. cerevisiae* ORC bound to 84 bp ARS1 DNA and Cdc6 (state 2) with flexible Orc6 N-terminal domain
Authors : Schmidt, J.M.; Yang, R.; Kumar, A.; Hunker, O.; Bleichert, F.
Deposited on : 2022-01-16
Resolution : 2.70 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 ⓘ 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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

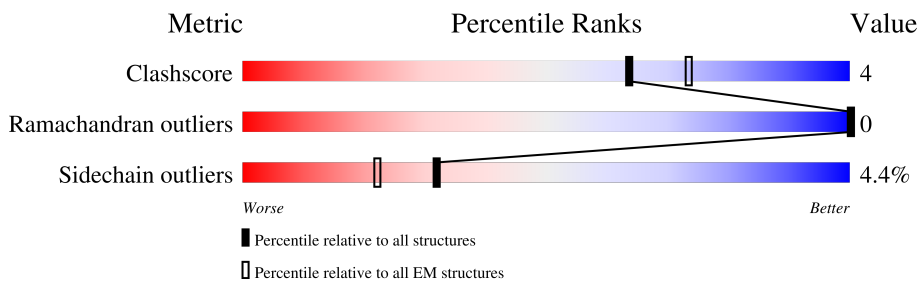
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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




Metric	Whole archive (#Entries)	EM structures (#Entries)
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 $\leq 5\%$. 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	917	
2	B	620	
3	C	616	
4	D	532	
5	E	479	
6	F	435	
7	G	84	
8	H	84	

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Mol	Chain	Length	Quality of chain
9	I	516	 <p>5% 58% 14% 27%</p>

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 23766 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	485	3885	2479	667	721	18	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P54784
A	-1	ASN	-	expression tag	UNP P54784
A	0	ALA	-	expression tag	UNP P54784

- Molecule 2 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	249	2066	1341	341	375	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	543	4497	2912	735	834	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	434	3543	2271	601	658	13	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP P54791

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASN	-	expression tag	UNP P54791
D	0	ALA	-	expression tag	UNP P54791

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	434	3562	2321	578	651	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	155	1300	837	220	232	11	0	0

- Molecule 7 is a DNA chain called DNA, 84 bp ARS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	G	41	832	405	132	255	40	0	0

- Molecule 8 is a DNA chain called DNA, 84 bp ARS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	H	41	846	405	165	235	41	0	0

- Molecule 9 is a protein called Cell division control protein 6.

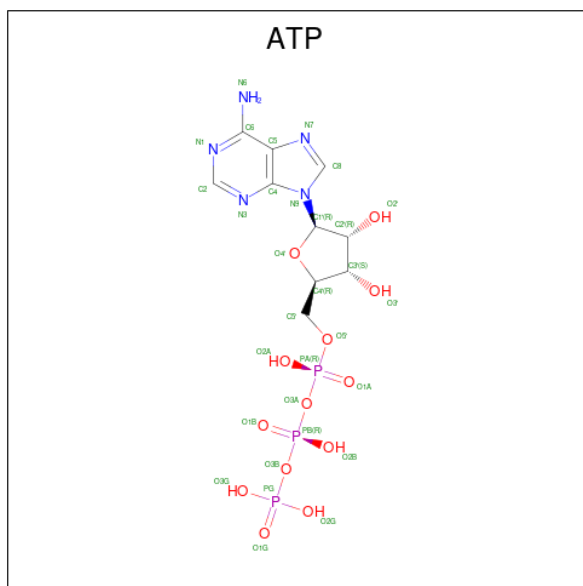
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	376	2995	1933	490	555	17	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	SER	-	expression tag	UNP P09119
I	-1	ASN	-	expression tag	UNP P09119
I	0	ALA	-	expression tag	UNP P09119

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
12	A	22	22	22	0

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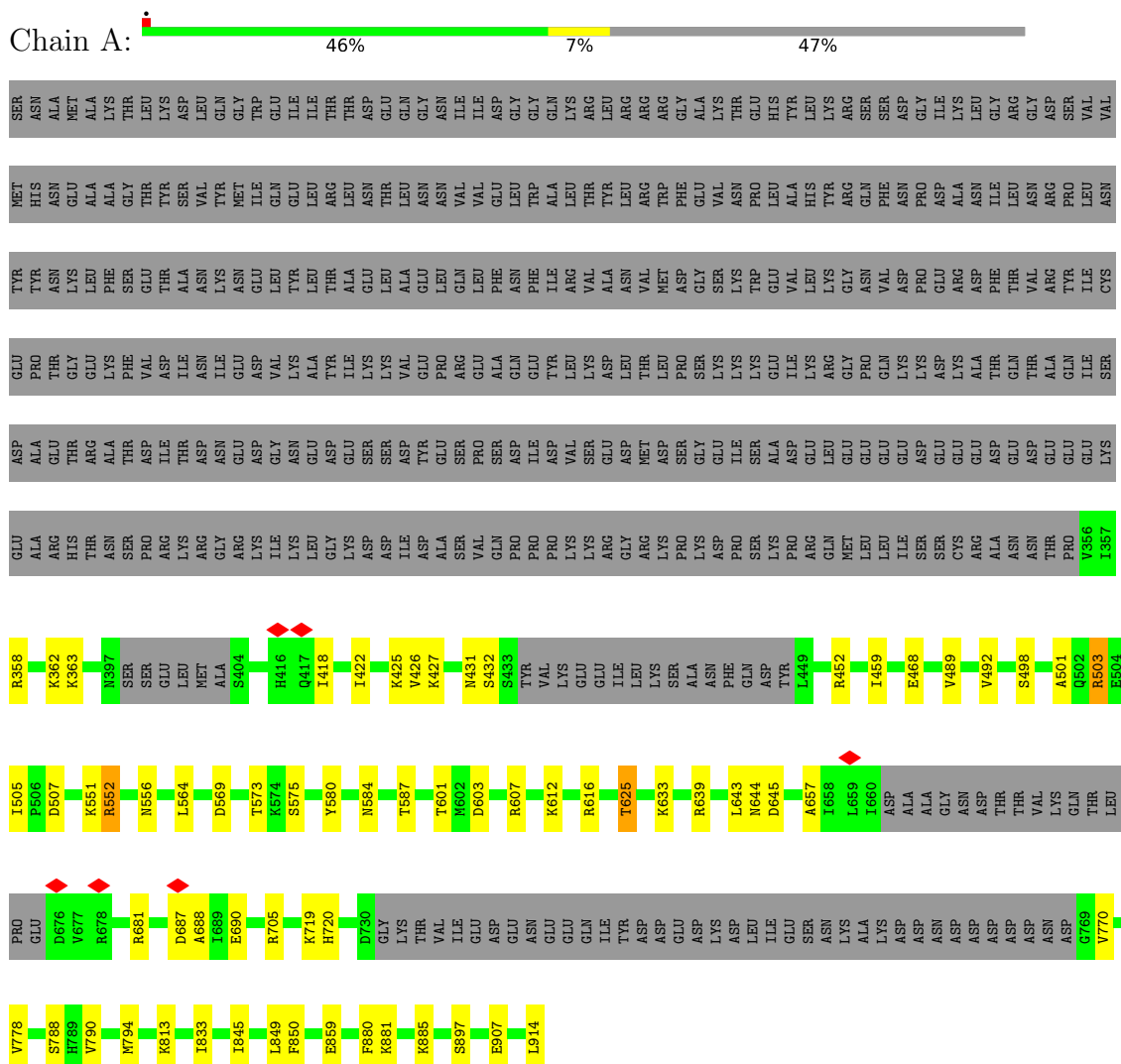
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Mol	Chain	Residues	Atoms		AltConf
12	B	5	Total 5	O 5	0
12	D	38	Total 38	O 38	0
12	E	30	Total 30	O 30	0
12	G	7	Total 7	O 7	0
12	H	6	Total 6	O 6	0
12	I	4	Total 4	O 4	0

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: Origin recognition complex subunit 1



- Molecule 2: Origin recognition complex subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	170092	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 ($e^-/\text{\AA}^2$)	6.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.30	0/3943	0.57	0/5301
2	B	0.33	0/2119	0.60	0/2865
3	C	0.32	0/4592	0.58	4/6193 (0.1%)
4	D	0.30	0/3605	0.54	0/4869
5	E	0.33	0/3644	0.59	2/4944 (0.0%)
6	F	0.27	0/1322	0.58	0/1781
7	G	0.64	0/928	1.09	0/1431
8	H	0.65	0/953	0.95	1/1468 (0.1%)
9	I	0.34	0/3038	0.62	1/4087 (0.0%)
All	All	0.35	0/24144	0.63	8/32939 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	111	ASP	CB-CG-OD1	8.25	125.72	118.30
5	E	195	ASP	CB-CG-OD1	6.47	124.13	118.30
3	C	268	VAL	CG1-CB-CG2	-6.46	100.57	110.90
9	I	248	LEU	CA-CB-CG	5.93	128.94	115.30
3	C	495	GLU	CA-CB-CG	5.71	125.95	113.40
8	H	44	DG	O4'-C1'-N9	5.24	111.67	108.00
3	C	526	LYS	CA-CB-CG	5.12	124.67	113.40
5	E	291	LEU	CA-CB-CG	5.02	126.84	115.30

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	3885	0	4002	33	0
2	B	2066	0	2038	25	0
3	C	4497	0	4465	53	0
4	D	3543	0	3603	21	0
5	E	3562	0	3605	31	0
6	F	1300	0	1338	18	0
7	G	832	0	474	7	0
8	H	846	0	462	3	0
9	I	2995	0	3113	47	0
10	A	31	0	12	0	0
10	D	31	0	12	0	0
10	E	31	0	12	0	0
10	I	31	0	12	0	0
11	A	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	I	1	0	0	0	0
12	A	22	0	0	0	0
12	B	5	0	0	0	0
12	D	38	0	0	0	0
12	E	30	0	0	0	0
12	G	7	0	0	0	0
12	H	6	0	0	0	0
12	I	4	0	0	0	0
All	All	23766	0	23148	202	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 (202) 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)
9:I:406:ARG:NH1	9:I:469:GLY:O	1.97	0.96
9:I:110:PRO:HD3	9:I:263:ASN:OD1	1.93	0.69
9:I:407:ILE:O	9:I:415:LYS:NZ	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:PHE:HB3	9:I:482:THR:HG21	1.77	0.65
1:A:468:GLU:HB3	1:A:505:ILE:HG22	1.80	0.62
3:C:145:ARG:NH2	7:G:36:DT:OP1	2.33	0.62
6:F:322:GLY:HA3	6:F:369:VAL:HG11	1.82	0.61
9:I:407:ILE:HG22	9:I:415:LYS:NZ	2.15	0.61
4:D:290:ASN:HA	4:D:295:ARG:HH22	1.64	0.61
9:I:155:PHE:O	9:I:162:LEU:HA	2.02	0.59
1:A:489:VAL:HG11	1:A:564:LEU:HD13	1.85	0.59
9:I:157:LEU:HB3	9:I:160:GLY:H	1.68	0.58
6:F:275:LYS:NZ	6:F:278:CYS:SG	2.68	0.58
9:I:422:ILE:HD13	9:I:495:MET:HE1	1.86	0.58
9:I:422:ILE:HD11	9:I:493:LEU:HD21	1.86	0.57
9:I:453:LEU:HB2	9:I:457:GLU:OE1	2.05	0.57
9:I:299:ILE:HG21	9:I:331:LEU:HD11	1.86	0.57
2:B:395:TYR:O	3:C:145:ARG:NH1	2.38	0.56
9:I:78:LEU:HB2	9:I:81:ARG:HB2	1.86	0.56
9:I:173:ILE:HA	9:I:227:ARG:HG2	1.87	0.56
1:A:681:ARG:HB3	1:A:770:VAL:HG22	1.86	0.56
4:D:315:ASP:O	4:D:321:ASN:ND2	2.38	0.56
5:E:138:LEU:HD23	5:E:140:ASP:O	2.06	0.56
5:E:68:VAL:O	5:E:138:LEU:HG	2.05	0.56
1:A:551:LYS:HG2	1:A:552:ARG:HD3	1.86	0.56
1:A:431:ASN:O	1:A:639:ARG:NH1	2.38	0.55
1:A:633:LYS:HE2	1:A:690:GLU:HG2	1.89	0.55
9:I:199:ILE:HG23	9:I:204:HIS:HB2	1.88	0.55
4:D:212:VAL:HB	4:D:245:VAL:HG12	1.90	0.54
3:C:426:GLU:O	3:C:430:ASN:ND2	2.40	0.54
4:D:409:ASN:OD1	4:D:453:LYS:NZ	2.41	0.54
9:I:407:ILE:HG22	9:I:415:LYS:HZ1	1.73	0.54
3:C:100:ARG:NH2	3:C:230:ASP:OD1	2.41	0.54
6:F:333:ASN:HD22	6:F:388:ASP:HB2	1.71	0.54
6:F:285:ILE:HD11	6:F:302:ILE:HG22	1.89	0.53
9:I:219:VAL:HG22	9:I:257:VAL:HB	1.91	0.53
5:E:274:THR:H	5:E:277:ASN:HB2	1.73	0.53
1:A:362:LYS:NZ	7:G:32:DT:O2	2.41	0.53
3:C:210:SER:HA	5:E:431:LYS:HD3	1.90	0.53
5:E:213:SER:O	5:E:217:LYS:HB2	2.08	0.53
3:C:190:ASN:OD1	3:C:193:ARG:NH1	2.41	0.53
5:E:360:ARG:NH2	7:G:57:DT:O2	2.40	0.53
3:C:482:SER:HB2	3:C:485:SER:HB2	1.91	0.53
1:A:881:LYS:O	9:I:484:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:122:LEU:HB2	5:E:161:LYS:HG2	1.90	0.52
3:C:398:ARG:O	3:C:398:ARG:NH1	2.42	0.52
4:D:399:LEU:HD23	4:D:529:LEU:HD13	1.89	0.52
9:I:265:LEU:HD12	9:I:265:LEU:N	2.23	0.52
5:E:216:ARG:HA	5:E:219:ILE:HD12	1.91	0.52
1:A:501:ALA:O	1:A:503:ARG:NH1	2.42	0.52
1:A:362:LYS:HB2	8:H:55:DA:H5''	1.91	0.52
5:E:133:ASP:HA	5:E:169:THR:HB	1.91	0.51
9:I:157:LEU:HD12	9:I:158:PRO:HD2	1.92	0.51
3:C:181:VAL:HG21	3:C:187:LEU:HD13	1.92	0.51
1:A:573:THR:OG1	1:A:575:SER:O	2.29	0.51
9:I:388:ASN:N	9:I:388:ASN:OD1	2.40	0.51
1:A:452:ARG:NH2	1:A:625:THR:O	2.43	0.51
2:B:319:VAL:HG11	3:C:491:LEU:HG	1.92	0.51
3:C:198:ASP:OD1	3:C:198:ASP:N	2.38	0.51
6:F:335:ARG:HG2	6:F:342:ILE:HG13	1.92	0.51
2:B:312:PHE:HE1	3:C:319:LYS:HG3	1.75	0.51
9:I:102:ASP:OD1	9:I:102:ASP:N	2.43	0.51
5:E:380:LEU:HB3	5:E:449:ARG:HB3	1.93	0.50
3:C:242:THR:HG22	5:E:430:LEU:HD22	1.94	0.50
3:C:358:PRO:HA	3:C:361:MET:HB2	1.93	0.49
1:A:459:ILE:HG22	1:A:492:VAL:HG11	1.94	0.49
3:C:238:PHE:HB3	3:C:240:ILE:CD1	2.43	0.49
9:I:425:LEU:HD13	9:I:491:VAL:HG12	1.93	0.49
2:B:282:ASN:HB3	2:B:485:PRO:HG3	1.95	0.49
2:B:262:THR:OG1	2:B:263:MET:N	2.46	0.48
3:C:288:VAL:HB	3:C:292:LEU:HB2	1.94	0.48
3:C:601:SER:OG	3:C:602:THR:N	2.46	0.48
9:I:109:PRO:HD2	9:I:112:THR:HG21	1.95	0.48
1:A:688:ALA:HB1	1:A:778:VAL:HG21	1.95	0.48
2:B:331:ILE:HG23	3:C:27:PRO:HB3	1.96	0.48
3:C:339:ASP:N	3:C:339:ASP:OD1	2.46	0.48
5:E:86:LYS:HA	5:E:86:LYS:HD2	1.58	0.48
4:D:105:GLN:HB3	4:D:335:PRO:HG2	1.96	0.48
3:C:224:LYS:HG3	3:C:258:LEU:HD11	1.94	0.48
9:I:97:SER:HB3	9:I:157:LEU:HD11	1.96	0.48
1:A:363:LYS:O	5:E:101:GLN:NE2	2.47	0.47
2:B:382:LEU:HD21	3:C:24:THR:HG21	1.95	0.47
5:E:360:ARG:HG2	7:G:58:DC:H5''	1.97	0.47
1:A:687:ASP:HA	1:A:690:GLU:HB2	1.97	0.47
2:B:467:ASN:ND2	3:C:309:ASN:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:518:ALA:HB3	3:C:523:GLN:HB2	1.96	0.47
1:A:845:ILE:HD11	4:D:329:GLU:HB3	1.96	0.47
2:B:374:ASP:HA	2:B:377:LYS:HD2	1.96	0.47
3:C:423:ASN:HB3	3:C:426:GLU:HB2	1.97	0.47
4:D:147:ALA:HB2	4:D:184:ILE:HD11	1.96	0.47
9:I:122:ILE:HD11	9:I:221:VAL:HG21	1.95	0.47
2:B:258:LYS:NZ	7:G:50:DT:OP2	2.40	0.47
3:C:470:ASN:HB3	3:C:475:LEU:HD12	1.96	0.47
9:I:443:ALA:HB1	9:I:511:PHE:CE1	2.50	0.47
9:I:443:ALA:HA	9:I:446:LYS:HE3	1.96	0.47
1:A:587:THR:HG21	1:A:616:ARG:HG2	1.98	0.46
3:C:185:LEU:HB3	5:E:66:GLU:HB3	1.97	0.46
6:F:329:PHE:O	6:F:336:ARG:NH2	2.43	0.46
3:C:256:ILE:HG23	5:E:299:LEU:HD22	1.96	0.46
5:E:337:ILE:HG23	5:E:341:LEU:HD12	1.97	0.46
6:F:366:VAL:HA	6:F:369:VAL:HG12	1.97	0.46
9:I:110:PRO:N	9:I:263:ASN:HD21	2.13	0.46
9:I:320:ALA:HB2	9:I:390:ILE:HD12	1.97	0.46
9:I:412:ILE:HD12	9:I:450:LEU:HD21	1.97	0.46
2:B:285:PHE:O	2:B:290:ARG:NH2	2.41	0.46
5:E:358:GLN:HG2	6:F:314:VAL:HG13	1.98	0.46
6:F:350:MET:HG2	6:F:354:MET:HG2	1.98	0.46
9:I:428:ASN:ND2	9:I:435:GLU:OE1	2.48	0.46
4:D:75:LEU:HD23	4:D:276:PRO:HG2	1.97	0.46
5:E:26:PRO:HG2	5:E:125:LYS:HB3	1.97	0.46
9:I:422:ILE:HG21	9:I:495:MET:HE2	1.98	0.46
4:D:299:SER:HB3	4:D:302:VAL:HG23	1.97	0.46
9:I:182:PHE:HA	9:I:185:ILE:HD12	1.97	0.46
5:E:356:ILE:HD11	6:F:368:LEU:HB3	1.96	0.46
2:B:269:VAL:HG12	3:C:578:LYS:HG2	1.97	0.46
4:D:97:SER:HB2	4:D:238:VAL:HG11	1.98	0.45
5:E:352:ARG:NH2	5:E:392:ALA:O	2.48	0.45
2:B:327:GLU:HG2	2:B:331:ILE:HD12	1.98	0.45
3:C:108:LEU:HB2	3:C:267:ASP:HA	1.99	0.45
3:C:469:ASP:OD1	3:C:470:ASN:N	2.48	0.45
8:H:24:DT:H2''	8:H:25:DT:H5''	1.97	0.45
1:A:612:LYS:HG3	9:I:266:ASP:OD2	2.17	0.45
2:B:369:SER:OG	3:C:21:SER:OG	2.33	0.45
6:F:277:TYR:OH	7:G:59:DA:OP2	2.33	0.45
6:F:330:ILE:HD13	6:F:382:LEU:HG	1.99	0.45
1:A:644:ASN:ND2	1:A:645:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:77:ILE:HG12	5:E:130:LEU:HD11	1.99	0.45
1:A:845:ILE:HG12	1:A:849:LEU:HD13	1.98	0.44
6:F:273:LEU:HD12	6:F:361:ASP:HB3	1.98	0.44
9:I:227:ARG:HA	9:I:227:ARG:HD2	1.70	0.44
2:B:357:SER:HB2	3:C:29:LEU:HD22	1.99	0.44
9:I:167:VAL:HG22	9:I:219:VAL:HB	1.98	0.44
6:F:330:ILE:HD11	6:F:383:GLN:HA	1.98	0.44
9:I:407:ILE:CG2	9:I:415:LYS:HZ2	2.30	0.44
2:B:274:PHE:HD1	3:C:582:ILE:HG23	1.82	0.44
5:E:205:ARG:NE	5:E:208:GLU:OE1	2.51	0.44
3:C:431:LEU:HD13	3:C:436:LEU:HD13	1.99	0.44
4:D:209:LYS:H	4:D:209:LYS:HG2	1.55	0.44
6:F:416:ASP:N	6:F:416:ASP:OD1	2.48	0.44
5:E:243:ILE:HG21	5:E:262:ILE:HG13	1.99	0.44
1:A:885:LYS:HB3	4:D:476:GLY:HA3	2.00	0.44
9:I:433:ILE:HG13	9:I:489:ILE:HD11	1.99	0.44
2:B:269:VAL:HG21	3:C:582:ILE:HD11	1.99	0.43
3:C:90:LEU:HD23	3:C:90:LEU:HA	1.88	0.43
9:I:265:LEU:N	9:I:265:LEU:CD1	2.80	0.43
1:A:790:VAL:O	1:A:794:MET:HG3	2.19	0.43
3:C:435:LYS:HG3	3:C:438:SER:HB3	2.00	0.43
9:I:349:LYS:HA	9:I:349:LYS:HD3	1.82	0.43
1:A:580:TYR:O	1:A:584:ASN:HB2	2.19	0.43
1:A:425:LYS:NZ	1:A:657:ALA:O	2.48	0.43
2:B:241:ASP:N	2:B:241:ASP:OD1	2.52	0.43
4:D:514:ARG:HH21	4:D:528:GLN:HB2	1.83	0.43
5:E:217:LYS:O	5:E:221:GLU:HB2	2.19	0.43
5:E:344:ARG:HH22	8:H:32:DG:H3'	1.83	0.43
6:F:298:VAL:O	6:F:302:ILE:HG12	2.19	0.43
2:B:299:LYS:HA	2:B:299:LYS:HD3	1.79	0.43
2:B:403:GLN:O	2:B:407:MET:HG3	2.19	0.43
3:C:56:LYS:HG2	3:C:336:VAL:HG13	2.01	0.43
3:C:83:LEU:HD11	3:C:268:VAL:HG21	2.01	0.42
9:I:477:LYS:HD2	9:I:483:LYS:HB3	2.01	0.42
1:A:427:LYS:HB2	1:A:427:LYS:HE3	1.91	0.42
9:I:460:GLU:O	9:I:464:ILE:N	2.51	0.42
4:D:349:LYS:HA	4:D:349:LYS:HD3	1.71	0.42
9:I:419:CYS:HG	9:I:498:PHE:HZ	1.63	0.42
1:A:788:SER:HB2	9:I:456:ASN:ND2	2.34	0.42
1:A:426:VAL:HG22	1:A:643:LEU:HD13	2.00	0.42
3:C:238:PHE:HB3	3:C:240:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:563:ASN:HB3	3:C:566:LEU:HB2	2.01	0.42
4:D:344:LEU:HD12	4:D:363:PHE:HB3	2.02	0.42
3:C:441:ASP:OD1	3:C:447:LYS:NZ	2.42	0.42
5:E:417:ASN:HD21	5:E:419:GLU:HG3	1.84	0.42
7:G:28:DT:H1'	7:G:29:DT:H5'	2.02	0.42
3:C:132:THR:HB	3:C:133:PRO:HD2	2.02	0.42
3:C:488:GLU:HB3	3:C:614:ARG:HG3	2.02	0.42
3:C:488:GLU:OE1	3:C:614:ARG:HA	2.19	0.42
1:A:418:ILE:HD12	4:D:92:GLN:HA	2.00	0.42
5:E:68:VAL:HG12	5:E:140:ASP:OD2	2.20	0.42
9:I:110:PRO:CA	9:I:263:ASN:HD21	2.32	0.42
4:D:55:ARG:HB2	4:D:298:ILE:HD11	2.01	0.41
2:B:247:PHE:HB3	5:E:347:ALA:HB2	2.01	0.41
3:C:39:ILE:HD11	3:C:54:VAL:HG12	2.03	0.41
2:B:376:PHE:HZ	2:B:403:GLN:HG2	1.85	0.41
3:C:498:LEU:HD23	3:C:498:LEU:HA	1.89	0.41
3:C:356:ARG:NH1	6:F:413:VAL:O	2.41	0.41
2:B:438:GLN:O	2:B:442:SER:OG	2.35	0.41
3:C:359:THR:HB	3:C:461:ILE:HD12	2.01	0.41
6:F:363:ILE:HA	6:F:366:VAL:HG12	2.02	0.41
2:B:321:SER:H	2:B:484:GLU:HB2	1.85	0.41
1:A:601:THR:HG22	1:A:603:ASP:H	1.86	0.41
1:A:833:ILE:HG21	1:A:850:PHE:HE2	1.86	0.41
3:C:17:ASP:OD1	3:C:17:ASP:N	2.53	0.41
3:C:57:ARG:HG3	3:C:336:VAL:HG22	2.02	0.41
4:D:59:GLN:HG2	4:D:64:LEU:HD11	2.02	0.41
1:A:719:LYS:HB3	1:A:719:LYS:HE2	1.67	0.41
4:D:214:PHE:HB2	4:D:247:ILE:HG12	2.02	0.41
5:E:5:THR:HG23	5:E:15:THR:HG22	2.03	0.41
4:D:346:ALA:HB3	5:E:20:SER:HB2	2.03	0.40
2:B:308:LEU:HD22	2:B:451:ALA:HB1	2.04	0.40
3:C:45:LEU:HD22	3:C:349:ASP:HB3	2.03	0.40
3:C:127:VAL:HG11	3:C:150:LEU:HD13	2.03	0.40
9:I:430:ASP:OD1	9:I:430:ASP:N	2.54	0.40
9:I:453:LEU:HD13	9:I:457:GLU:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	475/917 (52%)	463 (98%)	12 (2%)	0	100	100
2	B	245/620 (40%)	233 (95%)	12 (5%)	0	100	100
3	C	531/616 (86%)	515 (97%)	16 (3%)	0	100	100
4	D	426/532 (80%)	418 (98%)	8 (2%)	0	100	100
5	E	426/479 (89%)	413 (97%)	13 (3%)	0	100	100
6	F	153/435 (35%)	146 (95%)	7 (5%)	0	100	100
9	I	360/516 (70%)	349 (97%)	11 (3%)	0	100	100
All	All	2616/4115 (64%)	2537 (97%)	79 (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	A	430/815 (53%)	412 (96%)	18 (4%)	30	58
2	B	232/573 (40%)	218 (94%)	14 (6%)	19	42
3	C	507/576 (88%)	486 (96%)	21 (4%)	30	59
4	D	401/490 (82%)	380 (95%)	21 (5%)	23	49
5	E	401/440 (91%)	387 (96%)	14 (4%)	36	65
6	F	149/406 (37%)	146 (98%)	3 (2%)	55	81
9	I	341/472 (72%)	323 (95%)	18 (5%)	22	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2461/3772 (65%)	2352 (96%)	109 (4%)	32 56

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	ARG
1	A	422	ILE
1	A	432	SER
1	A	498	SER
1	A	503	ARG
1	A	507	ASP
1	A	552	ARG
1	A	556	ASN
1	A	569	ASP
1	A	607	ARG
1	A	625	THR
1	A	705	ARG
1	A	720	HIS
1	A	813	LYS
1	A	859	GLU
1	A	897	SER
1	A	907	GLU
1	A	914	LEU
2	B	255	THR
2	B	258	LYS
2	B	263	MET
2	B	271	ARG
2	B	272	GLU
2	B	281	PHE
2	B	288	ARG
2	B	369	SER
2	B	403	GLN
2	B	419	LYS
2	B	422	LEU
2	B	437	PHE
2	B	442	SER
2	B	495	VAL
3	C	25	VAL
3	C	59	GLU
3	C	99	ARG
3	C	230	ASP
3	C	247	ILE

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Mol	Chain	Res	Type
3	C	249	LYS
3	C	258	LEU
3	C	289	ASP
3	C	306	MET
3	C	310	THR
3	C	354	LEU
3	C	367	LEU
3	C	398	ARG
3	C	407	LYS
3	C	435	LYS
3	C	436	LEU
3	C	454	HIS
3	C	526	LYS
3	C	540	PHE
3	C	564	THR
3	C	608	VAL
4	D	77	ASP
4	D	97	SER
4	D	115	GLU
4	D	120	GLN
4	D	139	GLU
4	D	141	THR
4	D	151	GLU
4	D	209	LYS
4	D	216	PHE
4	D	236	ASP
4	D	241	SER
4	D	282	ASP
4	D	353	SER
4	D	362	SER
4	D	385	ASP
4	D	416	GLU
4	D	417	LYS
4	D	455	ASP
4	D	514	ARG
4	D	522	MET
4	D	528	GLN
5	E	3	VAL
5	E	130	LEU
5	E	142	ASP
5	E	210	MET
5	E	296	ASP

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Mol	Chain	Res	Type
5	E	339	SER
5	E	344	ARG
5	E	352	ARG
5	E	371	VAL
5	E	379	SER
5	E	425	SER
5	E	430	LEU
5	E	441	ILE
5	E	472	ASP
6	F	301	LYS
6	F	341	ARG
6	F	354	MET
9	I	81	ARG
9	I	89	MET
9	I	94	LYS
9	I	98	GLU
9	I	164	SER
9	I	169	SER
9	I	226	ASP
9	I	232	ASN
9	I	238	SER
9	I	239	VAL
9	I	302	GLN
9	I	309	THR
9	I	327	ASN
9	I	331	LEU
9	I	395	SER
9	I	425	LEU
9	I	430	ASP
9	I	462	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	248	HIS
5	E	253	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	I	1001	11	26,33,33	0.64	0	31,52,52	0.75	2 (6%)
10	ATP	A	1001	11	26,33,33	0.69	0	31,52,52	0.75	2 (6%)
10	ATP	E	1001	11	26,33,33	0.68	0	31,52,52	0.74	2 (6%)
10	ATP	D	1001	11	26,33,33	0.71	0	31,52,52	0.81	2 (6%)

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	I	1001	11	-	3/18/38/38	0/3/3/3
10	ATP	A	1001	11	-	1/18/38/38	0/3/3/3
10	ATP	E	1001	11	-	4/18/38/38	0/3/3/3
10	ATP	D	1001	11	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1001	ATP	C5-C6-N6	2.36	123.94	120.35
10	A	1001	ATP	C5-C6-N6	2.29	123.84	120.35
10	E	1001	ATP	C5-C6-N6	2.27	123.81	120.35
10	I	1001	ATP	C5-C6-N6	2.25	123.76	120.35
10	E	1001	ATP	PB-O3B-PG	2.11	140.06	132.83
10	D	1001	ATP	PB-O3B-PG	2.10	140.03	132.83
10	I	1001	ATP	PB-O3B-PG	2.05	139.87	132.83
10	A	1001	ATP	PB-O3B-PG	2.04	139.81	132.83

There are no chirality outliers.

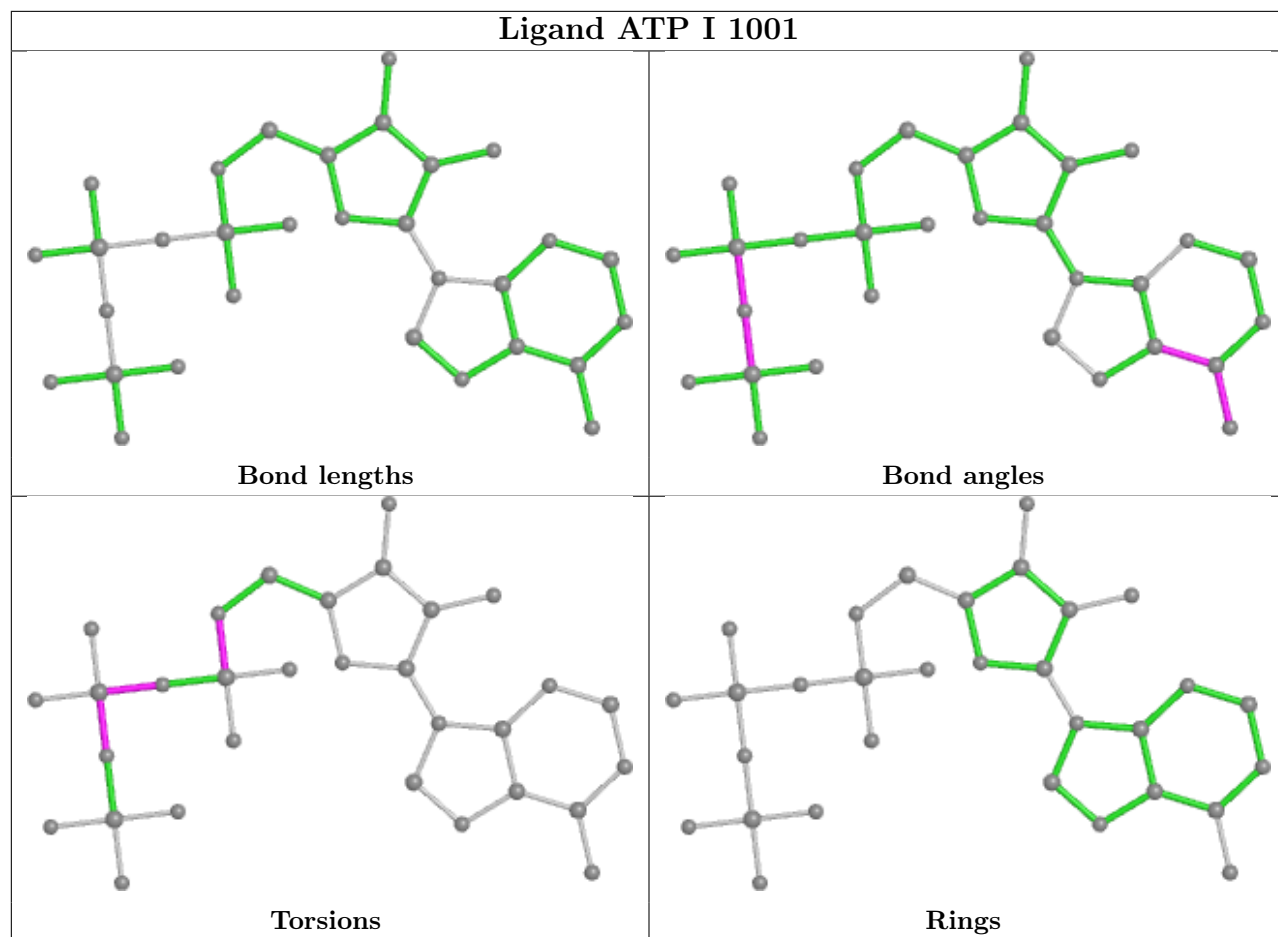
All (11) torsion outliers are listed below:

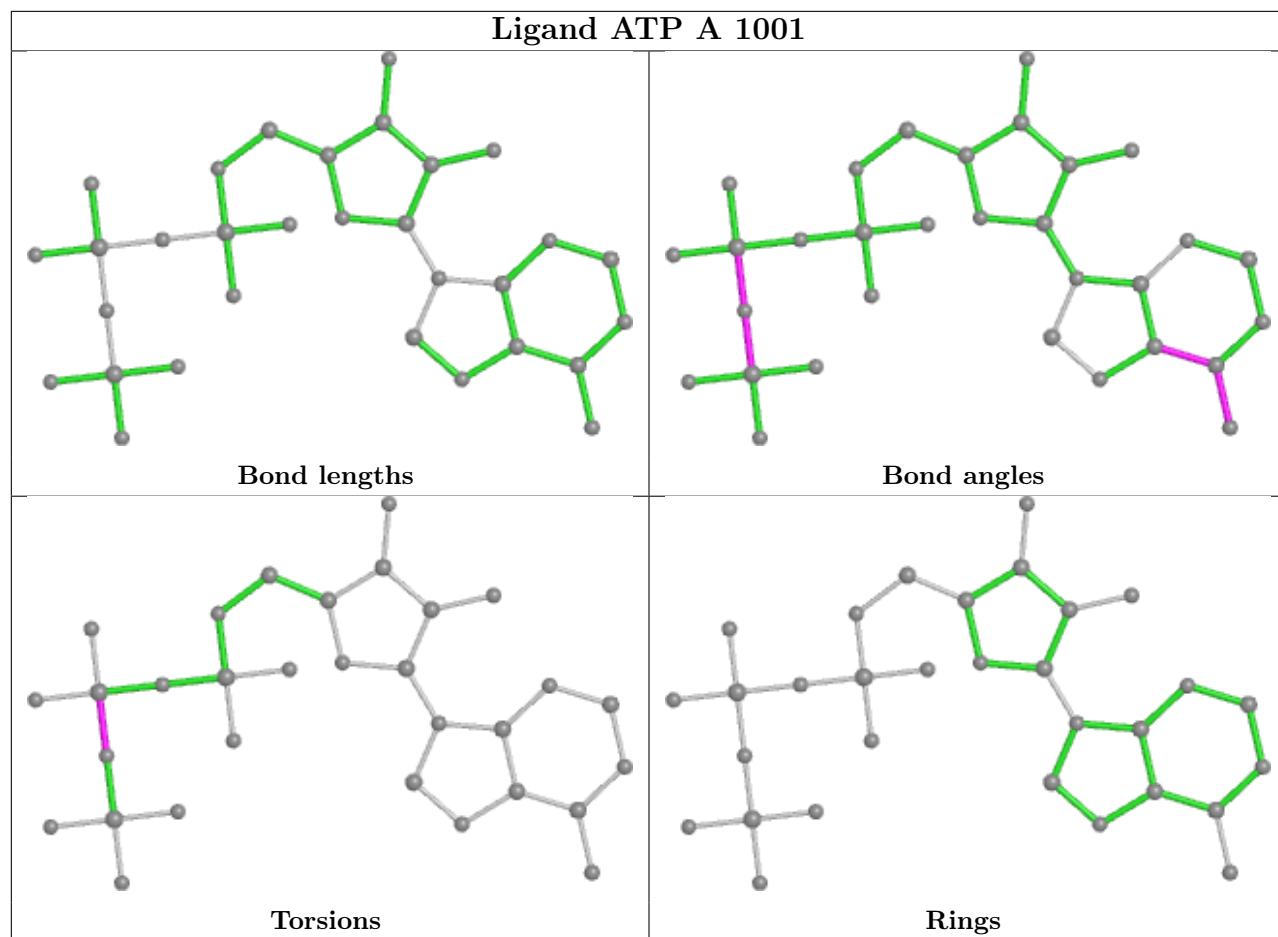
Mol	Chain	Res	Type	Atoms
10	D	1001	ATP	O4'-C4'-C5'-O5'
10	D	1001	ATP	C3'-C4'-C5'-O5'
10	I	1001	ATP	C5'-O5'-PA-O3A
10	A	1001	ATP	PG-O3B-PB-O1B
10	D	1001	ATP	PA-O3A-PB-O1B
10	E	1001	ATP	PA-O3A-PB-O2B
10	I	1001	ATP	PG-O3B-PB-O2B
10	I	1001	ATP	PA-O3A-PB-O2B
10	E	1001	ATP	C5'-O5'-PA-O3A
10	E	1001	ATP	O4'-C4'-C5'-O5'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

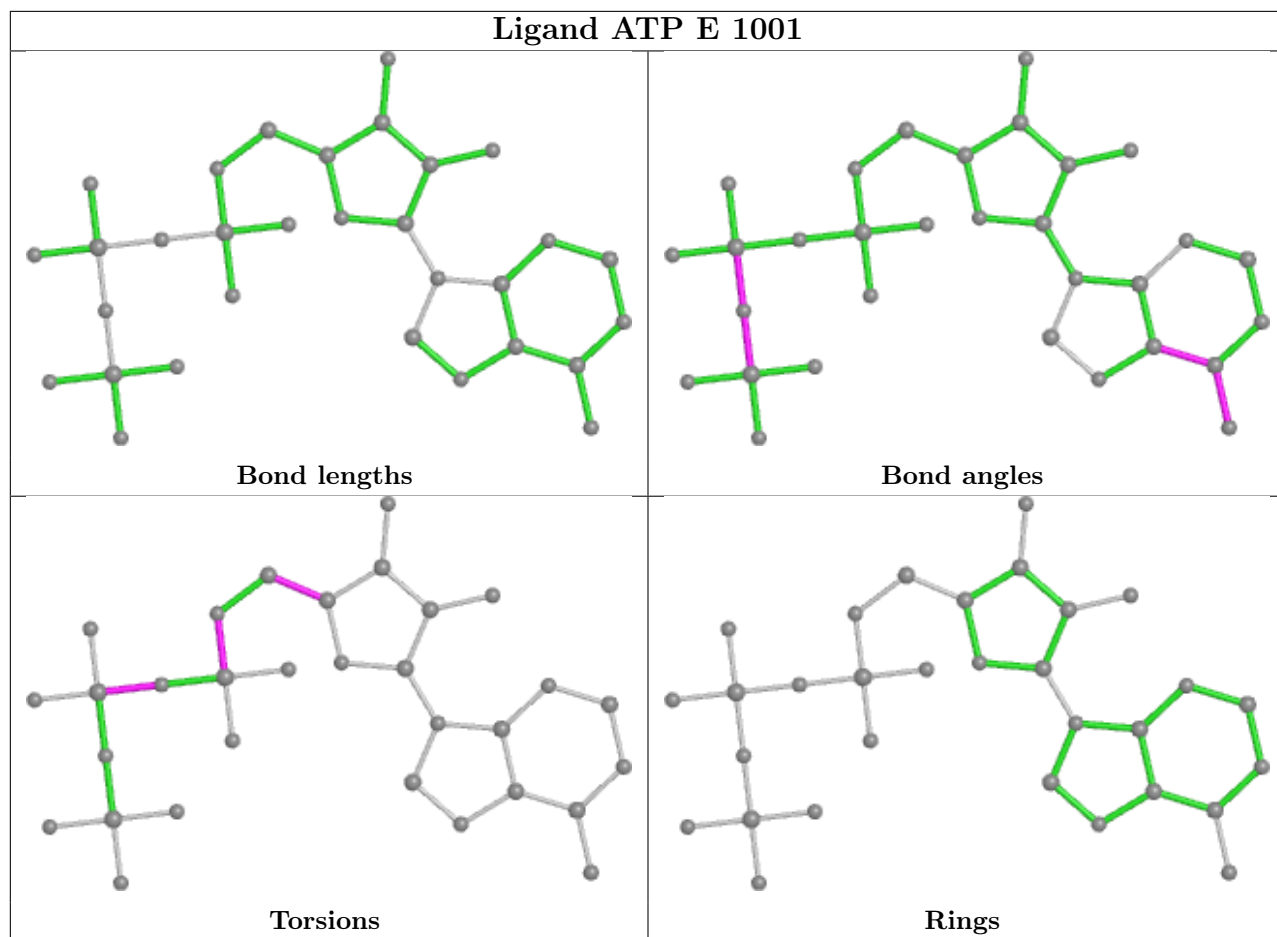
There are no ring outliers.

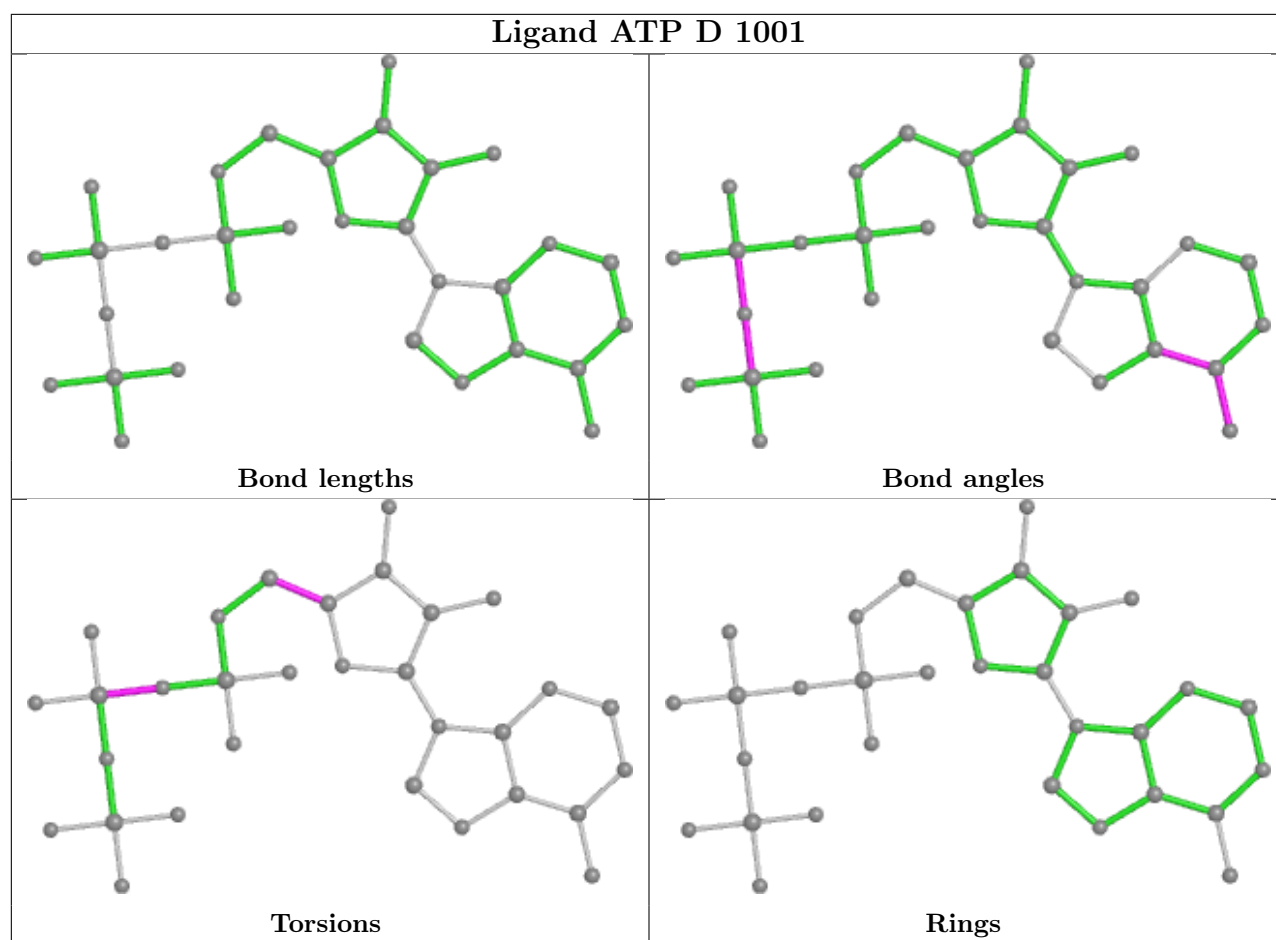
No monomer is involved in short contacts.

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.

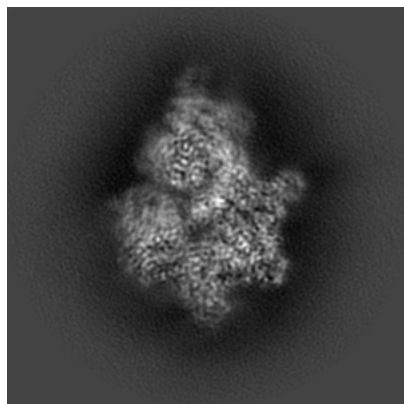
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25926. These allow visual inspection of the internal detail of the map and identification of artifacts.

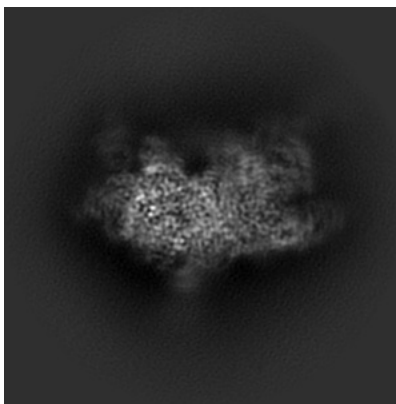
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

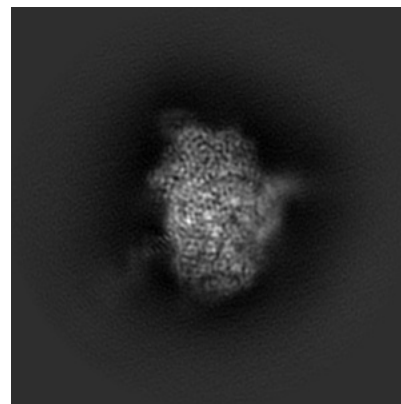
6.1.1 Primary map



X

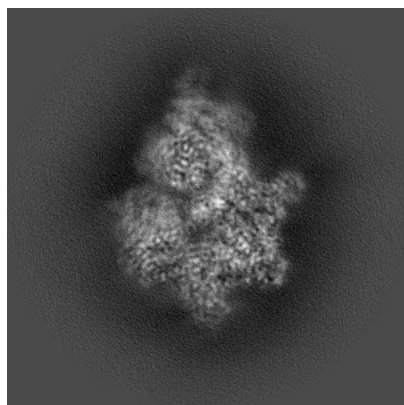


Y

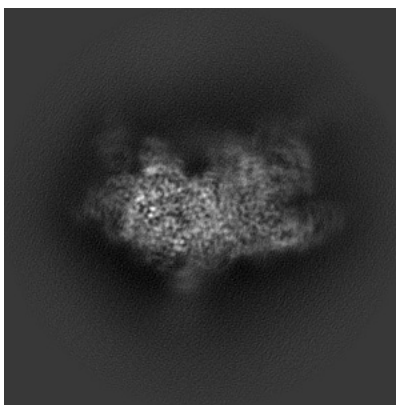


Z

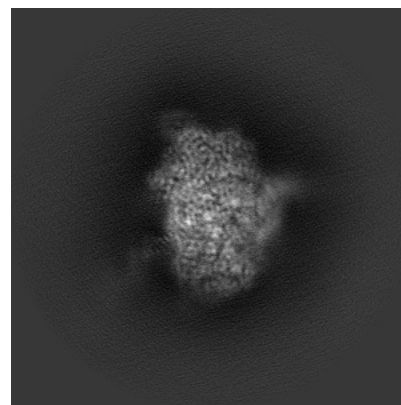
6.1.2 Raw map



X



Y

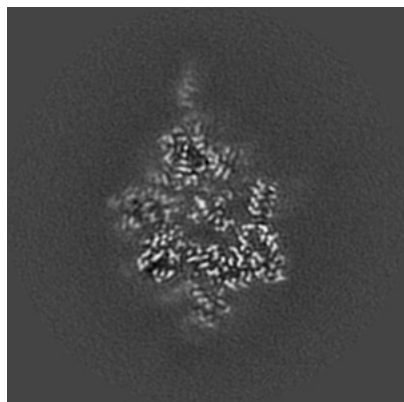


Z

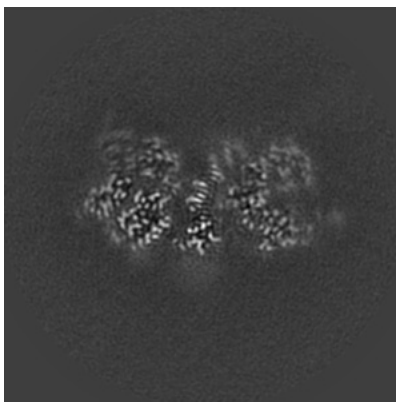
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

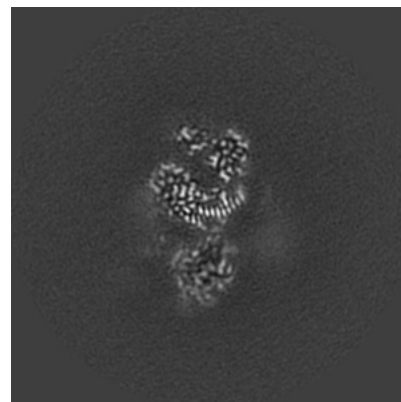
6.2.1 Primary map



X Index: 150

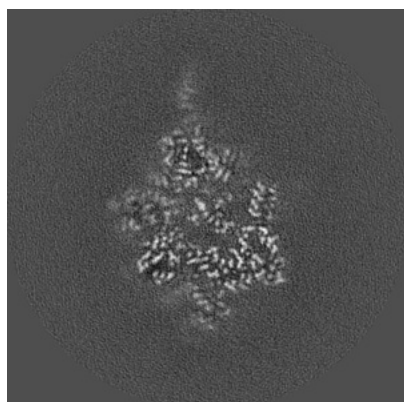


Y Index: 150

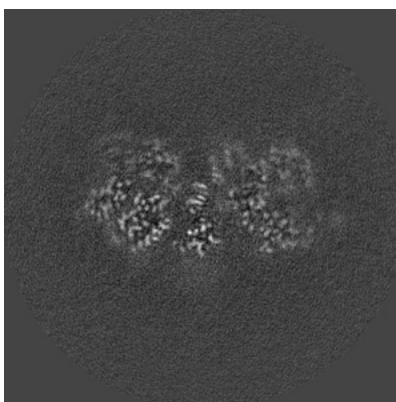


Z Index: 150

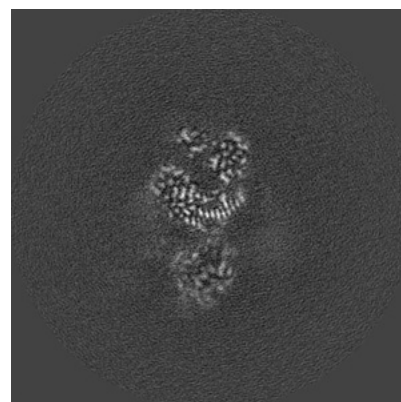
6.2.2 Raw map



X Index: 150



Y Index: 150

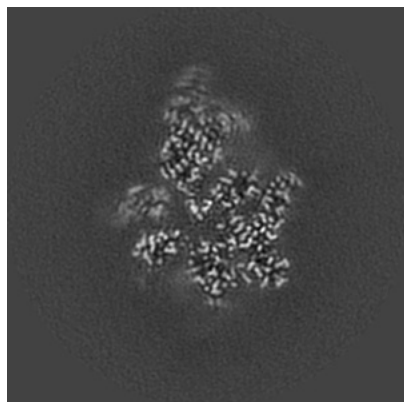


Z Index: 150

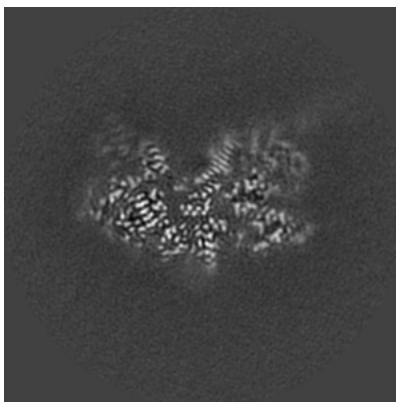
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

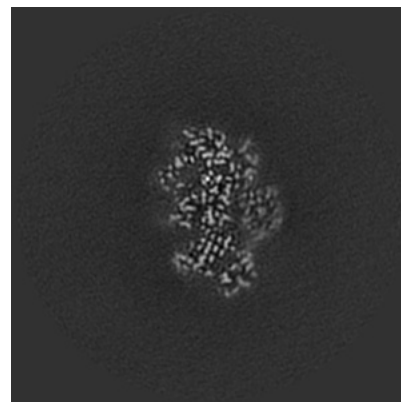
6.3.1 Primary map



X Index: 137

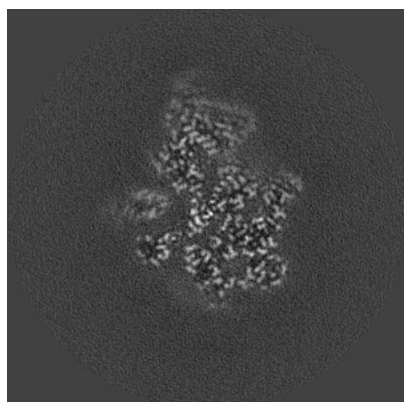


Y Index: 157

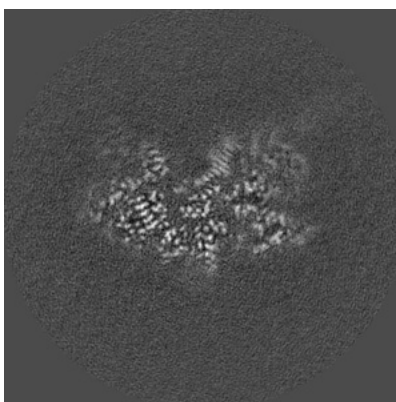


Z Index: 111

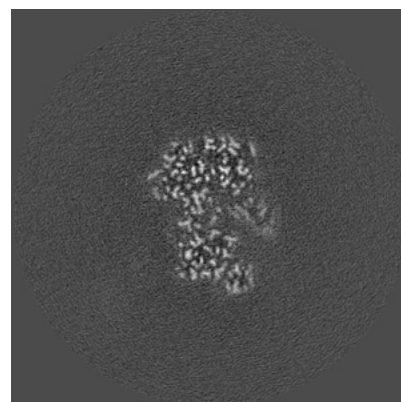
6.3.2 Raw map



X Index: 133



Y Index: 157

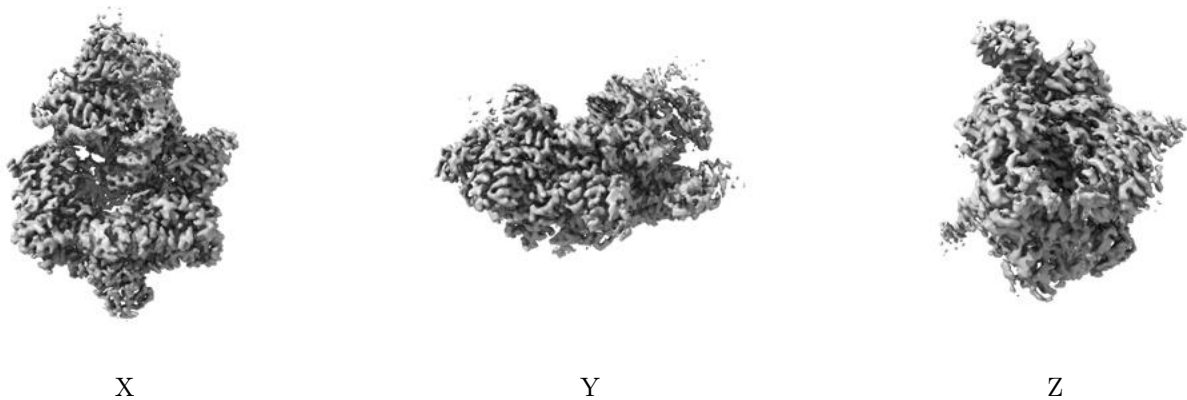


Z Index: 121

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

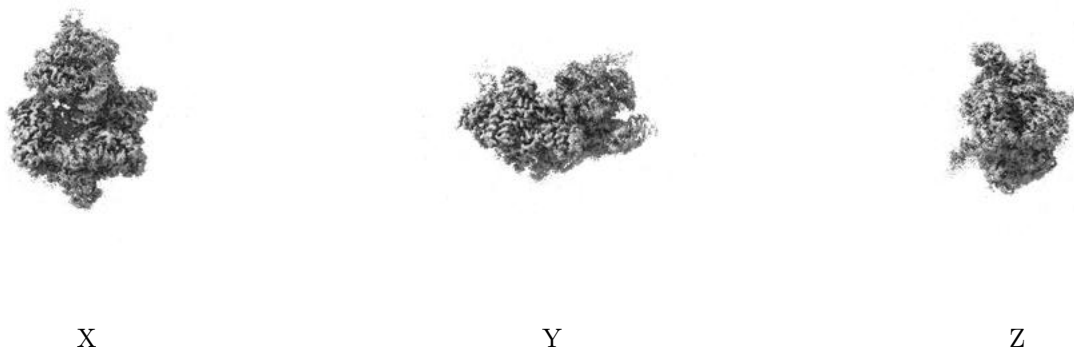
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

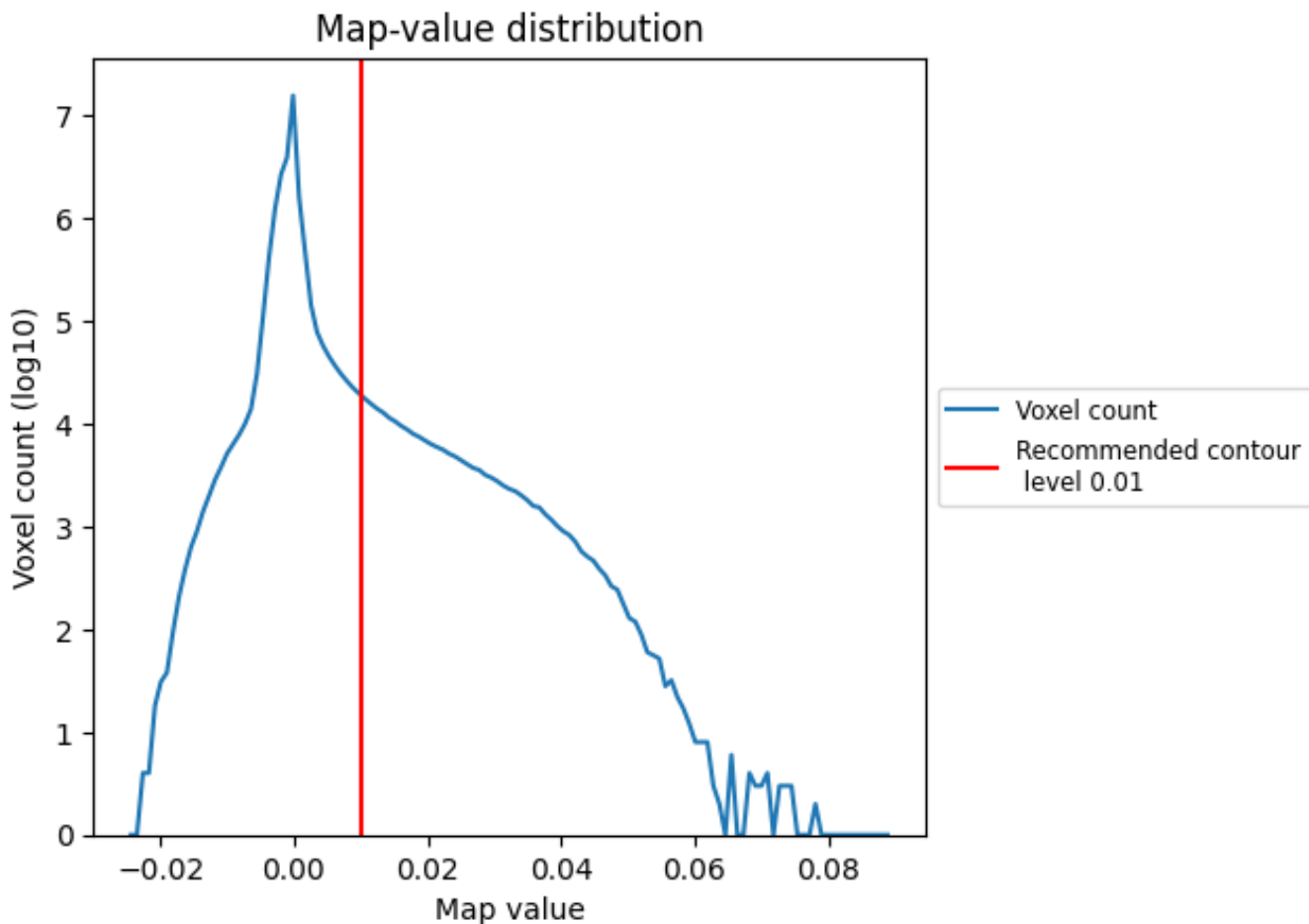
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

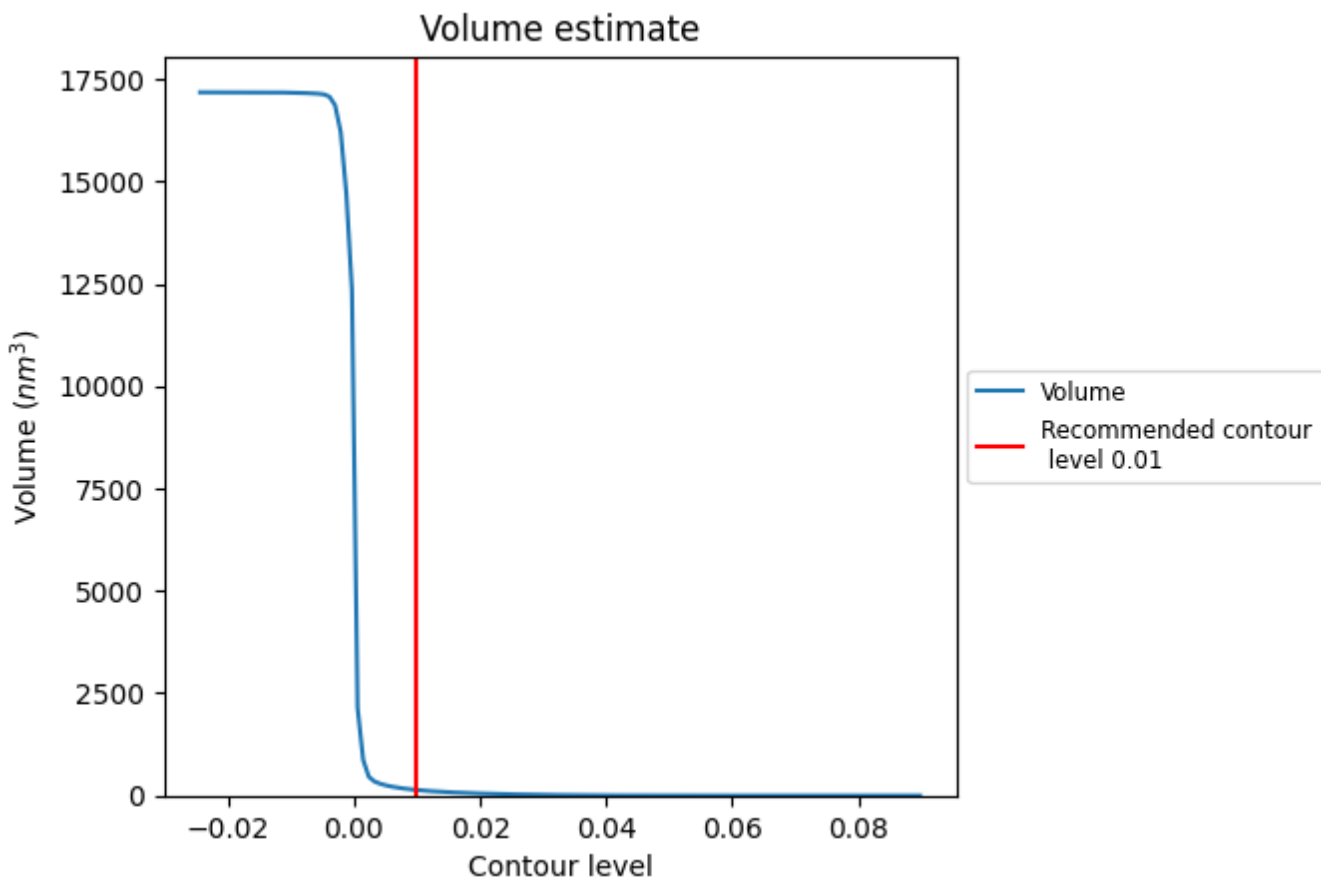
This section contains the results of statistical analysis of the map.

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.

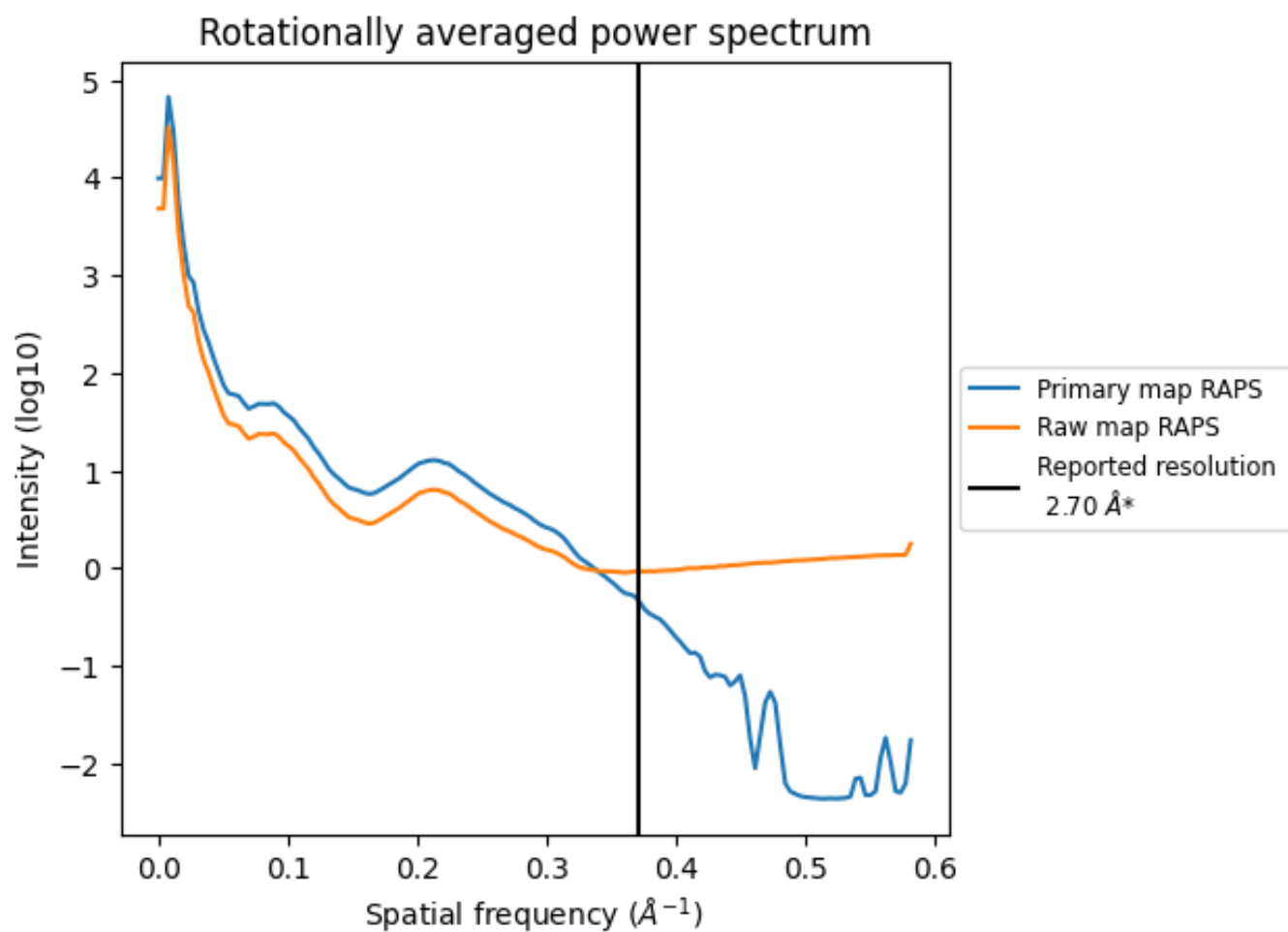
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm³; this corresponds to an approximate mass of 123 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

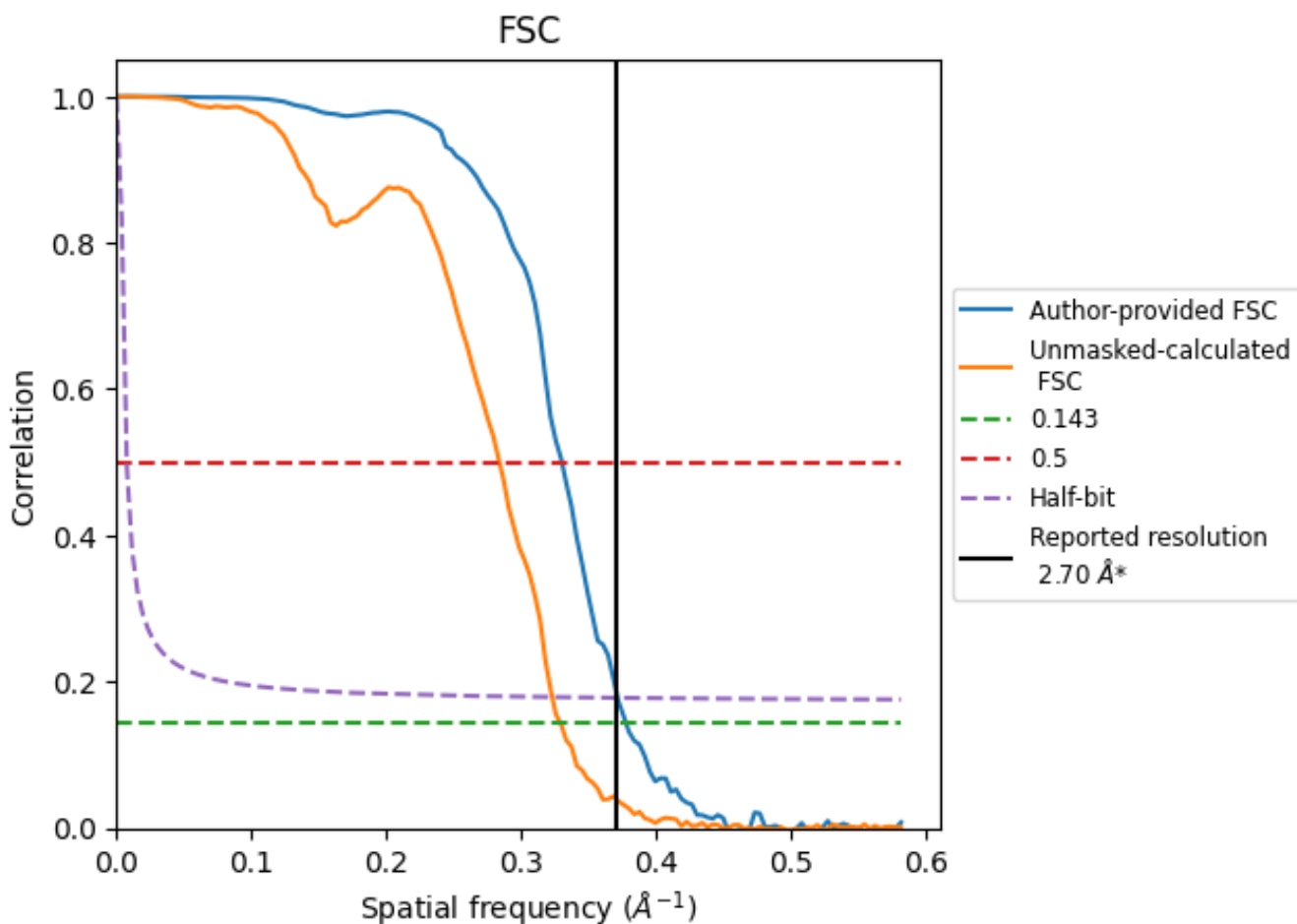


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

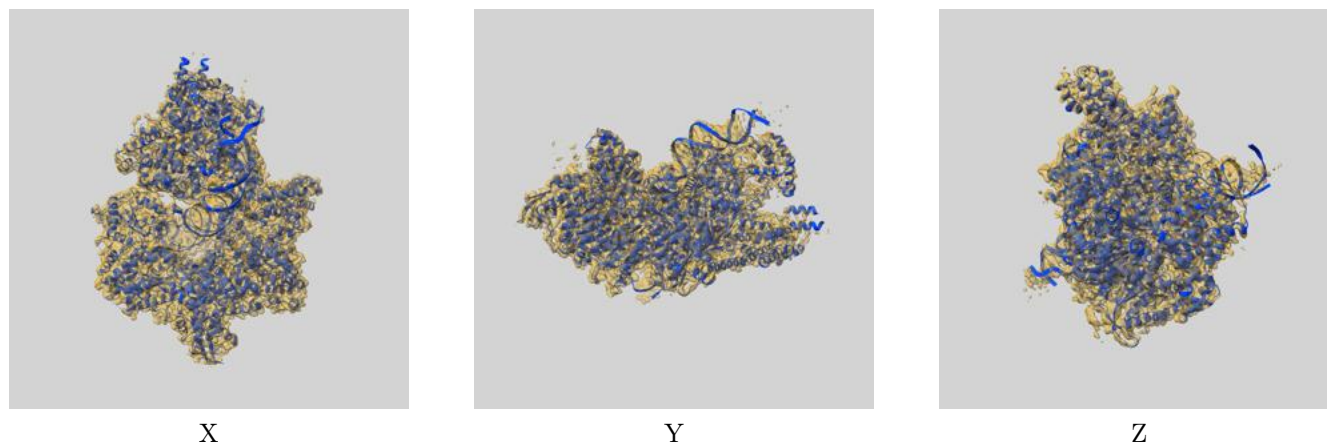
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.65	3.03	2.69
Unmasked-calculated*	3.04	3.52	3.10

*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 3.04 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

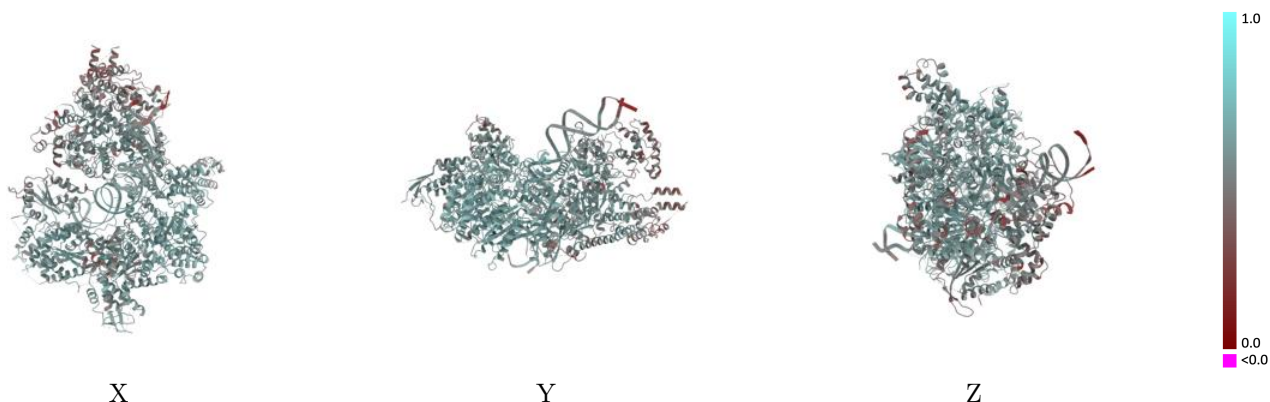
This section contains information regarding the fit between EMDB map EMD-25926 and PDB model 7TJI. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



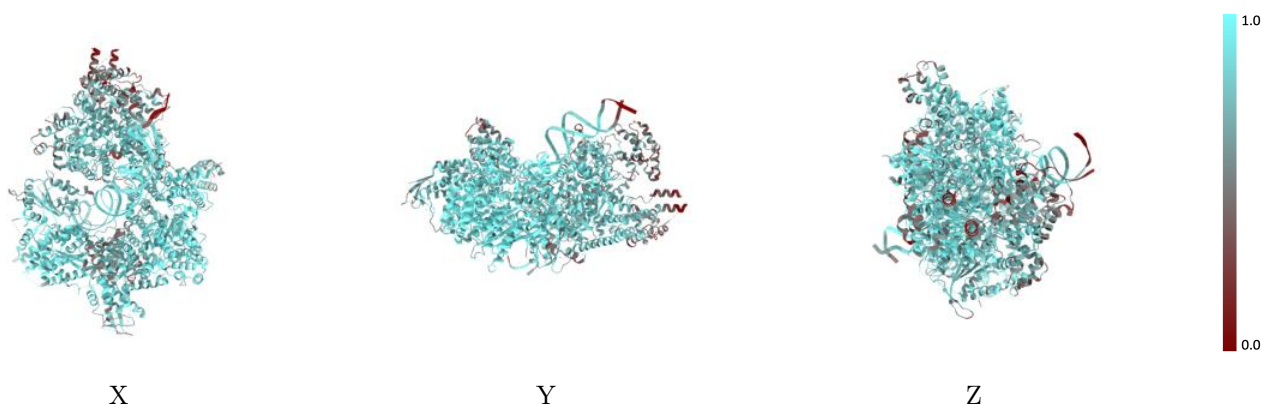
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



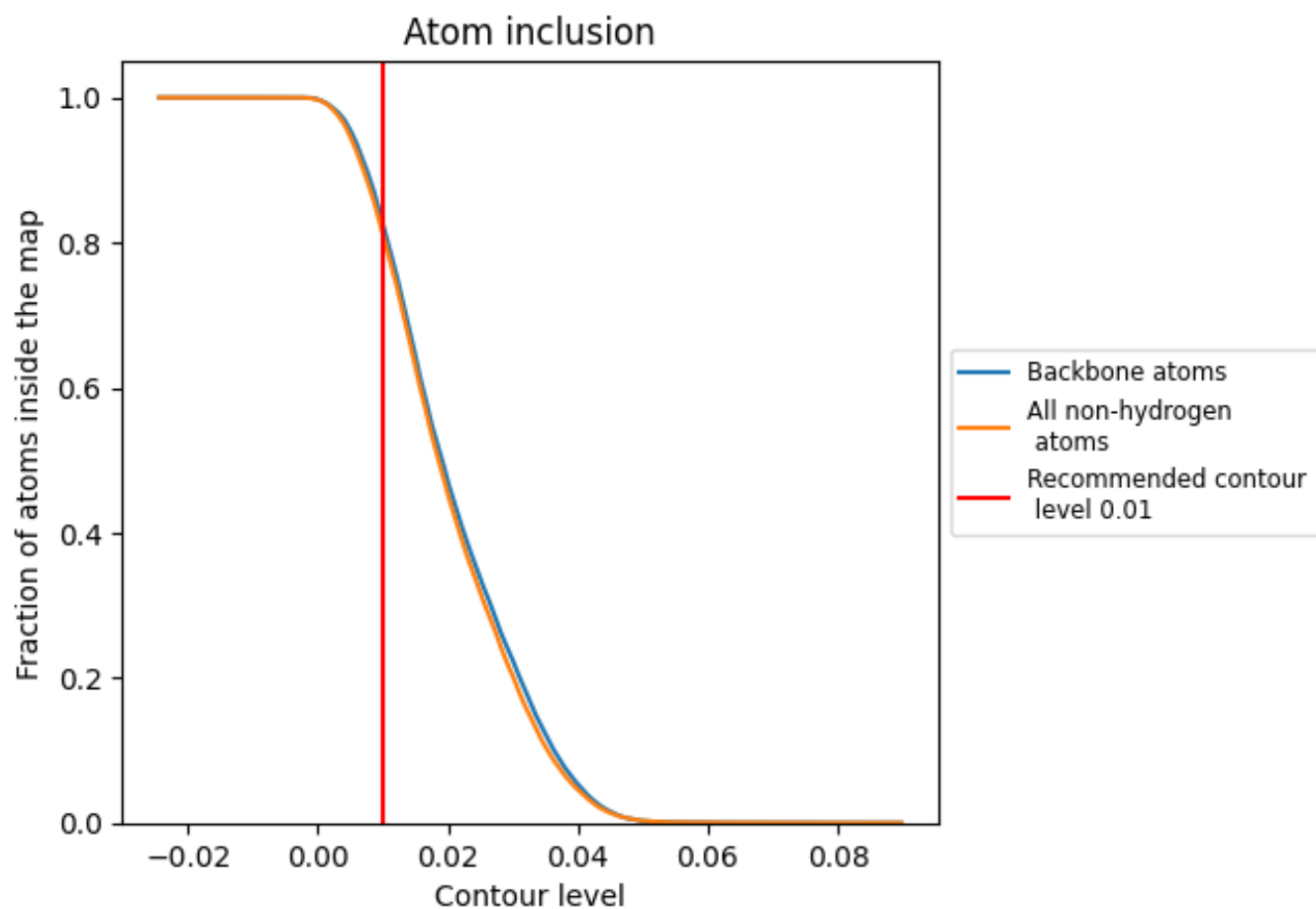
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 81% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8121	 0.5630
A	 0.8708	 0.5980
B	 0.8626	 0.5800
C	 0.7623	 0.5310
D	 0.9195	 0.6180
E	 0.8436	 0.5800
F	 0.5478	 0.4380
G	 0.8606	 0.5620
H	 0.8274	 0.5610
I	 0.7471	 0.5240

