



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:13 PM UTC

PDB ID : 7WIW / pdb_00007wiw
EMDB ID : EMD-32538
Title : Cryo-EM structure of Mycobacterium tuberculosis irtAB complexed with ATP
in an occluded conformation
Authors : Zhang, B.; Sun, S.; Yang, H.; Rao, Z.
Deposited on : 2022-01-05
Resolution : 3.12 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

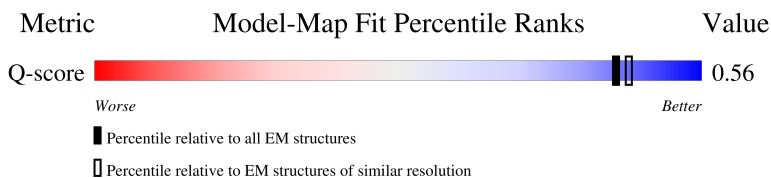
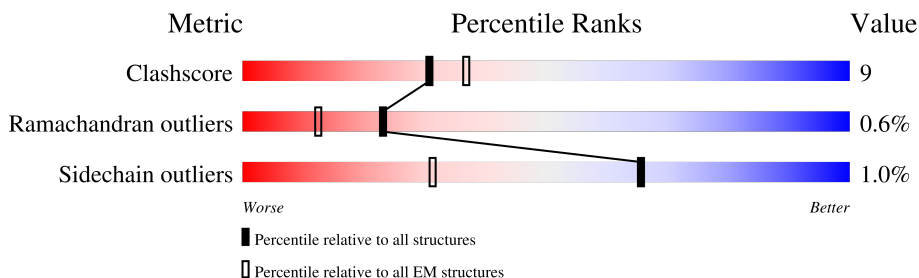
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.12 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14478 (2.62 - 3.62)

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	B	579	 75% 21% ..
2	A	859	 53% 13% . 34%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8603 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 Mycobactin import ATP-binding/permease protein IrtB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	567	Total	C	N	O	S	0	0
			4198	2670	754	764	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	495	GLN	GLU	conflict	UNP P9WQJ7

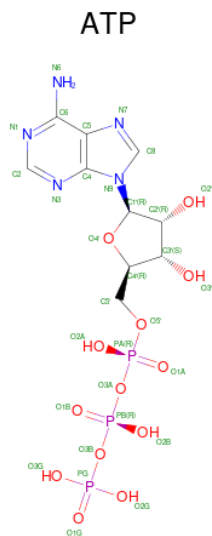
- Molecule 2 is a protein called Mycobactin import ATP-binding/permease protein IrtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	570	Total	C	N	O	S	0	0
			4340	2783	783	769	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	771	GLN	GLU	conflict	UNP P9WQJ9

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Mg 1 1	0
4	A	2	Total Mg 2 2	0



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101408	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.874	Depositor
Minimum map value	-1.174	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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	0.31	1/4273 (0.0%)	0.55	5/5844 (0.1%)
2	A	0.33	2/4425 (0.0%)	0.61	5/6036 (0.1%)
All	All	0.32	3/8698 (0.0%)	0.58	10/11880 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	493	VAL	C-O	-7.29	1.15	1.24
2	A	631	LEU	C-O	-6.54	1.15	1.24
2	A	629	VAL	C-O	-5.72	1.16	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	333	VAL	N-CA-C	-6.43	106.97	113.47
1	B	493	VAL	CA-C-O	-5.84	114.32	120.57
1	B	327	ALA	CA-C-N	5.75	132.32	121.97
1	B	327	ALA	C-N-CA	5.75	132.32	121.97
1	B	15	ALA	N-CA-C	-5.60	107.69	114.75
2	A	840	LEU	N-CA-C	-5.53	107.18	114.31
2	A	628	ASP	CA-C-N	-5.44	113.80	122.50
2	A	628	ASP	C-N-CA	-5.44	113.80	122.50
2	A	293	LEU	N-CA-C	-5.19	108.71	114.62
1	B	495	GLN	CB-CG-CD	-5.09	103.94	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4198	0	4318	84	0
2	A	4340	0	4496	79	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
All	All	8603	0	8838	155	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 9.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:O	1:B:328:VAL:HG23	1.70	0.92
2:A:771:GLN:NE2	2:A:802:HIS:HD2	1.70	0.89
1:B:323:TRP:HB3	1:B:326:GLY:O	1.77	0.83
2:A:612:PHE:HB2	2:A:630:SER:O	1.79	0.83
1:B:467:GLY:HA3	1:B:475:ARG:HD3	1.60	0.82
2:A:771:GLN:NE2	2:A:802:HIS:CD2	2.47	0.82
1:B:435:SER:H	1:B:438:GLN:HE21	1.27	0.80
1:B:531:ILE:HG13	1:B:532:ARG:H	1.46	0.79
1:B:203:GLN:HE21	1:B:207:ARG:HE	1.32	0.76
1:B:324:ARG:O	1:B:325:ASP:HB3	1.86	0.76
2:A:456:GLY:H	2:A:457:PRO:HD2	1.51	0.75
1:B:486:LYS:O	1:B:519:ARG:NH2	2.23	0.70
1:B:455:LEU:HD23	1:B:461:THR:HG21	1.73	0.69
2:A:697:HIS:HA	2:A:741:GLY:HA2	1.74	0.68
2:A:601:PRO:HA	2:A:672:GLN:HG2	1.76	0.68
2:A:599:ARG:HG3	2:A:600:GLU:H	1.59	0.67
1:B:503:GLU:OE1	2:A:836:ARG:NH1	2.26	0.67
2:A:476:TYR:O	2:A:480:GLN:NE2	2.27	0.67
1:B:96:ARG:NH2	1:B:313:ALA:O	2.28	0.66
2:A:763:ASP:HB2	2:A:795:ARG:HH12	1.61	0.66
1:B:86:LEU:HD13	1:B:125:VAL:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ASP:OD2	2:A:523:ARG:NH2	2.32	0.62
2:A:669:VAL:HG12	2:A:674:ILE:HG22	1.82	0.62
1:B:155:GLN:HB2	1:B:262:LEU:HD11	1.81	0.62
2:A:771:GLN:HE22	2:A:802:HIS:CD2	2.17	0.62
2:A:771:GLN:HE22	2:A:802:HIS:HD2	1.48	0.62
1:B:282:ARG:NH2	1:B:285:GLU:OE2	2.29	0.60
1:B:27:SER:OG	1:B:71:ASP:OD1	2.21	0.58
1:B:491:LEU:HB3	1:B:521:ARG:HG2	1.84	0.58
1:B:252:LEU:HB2	1:B:284:LEU:HD11	1.86	0.57
1:B:435:SER:OG	1:B:436:ASP:N	2.34	0.57
2:A:402:HIS:O	2:A:403:TYR:C	2.47	0.57
2:A:821:ILE:HG21	2:A:824:ARG:HH21	1.69	0.57
2:A:599:ARG:HG3	2:A:600:GLU:N	2.19	0.57
2:A:654:THR:HG23	2:A:659:PHE:HD2	1.70	0.57
2:A:370:LEU:HD11	2:A:583:LEU:HD22	1.87	0.56
2:A:418:ALA:HB3	2:A:419:PRO:HD3	1.87	0.56
2:A:459:ILE:HD12	2:A:574:ARG:HD2	1.87	0.56
2:A:406:THR:OG1	2:A:407:HIS:N	2.39	0.56
2:A:538:LEU:O	2:A:544:MET:N	2.29	0.56
1:B:448:VAL:HG13	1:B:451:LEU:HD23	1.88	0.56
2:A:703:ASN:HB3	2:A:754:LEU:HD21	1.87	0.55
2:A:827:HIS:HA	2:A:830:LEU:HB2	1.89	0.55
2:A:722:GLU:OE2	2:A:790:ARG:NH2	2.35	0.54
1:B:179:ARG:O	1:B:179:ARG:HG3	2.07	0.54
1:B:328:VAL:O	1:B:328:VAL:HG12	2.06	0.54
2:A:480:GLN:HG3	2:A:484:ARG:HE	1.71	0.54
2:A:401:LEU:O	2:A:402:HIS:O	2.26	0.53
1:B:457:ASP:OD1	1:B:457:ASP:N	2.41	0.53
1:B:238:ILE:HG13	1:B:239:PRO:HD3	1.91	0.53
2:A:349:ALA:HA	2:A:352:THR:HG22	1.91	0.53
2:A:616:THR:HB	2:A:664:ARG:HB2	1.90	0.53
1:B:531:ILE:O	1:B:533:HIS:N	2.42	0.52
1:B:57:LEU:HD22	2:A:536:THR:HG21	1.90	0.52
2:A:771:GLN:CD	2:A:802:HIS:HD2	2.18	0.52
2:A:724:GLN:O	2:A:753:ARG:NH2	2.42	0.52
1:B:450:GLU:OE2	1:B:477:ARG:NH1	2.42	0.52
1:B:189:ASN:O	1:B:193:THR:HG23	2.10	0.51
2:A:320:LEU:HD21	2:A:329:ARG:HG3	1.92	0.51
1:B:129:VAL:HG23	1:B:130:ASN:H	1.76	0.51
1:B:86:LEU:HD12	1:B:124:LEU:HB2	1.93	0.51
1:B:70:LEU:O	1:B:74:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:456:GLY:H	2:A:457:PRO:CD	2.21	0.51
2:A:640:ALA:HB3	2:A:813:ILE:HA	1.92	0.51
2:A:530:LEU:O	2:A:534:THR:HG22	2.12	0.50
1:B:148:ALA:O	1:B:151:PRO:HD2	2.12	0.50
1:B:370:CYS:HB2	1:B:542:ASP:H	1.76	0.50
2:A:750:GLU:HB3	2:A:753:ARG:HH11	1.76	0.50
1:B:497:THR:HG22	1:B:497:THR:O	2.11	0.50
2:A:606:ALA:O	2:A:609:THR:HG22	2.11	0.50
1:B:412:VAL:O	1:B:494:ASP:HB2	2.12	0.49
1:B:324:ARG:O	1:B:325:ASP:CB	2.54	0.49
1:B:163:GLY:HA2	1:B:166:LEU:HD12	1.94	0.49
1:B:214:PRO:HG3	2:A:371:LEU:HD12	1.95	0.49
2:A:830:LEU:HB3	2:A:837:TYR:CD1	2.47	0.49
2:A:641:LEU:HD23	2:A:800:ILE:HG12	1.95	0.48
2:A:291:LEU:C	2:A:293:LEU:H	2.22	0.48
2:A:774:ALA:O	2:A:803:ARG:NH2	2.47	0.48
2:A:419:PRO:HG3	2:A:559:PHE:HB2	1.95	0.48
1:B:363:ALA:HB3	1:B:537:VAL:HG22	1.95	0.47
1:B:531:ILE:C	1:B:533:HIS:H	2.22	0.47
2:A:612:PHE:CB	2:A:630:SER:O	2.55	0.47
1:B:39:VAL:HG22	1:B:40:PRO:HD3	1.95	0.47
1:B:296:ALA:O	1:B:300:THR:HG23	2.14	0.47
2:A:316:GLU:O	2:A:320:LEU:HB2	2.15	0.47
1:B:505:GLU:HG3	1:B:506:ALA:N	2.29	0.47
1:B:41:LEU:HD12	1:B:53:ALA:HB1	1.96	0.47
1:B:323:TRP:NE1	1:B:404:ALA:O	2.47	0.47
1:B:389:ARG:HE	1:B:391:LEU:HD21	1.80	0.47
1:B:43:ALA:HB2	1:B:272:GLU:HG2	1.97	0.46
1:B:81:LEU:HB2	1:B:128:VAL:HG21	1.97	0.46
1:B:440:ALA:HA	1:B:443:VAL:HG12	1.97	0.46
2:A:472:GLU:HB3	2:A:493:PHE:HD1	1.79	0.46
2:A:813:ILE:HD13	2:A:827:HIS:HB2	1.97	0.46
2:A:835:GLY:C	2:A:837:TYR:H	2.23	0.46
2:A:280:GLN:OE1	2:A:281:ALA:N	2.48	0.46
1:B:1:MET:N	1:B:1:MET:SD	2.88	0.46
1:B:422:THR:O	1:B:426:ASN:ND2	2.45	0.46
2:A:655:LEU:HD22	2:A:662:VAL:HG12	1.97	0.45
2:A:727:ASP:O	2:A:731:ARG:HG3	2.16	0.45
1:B:224:ALA:O	1:B:228:THR:HG23	2.16	0.45
2:A:459:ILE:HG22	2:A:578:LEU:HD12	1.99	0.45
1:B:85:VAL:O	1:B:89:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:ALA:H	2:A:288:PRO:HD3	1.82	0.45
1:B:129:VAL:HG23	1:B:130:ASN:N	2.31	0.44
1:B:2:ILE:C	1:B:4:THR:H	2.23	0.44
2:A:416:VAL:O	2:A:420:VAL:HB	2.17	0.44
1:B:9:VAL:HG11	1:B:17:LEU:HD22	1.97	0.44
1:B:531:ILE:HG13	1:B:532:ARG:N	2.23	0.44
2:A:596:GLU:HB2	2:A:675:ARG:HB3	1.99	0.44
2:A:752:GLN:HE22	2:A:775:PHE:H	1.65	0.44
2:A:419:PRO:HA	2:A:422:VAL:HG12	1.99	0.44
2:A:734:ASP:OD1	2:A:738:THR:OG1	2.25	0.44
1:B:501:ASP:OD2	1:B:504:ASN:ND2	2.50	0.44
1:B:133:THR:HB	1:B:134:PRO:HD3	2.00	0.43
1:B:146:ALA:HB1	1:B:161:LEU:HD22	2.00	0.43
1:B:236:MET:O	1:B:239:PRO:HD2	2.17	0.43
1:B:416:PRO:HB2	1:B:475:ARG:HG2	1.99	0.43
1:B:515:ASP:OD1	1:B:516:PRO:HD2	2.18	0.43
1:B:188:ALA:HB1	1:B:226:GLN:HA	2.00	0.43
3:B:601:ATP:O3G	2:A:749:GLY:HA3	2.19	0.43
2:A:457:PRO:O	2:A:461:GLN:HB2	2.19	0.43
1:B:292:GLU:N	1:B:292:GLU:OE1	2.51	0.43
1:B:45:LEU:HG	2:A:539:VAL:HG21	2.01	0.43
1:B:129:VAL:O	1:B:134:PRO:HD3	2.17	0.43
1:B:497:THR:O	1:B:497:THR:CG2	2.67	0.43
1:B:553:GLU:HA	1:B:556:THR:HG22	2.00	0.43
1:B:120:THR:HG21	1:B:307:ILE:HD11	2.01	0.43
1:B:250:LEU:O	1:B:254:VAL:HG23	2.18	0.43
2:A:443:VAL:O	2:A:447:ILE:HG13	2.18	0.43
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.85	0.42
2:A:530:LEU:HD23	2:A:530:LEU:HA	1.83	0.42
2:A:651:THR:O	2:A:655:LEU:HG	2.18	0.42
1:B:560:ARG:O	1:B:564:PHE:HB2	2.19	0.42
1:B:76:ARG:O	1:B:80:GLU:HG2	2.19	0.42
1:B:122:PRO:HA	1:B:125:VAL:HG22	2.00	0.42
2:A:515:LYS:O	2:A:568:TYR:OH	2.25	0.42
2:A:657:ALA:HB2	2:A:688:PHE:CZ	2.55	0.42
2:A:748:GLY:HA2	2:A:751:ARG:HG2	2.02	0.42
2:A:538:LEU:HB3	2:A:544:MET:HB2	2.02	0.42
1:B:1:MET:HE3	1:B:297:LEU:HG	2.02	0.41
1:B:331:ARG:O	1:B:331:ARG:HG3	2.21	0.41
1:B:491:LEU:HD22	1:B:519:ARG:HH11	1.85	0.41
1:B:212:VAL:HB	2:A:375:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:LEU:O	2:A:402:HIS:C	2.60	0.41
1:B:294:ALA:HB3	1:B:295:PRO:HD3	2.03	0.41
1:B:498:SER:O	2:A:771:GLN:OE1	2.38	0.41
2:A:537:LEU:O	2:A:541:THR:OG1	2.35	0.41
2:A:442:LEU:O	2:A:446:THR:HG23	2.21	0.40
2:A:813:ILE:O	2:A:824:ARG:HA	2.20	0.40
1:B:408:VAL:O	1:B:490:VAL:HB	2.22	0.40
1:B:538:LEU:HD23	1:B:548:ASP:HB3	2.03	0.40
2:A:782:TYR:O	2:A:786:GLN:HB2	2.22	0.40
2:A:778:PRO:HA	2:A:781:GLU:HG2	2.04	0.40
1:B:498:SER:HB2	2:A:774:ALA:HB1	2.03	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	565/579 (98%)	529 (94%)	33 (6%)	3 (0%)	24	55
2	A	568/859 (66%)	517 (91%)	47 (8%)	4 (1%)	18	47
All	All	1133/1438 (79%)	1046 (92%)	80 (7%)	7 (1%)	23	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	328	VAL
1	B	497	THR
2	A	402	HIS
2	A	631	LEU
1	B	532	ARG
2	A	712	PRO
2	A	771	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	426/435 (98%)	422 (99%)	4 (1%)	70	78
2	A	448/674 (66%)	443 (99%)	5 (1%)	65	76
All	All	874/1109 (79%)	865 (99%)	9 (1%)	65	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39	VAL
1	B	216	ARG
1	B	495	GLN
1	B	542	ASP
2	A	291	LEU
2	A	407	HIS
2	A	629	VAL
2	A	630	SER
2	A	771	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	109	ASN
1	B	203	GLN
1	B	249	GLN
1	B	383	HIS
1	B	438	GLN
1	B	476	GLN
1	B	504	ASN
1	B	526	HIS
2	A	461	GLN
2	A	480	GLN
2	A	508	GLN
2	A	717	GLN
2	A	752	GLN

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Mol	Chain	Res	Type
2	A	771	GLN
2	A	802	HIS
2	A	827	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	901	4	32,33,33	1.33	5 (15%)	48,52,52	1.74	9 (18%)
3	ATP	B	601	4	32,33,33	1.31	4 (12%)	48,52,52	1.78	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	901	4	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	601	4	-	3/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	ATP	C5-C4	4.46	1.47	1.39
3	A	901	ATP	C5-C4	4.42	1.47	1.39
3	A	901	ATP	C5-C6	2.61	1.48	1.41
3	B	601	ATP	C5-C6	2.51	1.48	1.41
3	B	601	ATP	C5-N7	-2.49	1.34	1.39
3	A	901	ATP	C5-N7	-2.37	1.34	1.39
3	B	601	ATP	C8-N7	2.23	1.36	1.31
3	A	901	ATP	C8-N7	2.22	1.35	1.31
3	A	901	ATP	C4-N9	-2.06	1.33	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	ATP	C5-C4-N3	-5.84	118.68	126.72
3	A	901	ATP	C5-C4-N3	-5.78	118.76	126.72
3	B	601	ATP	N3-C4-N9	4.62	135.03	127.17
3	A	901	ATP	N3-C4-N9	4.52	134.86	127.17
3	A	901	ATP	C2-N3-C4	3.73	120.94	111.83
3	B	601	ATP	C2-N3-C4	3.70	120.87	111.83
3	A	901	ATP	C4-C5-N7	-3.48	106.60	110.58
3	B	601	ATP	C4-C5-N7	-3.38	106.72	110.58
3	A	901	ATP	N3-C2-N1	-3.31	123.57	128.58
3	B	601	ATP	N3-C2-N1	-3.29	123.60	128.58
3	A	901	ATP	C4-N9-C8	2.68	108.55	105.74
3	B	601	ATP	C4-N9-C8	2.60	108.47	105.74
3	A	901	ATP	C5-N7-C8	2.47	107.34	103.45
3	B	601	ATP	C5-N7-C8	2.45	107.30	103.45
3	B	601	ATP	C3'-C2'-C1'	2.21	105.64	101.46
3	A	901	ATP	C6-C5-N7	2.13	136.20	132.09
3	A	901	ATP	C3'-C2'-C1'	2.04	105.31	101.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	ATP	C5'-O5'-PA-O2A

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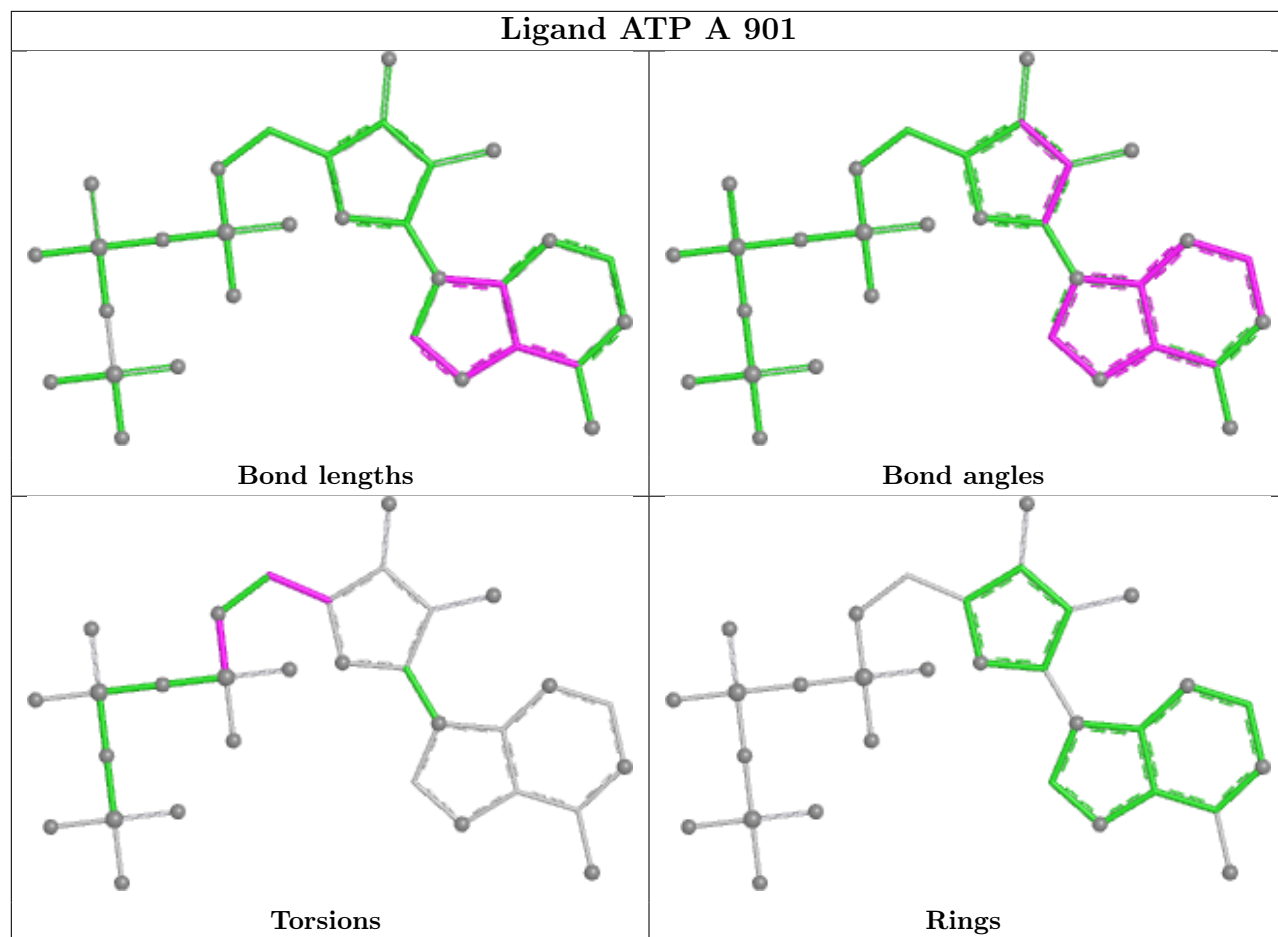
Mol	Chain	Res	Type	Atoms
3	B	601	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C5'-O5'-PA-O2A
3	A	901	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	O4'-C4'-C5'-O5'
3	A	901	ATP	C3'-C4'-C5'-O5'
3	B	601	ATP	C5'-O5'-PA-O1A

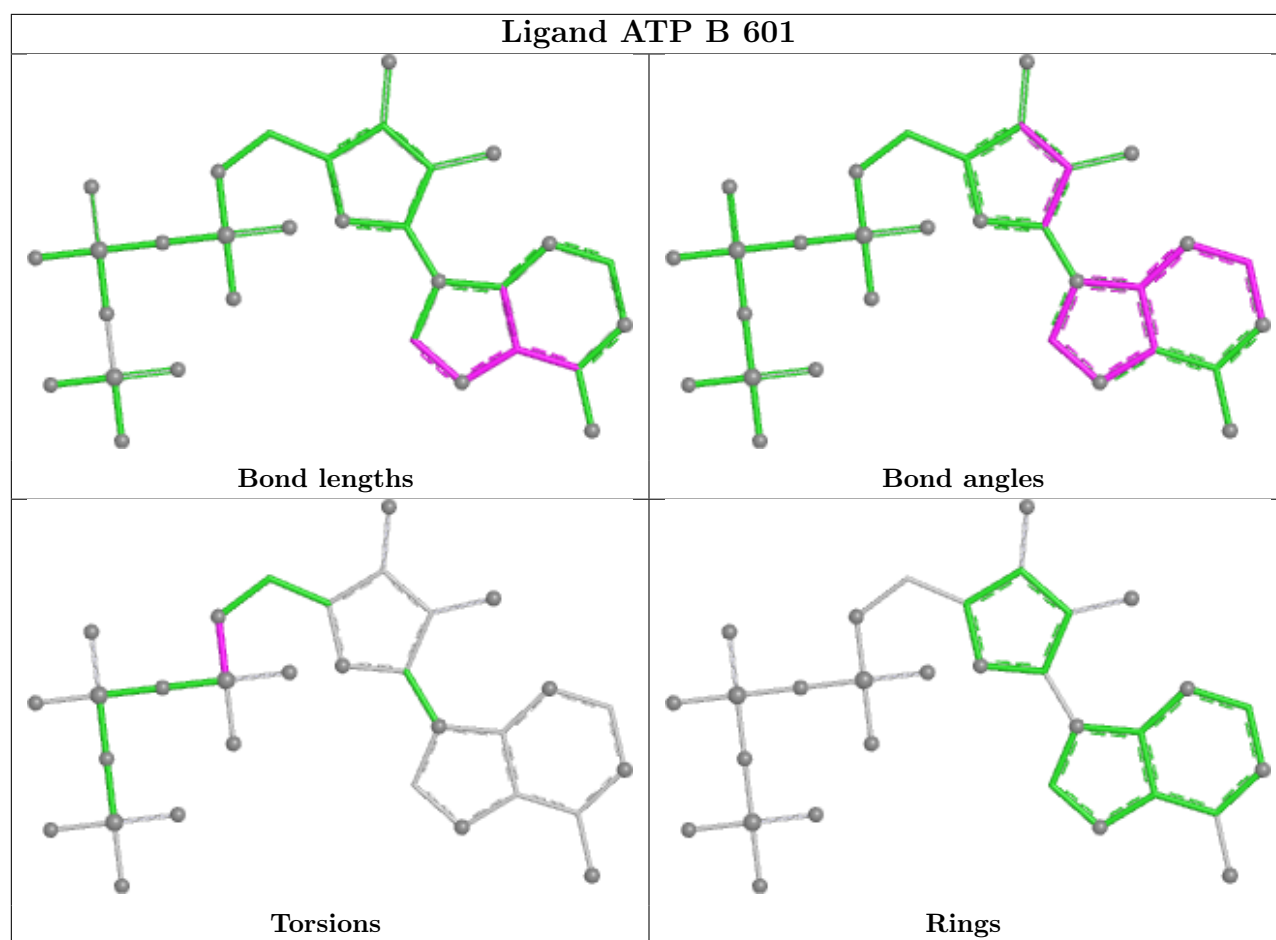
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ATP	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 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.

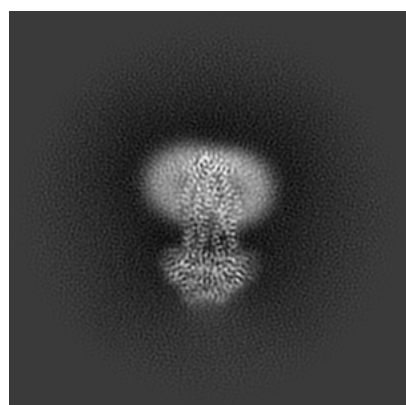
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32538. These allow visual inspection of the internal detail of the map and identification of artifacts.

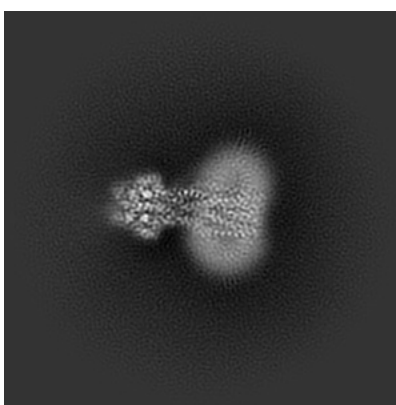
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

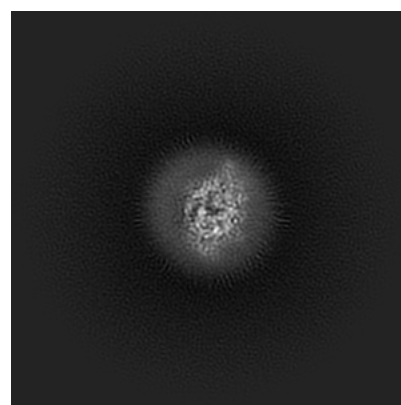
6.1.1 Primary map



X



Y

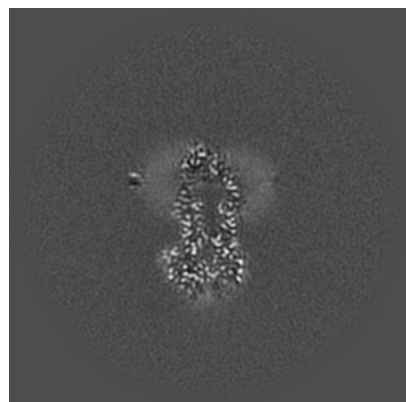


Z

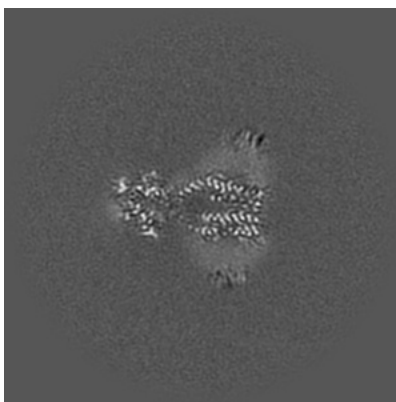
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

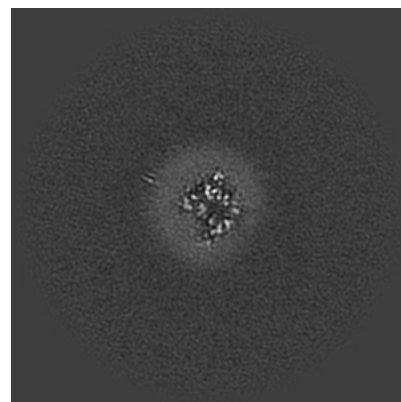
6.2.1 Primary map



X Index: 192



Y Index: 192

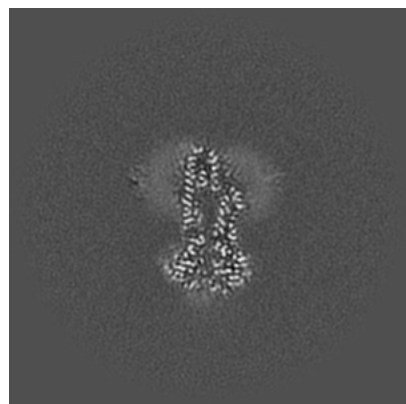


Z Index: 192

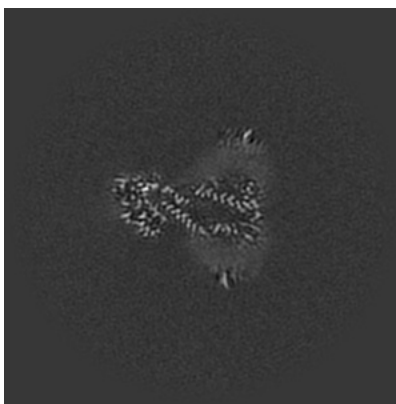
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

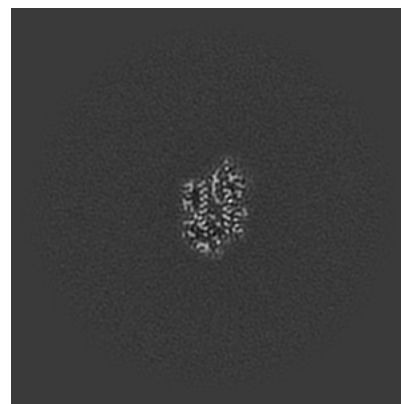
6.3.1 Primary map



X Index: 197



Y Index: 198

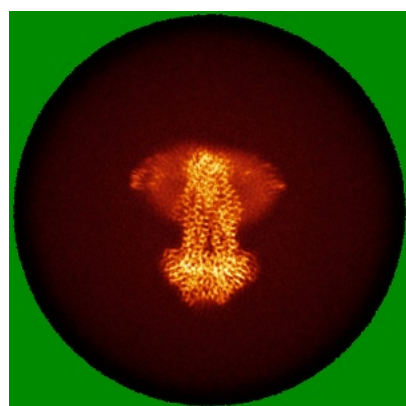


Z Index: 136

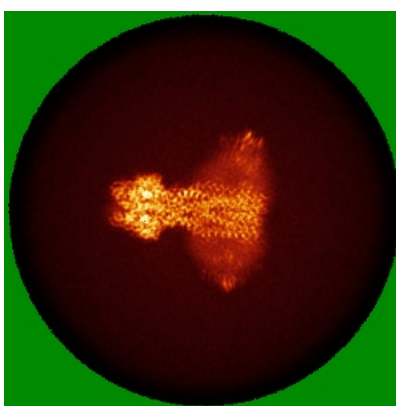
The images above show the largest variance slices of the map in three orthogonal directions.

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

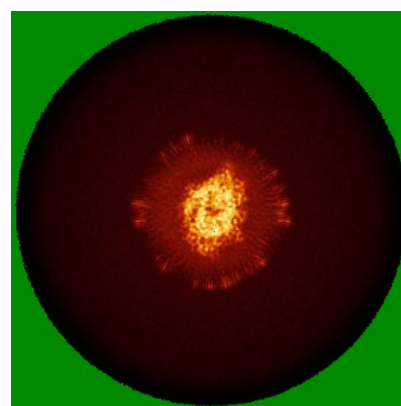
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

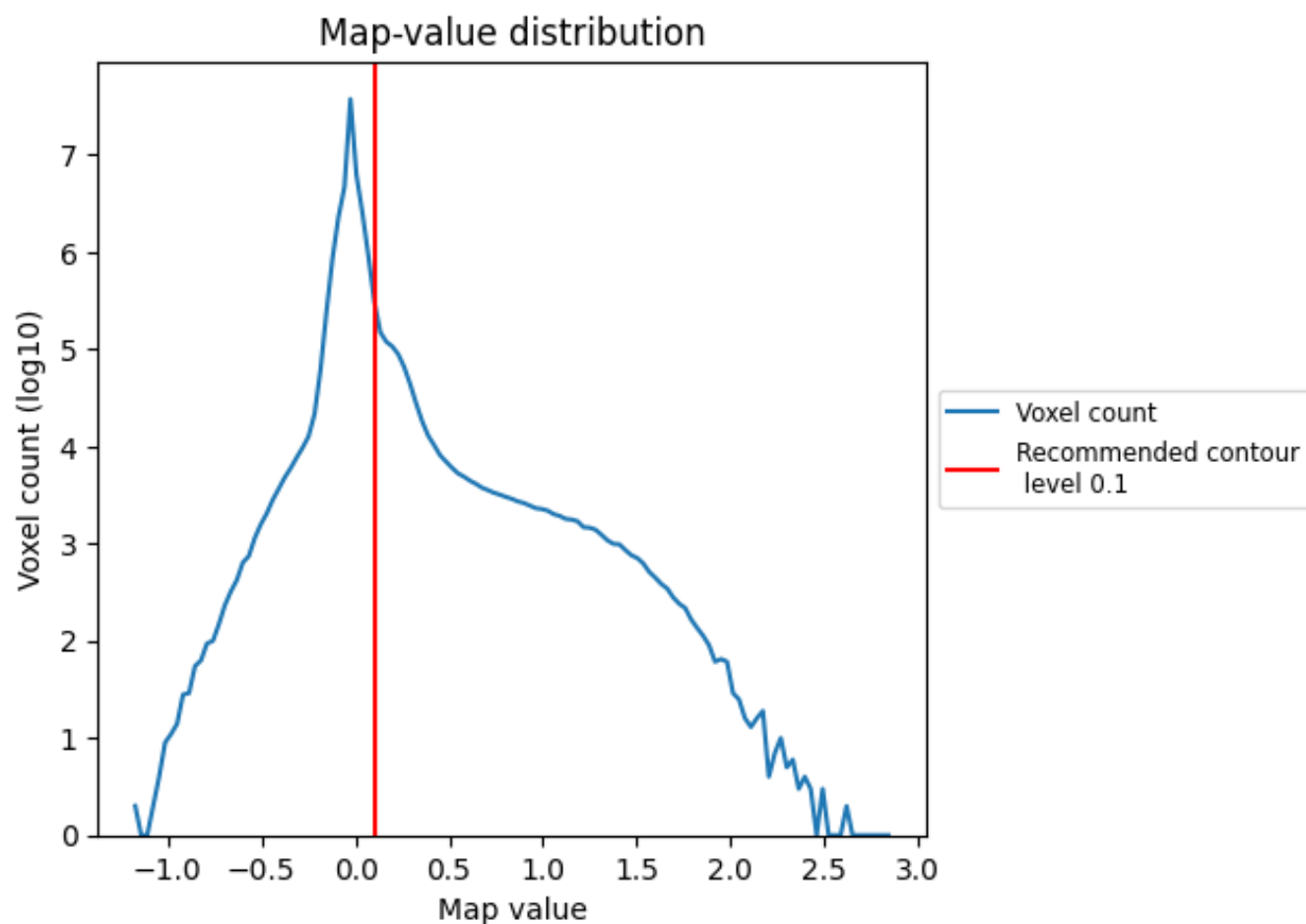
6.6 Mask visualisation

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

7 Map analysis [i](#)

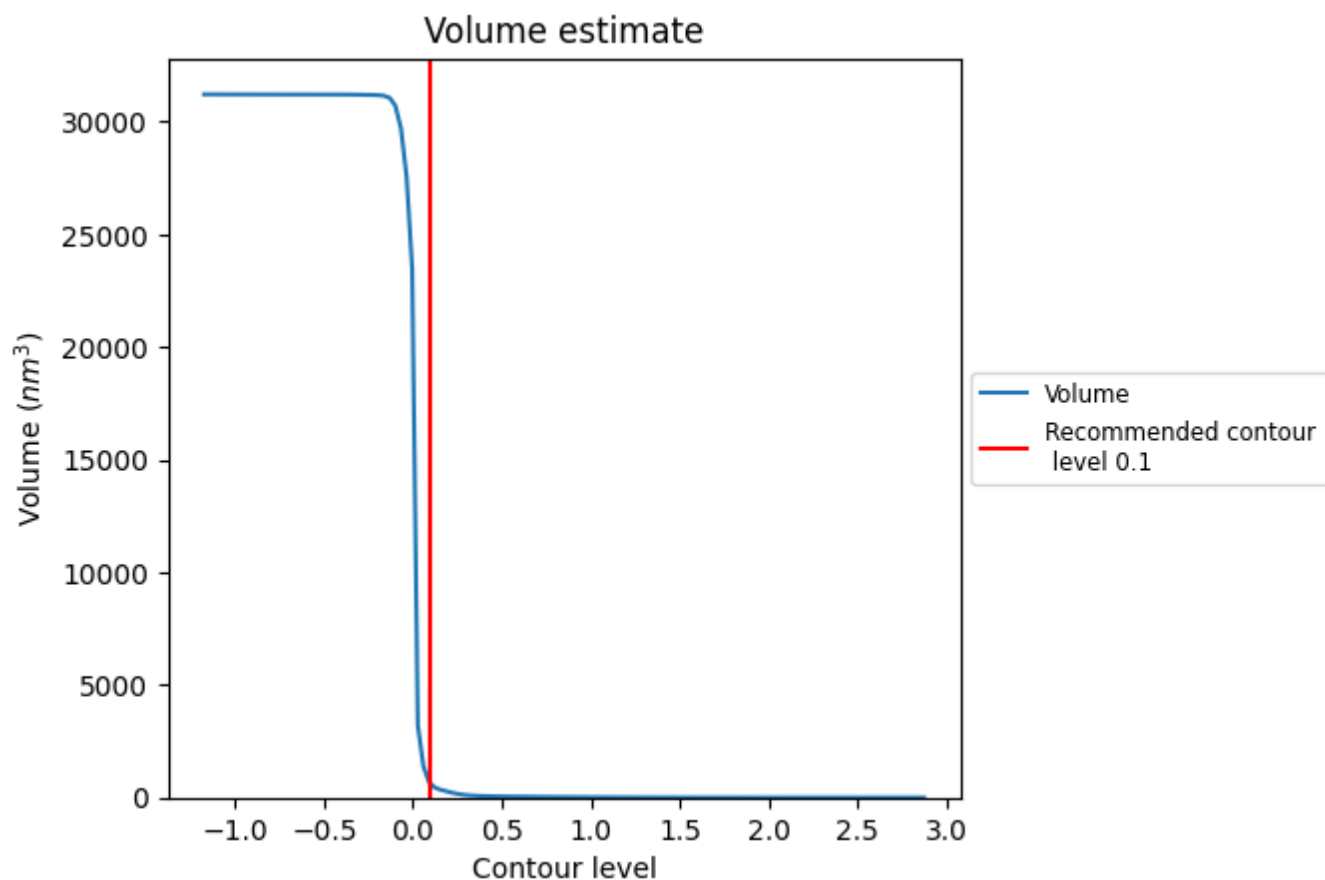
This section contains the results of statistical analysis of the map.

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.

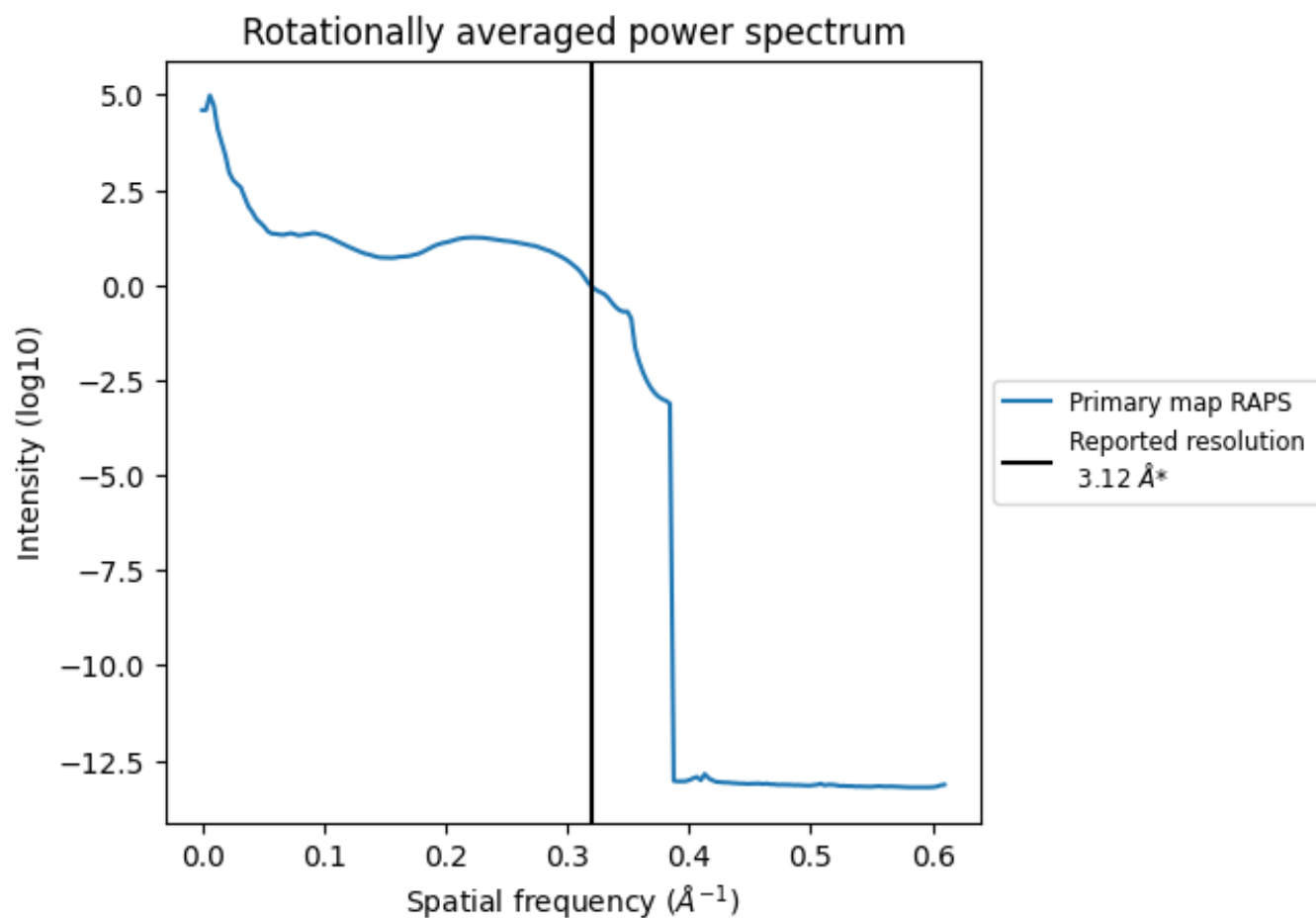
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 616 nm^3 ; this corresponds to an approximate mass of 556 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.321 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

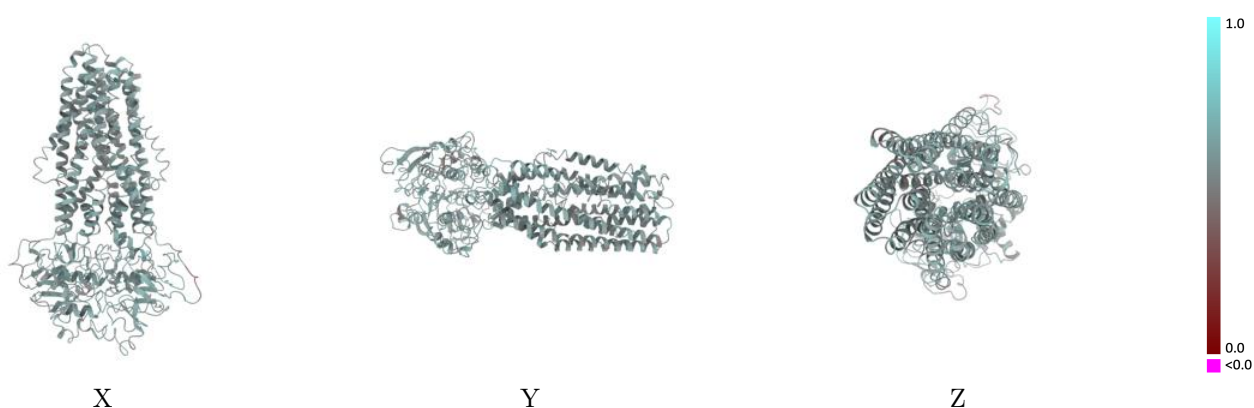
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32538 and PDB model 7WIW. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)

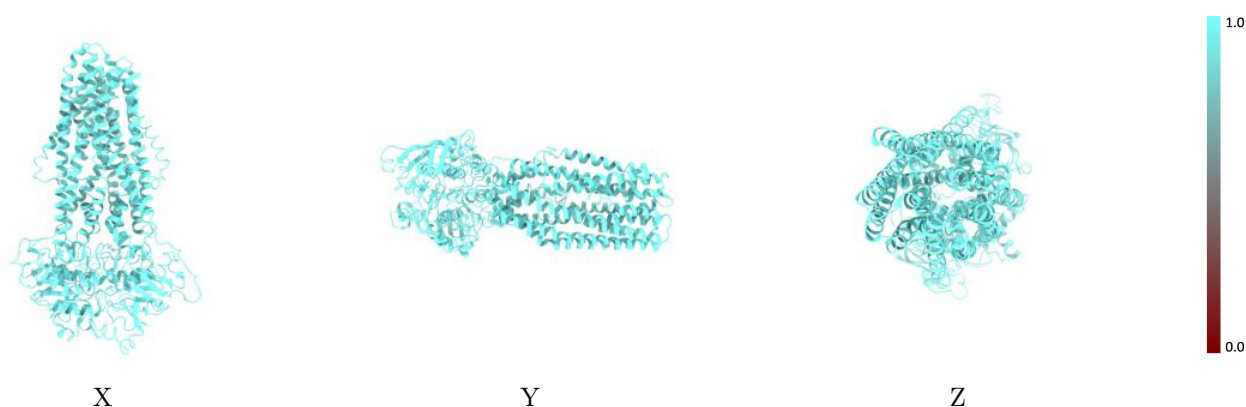
This section was not generated.

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



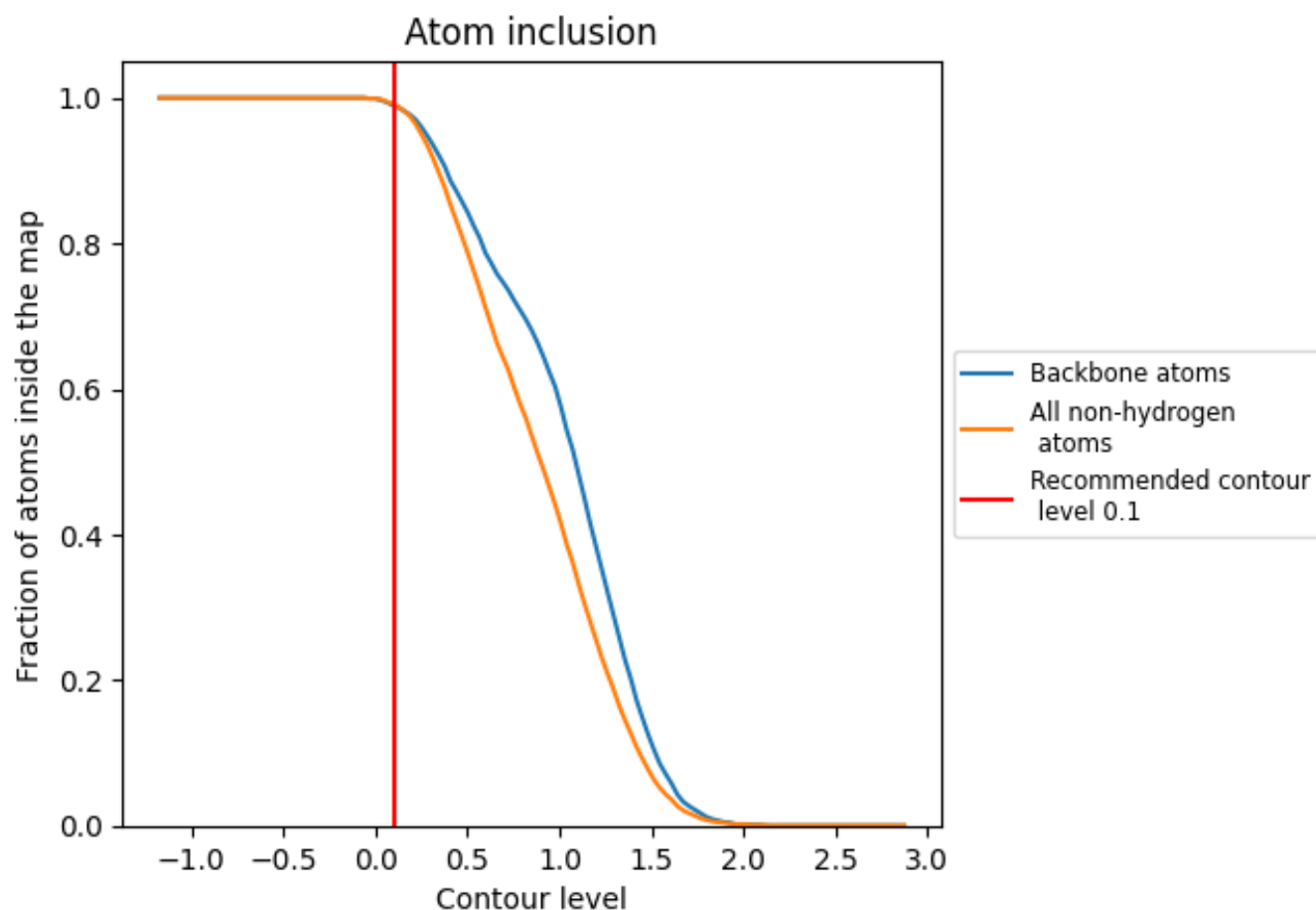
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9910	0.5600
A	0.9920	0.5630
B	0.9900	0.5560

