



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:47 AM UTC

PDB ID : 9KKM / pdb_00009kkm
EMDB ID : EMD-62392
Title : cryo-EM structure of acetyl-CoA carboxyltransferase holoenzyme dimer from *Shewanella oneidensis*, mutant E1238A, complexed with ADP
Authors : Wang, W.; Han, S.R.; Xu, Y.Y.; Gao, H.C.
Deposited on : 2024-11-13
Resolution : 4.14 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

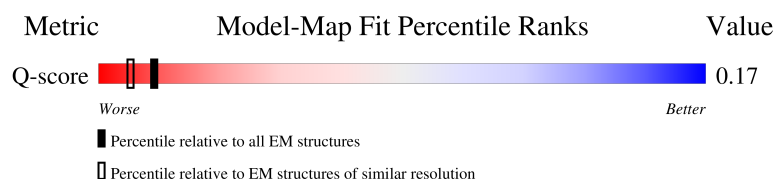
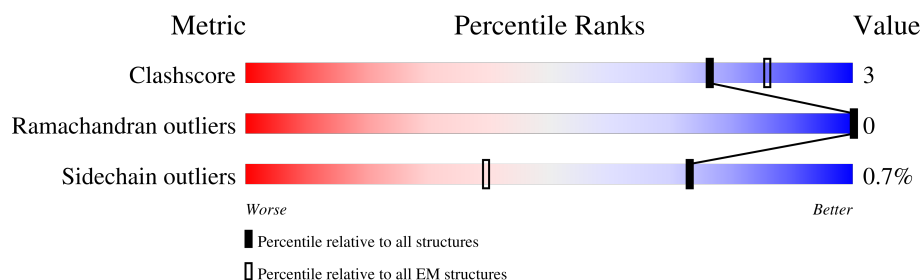
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.14 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	5577 (3.64 - 4.64)

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	1517	
1	B	1517	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	1601	-	-	X	-
2	ADP	B	1601	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21254 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.

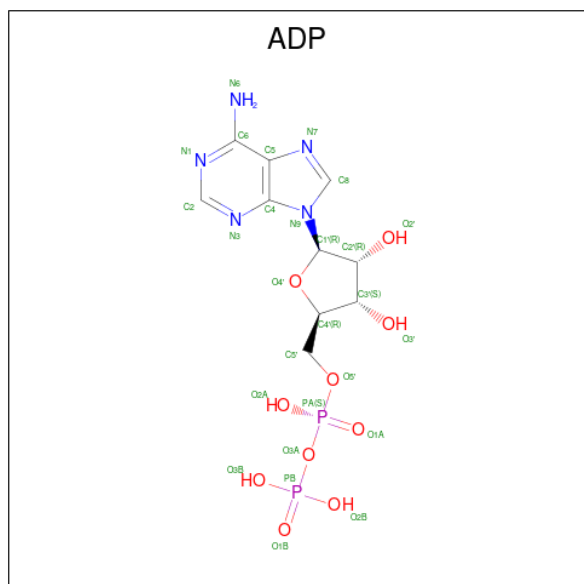
- Molecule 1 is a protein called Acetyl-CoA carboxylase multifunctional enzyme AccADCB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1361	Total	C	N	O	S	0	0
			10599	6716	1838	2001	44		
1	B	1361	Total	C	N	O	S	0	0
			10599	6716	1838	2001	44		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1238	ALA	GLU	engineered mutation	UNP Q8EIJ9
B	1238	ALA	GLU	engineered mutation	UNP Q8EIJ9

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

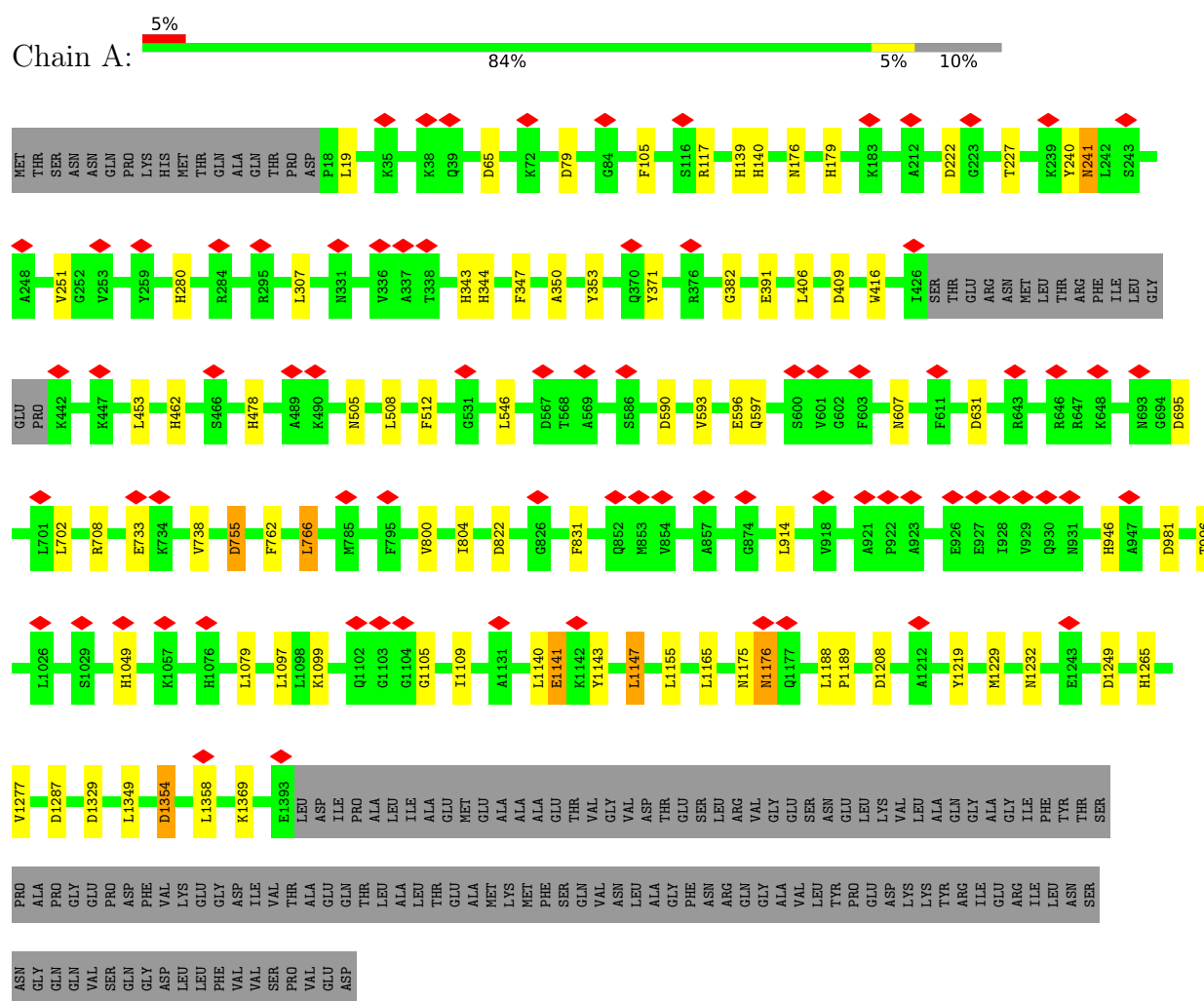
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

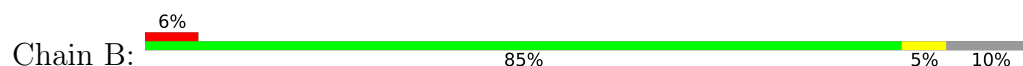
3 Residue-property plots

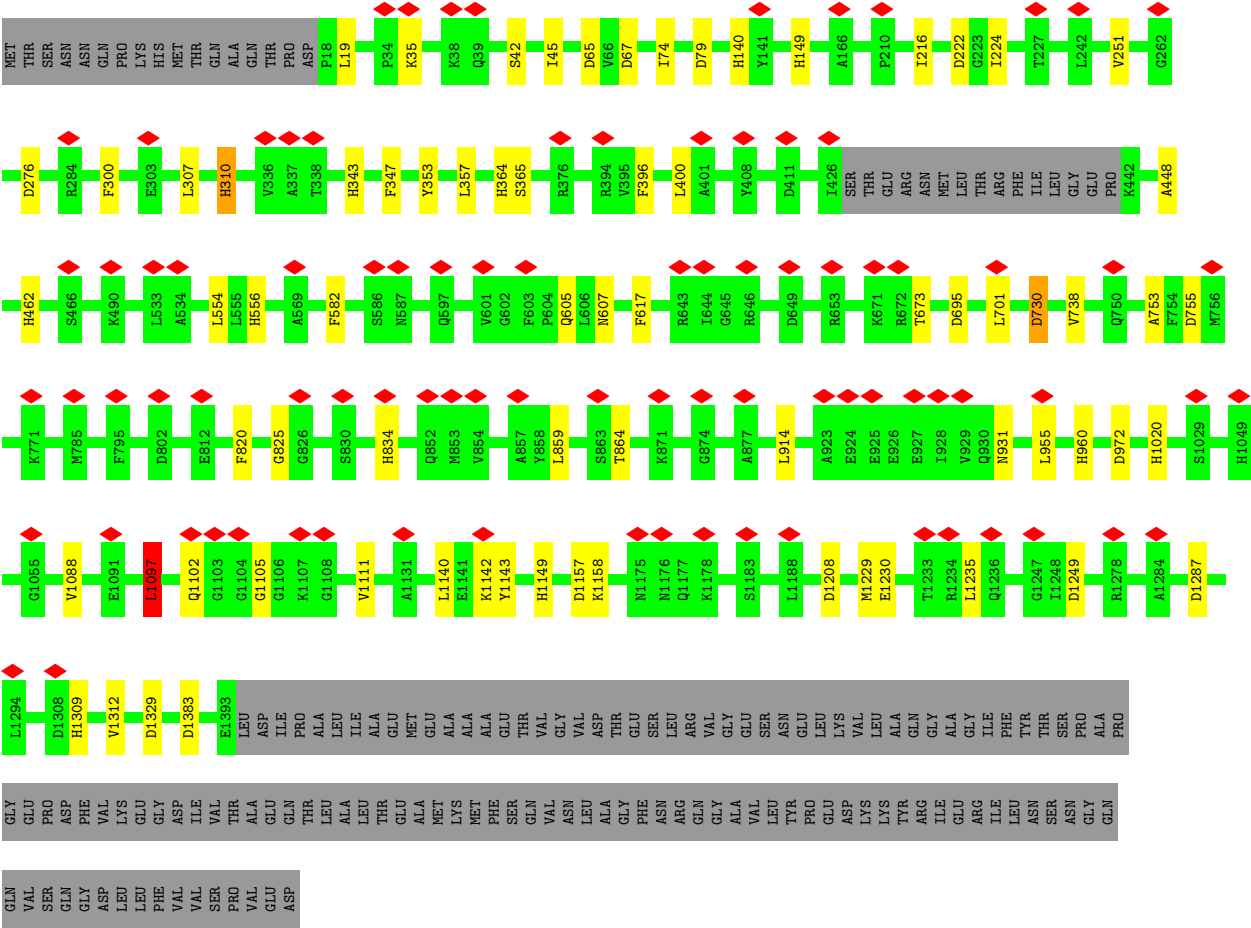
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Acetyl-CoA carboxylase multifunctional enzyme AccADCB



- Molecule 1: Acetyl-CoA carboxylase multifunctional enzyme AccADCB





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	146508	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.847	Depositor
Minimum map value	-2.993	Depositor
Average map value	-0.026	Depositor
Map value standard deviation	0.797	Depositor
Recommended contour level	3.68	Depositor
Map size ($\text{\AA}$)	261.4, 261.4, 261.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3069999, 1.3069999, 1.3069999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	0.90	0/10808	1.61	46/14642 (0.3%)
1	B	0.89	0/10808	1.59	50/14642 (0.3%)
All	All	0.89	0/21616	1.60	96/29284 (0.3%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1141	GLU	CB-CA-C	-14.79	77.53	110.07
1	B	1097	LEU	N-CA-CB	14.78	136.55	110.83
1	B	972	ASP	CA-CB-CG	9.19	121.79	112.60
1	A	1287	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	607	ASN	CA-CB-CG	7.77	120.37	112.60
1	B	730	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	1176	ASN	N-CA-CB	-7.65	97.56	110.49
1	B	607	ASN	CA-CB-CG	7.65	120.25	112.60
1	B	1287	ASP	CA-CB-CG	7.08	119.68	112.60
1	A	1329	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	825	GLY	CA-C-N	6.99	127.86	120.03
1	B	825	GLY	C-N-CA	6.99	127.86	120.03
1	B	1329	ASP	CA-CB-CG	6.96	119.56	112.60
1	B	65	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	695	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	695	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	105	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	241	ASN	N-CA-CB	6.38	122.48	112.46
1	A	505	ASN	CA-C-N	6.14	128.79	120.38
1	A	505	ASN	C-N-CA	6.14	128.79	120.38
1	A	1249	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	1232	ASN	CA-CB-CG	6.12	118.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	65	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	1157	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	582	PHE	CA-CB-CG	5.87	119.67	113.80
1	A	79	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	222	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	364	HIS	CA-CB-CG	5.77	119.57	113.80
1	A	755	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	347	PHE	CA-C-N	5.74	126.32	119.94
1	A	347	PHE	C-N-CA	5.74	126.32	119.94
1	B	79	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	1102	GLN	CA-C-N	5.64	125.69	120.34
1	B	1102	GLN	C-N-CA	5.64	125.69	120.34
1	A	179	HIS	CE1-NE2-CD2	-5.62	103.38	109.00
1	A	1208	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	276	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	222	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	347	PHE	CA-C-N	5.50	126.08	119.98
1	B	347	PHE	C-N-CA	5.50	126.08	119.98
1	A	831	PHE	N-CA-C	5.49	118.78	111.75
1	A	382	GLY	CA-C-N	5.49	127.90	120.38
1	A	382	GLY	C-N-CA	5.49	127.90	120.38
1	A	179	HIS	ND1-CE1-NE2	5.47	113.87	108.40
1	B	755	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	67	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	35	LYS	N-CA-C	5.43	116.89	111.07
1	B	1249	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	1149	HIS	ND1-CE1-NE2	5.37	113.77	108.40
1	A	946	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
1	B	1208	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	462	HIS	ND1-CE1-NE2	5.33	113.73	108.40
1	B	310	HIS	ND1-CE1-NE2	5.31	113.71	108.40
1	B	960	HIS	ND1-CE1-NE2	5.30	113.70	108.40
1	A	996	THR	CA-C-N	5.29	127.63	120.38
1	A	996	THR	C-N-CA	5.29	127.63	120.38
1	A	822	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	931	ASN	CA-C-N	5.28	128.59	121.20
1	B	931	ASN	C-N-CA	5.28	128.59	121.20
1	B	1383	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	766	LEU	N-CA-CB	5.25	118.30	110.22
1	A	981	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	946	HIS	ND1-CE1-NE2	5.21	113.61	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ASN	CA-C-N	5.19	127.55	120.54
1	A	176	ASN	C-N-CA	5.19	127.55	120.54
1	B	310	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
1	A	140	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
1	A	478	HIS	ND1-CE1-NE2	5.10	113.50	108.40
1	B	556	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
1	B	673	THR	CA-C-N	5.09	127.80	120.11
1	B	673	THR	C-N-CA	5.09	127.80	120.11
1	A	462	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
1	A	631	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	343	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
1	A	462	HIS	ND1-CE1-NE2	5.08	113.48	108.40
1	B	149	HIS	ND1-CE1-NE2	5.08	113.48	108.40
1	A	139	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
1	A	344	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
1	B	343	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
1	B	448	ALA	CA-C-N	5.06	127.02	120.44
1	B	448	ALA	C-N-CA	5.06	127.02	120.44
1	B	753	ALA	CA-C-N	5.05	127.95	120.82
1	B	753	ALA	C-N-CA	5.05	127.95	120.82
1	A	409	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	364	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
1	B	556	HIS	ND1-CE1-NE2	5.05	113.45	108.40
1	B	1020	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
1	B	820	PHE	CA-CB-CG	5.02	118.82	113.80
1	B	140	HIS	CE1-NE2-CD2	-5.02	103.98	109.00
1	B	1309	HIS	ND1-CE1-NE2	5.01	113.41	108.40
1	B	834	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
1	B	834	HIS	ND1-CE1-NE2	5.01	113.41	108.40
1	A	1265	HIS	ND1-CE1-NE2	5.01	113.41	108.40
1	A	280	HIS	CE1-NE2-CD2	-5.00	104.00	109.00
1	A	478	HIS	CE1-NE2-CD2	-5.00	104.00	109.00

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	10599	0	10598	83	0
1	B	10599	0	10598	39	0
2	A	27	0	12	28	0
2	B	27	0	12	22	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	21254	0	21220	127	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 3.

All (127) 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:1097:LEU:HD11	2:B:1601:ADP:C2	1.54	1.41
1:A:762:PHE:CE2	1:A:804:ILE:HD11	1.67	1.29
1:A:762:PHE:CZ	1:A:804:ILE:HD11	1.68	1.28
1:A:762:PHE:HZ	1:A:804:ILE:CG1	1.47	1.26
1:A:762:PHE:CZ	1:A:804:ILE:CD1	2.25	1.20
1:A:762:PHE:CE1	1:A:766:LEU:CD1	2.26	1.19
1:A:1229:MET:CE	2:A:1601:ADP:H5'1	1.73	1.17
1:A:1229:MET:SD	2:A:1601:ADP:H5'1	1.87	1.15
1:A:762:PHE:CE1	1:A:766:LEU:HD12	1.81	1.14
1:A:762:PHE:CZ	1:A:804:ILE:CG1	2.34	1.10
1:A:1097:LEU:HD12	1:A:1141:GLU:OE1	1.48	1.09
1:A:762:PHE:HE1	1:A:766:LEU:HD12	1.12	1.09
1:A:241:ASN:HD21	1:A:391:GLU:HB2	1.19	1.06
1:A:762:PHE:CZ	1:A:804:ILE:HG13	1.91	1.06
1:A:1097:LEU:HD11	2:A:1601:ADP:HN61	1.22	1.05
1:A:762:PHE:HE1	1:A:766:LEU:CD1	1.66	1.04
1:B:1097:LEU:CD1	2:B:1601:ADP:C2	2.41	1.02
1:A:762:PHE:CE1	1:A:766:LEU:HD11	1.95	1.01
1:A:1229:MET:SD	2:A:1601:ADP:C5'	2.48	1.00
2:A:1601:ADP:N3	2:A:1601:ADP:H3'	1.77	0.99
1:A:762:PHE:HZ	1:A:804:ILE:CD1	1.67	0.98
1:B:1097:LEU:HD11	2:B:1601:ADP:N1	1.79	0.97
1:B:1097:LEU:CD1	2:B:1601:ADP:N1	2.28	0.97
1:A:1097:LEU:HD11	2:A:1601:ADP:N6	1.80	0.95
1:B:1097:LEU:HD21	1:B:1143:TYR:CD1	2.04	0.93
1:A:1229:MET:HE1	2:A:1601:ADP:H5'1	1.49	0.92
1:A:241:ASN:ND2	1:A:391:GLU:HB2	1.86	0.91
1:B:1143:TYR:HD1	2:B:1601:ADP:N1	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:PHE:HE2	1:A:804:ILE:HD11	1.38	0.87
1:A:762:PHE:CZ	1:A:766:LEU:HD11	2.14	0.82
2:A:1601:ADP:N3	2:A:1601:ADP:C3'	2.43	0.80
1:A:241:ASN:HD21	1:A:391:GLU:CB	1.94	0.80
1:B:1097:LEU:HG	2:B:1601:ADP:N1	1.96	0.80
1:B:1143:TYR:CE1	2:B:1601:ADP:H2	2.00	0.79
1:A:241:ASN:ND2	1:A:391:GLU:CB	2.46	0.79
1:A:762:PHE:CE2	1:A:804:ILE:CD1	2.56	0.78
1:B:1097:LEU:CG	2:B:1601:ADP:N1	2.46	0.78
1:B:1143:TYR:CD1	2:B:1601:ADP:C2	2.70	0.78
1:A:1097:LEU:CD1	1:A:1141:GLU:OE1	2.29	0.78
1:A:1189:PRO:HD3	1:A:1219:TYR:OH	1.84	0.77
1:B:1143:TYR:CD1	2:B:1601:ADP:N1	2.56	0.72
1:B:1229:MET:SD	2:B:1601:ADP:H3'	2.30	0.71
1:A:1229:MET:SD	2:A:1601:ADP:H5'2	2.29	0.71
1:B:1143:TYR:CE1	2:B:1601:ADP:C2	2.80	0.70
2:A:1601:ADP:N3	2:A:1601:ADP:C2'	2.54	0.69
1:A:593:VAL:HA	1:A:596:GLU:HG3	1.73	0.68
1:B:1143:TYR:HE1	2:B:1601:ADP:H2	1.43	0.67
1:A:593:VAL:HA	1:A:596:GLU:CG	2.25	0.66
1:B:1143:TYR:HD1	2:B:1601:ADP:C2	2.10	0.66
1:A:1229:MET:CE	2:A:1601:ADP:C5'	2.65	0.65
1:A:1097:LEU:HD11	2:A:1601:ADP:C6	2.30	0.65
1:B:1097:LEU:HD22	1:B:1111:VAL:HA	1.79	0.65
2:A:1601:ADP:N3	2:A:1601:ADP:H2'	2.13	0.63
1:A:593:VAL:O	1:A:596:GLU:HG3	1.98	0.62
1:A:702:LEU:HD23	1:A:702:LEU:H	1.65	0.62
1:A:1079:LEU:HD11	1:A:1140:LEU:HB2	1.83	0.61
1:A:762:PHE:C	1:A:762:PHE:CD1	2.78	0.60
1:A:1097:LEU:CD1	2:A:1601:ADP:HN61	2.04	0.60
1:A:596:GLU:OE2	1:A:597:GLN:HG3	2.01	0.60
1:A:1097:LEU:CD1	2:A:1601:ADP:N6	2.63	0.60
1:A:762:PHE:CE1	1:A:804:ILE:HG13	2.36	0.59
1:A:1097:LEU:HB2	1:A:1141:GLU:HB2	1.84	0.58
1:A:1188:LEU:HA	1:A:1219:TYR:CZ	2.38	0.58
1:B:1142:LYS:O	2:B:1601:ADP:N6	2.37	0.58
1:A:1097:LEU:HD11	2:A:1601:ADP:C5	2.39	0.57
1:B:1097:LEU:HG	2:B:1601:ADP:C6	2.39	0.57
1:A:371:TYR:OH	1:A:708:ARG:CG	2.52	0.56
1:A:1354:ASP:OD1	1:A:1369:LYS:HE3	2.04	0.56
1:A:762:PHE:CD2	1:A:800:VAL:HG13	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:PHE:CG	1:A:800:VAL:HG13	2.41	0.55
1:A:1097:LEU:HD11	2:A:1601:ADP:N7	2.22	0.55
1:B:1230:GLU:OE2	2:B:1601:ADP:O1A	2.24	0.55
1:B:1097:LEU:HD11	2:B:1601:ADP:H2	1.59	0.54
1:A:406:LEU:C	1:A:406:LEU:HD23	2.33	0.54
1:A:371:TYR:OH	1:A:708:ARG:HG3	2.08	0.53
1:B:1097:LEU:HD21	1:B:1143:TYR:CG	2.42	0.53
1:A:1189:PRO:CD	1:A:1219:TYR:OH	2.55	0.52
1:A:453:LEU:HD22	1:A:512:PHE:HB2	1.91	0.52
1:A:1105:GLY:N	2:A:1601:ADP:O2B	2.41	0.52
1:A:593:VAL:CA	1:A:596:GLU:HG3	2.38	0.52
1:B:738:VAL:HG11	1:B:914:LEU:HD22	1.92	0.51
1:A:1147:LEU:HD22	2:A:1601:ADP:C2	2.46	0.51
1:A:1143:TYR:HA	2:A:1601:ADP:N6	2.26	0.51
1:A:240:TYR:O	1:A:241:ASN:OD1	2.29	0.51
1:A:1143:TYR:HD1	2:A:1601:ADP:N6	2.09	0.50
1:A:307:LEU:HD21	1:A:350:ALA:HB2	1.91	0.50
1:A:593:VAL:C	1:A:596:GLU:HG3	2.36	0.50
1:A:1155:LEU:HD11	1:A:1165:LEU:HD11	1.94	0.50
1:B:74:ILE:HA	1:B:224:ILE:HD11	1.94	0.50
1:A:241:ASN:ND2	1:A:391:GLU:HB3	2.24	0.50
1:A:1147:LEU:CD2	2:A:1601:ADP:C2	2.94	0.50
1:A:453:LEU:HD21	1:A:508:LEU:HB3	1.95	0.48
1:B:1097:LEU:HD22	1:B:1111:VAL:HG22	1.95	0.48
1:B:42:SER:HA	1:B:45:ILE:HD12	1.96	0.48
1:A:19:LEU:HD11	1:A:353:TYR:CE2	2.48	0.47
1:A:1188:LEU:HA	1:A:1219:TYR:OH	2.14	0.47
1:A:1097:LEU:CD1	2:A:1601:ADP:N7	2.77	0.47
1:A:593:VAL:O	1:A:596:GLU:OE2	2.32	0.46
1:A:1277:VAL:HG13	1:A:1349:LEU:HD21	1.96	0.46
1:A:1143:TYR:HA	2:A:1601:ADP:HN62	1.80	0.46
1:A:1175:ASN:O	1:A:1176:ASN:HB3	2.15	0.46
1:A:406:LEU:HD11	1:A:416:TRP:HB2	1.97	0.46
1:A:406:LEU:HD23	1:A:406:LEU:O	2.15	0.46
1:B:1088:VAL:HG12	1:B:1140:LEU:HD22	1.99	0.45
1:B:300:PHE:CE2	1:B:307:LEU:HD22	2.50	0.45
2:A:1601:ADP:C3'	2:A:1601:ADP:C4	3.00	0.45
1:A:1099:LYS:HE3	1:A:1109:ILE:CD1	2.47	0.44
1:A:1176:ASN:ND2	2:A:1601:ADP:O1A	2.50	0.44
1:B:859:LEU:HB3	1:B:864:THR:HG21	1.99	0.44
1:B:353:TYR:CE1	1:B:357:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:PHE:CE2	1:B:400:LEU:HD11	2.53	0.44
1:A:251:VAL:HA	1:A:702:LEU:HD12	1.99	0.43
1:B:955:LEU:HD21	1:B:1235:LEU:HD22	1.98	0.43
1:A:702:LEU:H	1:A:702:LEU:CD2	2.29	0.43
1:A:738:VAL:HG11	1:A:914:LEU:HD22	1.99	0.43
1:A:593:VAL:HA	1:A:596:GLU:HG2	2.01	0.43
1:B:19:LEU:HD22	1:B:310:HIS:CD2	2.54	0.43
1:A:1099:LYS:HG2	1:A:1109:ILE:HG12	2.01	0.42
1:A:1143:TYR:HD1	2:A:1601:ADP:HN61	1.68	0.42
1:B:19:LEU:HD22	1:B:310:HIS:CG	2.55	0.41
1:B:1097:LEU:CD1	2:B:1601:ADP:C6	2.99	0.41
1:B:1105:GLY:N	2:B:1601:ADP:O2B	2.53	0.41
1:A:1147:LEU:HD13	2:A:1601:ADP:H2	1.86	0.41
1:B:554:LEU:HD23	1:B:617:PHE:CE1	2.56	0.40
1:B:45:ILE:HD11	1:B:216:ILE:HD13	2.02	0.40
1:B:1143:TYR:HE1	2:B:1601:ADP:C2	2.29	0.40
1:B:1097:LEU:HG	2:B:1601:ADP:N6	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1357/1517 (90%)	1307 (96%)	50 (4%)	0	100	100
1	B	1357/1517 (90%)	1310 (96%)	47 (4%)	0	100	100
All	All	2714/3034 (90%)	2617 (96%)	97 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1146/1277 (90%)	1137 (99%)	9 (1%)	73	77
1	B	1146/1277 (90%)	1138 (99%)	8 (1%)	76	79
All	All	2292/2554 (90%)	2275 (99%)	17 (1%)	73	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ARG
1	A	227	THR
1	A	546	LEU
1	A	733	GLU
1	A	755	ASP
1	A	1049	HIS
1	A	1147	LEU
1	A	1354	ASP
1	A	1358	LEU
1	B	251	VAL
1	B	365	SER
1	B	605	GLN
1	B	701	LEU
1	B	730	ASP
1	B	1097	LEU
1	B	1158	LYS
1	B	1312	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	78	GLN
1	A	175	GLN
1	A	241	ASN
1	A	320	ASN

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Mol	Chain	Res	Type
1	A	413	ASN
1	A	418	ASN
1	A	462	HIS
1	A	467	ASN
1	A	470	ASN
1	A	496	GLN
1	A	505	ASN
1	A	528	ASN
1	A	561	HIS
1	A	570	ASN
1	A	640	ASN
1	A	750	GLN
1	A	891	GLN
1	A	931	ASN
1	A	962	ASN
1	A	995	ASN
1	A	1067	GLN
1	A	1081	ASN
1	A	1102	GLN
1	A	1135	ASN
1	A	1220	ASN
1	A	1341	ASN
1	B	22	GLN
1	B	25	HIS
1	B	78	GLN
1	B	279	GLN
1	B	368	GLN
1	B	467	ASN
1	B	478	HIS
1	B	505	ASN
1	B	552	ASN
1	B	566	GLN
1	B	640	ASN
1	B	684	GLN
1	B	887	ASN
1	B	963	ASN
1	B	1003	ASN
1	B	1056	ASN
1	B	1065	GLN
1	B	1224	ASN
1	B	1236	GLN
1	B	1309	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
2	ADP	A	1601	3	28,29,29	0.45	0	43,45,45	0.91	1 (2%)
2	ADP	B	1601	3	28,29,29	0.45	0	43,45,45	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1601	3	-	8/16/32/32	0/3/3/3
2	ADP	B	1601	3	-	4/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1601	ADP	C2'-C1'-N9	-4.89	101.15	113.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

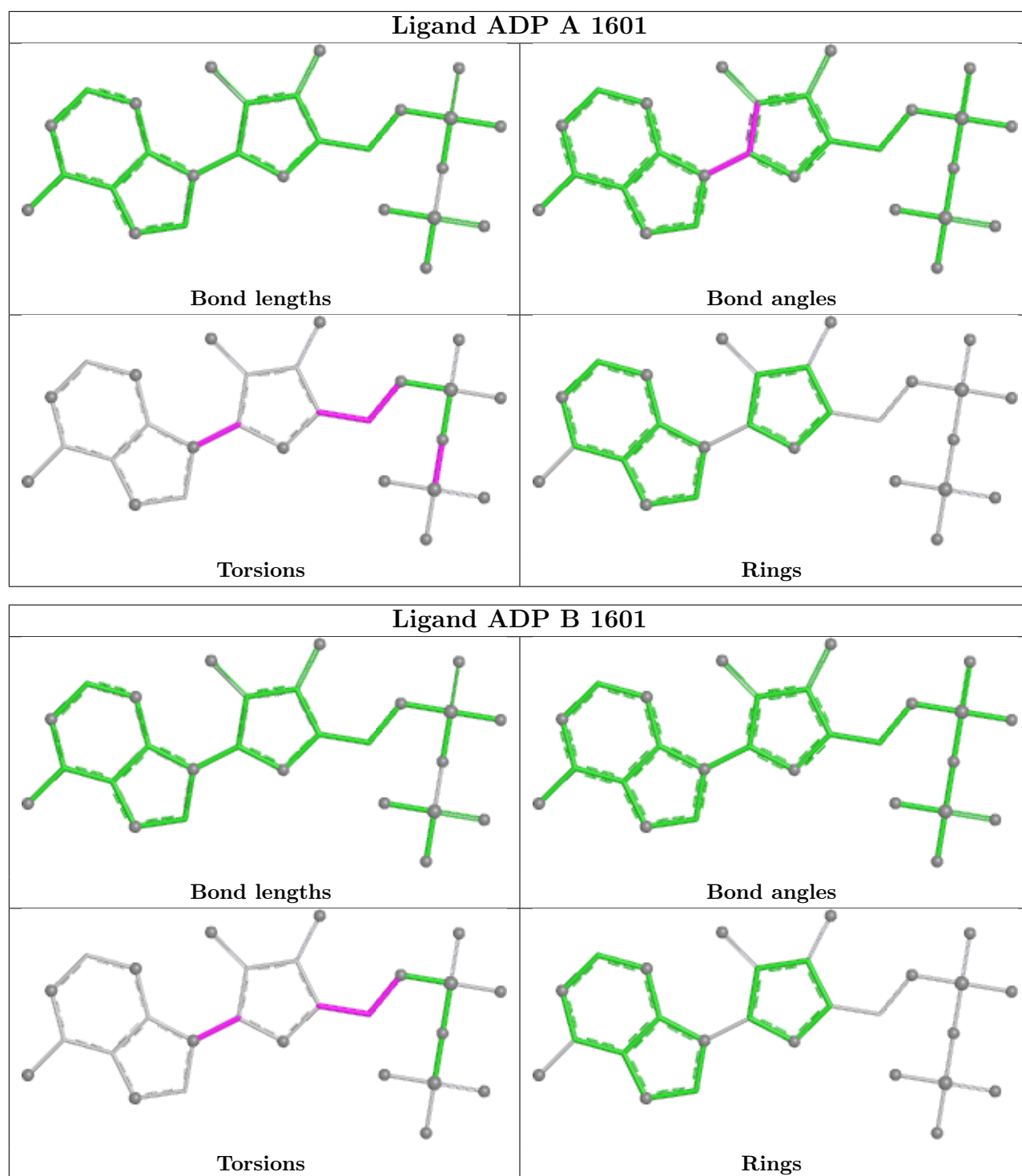
Mol	Chain	Res	Type	Atoms
2	A	1601	ADP	PA-O3A-PB-O2B
2	A	1601	ADP	C4'-C5'-O5'-PA
2	B	1601	ADP	O4'-C4'-C5'-O5'
2	A	1601	ADP	C3'-C4'-C5'-O5'
2	B	1601	ADP	C3'-C4'-C5'-O5'
2	A	1601	ADP	O4'-C4'-C5'-O5'
2	A	1601	ADP	C2'-C1'-N9-C4
2	A	1601	ADP	C2'-C1'-N9-C8
2	B	1601	ADP	C4'-C5'-O5'-PA
2	A	1601	ADP	PA-O3A-PB-O1B
2	B	1601	ADP	C2'-C1'-N9-C8
2	A	1601	ADP	O4'-C1'-N9-C8

There are no ring outliers.

2 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	ADP	28	0
2	B	1601	ADP	22	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

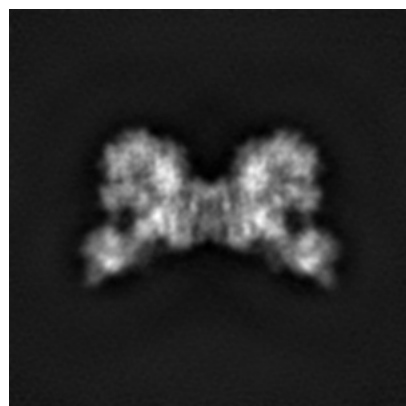
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62392. These allow visual inspection of the internal detail of the map and identification of artifacts.

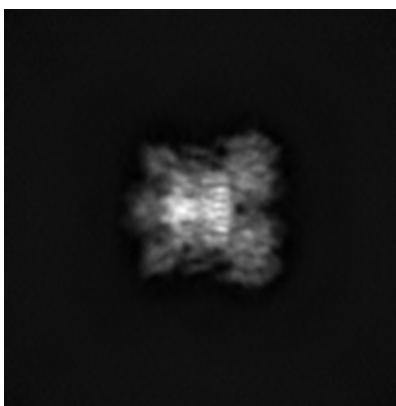
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

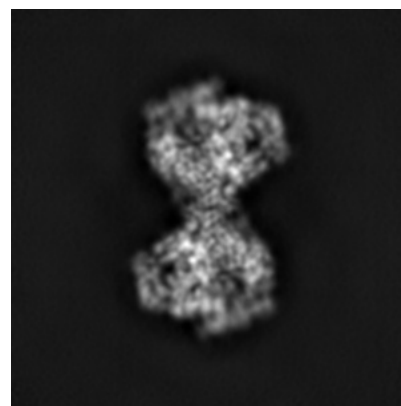
6.1.1 Primary map



X

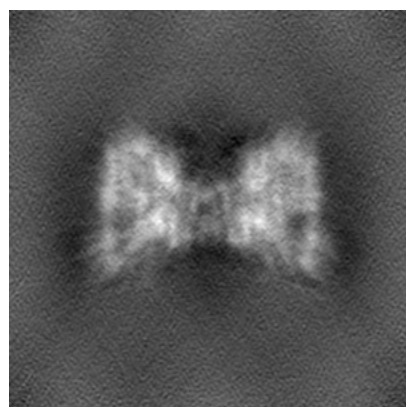


Y

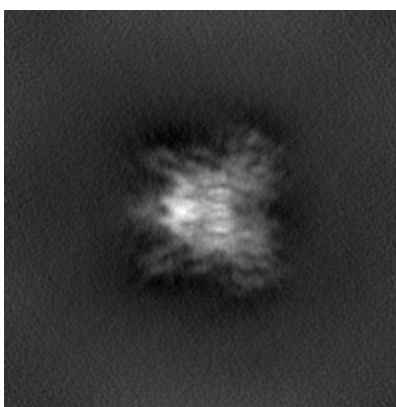


Z

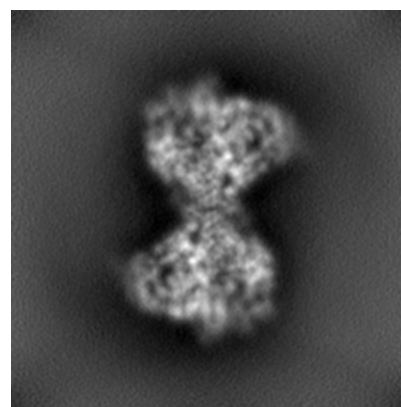
6.1.2 Raw map



X



Y

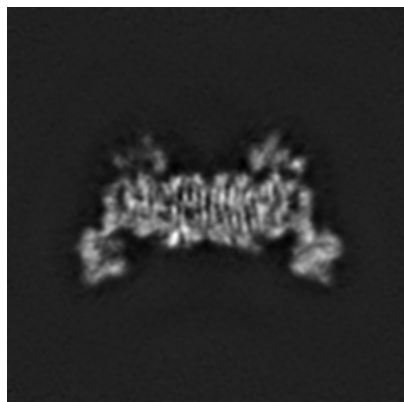


Z

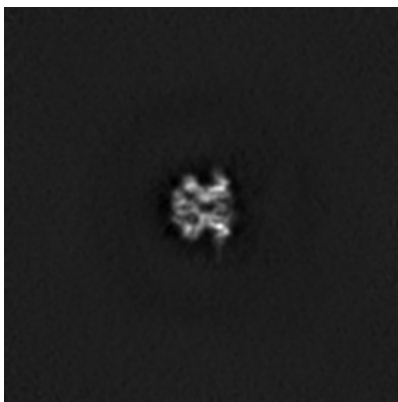
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

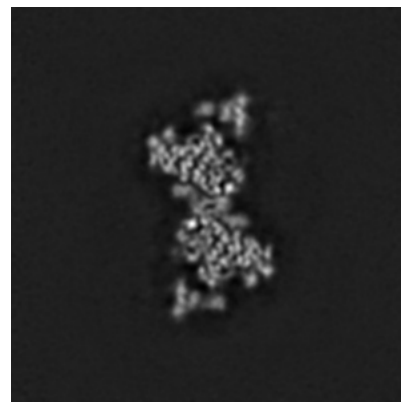
6.2.1 Primary map



X Index: 100

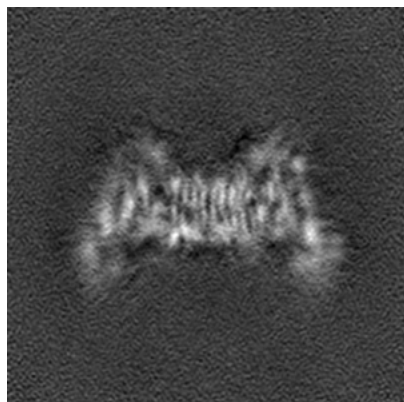


Y Index: 100

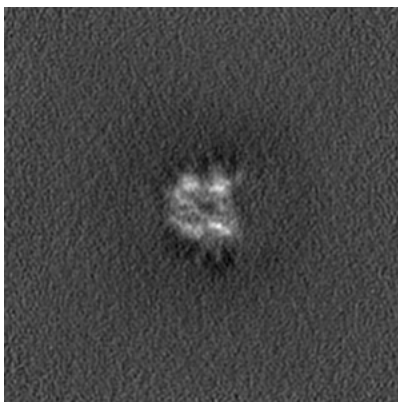


Z Index: 100

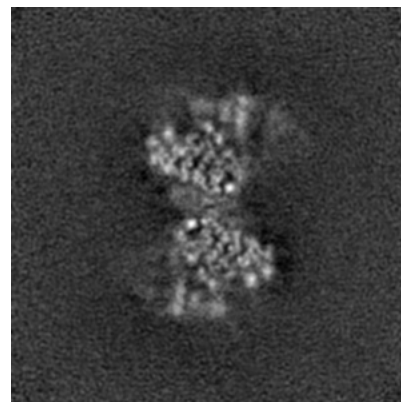
6.2.2 Raw map



X Index: 100



Y Index: 100

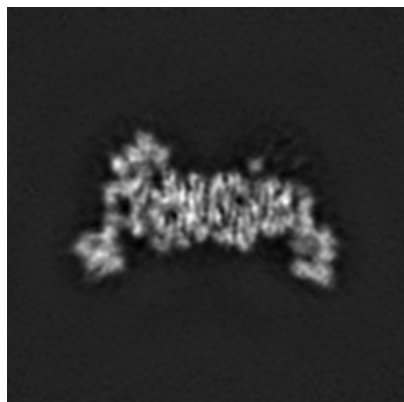


Z Index: 100

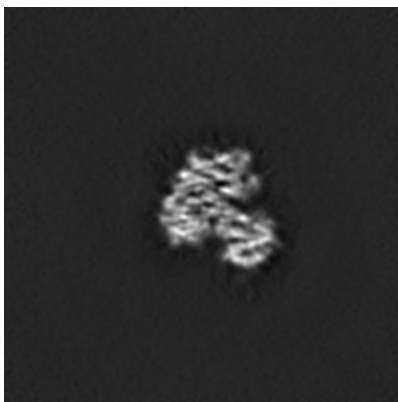
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

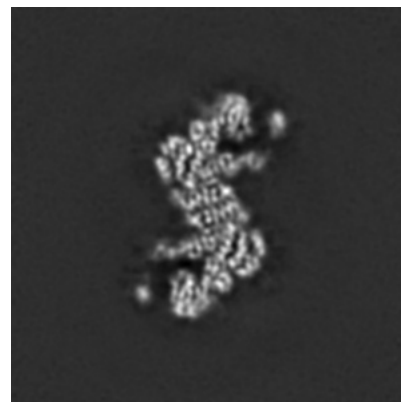
6.3.1 Primary map



X Index: 97

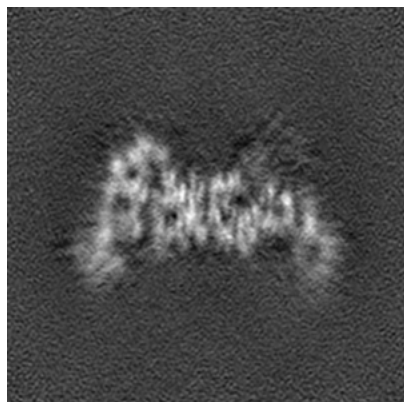


Y Index: 81

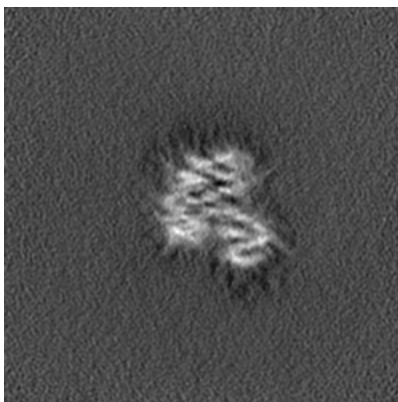


Z Index: 109

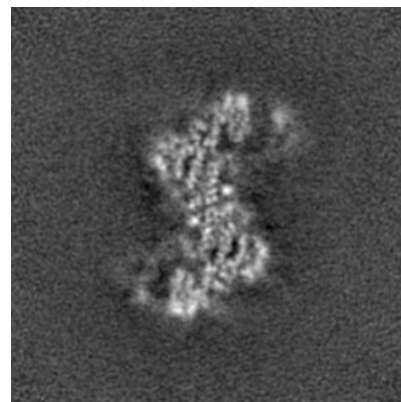
6.3.2 Raw map



X Index: 97



Y Index: 81

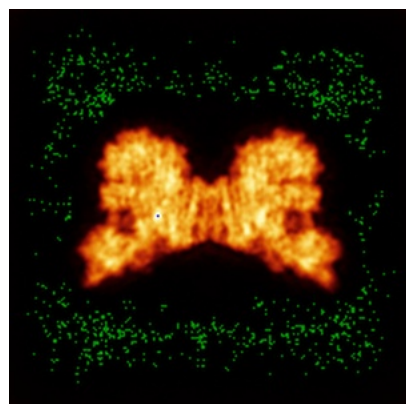


Z Index: 107

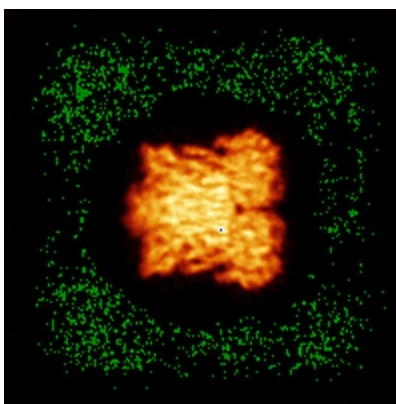
The images above show the largest variance slices of the map in three orthogonal directions.

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

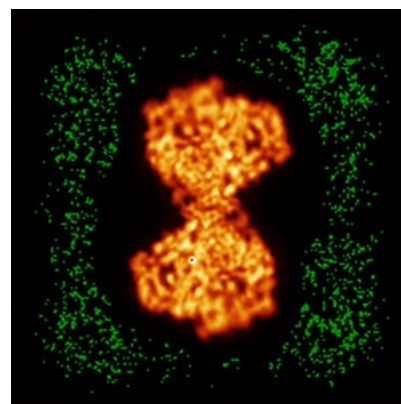
6.4.1 Primary map



X

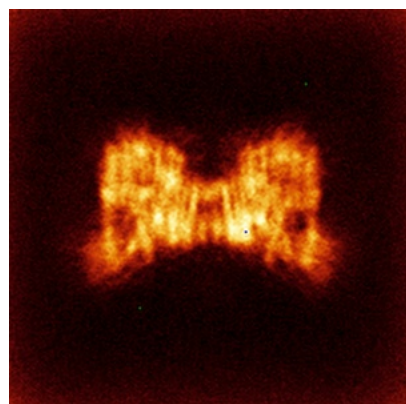


Y

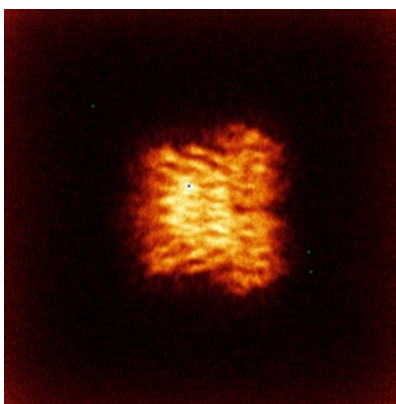


Z

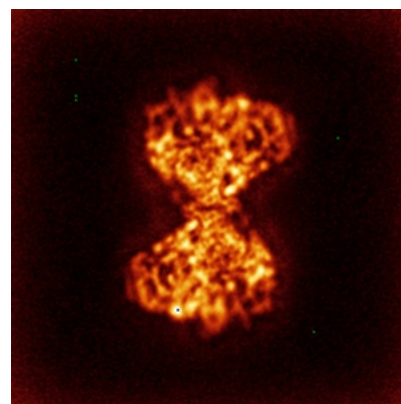
6.4.2 Raw map



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.

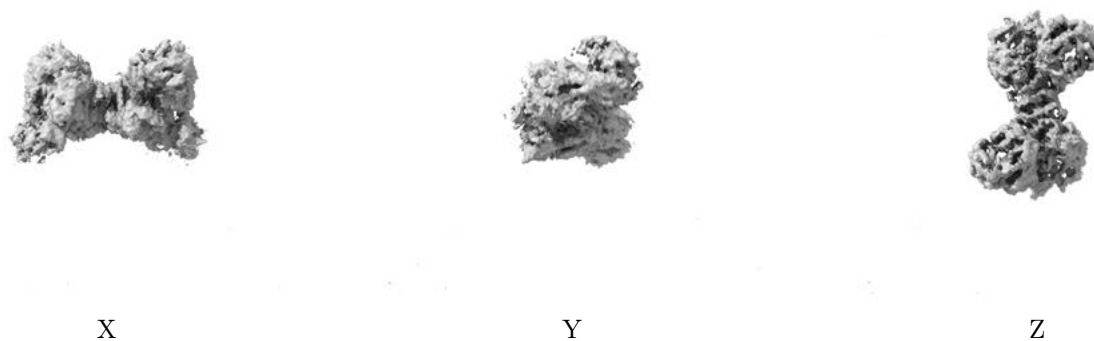
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.68. 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



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.

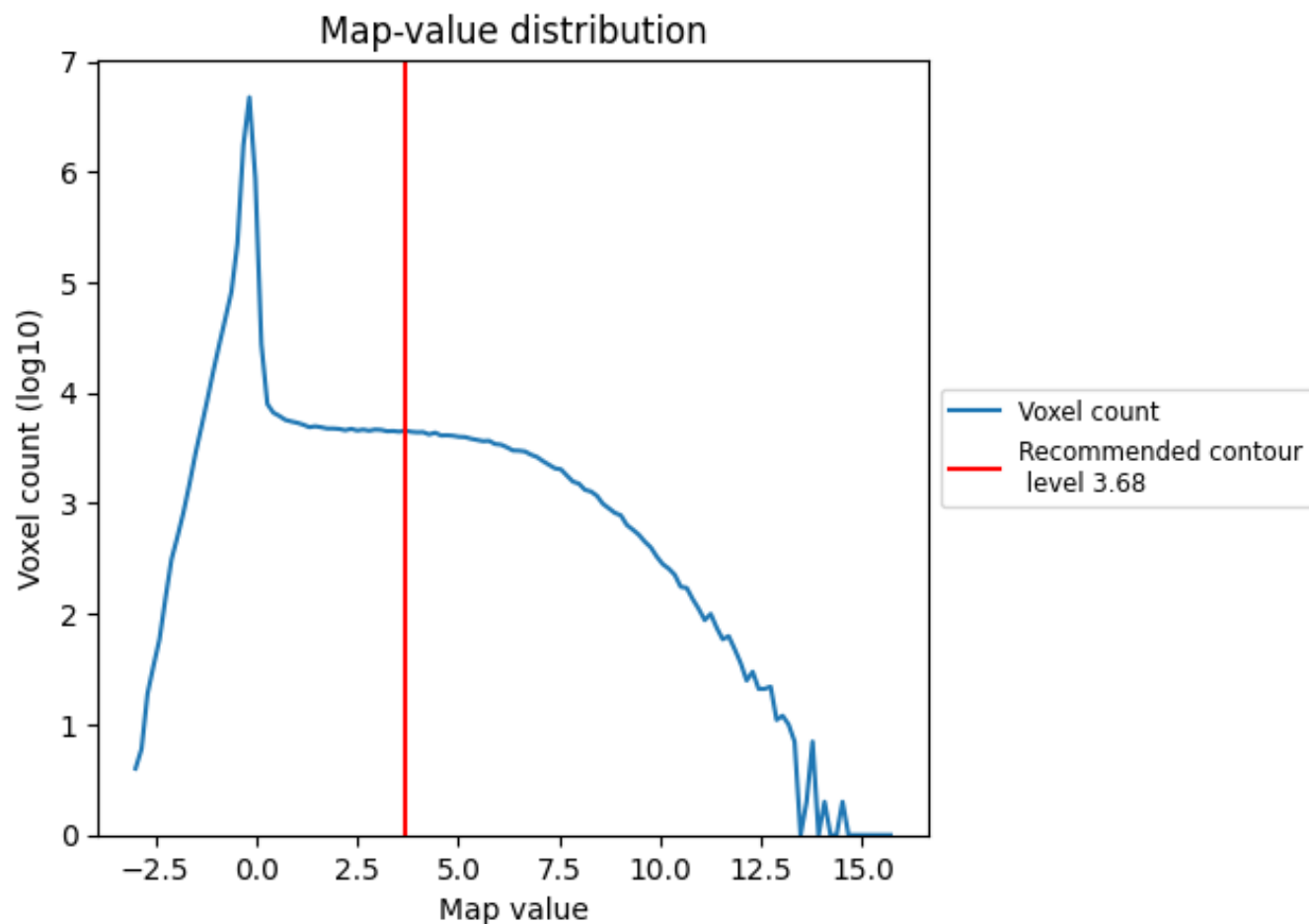
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

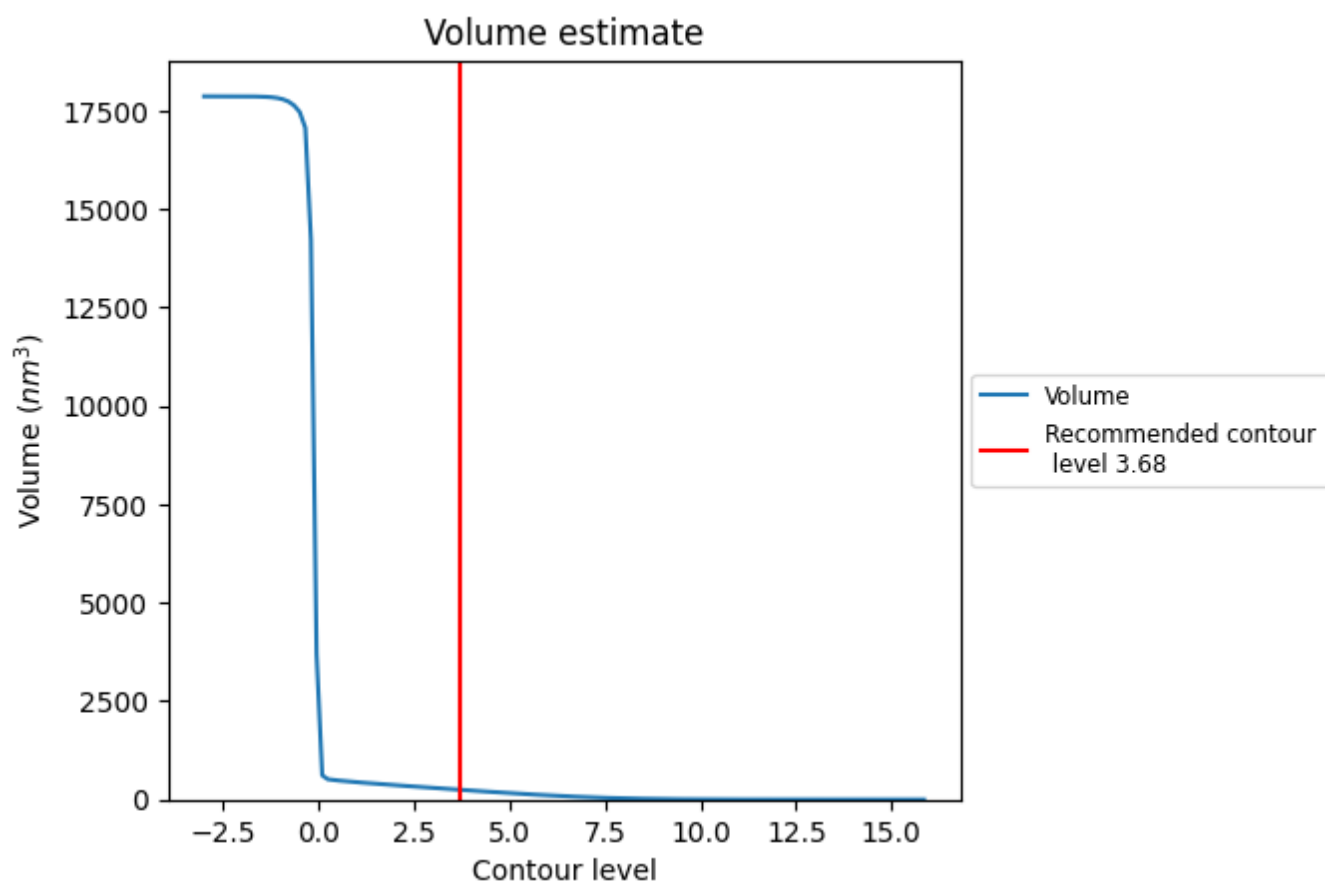
This section contains the results of statistical analysis of the map.

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.

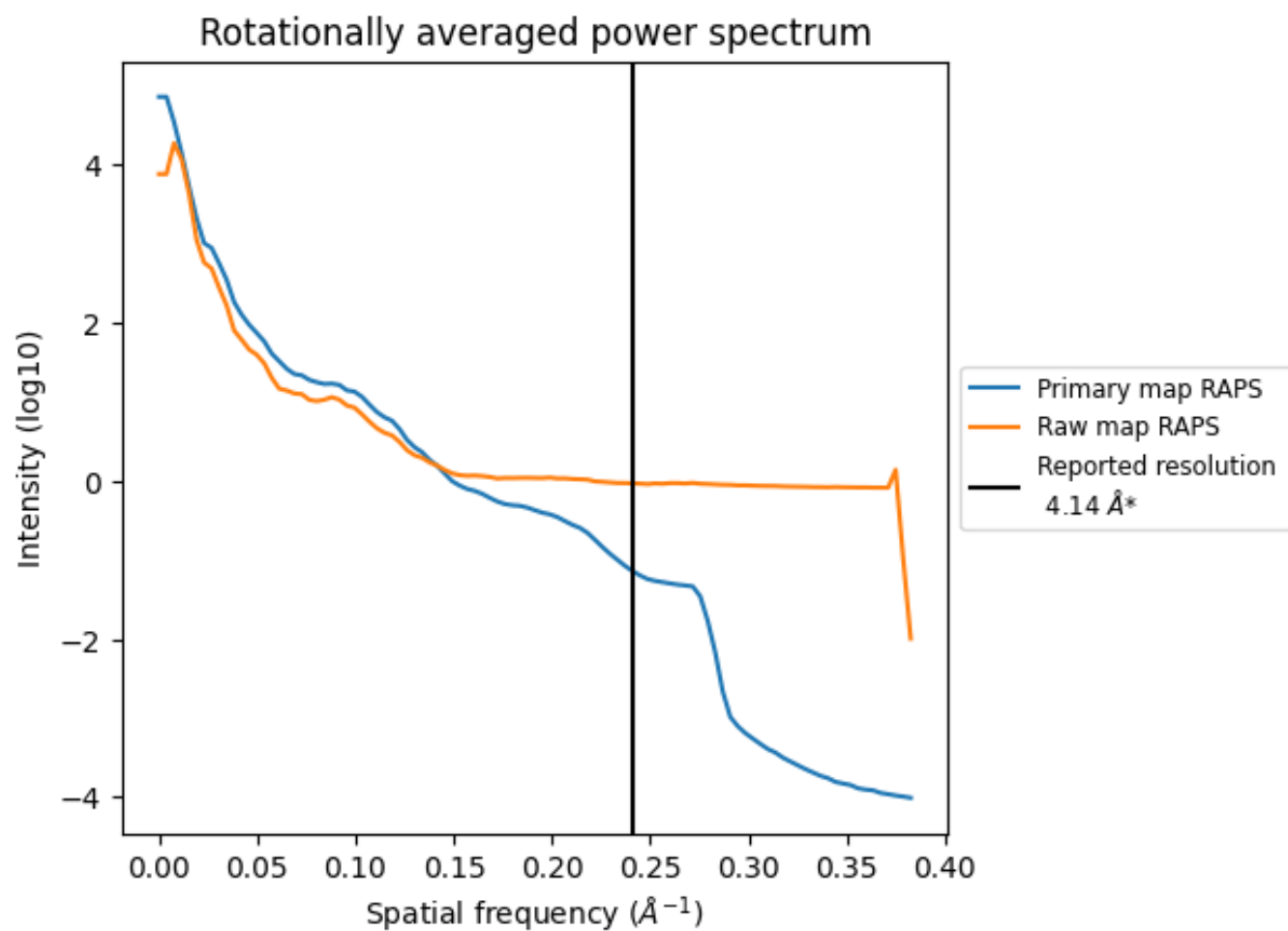
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm^3 ; this corresponds to an approximate mass of 226 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 ⓘ

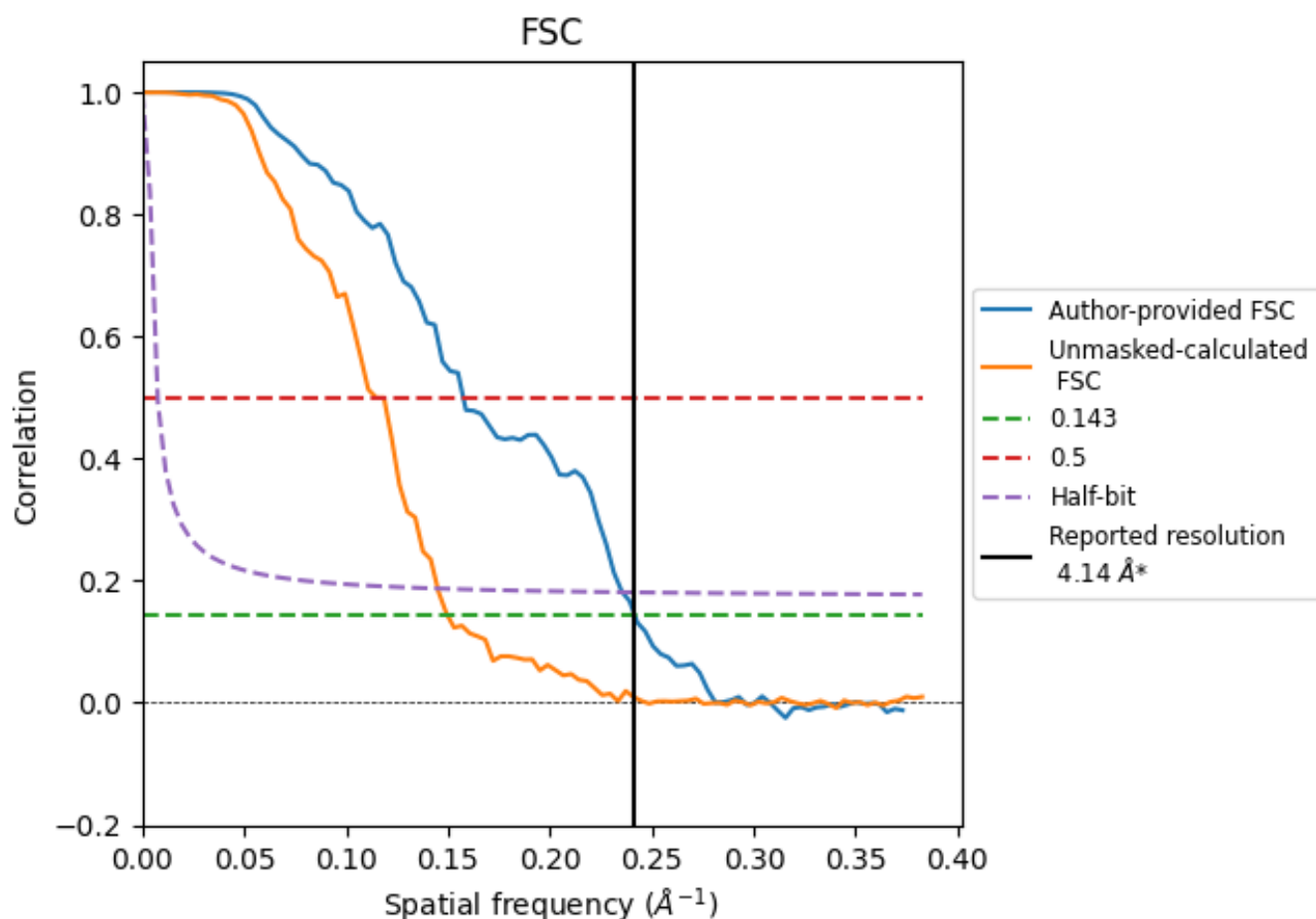


*Reported resolution corresponds to spatial frequency of 0.242 $\text{\AA}^{-1}$

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 0.242 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

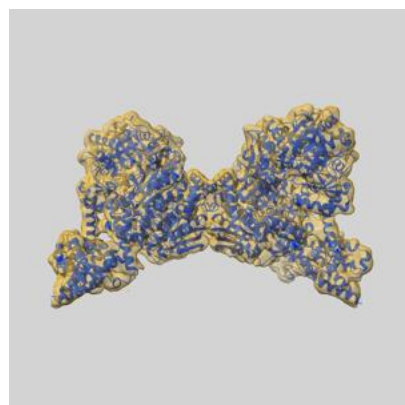
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	4.14	6.35	4.25
Unmasked-calculated*	6.68	8.72	6.90

*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 6.68 differs from the reported value 4.14 by more than 10 %

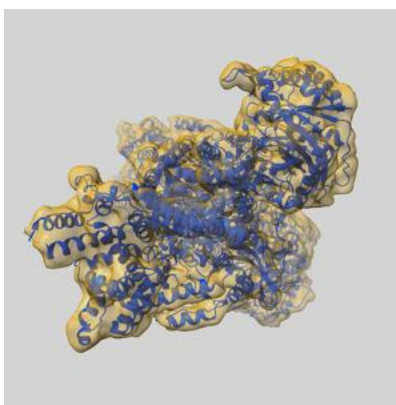
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62392 and PDB model 9KKM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

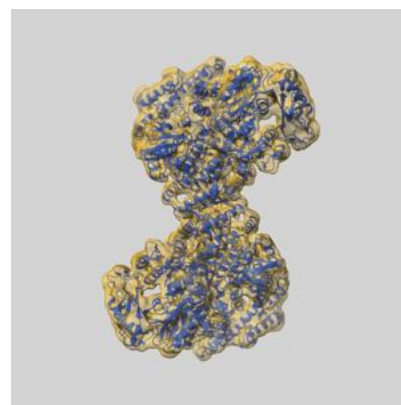
9.1 Map-model overlay [i](#)



X



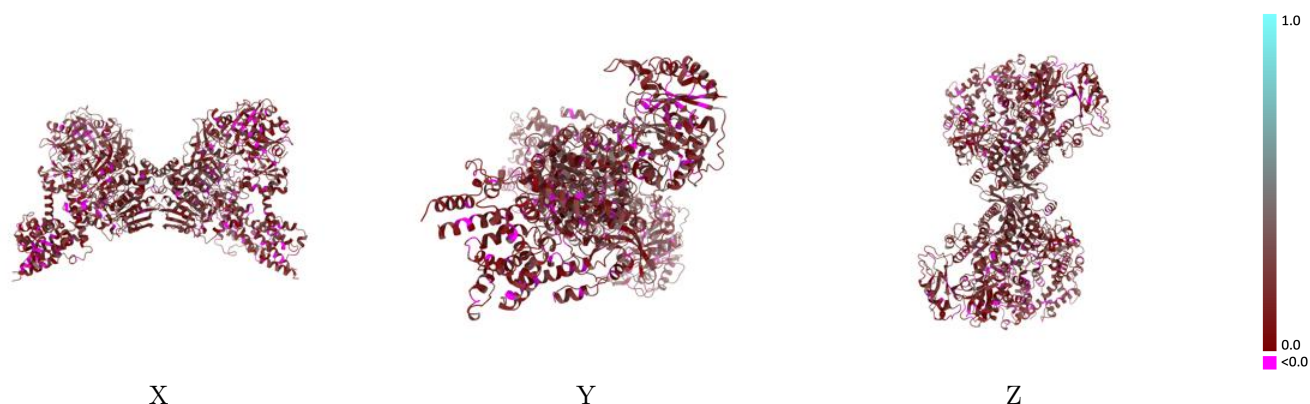
Y



Z

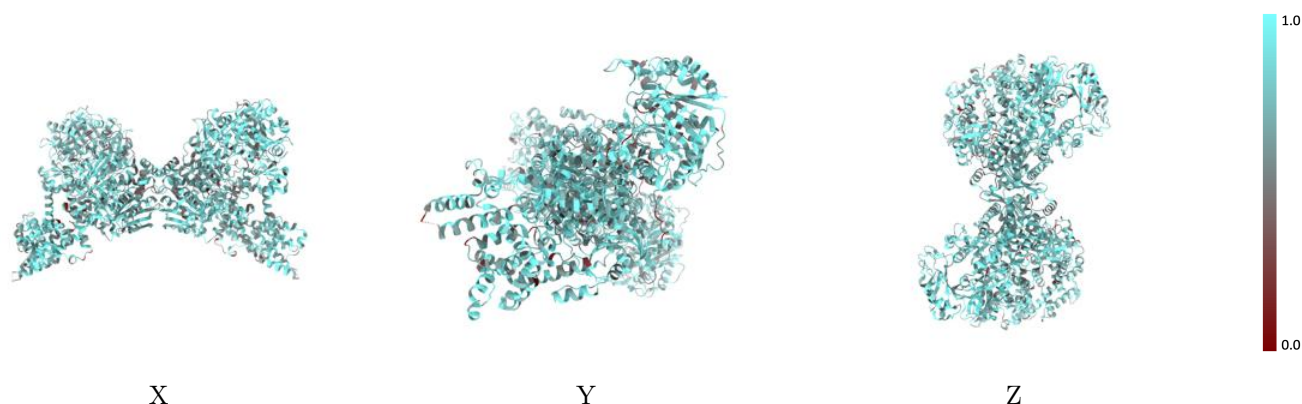
The images above show the 3D surface view of the map at the recommended contour level 3.68 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



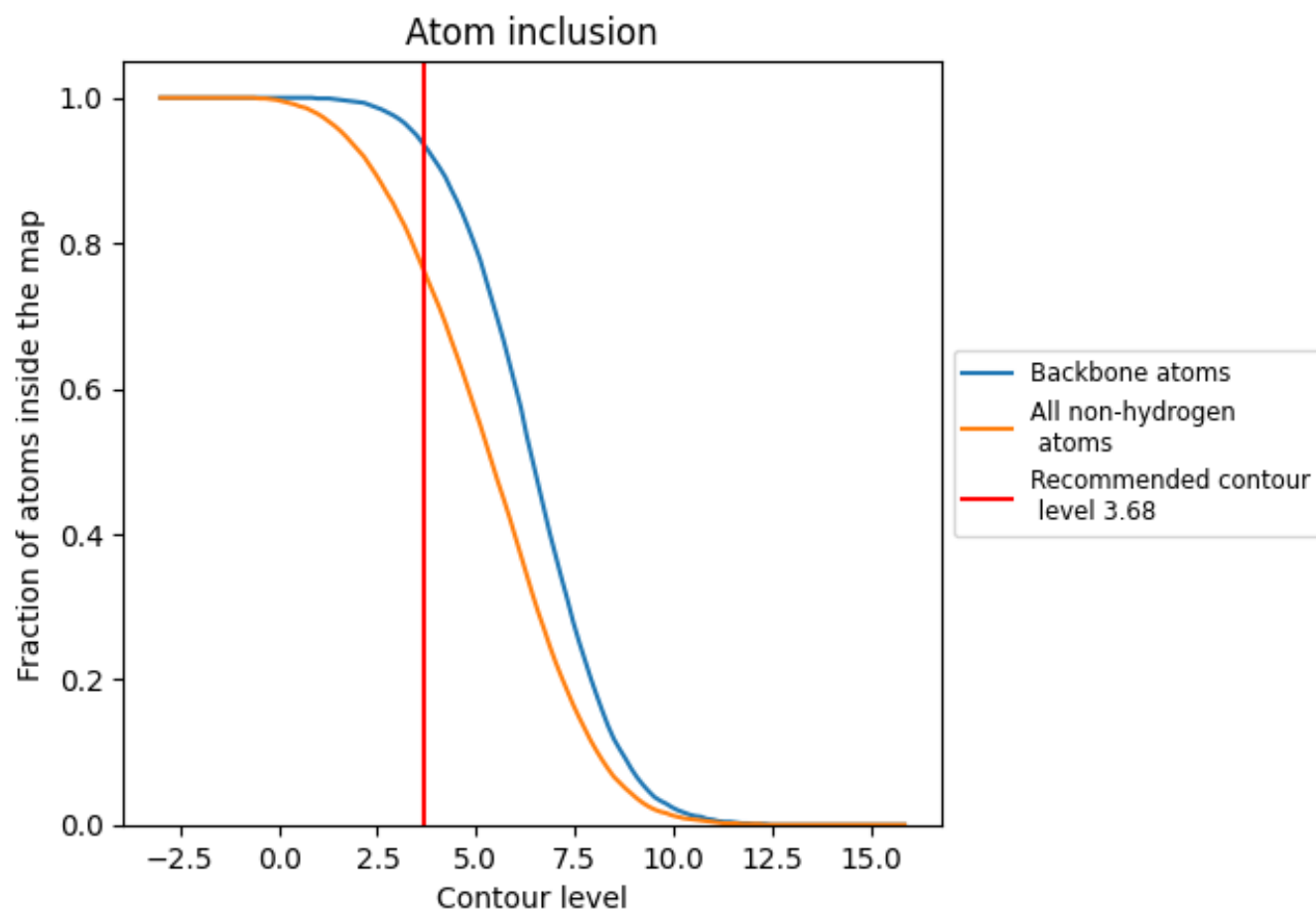
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.68).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 76% 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 (3.68) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7620	0.1700
A	0.7630	0.1710
B	0.7600	0.1680

