



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:54 PM UTC

PDB ID : 7EN1 / pdb_00007en1
EMDB ID : EMD-31199
Title : Pyochelin synthetase, a dimeric nonribosomal peptide synthetase elongation module-after-condensation
Authors : Wang, J.L.; Wang, Z.J.
Deposited on : 2021-04-15
Resolution : 3.47 Å(reported)

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

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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

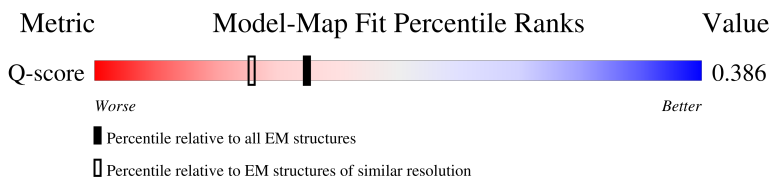
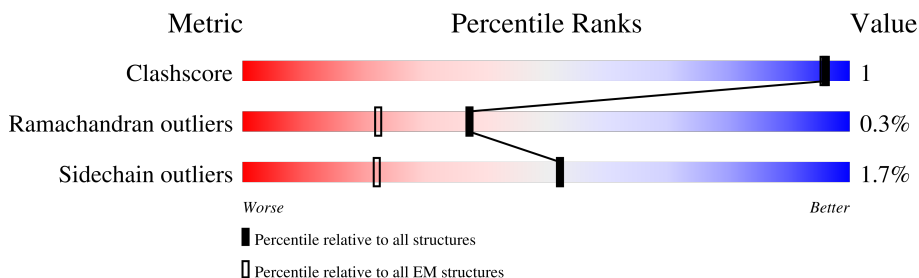
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 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	13733 (2.97 - 3.97)

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	1455	 86% 5% 9%
1	B	1455	 87% 5% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 40939 atoms, of which 20496 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 Dihydroaeruginosic acid synthetase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1320	Total	C	H	N	O	S	0	0
			20280	6384	10162	1874	1829	31		
1	B	1334	Total	C	H	N	O	S	0	0
			20444	6431	10245	1881	1854	33		

There are 34 discrepancies between the modelled and reference sequences:

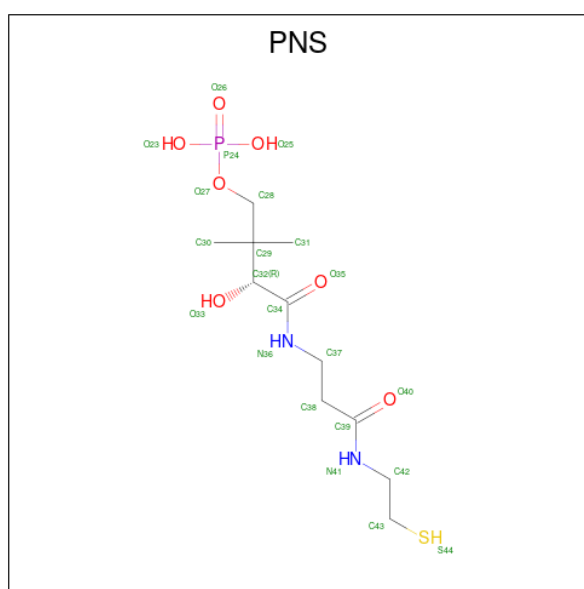
Chain	Residue	Modelled	Actual	Comment	Reference
A	1439	HIS	-	expression tag	UNP G3XCV2
A	1440	HIS	-	expression tag	UNP G3XCV2
A	1441	HIS	-	expression tag	UNP G3XCV2
A	1442	HIS	-	expression tag	UNP G3XCV2
A	1443	HIS	-	expression tag	UNP G3XCV2
A	1444	HIS	-	expression tag	UNP G3XCV2
A	1445	LEU	-	expression tag	UNP G3XCV2
A	1446	PRO	-	expression tag	UNP G3XCV2
A	1447	SER	-	expression tag	UNP G3XCV2
A	1448	TRP	-	expression tag	UNP G3XCV2
A	1449	SER	-	expression tag	UNP G3XCV2
A	1450	HIS	-	expression tag	UNP G3XCV2
A	1451	PRO	-	expression tag	UNP G3XCV2
A	1452	GLN	-	expression tag	UNP G3XCV2
A	1453	PHE	-	expression tag	UNP G3XCV2
A	1454	GLU	-	expression tag	UNP G3XCV2
A	1455	LYS	-	expression tag	UNP G3XCV2
B	1439	HIS	-	expression tag	UNP G3XCV2
B	1440	HIS	-	expression tag	UNP G3XCV2
B	1441	HIS	-	expression tag	UNP G3XCV2
B	1442	HIS	-	expression tag	UNP G3XCV2
B	1443	HIS	-	expression tag	UNP G3XCV2
B	1444	HIS	-	expression tag	UNP G3XCV2
B	1445	LEU	-	expression tag	UNP G3XCV2
B	1446	PRO	-	expression tag	UNP G3XCV2
B	1447	SER	-	expression tag	UNP G3XCV2

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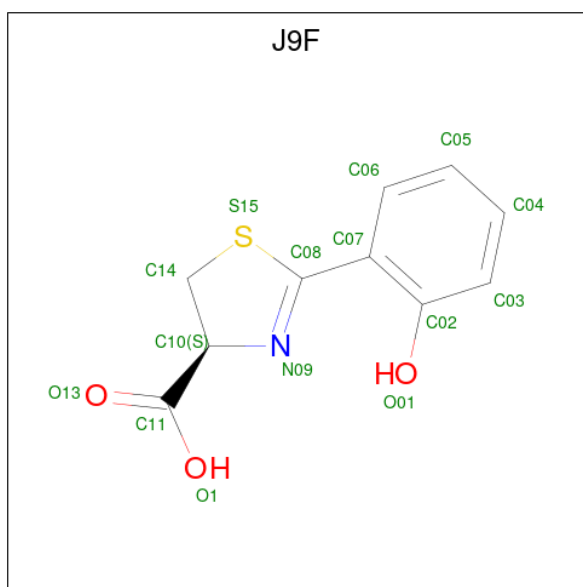
Chain	Residue	Modelled	Actual	Comment	Reference
B	1448	TRP	-	expression tag	UNP G3XCV2
B	1449	SER	-	expression tag	UNP G3XCV2
B	1450	HIS	-	expression tag	UNP G3XCV2
B	1451	PRO	-	expression tag	UNP G3XCV2
B	1452	GLN	-	expression tag	UNP G3XCV2
B	1453	PHE	-	expression tag	UNP G3XCV2
B	1454	GLU	-	expression tag	UNP G3XCV2
B	1455	LYS	-	expression tag	UNP G3XCV2

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues	Atoms							AltConf
2	A	1	Total	C	H	N	O	P	S	0
			41	11	20	2	6	1	1	
2	B	1	Total	C	H	N	O	P	S	0
			41	11	20	2	6	1	1	

- Molecule 3 is (4S)-2-(2-hydroxyphenyl)-4,5-dihydro-1,3-thiazole-4-carboxylic acid (CCD ID: J9F) (formula: $C_{10}H_9NO_3S$) (labeled as "Ligand of Interest" by depositor).

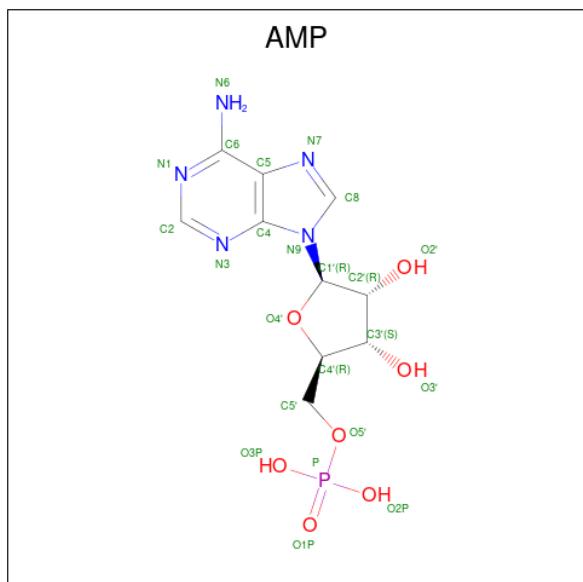


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	S	0
			22	10	8	1	2	1	

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

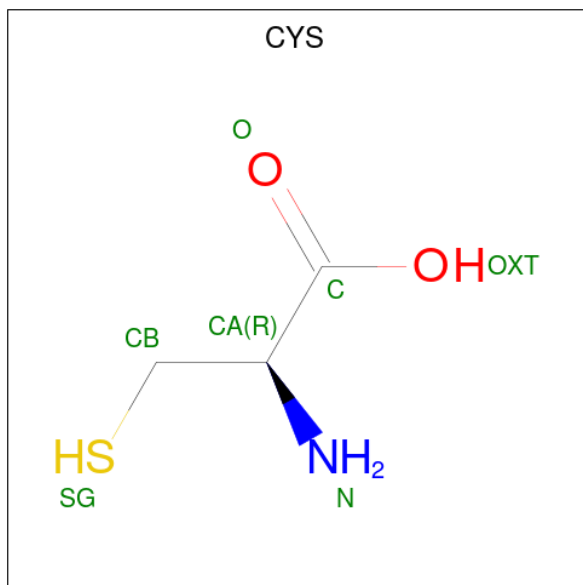
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



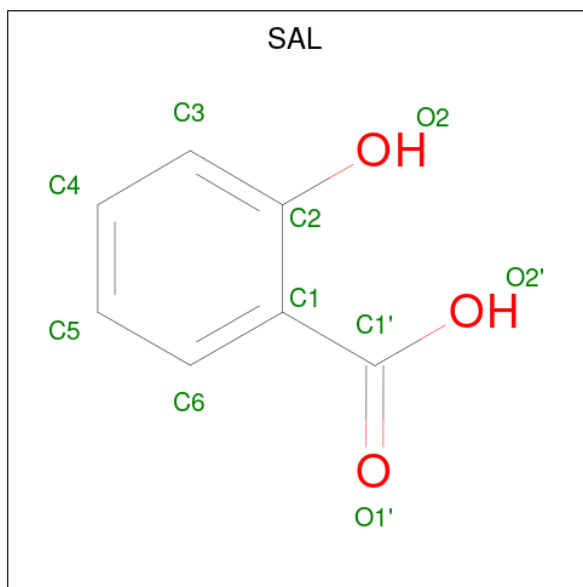
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			35	10	12	5	7	1	
5	B	1	Total	C	H	N	O	P	0
			35	10	12	5	7	1	

- Molecule 6 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).

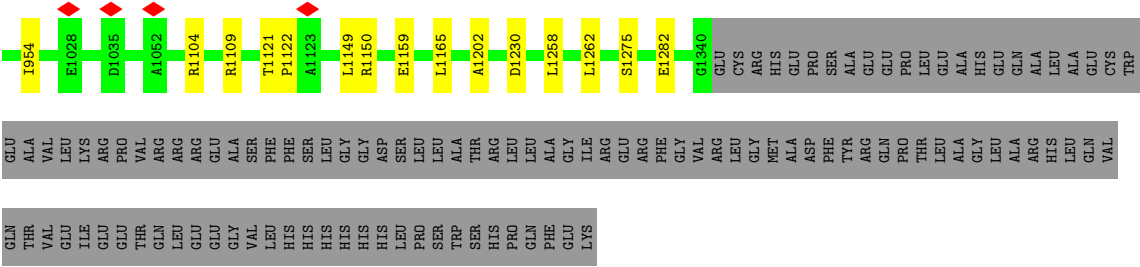


Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	S	0
			12	3	6	1	1	1	
6	B	1	Total	C	H	N	O	S	0
			13	3	6	1	2	1	

- Molecule 7 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
7	B	1	14	7	5	2	0



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58112	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 ($e^-/\text{\AA}^2$)	60.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	250.0, 250.0, 250.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, SAL, J9F, AMP, 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	0.83	0/10332	1.35	19/14069 (0.1%)
1	B	0.83	0/10412	1.34	20/14189 (0.1%)
All	All	0.83	0/20744	1.34	39/28258 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	10
All	All	0	20

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	PHE	CA-CB-CG	8.47	122.27	113.80
1	B	174	PRO	N-CA-CB	7.44	107.09	103.22
1	A	807	LEU	CA-C-N	6.76	129.65	120.38
1	A	807	LEU	C-N-CA	6.76	129.65	120.38
1	B	128	SER	N-CA-C	6.47	118.34	111.28
1	B	235	ASP	CA-CB-CG	-6.37	106.23	112.60
1	A	927	ASP	CA-CB-CG	5.97	118.58	112.60
1	B	689	GLN	N-CA-C	5.87	120.17	113.19
1	B	747	ASP	CA-C-N	5.67	128.13	120.65
1	B	747	ASP	C-N-CA	5.67	128.13	120.65
1	A	235	ASP	CA-CB-CG	-5.63	106.97	112.60
1	B	477	VAL	CA-C-N	5.61	128.26	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	477	VAL	C-N-CA	5.61	128.26	120.29
1	A	711	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	190	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	832	GLY	CA-C-N	5.48	127.89	120.38
1	B	832	GLY	C-N-CA	5.48	127.89	120.38
1	A	199	LEU	CA-C-N	5.40	127.78	120.65
1	A	199	LEU	C-N-CA	5.40	127.78	120.65
1	B	127	VAL	CA-C-N	5.34	127.44	120.28
1	B	127	VAL	C-N-CA	5.34	127.44	120.28
1	B	130	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	B	711	HIS	CB-CG-CD2	-5.28	124.33	131.20
1	A	481	HIS	CB-CG-CD2	-5.26	124.37	131.20
1	A	639	PRO	N-CA-CB	5.25	105.95	103.22
1	A	130	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	A	276	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	A	1245	LEU	CA-C-N	5.23	129.78	122.36
1	A	1245	LEU	C-N-CA	5.23	129.78	122.36
1	B	168	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	1006	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	B	833	CYS	N-CA-C	5.16	117.58	111.33
1	A	168	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	1422	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	1275	SER	N-CA-C	5.09	115.53	108.00
1	A	924	ARG	N-CA-CB	-5.04	103.03	110.49
1	A	128	SER	N-CA-C	5.03	117.65	111.82
1	B	807	LEU	CA-C-N	5.01	128.34	120.82
1	B	807	LEU	C-N-CA	5.01	128.34	120.82

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	TYR	Sidechain
1	A	1150	ARG	Sidechain
1	A	1274	ARG	Sidechain
1	A	1390	ARG	Sidechain
1	A	167	ARG	Sidechain
1	A	203	ARG	Sidechain
1	A	255	TYR	Sidechain
1	A	440	ARG	Sidechain
1	A	591	ARG	Sidechain
1	A	928	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	1104	ARG	Sidechain
1	B	1150	ARG	Sidechain
1	B	12	ARG	Sidechain
1	B	203	ARG	Sidechain
1	B	255	TYR	Sidechain
1	B	332	ARG	Sidechain
1	B	372	PHE	Sidechain
1	B	826	ARG	Sidechain
1	B	865	TYR	Sidechain
1	B	923	TYR	Sidechain

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	10118	10162	10159	16	0
1	B	10199	10245	10241	20	0
2	A	21	20	20	0	0
2	B	21	20	20	0	0
3	A	14	8	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	23	12	12	0	0
5	B	23	12	12	0	0
6	A	6	6	4	1	0
6	B	7	6	4	0	0
7	B	9	5	4	0	0
All	All	20443	20496	20476	35	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 1.

All (35) 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:846:ILE:H	1:B:846:ILE:HD12	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:ILE:H	1:A:846:ILE:HD12	1.65	0.61
1:A:474:THR:OG1	3:A:1502:J9F:O01	2.19	0.59
1:B:621:VAL:HG21	1:B:748:LEU:HD21	1.85	0.58
1:B:630:CYS:SG	1:B:694:VAL:HG23	2.45	0.57
1:A:1325:LYS:HZ1	6:A:1505:CYS:N	2.07	0.53
1:A:196:TRP:CD1	1:A:229:ARG:HH11	2.28	0.52
1:B:668:ARG:C	1:B:669:LEU:HD12	2.36	0.51
1:B:1121:THR:HG23	1:B:1122:PRO:HD3	1.94	0.50
1:A:1023:LEU:HD23	1:A:1041:TRP:CE3	2.47	0.49
1:A:668:ARG:C	1:A:669:LEU:HD12	2.38	0.49
1:B:1258:LEU:C	1:B:1258:LEU:HD23	2.39	0.48
1:A:877:VAL:HG21	1:A:893:TRP:CE2	2.50	0.47
1:B:513:TYR:CZ	1:B:517:LEU:HD11	2.50	0.46
1:B:1262:LEU:C	1:B:1262:LEU:HD23	2.40	0.46
1:B:893:TRP:CD1	1:B:924:ARG:HA	2.51	0.46
1:B:196:TRP:CD1	1:B:229:ARG:HH11	2.34	0.45
1:B:846:ILE:H	1:B:846:ILE:CD1	2.27	0.45
1:A:696:TYR:CZ	1:A:706:GLY:HA3	2.52	0.44
1:B:241:VAL:HG21	1:B:449:ASN:CG	2.43	0.43
1:B:849:ASN:ND2	1:B:874:TYR:CE1	2.86	0.43
1:A:513:TYR:CZ	1:A:517:LEU:HD11	2.53	0.43
1:A:874:TYR:CZ	1:A:894:ILE:HG12	2.53	0.43
1:A:535:TRP:CD2	1:B:896:GLY:HA2	2.54	0.43
1:A:849:ASN:ND2	1:A:874:TYR:CE1	2.86	0.42
1:B:874:TYR:CZ	1:B:894:ILE:HG12	2.55	0.42
1:A:923:TYR:CE2	1:A:925:THR:HA	2.55	0.41
1:A:196:TRP:CE3	1:A:221:VAL:HG11	2.55	0.41
1:B:625:LEU:CD1	1:B:749:PHE:CZ	3.03	0.41
1:B:693:TYR:CZ	1:B:709:VAL:HG21	2.56	0.41
1:B:196:TRP:CE3	1:B:221:VAL:HG11	2.55	0.41
1:A:687:ALA:HA	1:A:688:PRO:HD3	1.92	0.41
1:B:837:VAL:C	1:B:838:LEU:HD12	2.46	0.40
1:B:717:THR:HG21	1:B:846:ILE:HB	2.03	0.40
1:A:238:ALA:O	1:A:386:ALA:HA	2.22	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	1316/1455 (90%)	1241 (94%)	71 (5%)	4 (0%)	36	67
1	B	1332/1455 (92%)	1263 (95%)	66 (5%)	3 (0%)	43	74
All	All	2648/2910 (91%)	2504 (95%)	137 (5%)	7 (0%)	37	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	897	ALA
1	A	701	THR
1	B	467	LEU
1	B	1202	ALA
1	A	1382	GLY
1	B	104	PRO
1	A	1309	PRO

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	1008/1122 (90%)	989 (98%)	19 (2%)	50	67
1	B	1019/1122 (91%)	1003 (98%)	16 (2%)	55	70
All	All	2027/2244 (90%)	1992 (98%)	35 (2%)	52	69

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	VAL
1	A	215	VAL
1	A	241	VAL
1	A	276	ARG
1	A	313	ILE
1	A	445	VAL
1	A	449	ASN
1	A	471	LEU
1	A	587	GLU
1	A	652	VAL
1	A	717	THR
1	A	1011	LEU
1	A	1055	SER
1	A	1109	ARG
1	A	1148	LEU
1	A	1207	GLU
1	A	1237	LEU
1	A	1273	TRP
1	A	1305	GLN
1	B	138	ARG
1	B	154	GLN
1	B	216	PHE
1	B	295	LEU
1	B	374	ARG
1	B	505	LEU
1	B	603	PRO
1	B	695	ILE
1	B	716	ASN
1	B	954	ILE
1	B	1109	ARG
1	B	1149	LEU
1	B	1159	GLU
1	B	1165	LEU
1	B	1230	ASP
1	B	1282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	HIS
1	A	421	HIS
1	A	538	GLN
1	A	578	GLN

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Mol	Chain	Res	Type
1	A	616	GLN
1	A	617	GLN
1	A	638	GLN
1	A	672	GLN
1	A	779	HIS
1	A	851	GLN
1	A	1223	GLN
1	B	538	GLN
1	B	672	GLN
1	B	851	GLN
1	B	1066	GLN
1	B	1099	GLN
1	B	1204	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
5	AMP	B	1504	4	25,25,25	1.11	2 (8%)	37,38,38	1.65	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYS	A	1505	5	4,5,6	1.20	1 (25%)	1,5,7	1.68	0
7	SAL	B	1502	2	9,9,10	0.60	0	11,11,13	0.62	0
2	PNS	B	1501	1,7	14,20,21	0.93	0	18,26,29	1.12	1 (5%)
5	AMP	A	1504	4,6	25,25,25	1.17	3 (12%)	37,38,38	1.45	10 (27%)
2	PNS	A	1501	1,3	14,20,21	1.17	1 (7%)	18,26,29	1.14	1 (5%)
3	J9F	A	1502	2	15,15,16	1.00	1 (6%)	15,20,22	1.44	3 (20%)
6	CYS	B	1505	-	5,6,6	0.96	0	3,7,7	1.75	1 (33%)

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
5	AMP	B	1504	4	-	6/10/26/26	0/3/3/3
6	CYS	A	1505	5	-	0/1/4/6	-
7	SAL	B	1502	2	-	2/2/2/4	0/1/1/1
2	PNS	B	1501	1,7	-	5/24/26/27	-
5	AMP	A	1504	4,6	-	6/10/26/26	0/3/3/3
2	PNS	A	1501	1,3	-	9/24/26/27	-
3	J9F	A	1502	2	-	4/4/15/17	0/2/2/2
6	CYS	B	1505	-	-	4/6/6/6	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1504	AMP	C5-C4	-2.70	1.34	1.39
5	B	1504	AMP	C5-C4	-2.53	1.34	1.39
6	A	1505	CYS	CB-SG	2.31	1.86	1.81
3	A	1502	J9F	C08-N09	2.26	1.29	1.27
2	A	1501	PNS	C28-C29	2.20	1.56	1.52
5	A	1504	AMP	P-O2P	-2.11	1.46	1.54
5	B	1504	AMP	C5-N7	-2.06	1.35	1.39
5	A	1504	AMP	P-O3P	-2.01	1.47	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1504	AMP	O5'-P-O1P	4.60	118.88	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1502	J9F	S15-C08-N09	-3.57	111.77	117.94
2	B	1501	PNS	C42-N41-C39	3.43	129.21	122.82
2	A	1501	PNS	C30-C29-C32	3.06	113.98	108.77
5	B	1504	AMP	C5-C4-N3	-3.01	122.57	126.72
5	B	1504	AMP	C4-C5-N7	2.94	113.94	110.58
6	B	1505	CYS	CB-CA-C	2.87	112.75	109.89
3	A	1502	J9F	C07-C08-S15	-2.83	114.55	120.08
5	A	1504	AMP	C5-C4-N3	-2.81	122.85	126.72
5	A	1504	AMP	C4-C5-N7	2.63	113.59	110.58
3	A	1502	J9F	C14-S15-C08	2.55	91.83	89.40
5	B	1504	AMP	O3P-P-O5'	2.52	113.25	106.67
5	A	1504	AMP	O3P-P-O2P	-2.47	98.53	107.80
5	A	1504	AMP	O2P-P-O5'	2.41	112.95	106.67
5	B	1504	AMP	C2-N1-C6	-2.39	114.81	118.73
5	B	1504	AMP	O2P-P-O5'	2.38	112.87	106.67
5	B	1504	AMP	N3-C4-N9	2.36	131.18	127.17
5	A	1504	AMP	C2-N1-C6	-2.30	114.96	118.73
5	A	1504	AMP	C2'-C3'-C4'	-2.19	98.38	102.61
5	A	1504	AMP	C5-C6-N1	2.17	123.02	117.51
5	A	1504	AMP	N6-C6-N1	-2.10	113.69	118.38
5	B	1504	AMP	O3P-P-O1P	-2.07	102.78	110.83
5	A	1504	AMP	N3-C4-N9	2.02	130.61	127.17
5	A	1504	AMP	O2'-C2'-C1'	2.02	117.05	110.10
5	B	1504	AMP	C5-C6-N1	2.01	122.62	117.51

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	PNS	O27-C28-C29-C31
2	A	1501	PNS	C28-C29-C32-C34
2	A	1501	PNS	C30-C29-C32-C34
2	A	1501	PNS	O33-C32-C34-O35
2	B	1501	PNS	O33-C32-C34-O35
2	B	1501	PNS	O33-C32-C34-N36
2	B	1501	PNS	C43-C42-N41-C39
3	A	1502	J9F	C02-C07-C08-N09
3	A	1502	J9F	C02-C07-C08-S15
5	A	1504	AMP	C5'-O5'-P-O2P
5	B	1504	AMP	C5'-O5'-P-O2P
5	B	1504	AMP	C5'-O5'-P-O3P
5	B	1504	AMP	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
6	B	1505	CYS	O-C-CA-CB
7	B	1502	SAL	C2-C1-C1'-O1'
5	A	1504	AMP	C2'-C1'-N9-C8
3	A	1502	J9F	C06-C07-C08-S15
5	A	1504	AMP	O4'-C4'-C5'-O5'
7	B	1502	SAL	C6-C1-C1'-O1'
5	B	1504	AMP	C5'-O5'-P-O1P
2	B	1501	PNS	C29-C32-C34-O35
6	B	1505	CYS	OXT-C-CA-CB
2	A	1501	PNS	C29-C28-O27-P24
6	B	1505	CYS	C-CA-CB-SG
2	A	1501	PNS	C31-C29-C32-C34
2	A	1501	PNS	O27-C28-C29-C30
2	A	1501	PNS	O27-C28-C29-C32
5	A	1504	AMP	C4'-C5'-O5'-P
5	B	1504	AMP	C4'-C5'-O5'-P
5	A	1504	AMP	C5'-O5'-P-O1P
5	A	1504	AMP	C2'-C1'-N9-C4
5	B	1504	AMP	C2'-C1'-N9-C4
2	B	1501	PNS	C29-C32-C34-N36
3	A	1502	J9F	C06-C07-C08-N09
2	A	1501	PNS	O33-C32-C34-N36
6	B	1505	CYS	OXT-C-CA-N

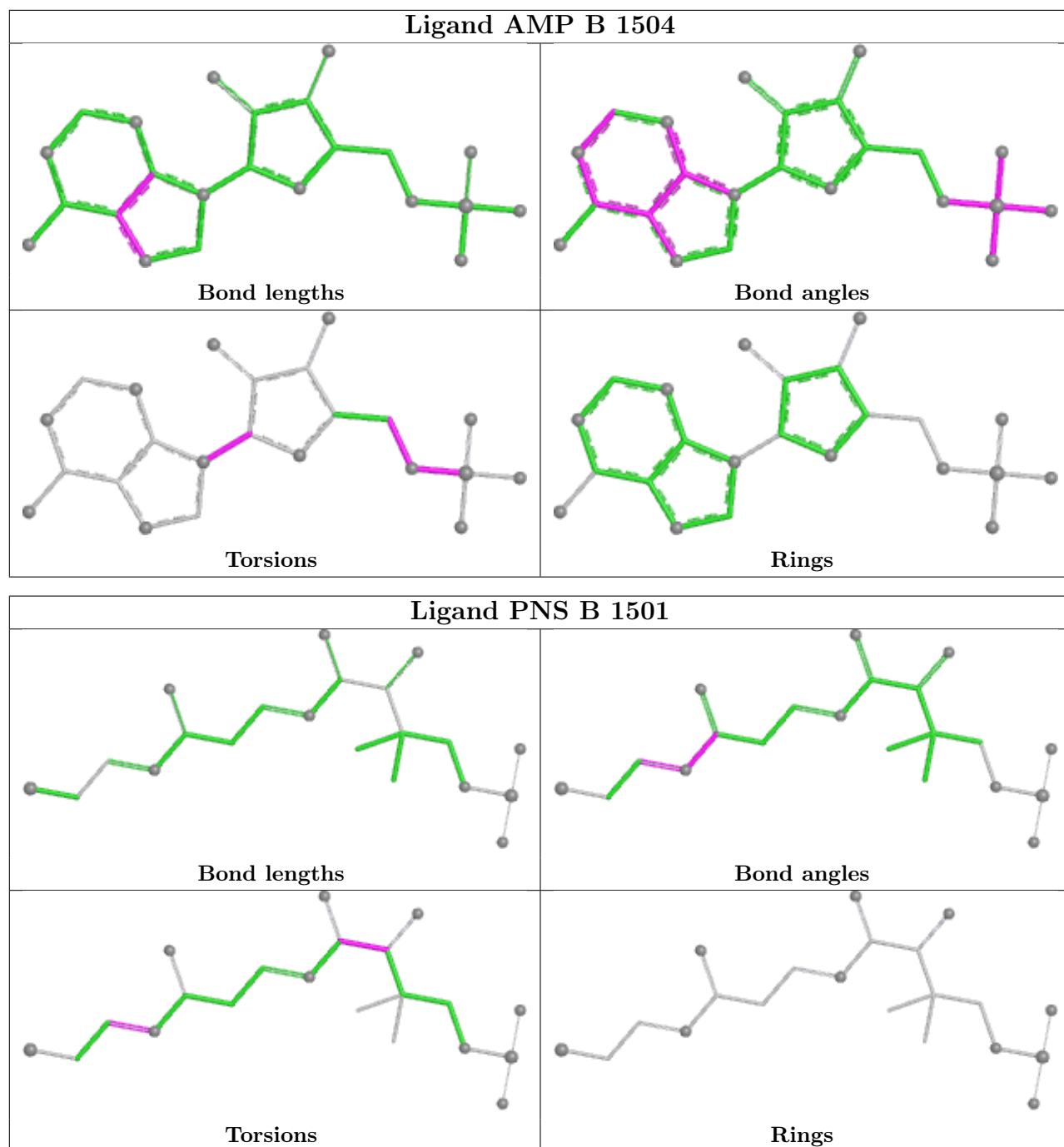
There are no ring outliers.

2 monomers are involved in 2 short contacts:

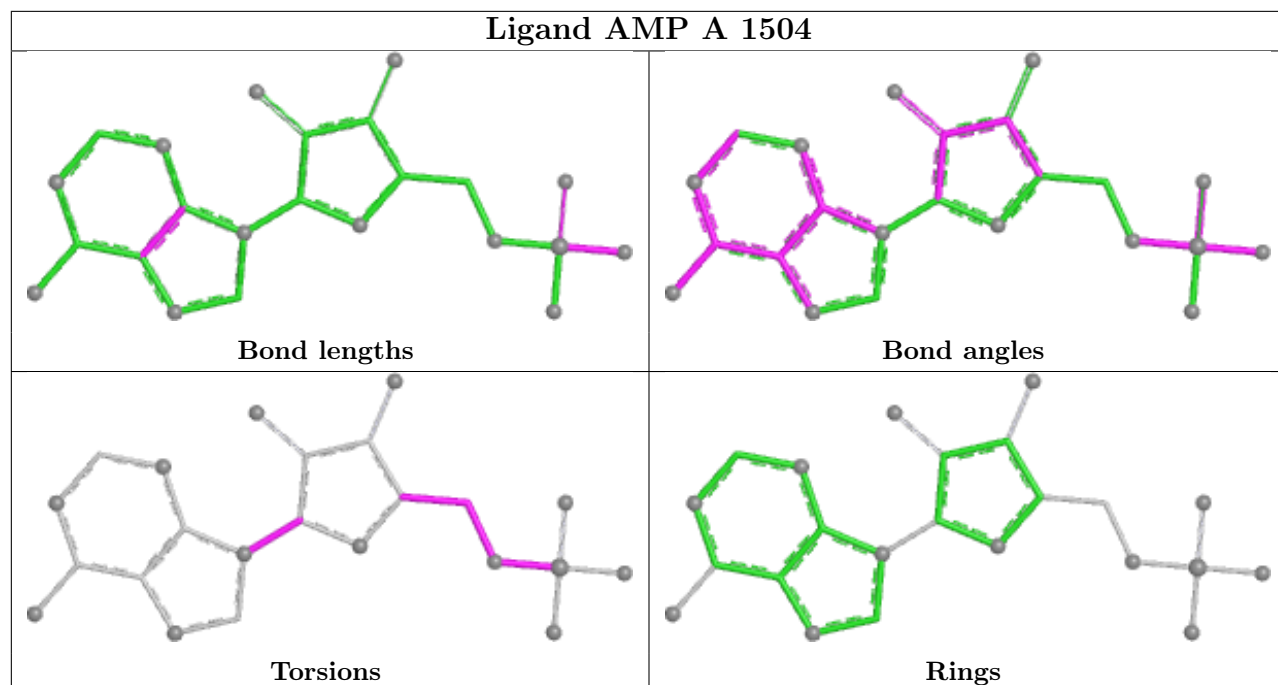
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1505	CYS	1	0
3	A	1502	J9F	1	0

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

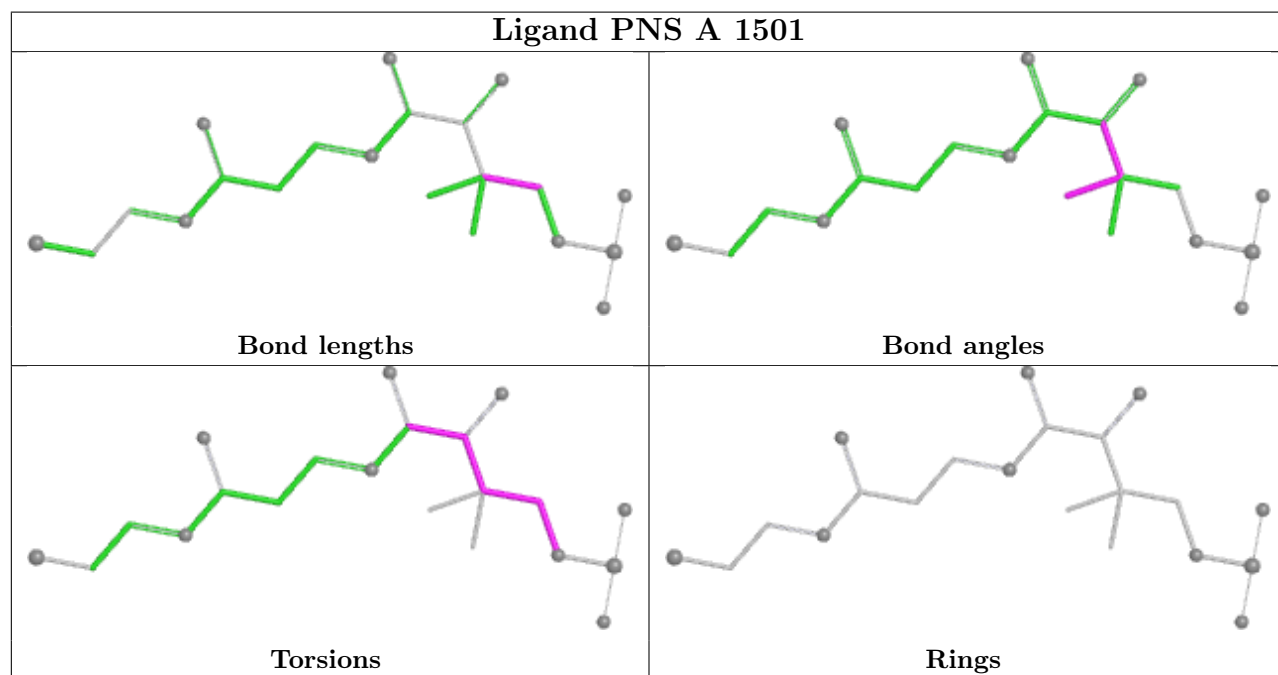
equivalents in the CSD to analyse the geometry.

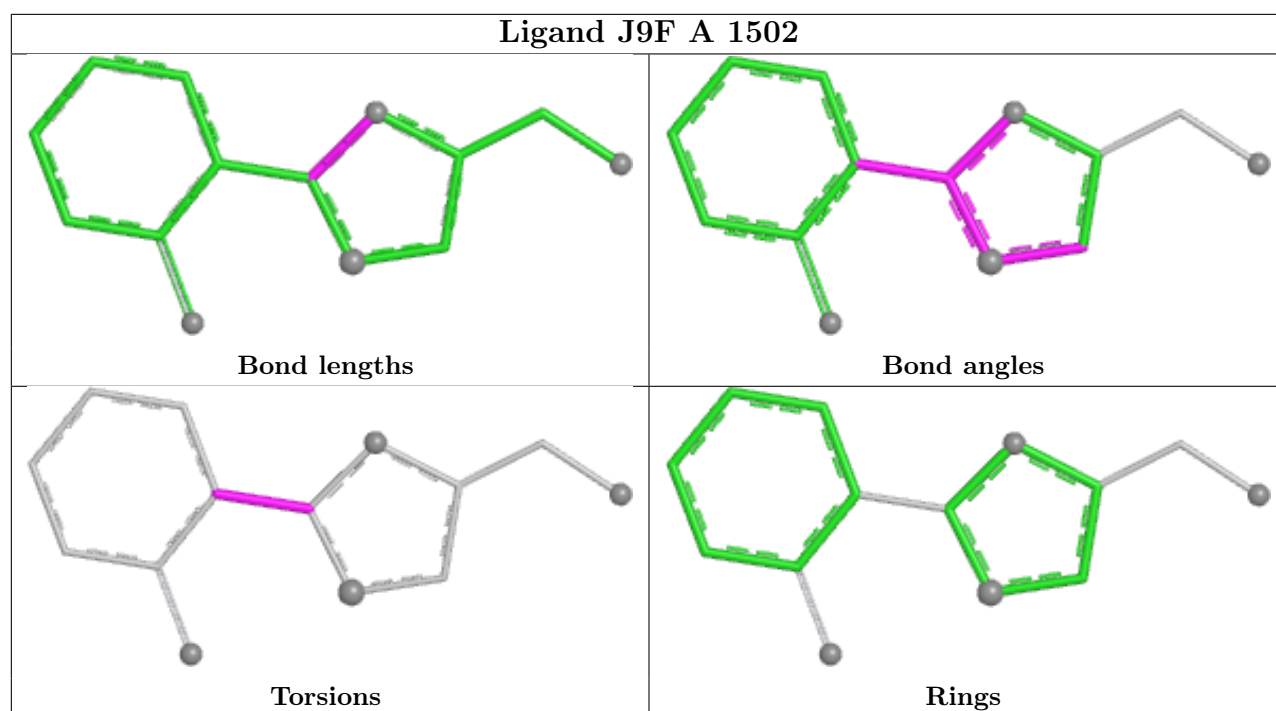


Ligand AMP A 1504



Ligand PNS A 1501





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.

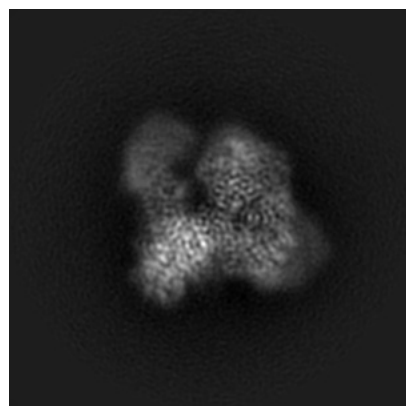
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31199. These allow visual inspection of the internal detail of the map and identification of artifacts.

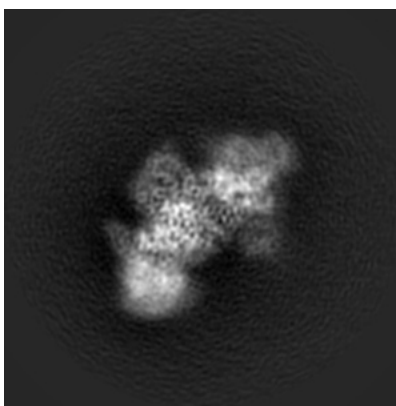
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

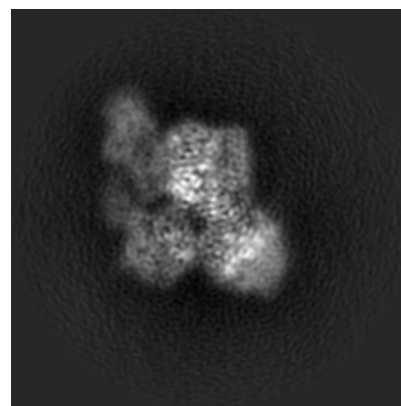
6.1.1 Primary map



X

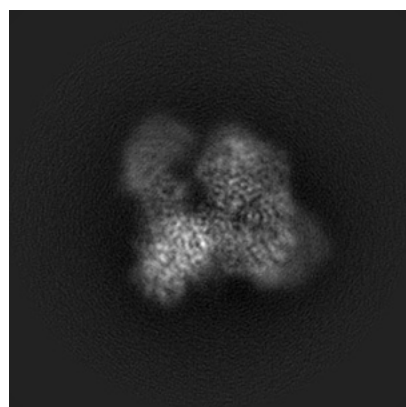


Y

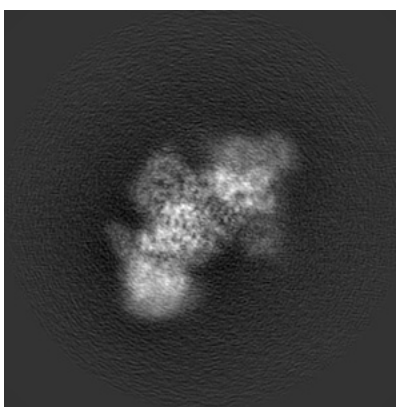


Z

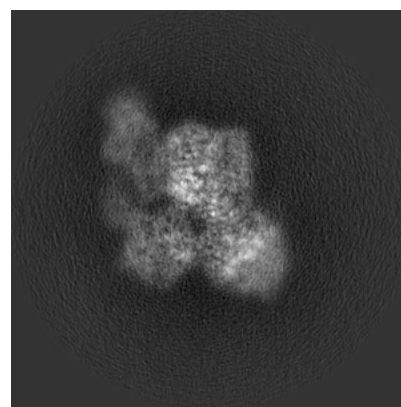
6.1.2 Raw map



X



Y

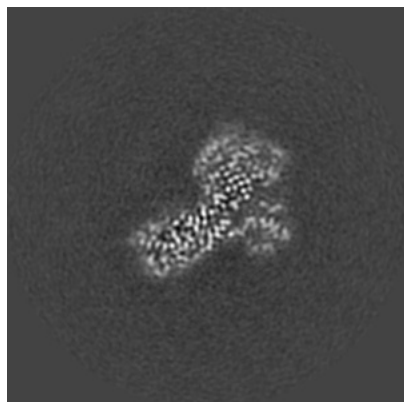


Z

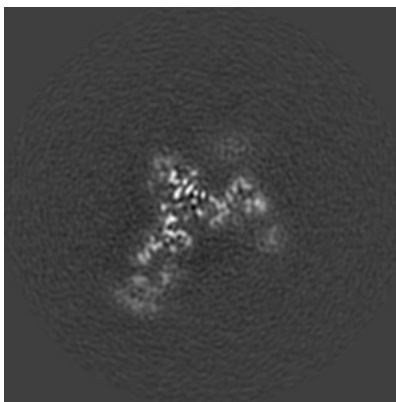
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

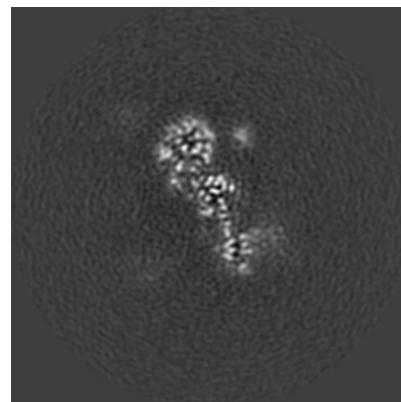
6.2.1 Primary map



X Index: 125

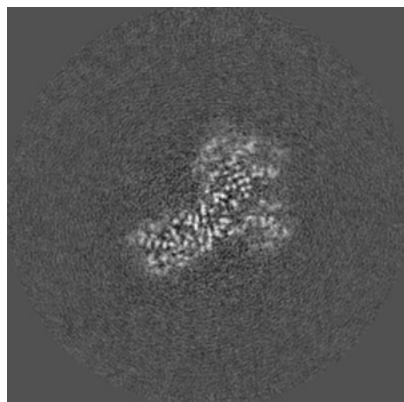


Y Index: 125

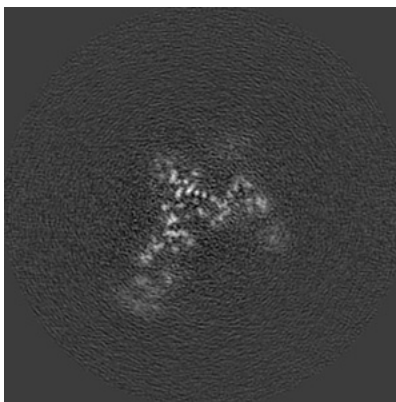


Z Index: 125

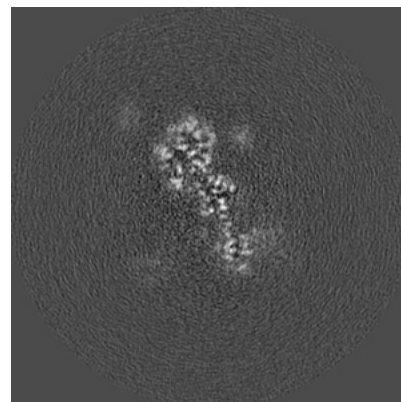
6.2.2 Raw map



X Index: 125



Y Index: 125

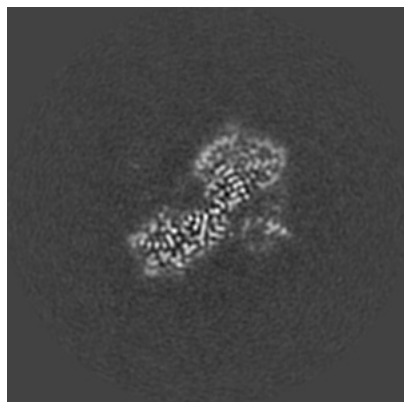


Z Index: 125

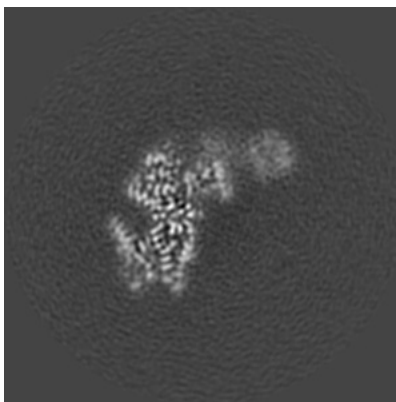
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

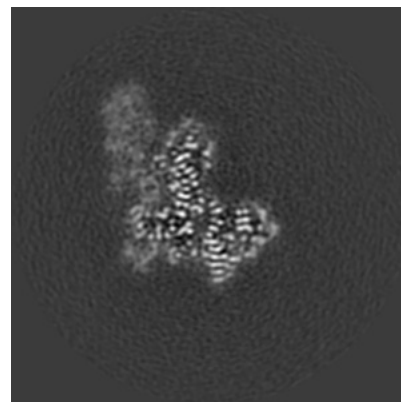
6.3.1 Primary map



X Index: 127

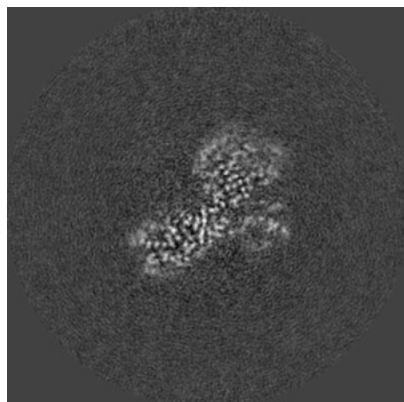


Y Index: 106

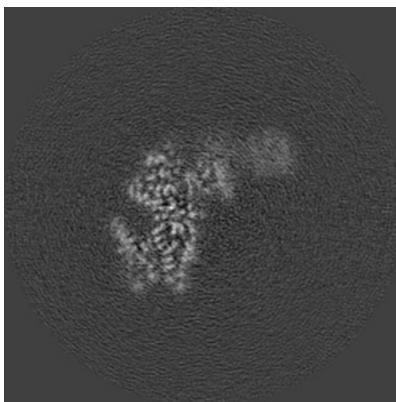


Z Index: 101

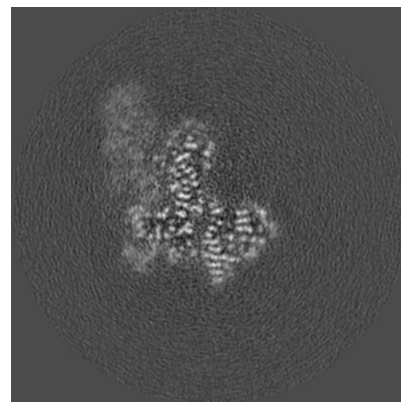
6.3.2 Raw map



X Index: 126



Y Index: 106

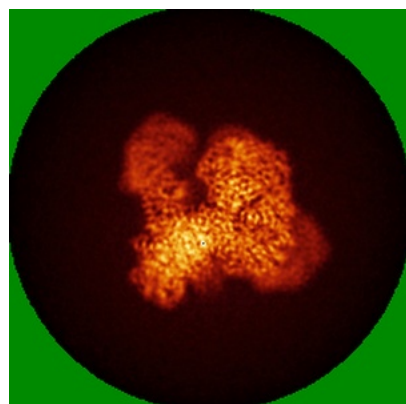


Z Index: 102

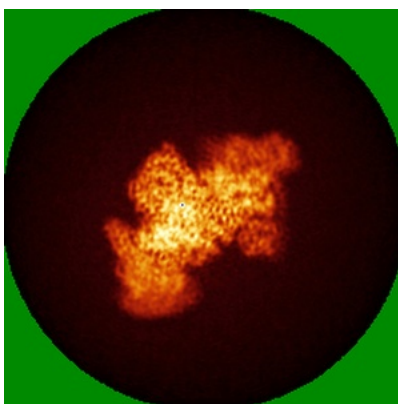
The images above show the largest variance slices of the map in three orthogonal directions.

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

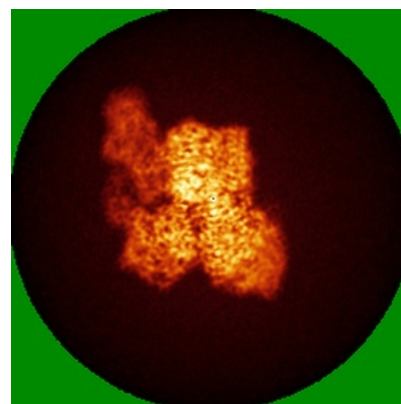
6.4.1 Primary map



X

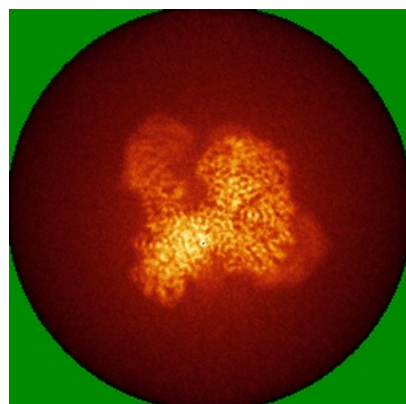


Y

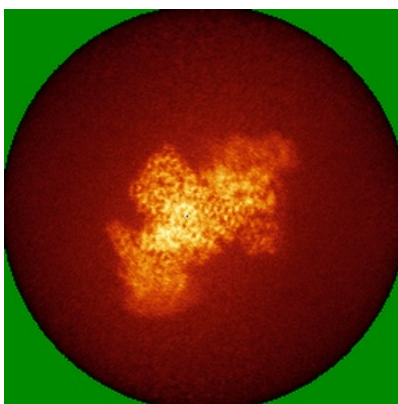


Z

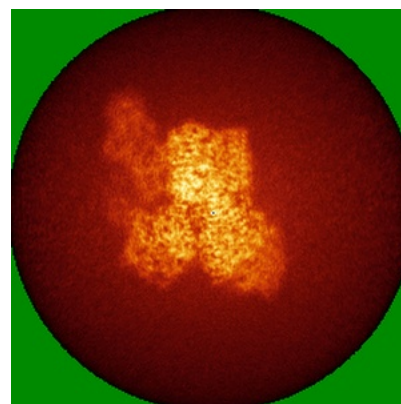
6.4.2 Raw map



X



Y

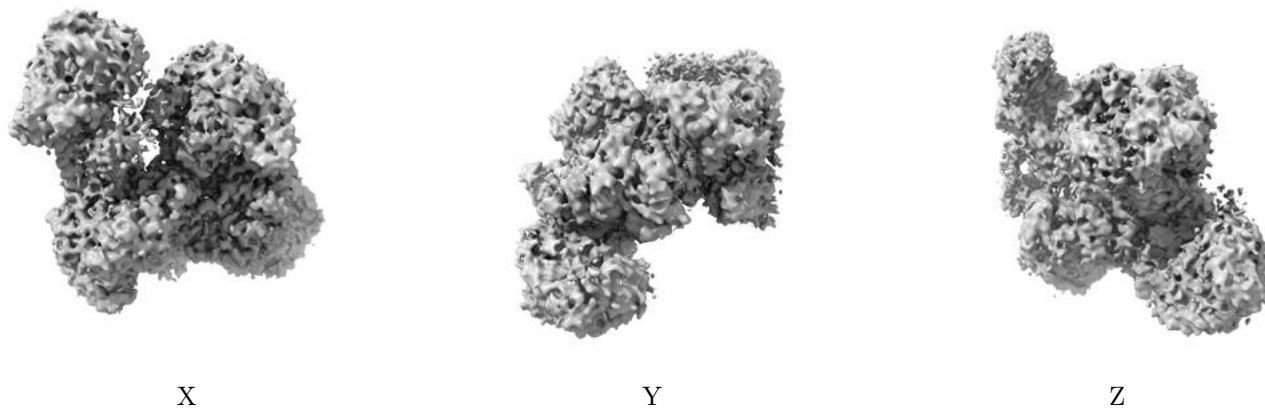


Z

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.

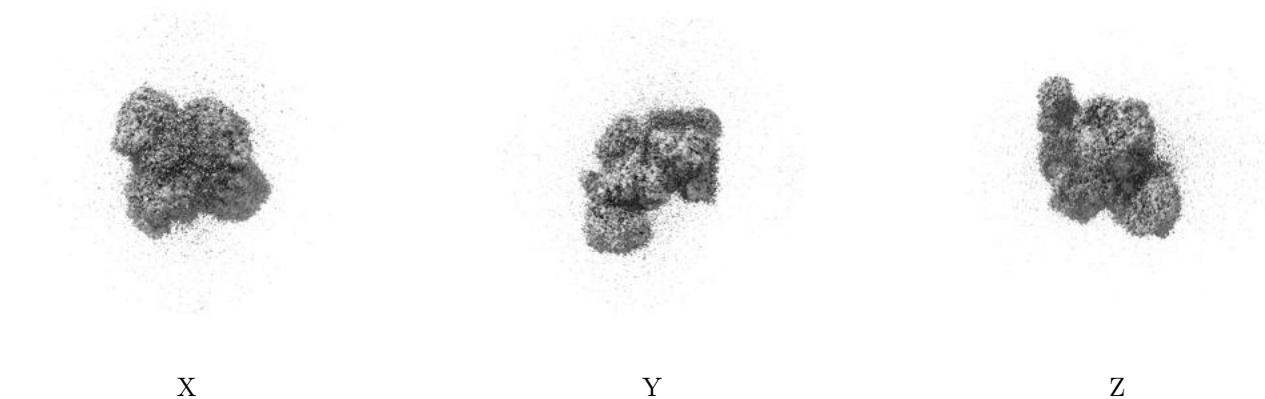
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

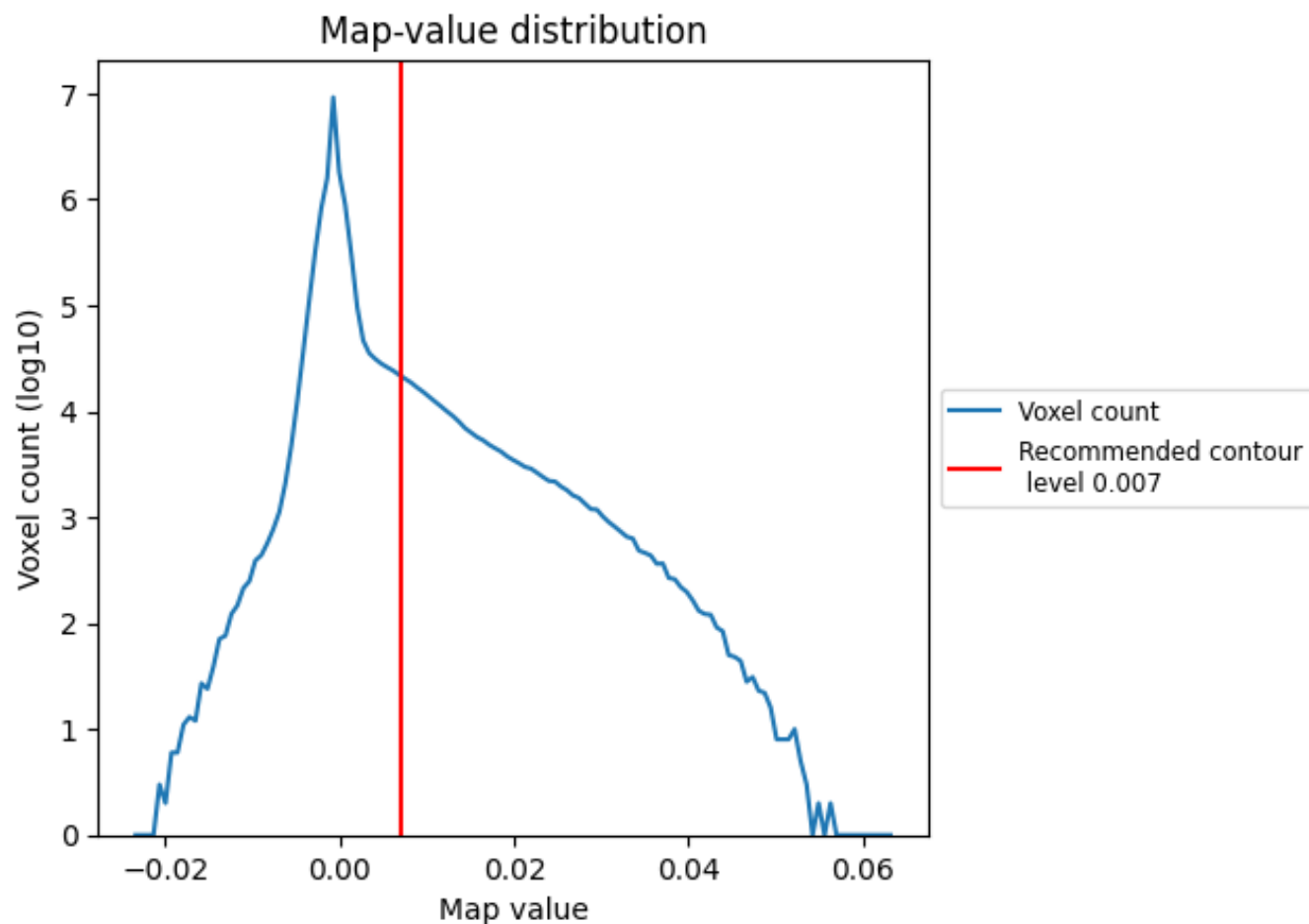
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

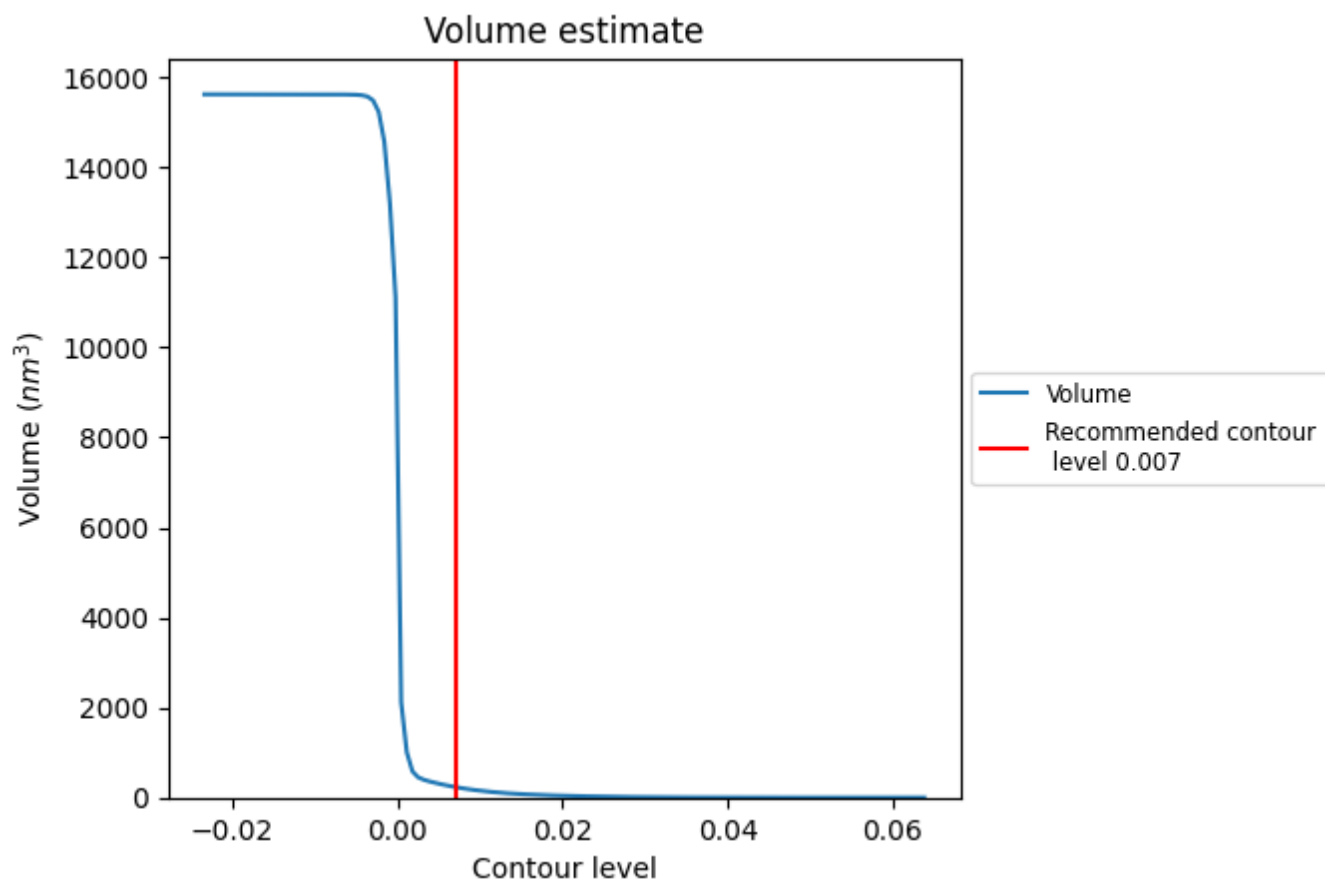
This section contains the results of statistical analysis of the map.

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.

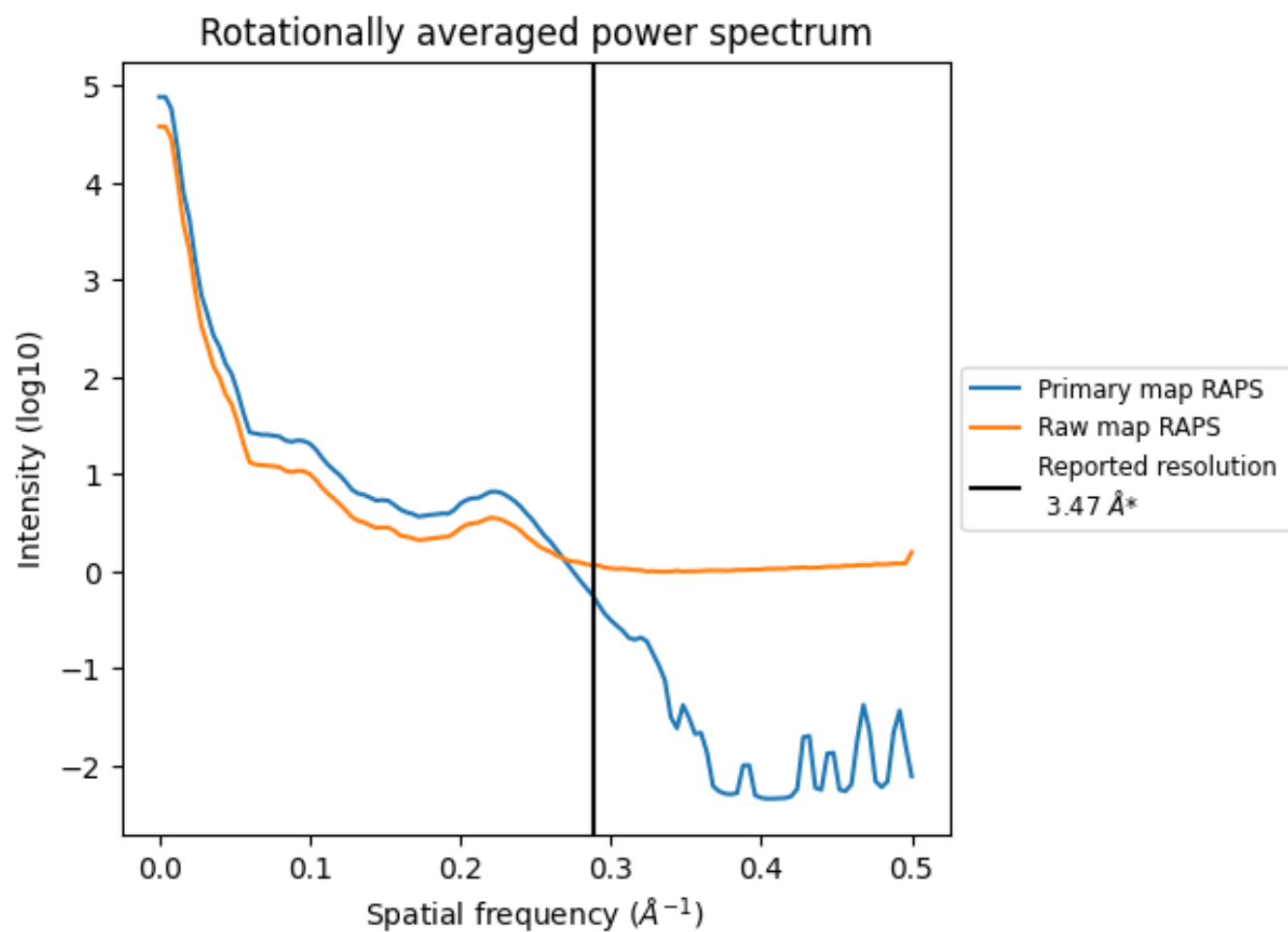
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 235 nm^3 ; this corresponds to an approximate mass of 212 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 ⓘ

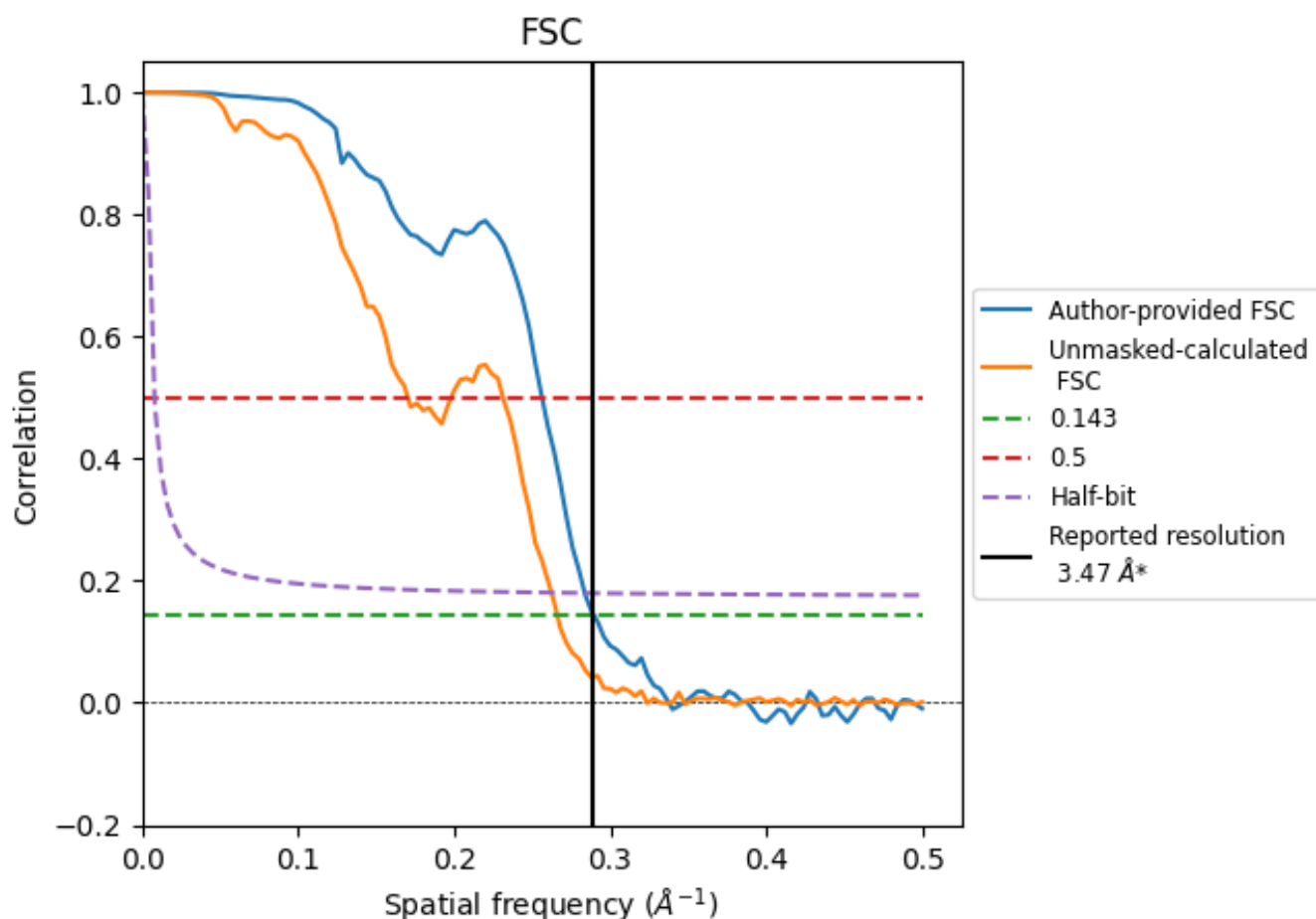


*Reported resolution corresponds to spatial frequency of 0.288 Å⁻¹

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 0.288 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

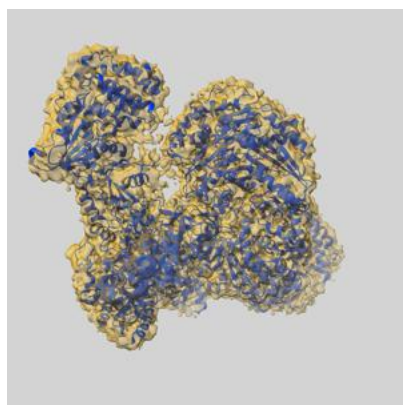
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.45	3.90	3.52
Unmasked-calculated*	3.76	5.87	3.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

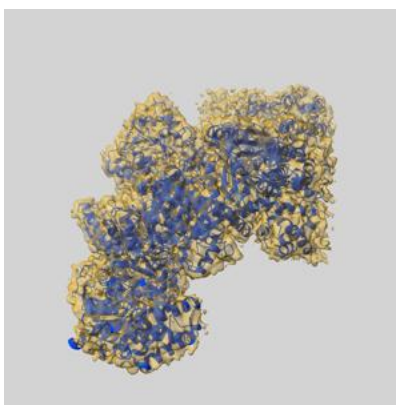
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31199 and PDB model 7EN1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

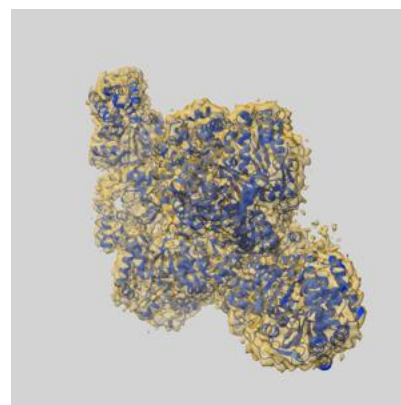
9.1 Map-model overlay [i](#)



X



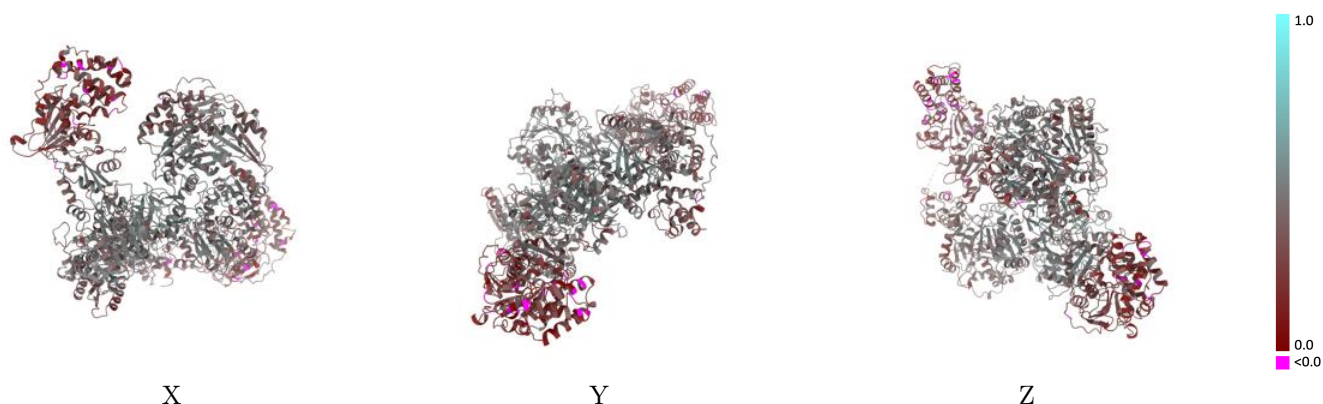
Y



Z

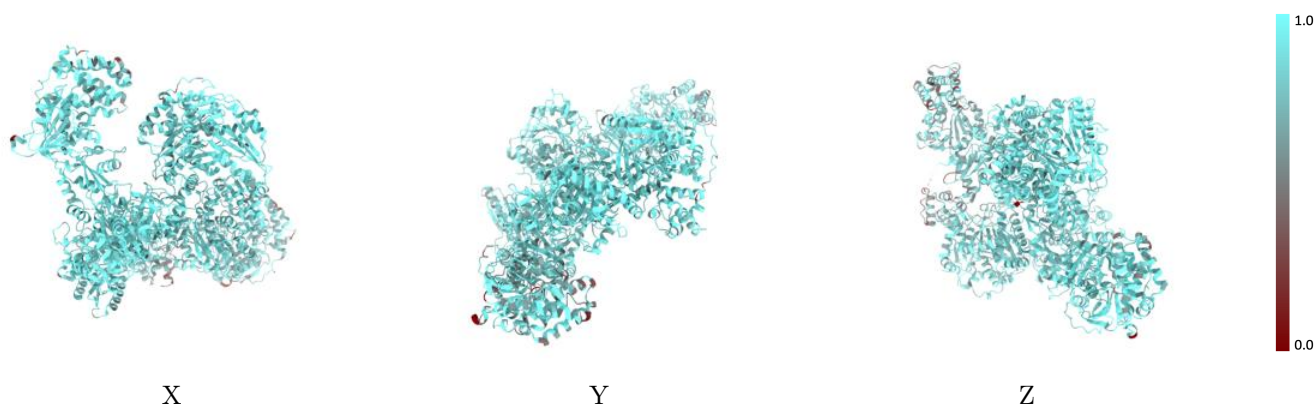
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



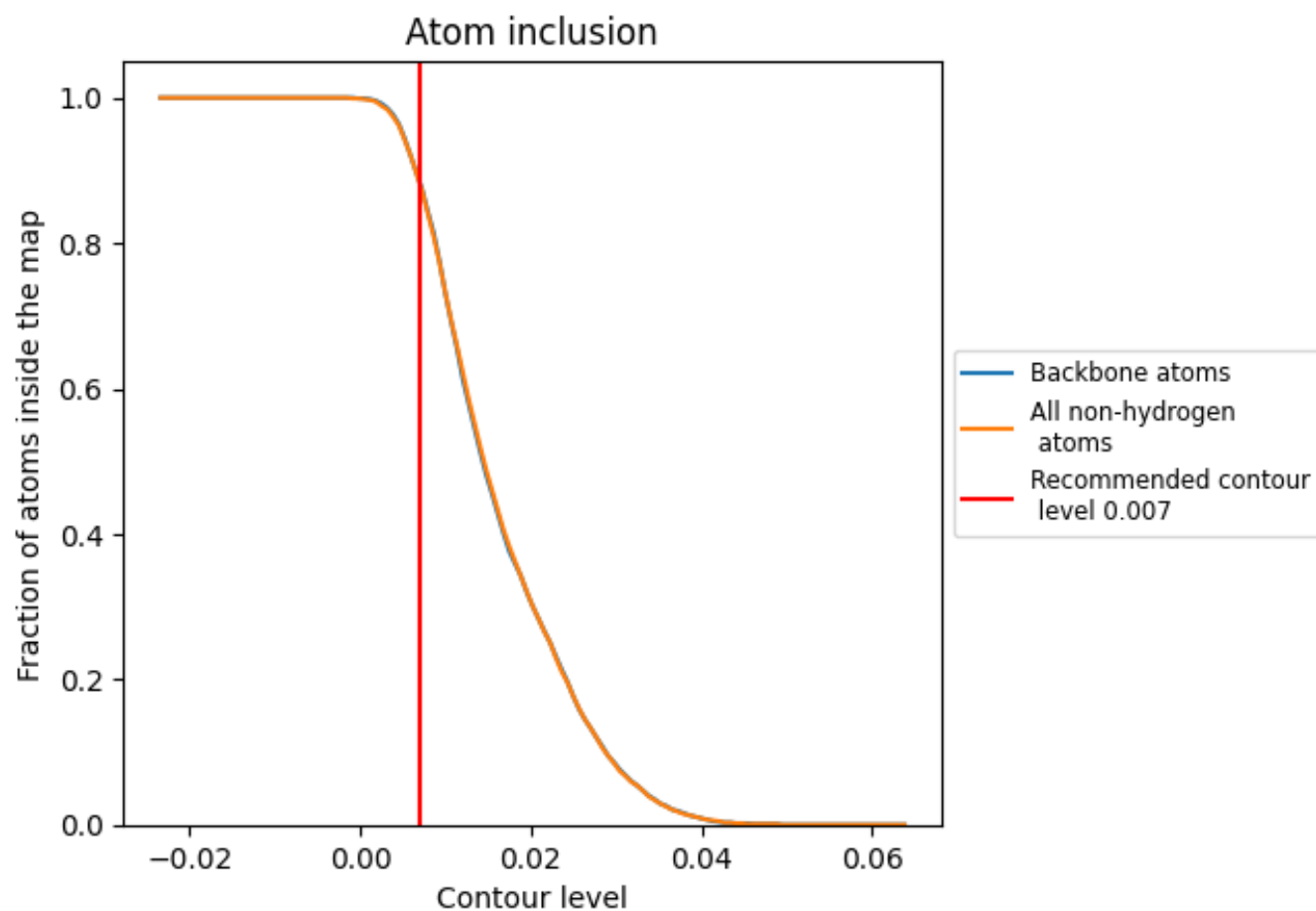
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8820	0.3860
A	0.8630	0.3700
B	0.9230	0.4020

