



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 03:27 PM JST

PDB ID : 7EN1
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.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

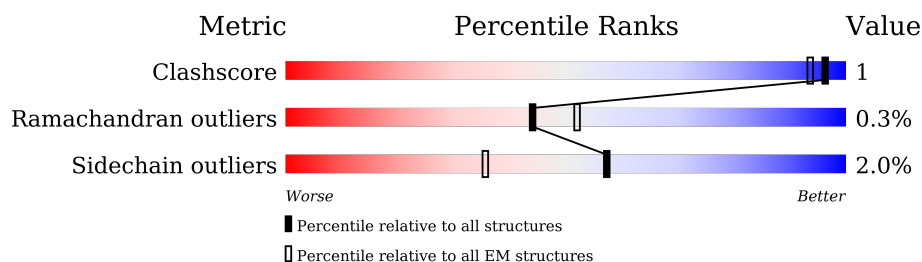
1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1455	 82% 9% 9%
1	B	1455	 83% 9% 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:

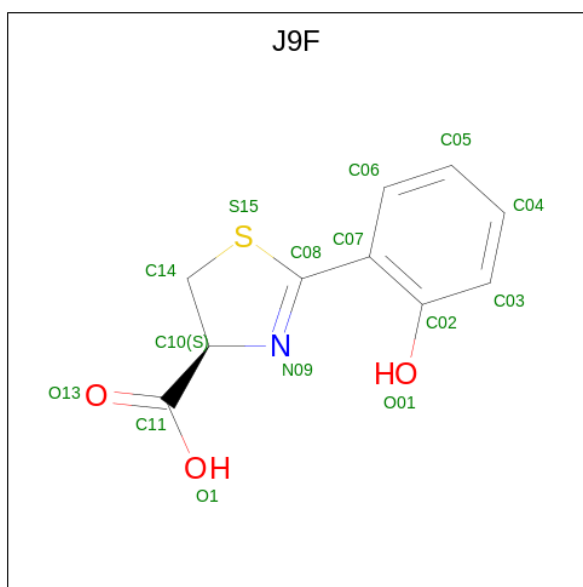
Chain	Residue	Modelled	Actual	Comment	Reference
A	1439	HIS	-	expression tag	UNP G3XCV2
A	1440	HIS	-	expression tag	UNP G3XCV2
A	1441	HIS	-	expression tag	UNP G3XCV2
A	1442	HIS	-	expression tag	UNP G3XCV2
A	1443	HIS	-	expression tag	UNP G3XCV2
A	1444	HIS	-	expression tag	UNP G3XCV2
A	1445	LEU	-	expression 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

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- Chemical structure of a protein-ligand complex, specifically a phosphonate derivative. The structure shows a central phosphorus atom (P24) bonded to three oxygen atoms (O26, O25, O27) and a carbon atom (C28). The carbon atom (C28) is part of a chain that includes a carboxylic acid group (C30, O33, O35) and a thiol group (C42, S44). The structure is labeled with atom names and numbers, and the overall molecule is identified as PNS.

- Molecule 3 is (4S)-2-(2-hydroxyphenyl)-4,5-dihydro-1,3-thiazole-4-carboxylic acid (three-letter code: J9F) (formula: C₁₀H₉NO₃S) (labeled as "Ligand of Interest" by depositor).

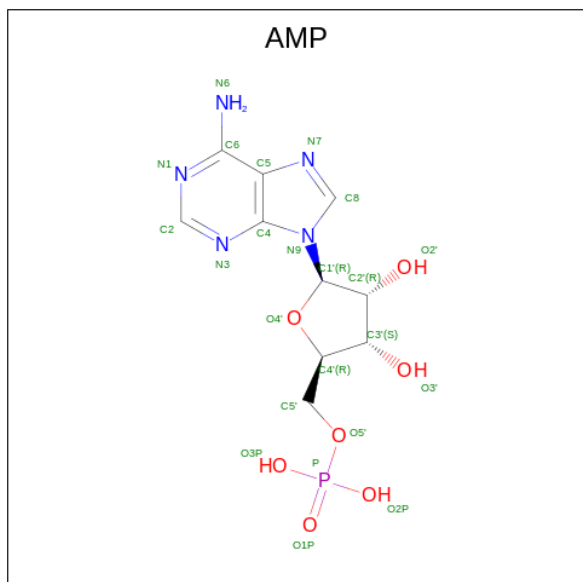


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	S	0
			22	10	8	1	2	1	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

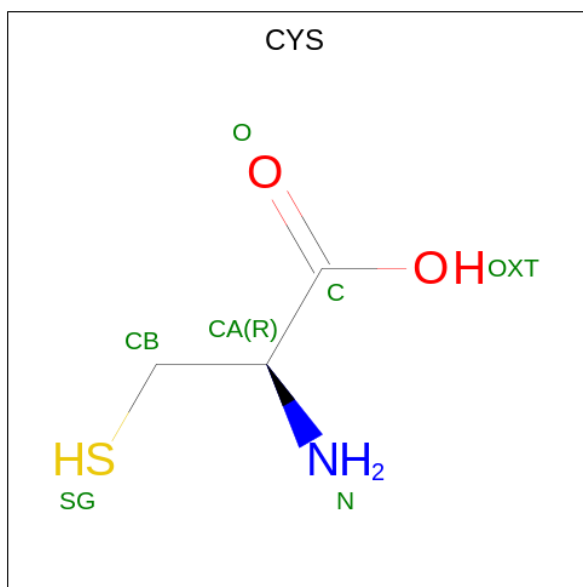
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



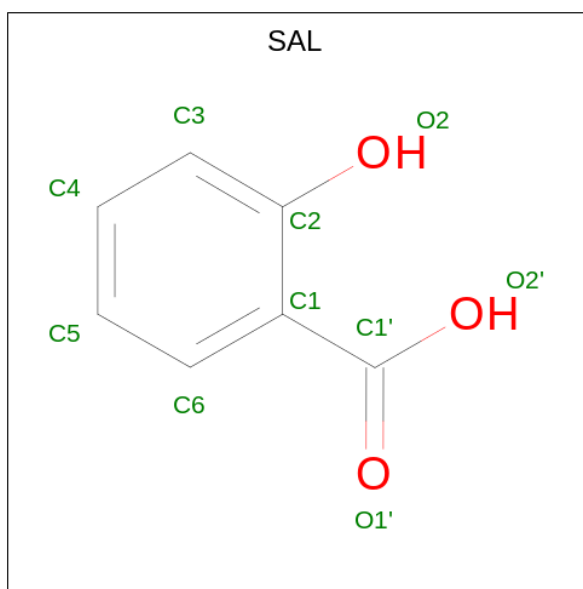
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			35	10	12	5	7	1	
5	B	1	Total	C	H	N	O	P	0
			35	10	12	5	7	1	

- Molecule 6 is CYSTEINE (three-letter code: 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 (three-letter code: SAL) (formula: $C_7H_6O_3$).

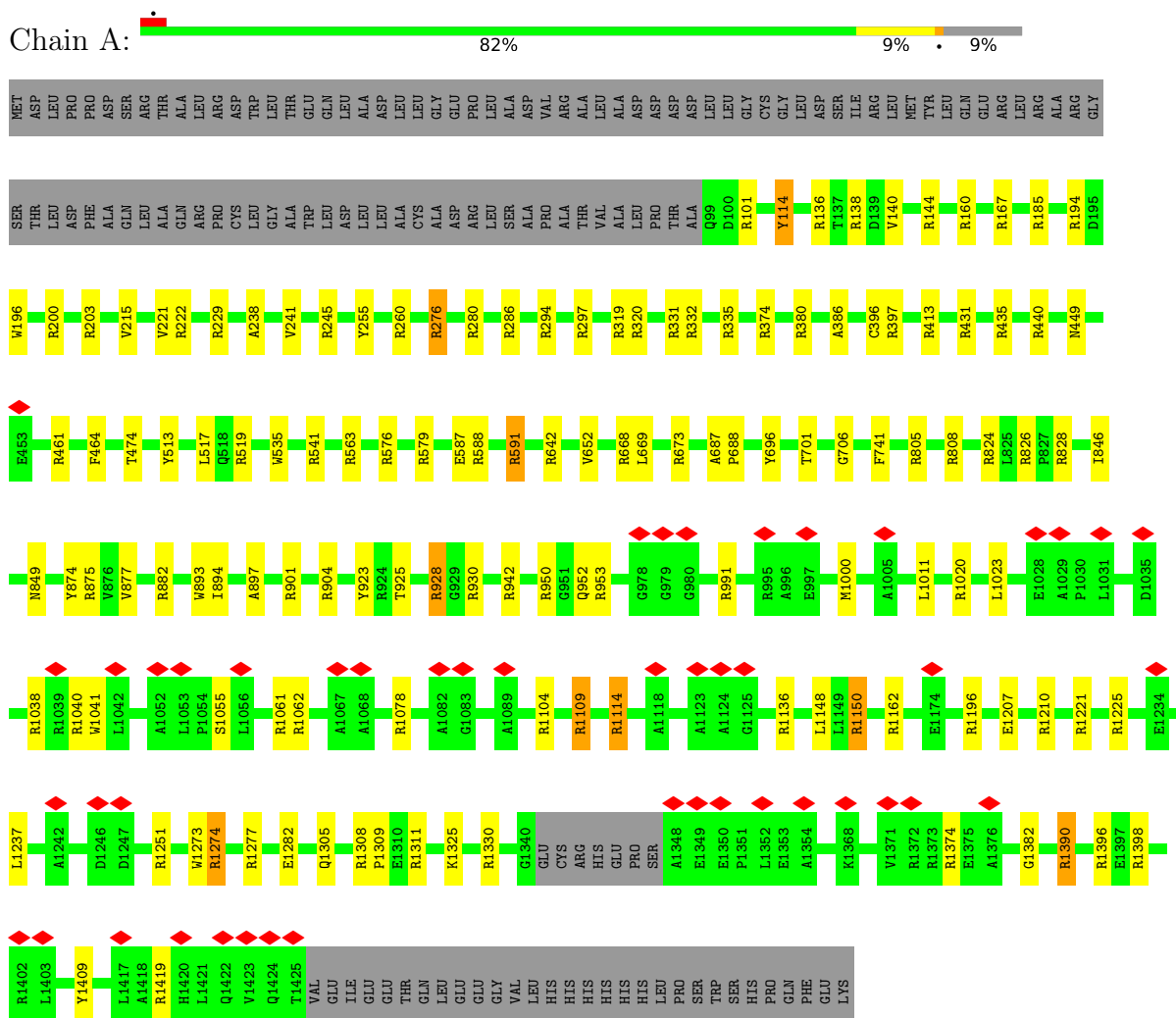


Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
7	B	1	14	7	5	2	0

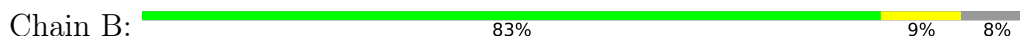
3 Residue-property plots [i](#)

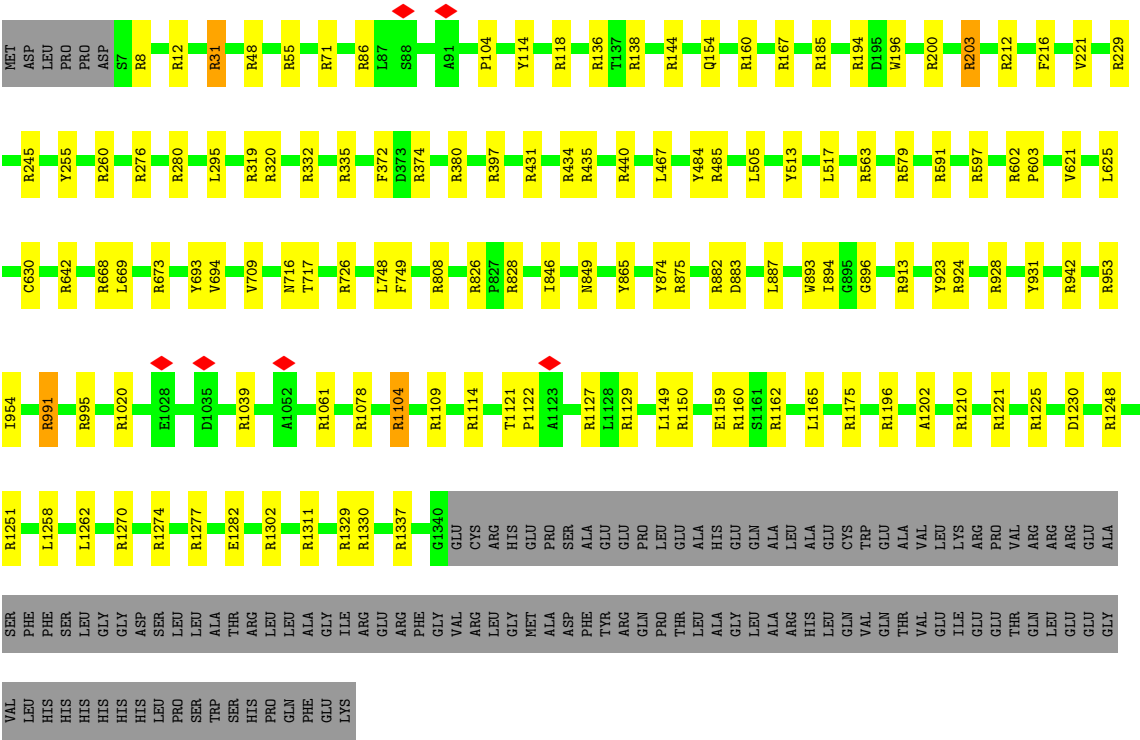
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dihydroaeruginosic acid synthetase



• Molecule 1: Dihydroaeruginosic acid synthetase





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: J9F, SAL, MG, AMP, PNS

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	0.69	0/10332	1.17	89/14069 (0.6%)
1	B	0.69	0/10412	1.16	82/14189 (0.6%)
All	All	0.69	0/20744	1.17	171/28258 (0.6%)

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 (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	A	901	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	A	1251	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	431	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	1150	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	A	200	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	824	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	B	1251	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	435	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	950	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	B	200	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	B	1160	ARG	NE-CZ-NH1	8.72	124.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	B	167	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	B	8	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	319	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	1277	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	1221	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	1277	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	882	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	245	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	B	319	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	B	136	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	280	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	222	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	245	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	114	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	B	942	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	1398	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	1162	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	276	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	B	1061	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	136	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	1104	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	144	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	991	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	953	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	229	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	875	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	397	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	1038	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	991	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	1396	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	1337	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	591	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	1127	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	B	1274	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	440	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	1311	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	519	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	1039	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	579	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	1329	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	A	461	ARG	NE-CZ-NH1	6.36	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1062	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	741	PHE	CB-CG-CD2	-6.28	116.41	120.80
1	A	808	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	1225	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	1020	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	1078	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	144	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	101	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	579	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	1210	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	931	TYR	CB-CG-CD1	-6.09	117.35	121.00
1	A	882	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	591	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	86	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	332	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	331	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	1330	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	928	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	55	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	1419	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	335	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	875	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	194	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	435	ARG	NH1-CZ-NH2	-5.88	112.94	119.40
1	A	1221	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	808	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	280	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	904	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	31	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	602	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	673	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	995	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	1104	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	297	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	1196	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	541	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	1374	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	576	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	1302	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	185	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	1020	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	563	ARG	NE-CZ-NH1	5.70	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	673	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	434	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	942	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	212	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	597	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	1162	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	114	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	B	1225	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	229	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	913	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	1398	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	203	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	1061	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	1270	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	380	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	1274	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	826	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	1040	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	928	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	1248	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	484	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	B	71	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	380	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	194	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	642	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	260	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	828	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	485	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	642	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	930	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	1210	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	588	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	160	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	320	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	118	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	431	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	374	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	805	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	1409	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	B	48	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	930	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	1302	ARG	NE-CZ-NH2	-5.30	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	222	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	397	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	286	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	229	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	320	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	1129	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	136	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	1390	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	1114	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	1078	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	1308	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	1311	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	1330	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	953	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	563	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	726	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	1114	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	294	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	114	TYR	CB-CG-CD1	5.14	124.09	121.00
1	A	431	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	1196	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	335	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	276	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	332	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	245	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	1109	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	828	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	320	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	260	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	1136	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	413	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	1175	ARG	NE-CZ-NH1	5.04	122.82	120.30

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

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Mol	Chain	Res	Type	Group
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
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

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	15	0
1	B	10199	10245	10241	17	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	31	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 (31) 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
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:A:1325:LYS:HZ1	6:A:1505:CYS:N	2.00	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: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: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:668:ARG:C	1:B:669:LEU:HD12	2.36	0.46
1:B:893:TRP:CD1	1:B:924:ARG:HA	2.51	0.46
1:B:846:ILE:H	1:B:846:ILE:CD1	2.27	0.45
1:A:668:ARG:C	1:A:669:LEU:HD12	2.38	0.44
1:A:696:TYR:CZ	1:A:706:GLY:HA3	2.52	0.44
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:B:1258:LEU:C	1:B:1258:LEU:HD23	2.39	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:B:1262:LEU:C	1:B:1262:LEU:HD23	2.40	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: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%)	41	75
1	B	1332/1455 (92%)	1263 (95%)	66 (5%)	3 (0%)	47	80
All	All	2648/2910 (91%)	2504 (95%)	137 (5%)	7 (0%)	44	75

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%)	986 (98%)	22 (2%)	52	77
1	B	1019/1122 (91%)	1000 (98%)	19 (2%)	57	80
All	All	2027/2244 (90%)	1986 (98%)	41 (2%)	57	79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ARG
1	A	140	VAL
1	A	215	VAL
1	A	241	VAL
1	A	276	ARG

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Mol	Chain	Res	Type
1	A	396	CYS
1	A	449	ASN
1	A	464	PHE
1	A	587	GLU
1	A	652	VAL
1	A	952	GLN
1	A	1000	MET
1	A	1011	LEU
1	A	1055	SER
1	A	1109	ARG
1	A	1114	ARG
1	A	1148	LEU
1	A	1207	GLU
1	A	1237	LEU
1	A	1273	TRP
1	A	1282	GLU
1	A	1305	GLN
1	B	31	ARG
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	716	ASN
1	B	883	ASP
1	B	887	LEU
1	B	954	ILE
1	B	991	ARG
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	449	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	1504	6,4	22,25,25	1.29	3 (13%)	25,38,38	1.64	6 (24%)
2	PNS	B	1501	7,1	13,20,21	1.00	0	18,26,29	1.14	1 (5%)
5	AMP	B	1504	4	22,25,25	1.14	2 (9%)	25,38,38	1.92	8 (32%)
3	J9F	A	1502	2	14,15,16	0.83	1 (7%)	13,20,22	0.55	0
6	CYS	B	1505	-	5,6,6	0.92	0	5,7,7	1.66	1 (20%)
7	SAL	B	1502	2	9,9,10	0.54	0	11,11,13	0.61	0
6	CYS	A	1505	5	4,5,6	1.16	1 (25%)	1,5,7	1.68	0
2	PNS	A	1501	3,1	13,20,21	1.06	0	18,26,29	1.13	1 (5%)

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	A	1504	6,4	-	4/6/26/26	0/3/3/3
2	PNS	B	1501	7,1	-	5/24/26/27	-
5	AMP	B	1504	4	-	4/6/26/26	0/3/3/3
3	J9F	A	1502	2	-	3/4/15/17	0/2/2/2
6	CYS	B	1505	-	-	4/6/6/6	-
7	SAL	B	1502	2	-	2/2/2/4	0/1/1/1
6	CYS	A	1505	5	-	0/1/4/6	-
2	PNS	A	1501	3,1	-	8/24/26/27	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1504	AMP	C5-C4	-2.51	1.34	1.40
5	B	1504	AMP	C5-C4	-2.40	1.34	1.40
5	A	1504	AMP	O4'-C1'	2.39	1.44	1.41
6	A	1505	CYS	CB-SG	2.23	1.86	1.81
5	A	1504	AMP	P-O2P	-2.05	1.46	1.54
5	B	1504	AMP	C4-N3	-2.03	1.32	1.35
3	A	1502	J9F	C08-N09	2.03	1.29	1.27

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1504	AMP	O5'-P-O1P	4.42	118.88	106.47
5	B	1504	AMP	C4-C5-N7	4.36	113.94	109.40
5	A	1504	AMP	C4-C5-N7	4.02	113.59	109.40
2	B	1501	PNS	C42-N41-C39	3.43	129.21	122.84
5	B	1504	AMP	O4'-C1'-C2'	-3.08	102.42	106.93
2	A	1501	PNS	C30-C29-C32	2.97	113.98	108.82
6	B	1505	CYS	CB-CA-C	2.87	112.75	109.89
5	B	1504	AMP	O3P-P-O5'	2.45	113.25	106.73
5	A	1504	AMP	O3P-P-O2P	-2.38	98.53	107.64
5	A	1504	AMP	N6-C6-N1	-2.35	113.69	118.57
5	B	1504	AMP	C3'-C2'-C1'	2.35	104.51	100.98
5	A	1504	AMP	O2P-P-O5'	2.34	112.95	106.73
5	B	1504	AMP	O2P-P-O5'	2.31	112.87	106.73
5	B	1504	AMP	C2-N1-C6	-2.30	114.81	118.75
5	A	1504	AMP	C2-N1-C6	-2.22	114.96	118.75
5	A	1504	AMP	C2'-C3'-C4'	-2.20	98.38	102.64
5	B	1504	AMP	O3P-P-O1P	-2.02	102.78	110.68

There are no chirality outliers.

All (30) torsion outliers are listed below:

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

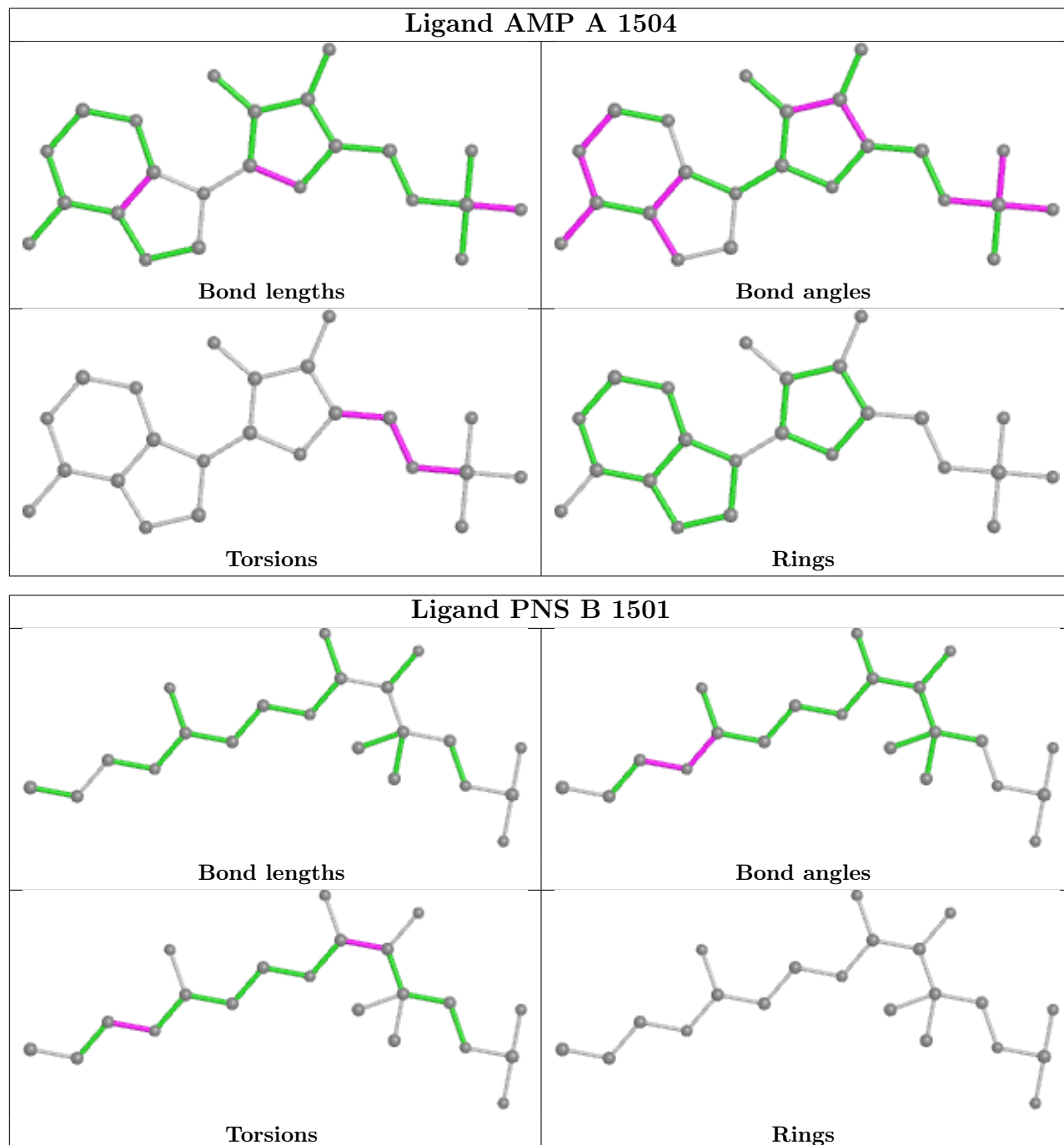
There are no ring outliers.

2 monomers are involved in 2 short contacts:

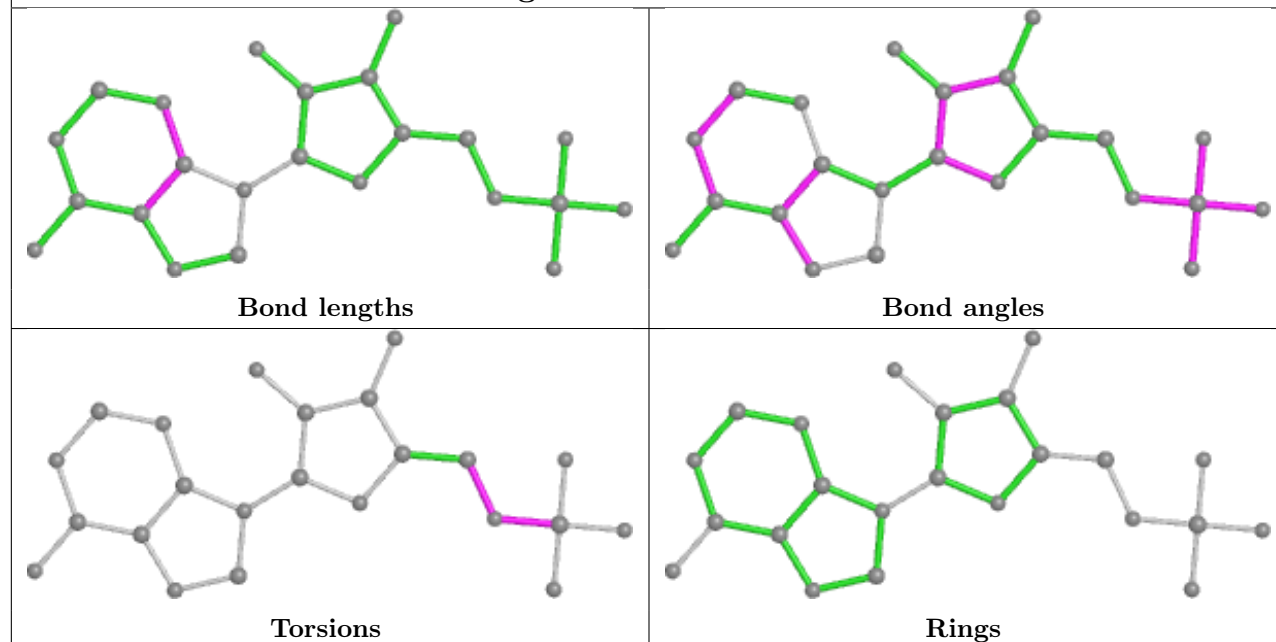
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	J9F	1	0
6	A	1505	CYS	1	0

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

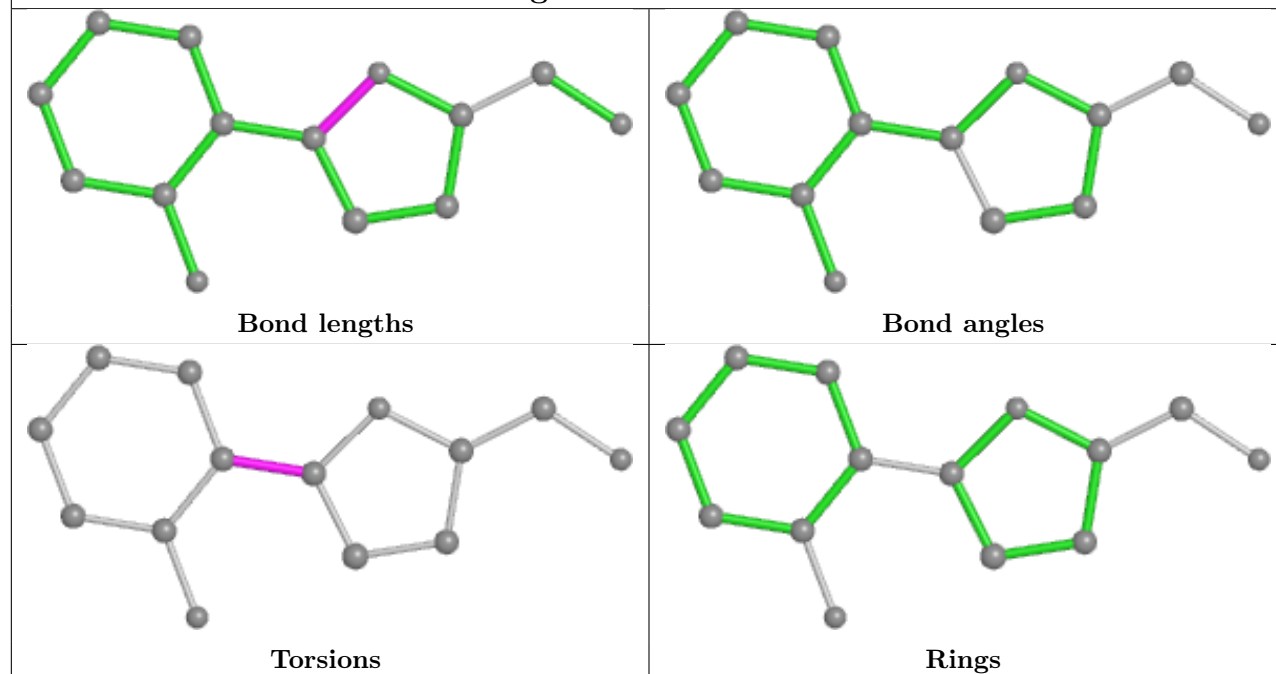
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

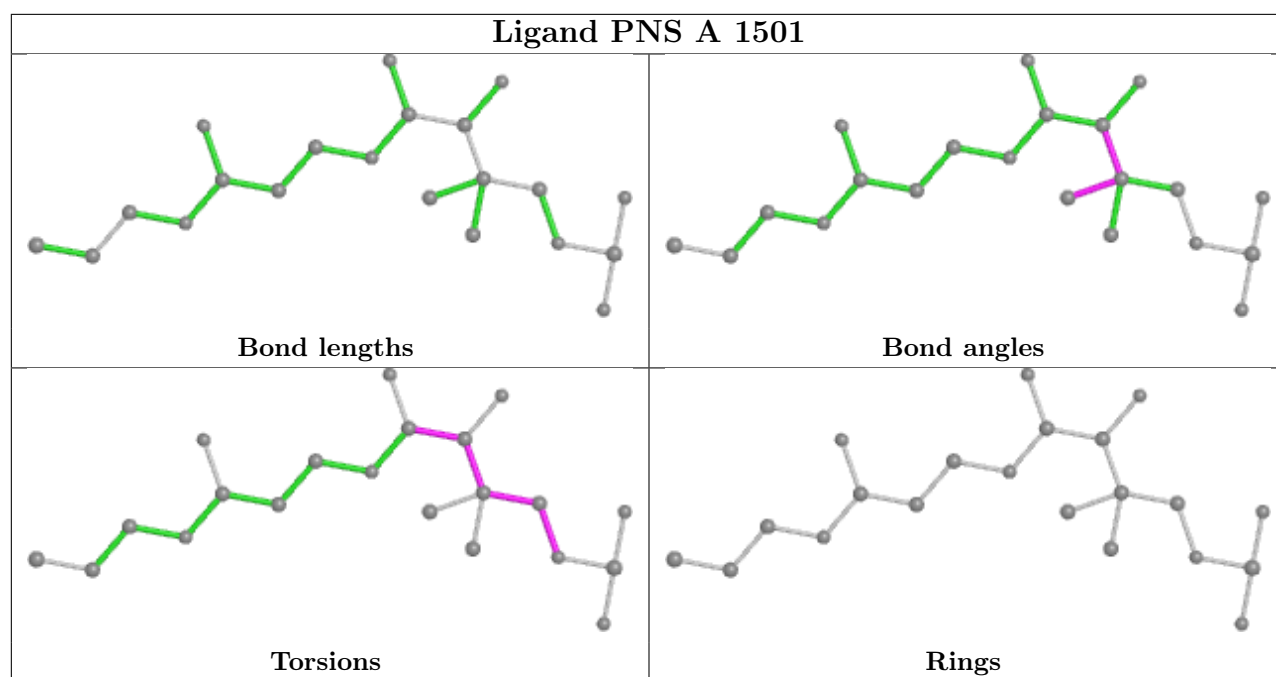


Ligand AMP B 1504



Ligand J9F A 1502





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.

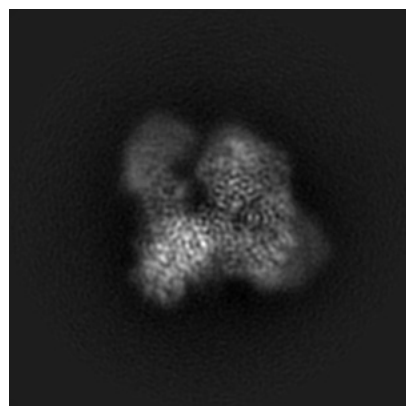
6 Map visualisation [i](#)

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.

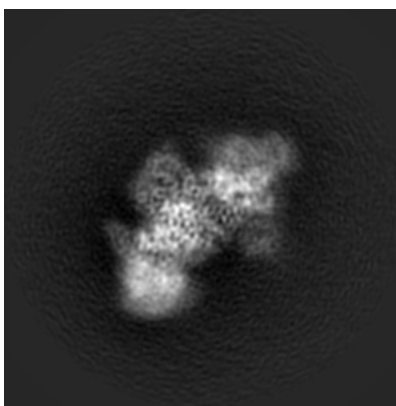
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

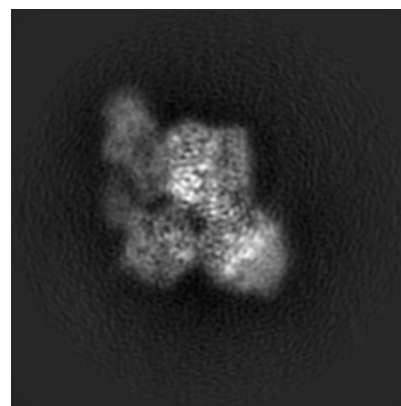
6.1.1 Primary map



X

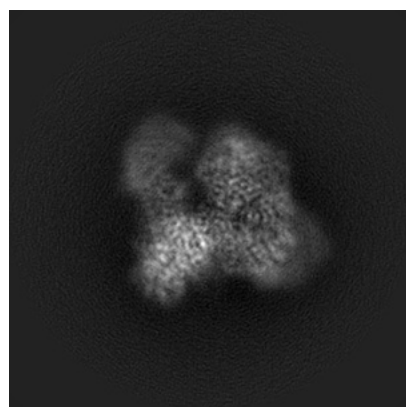


Y

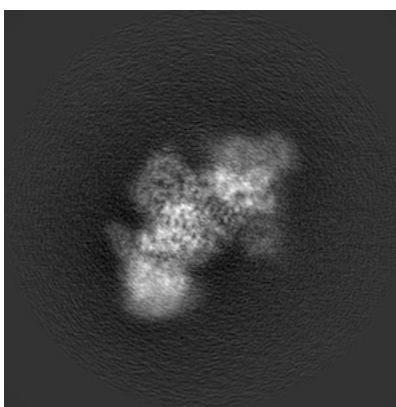


Z

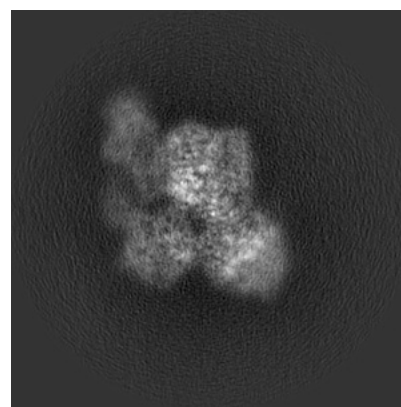
6.1.2 Raw map



X



Y

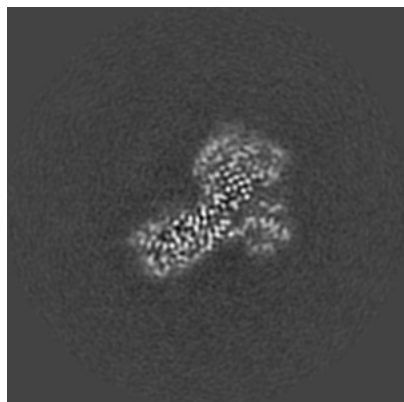


Z

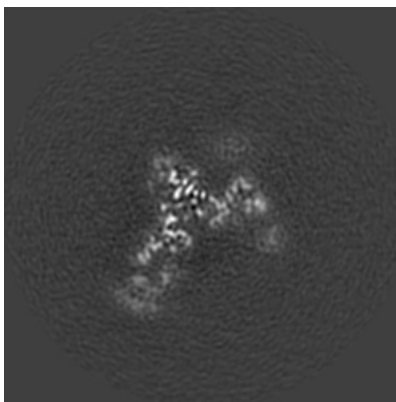
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

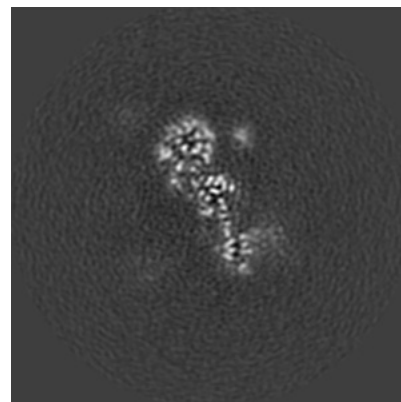
6.2.1 Primary map



X Index: 125

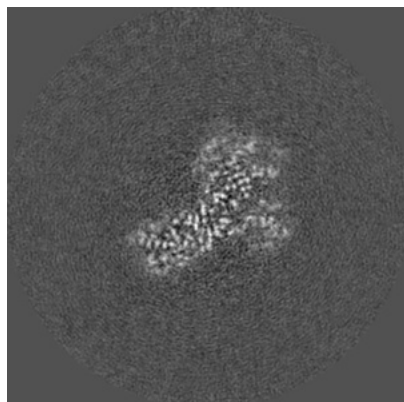


Y Index: 125

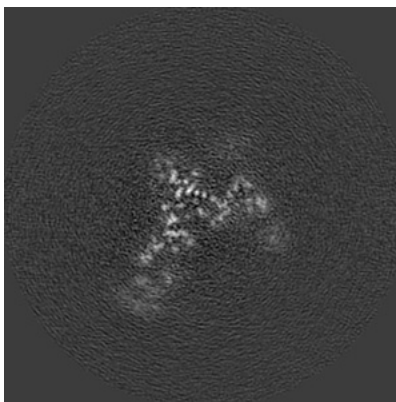


Z Index: 125

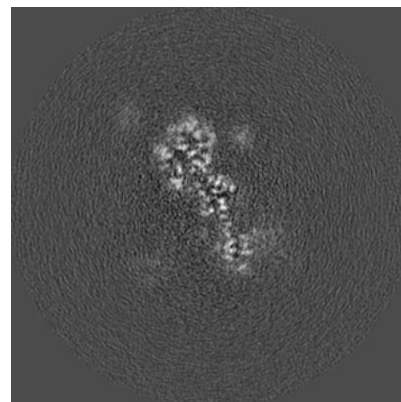
6.2.2 Raw map



X Index: 125



Y Index: 125

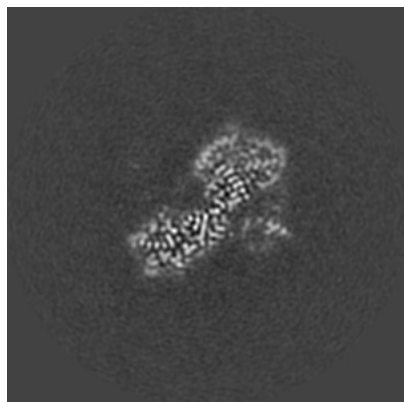


Z Index: 125

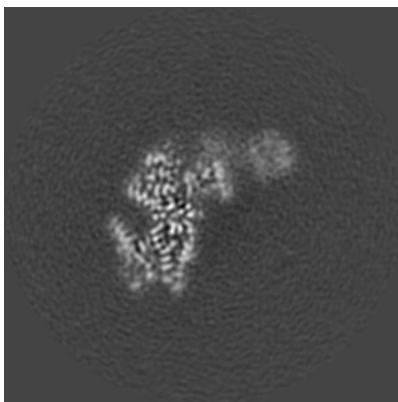
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

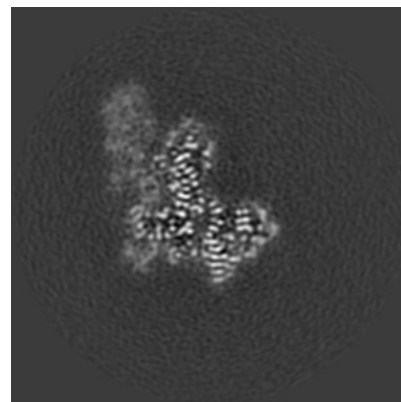
6.3.1 Primary map



X Index: 127

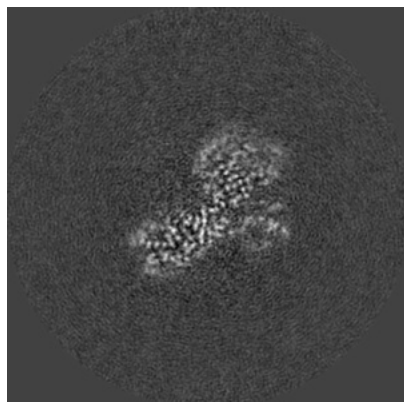


Y Index: 106

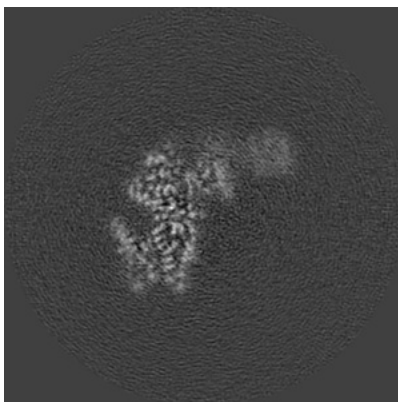


Z Index: 101

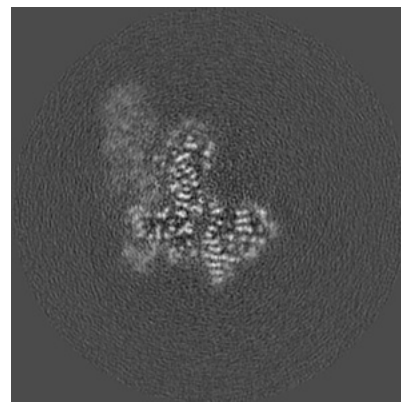
6.3.2 Raw map



X Index: 126



Y Index: 106



Z Index: 102

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

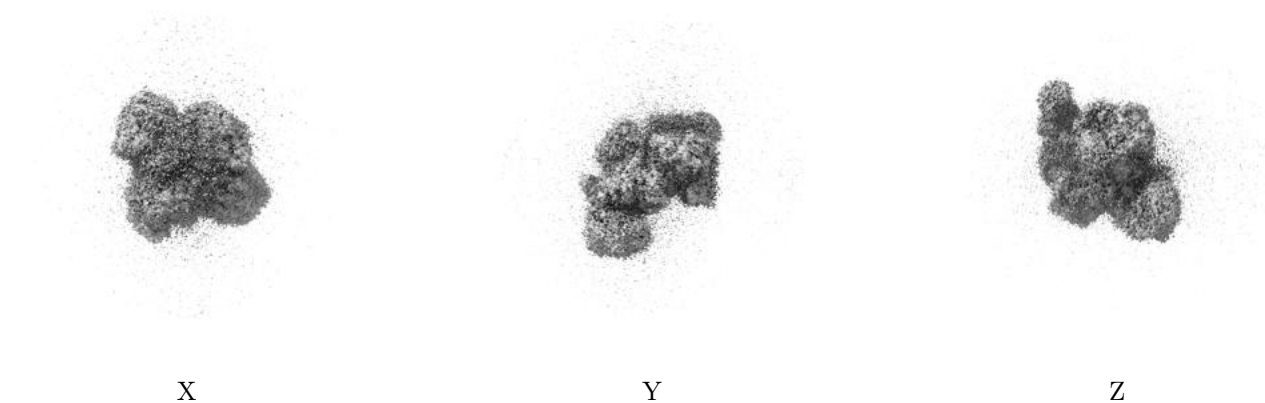
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

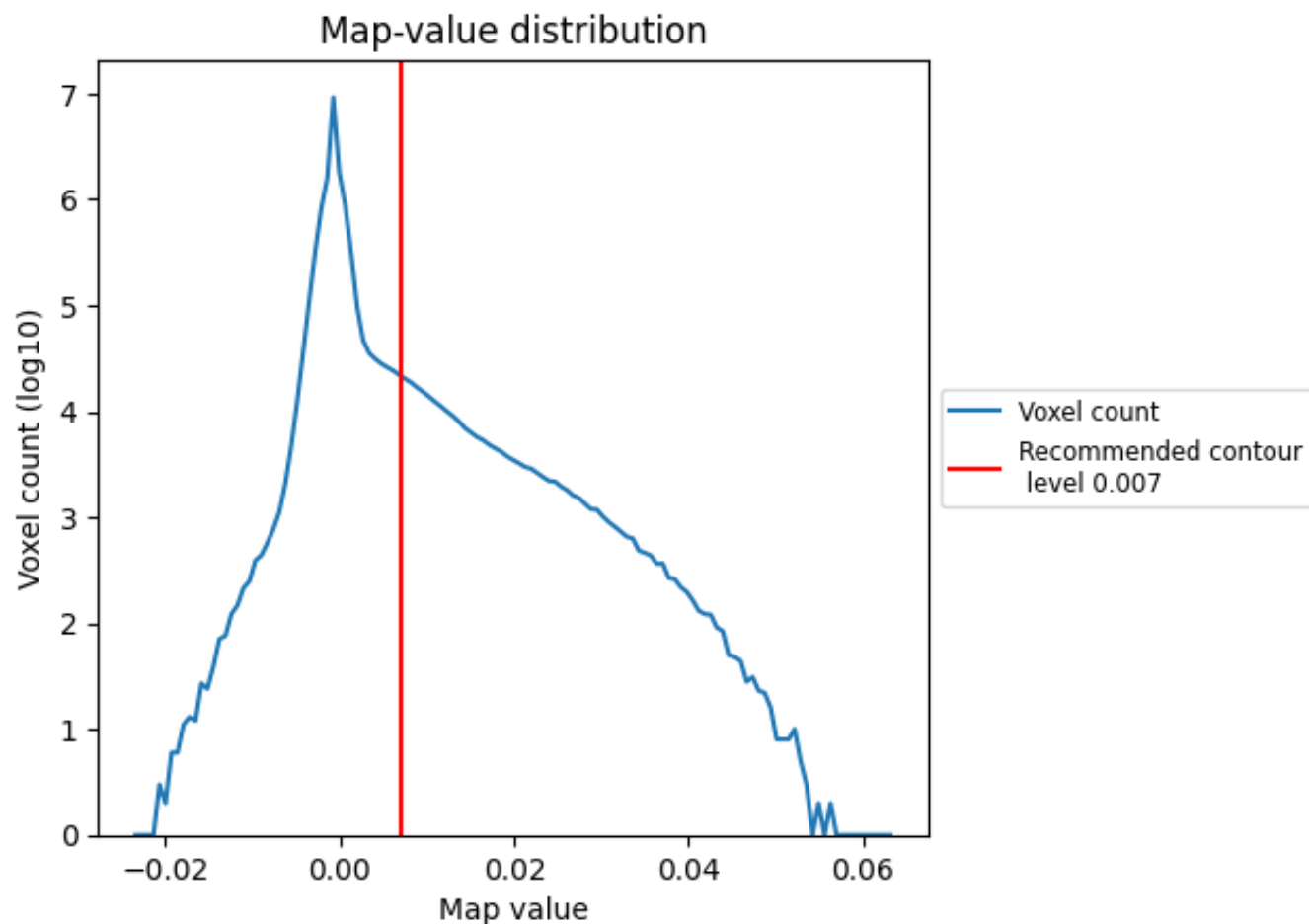
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

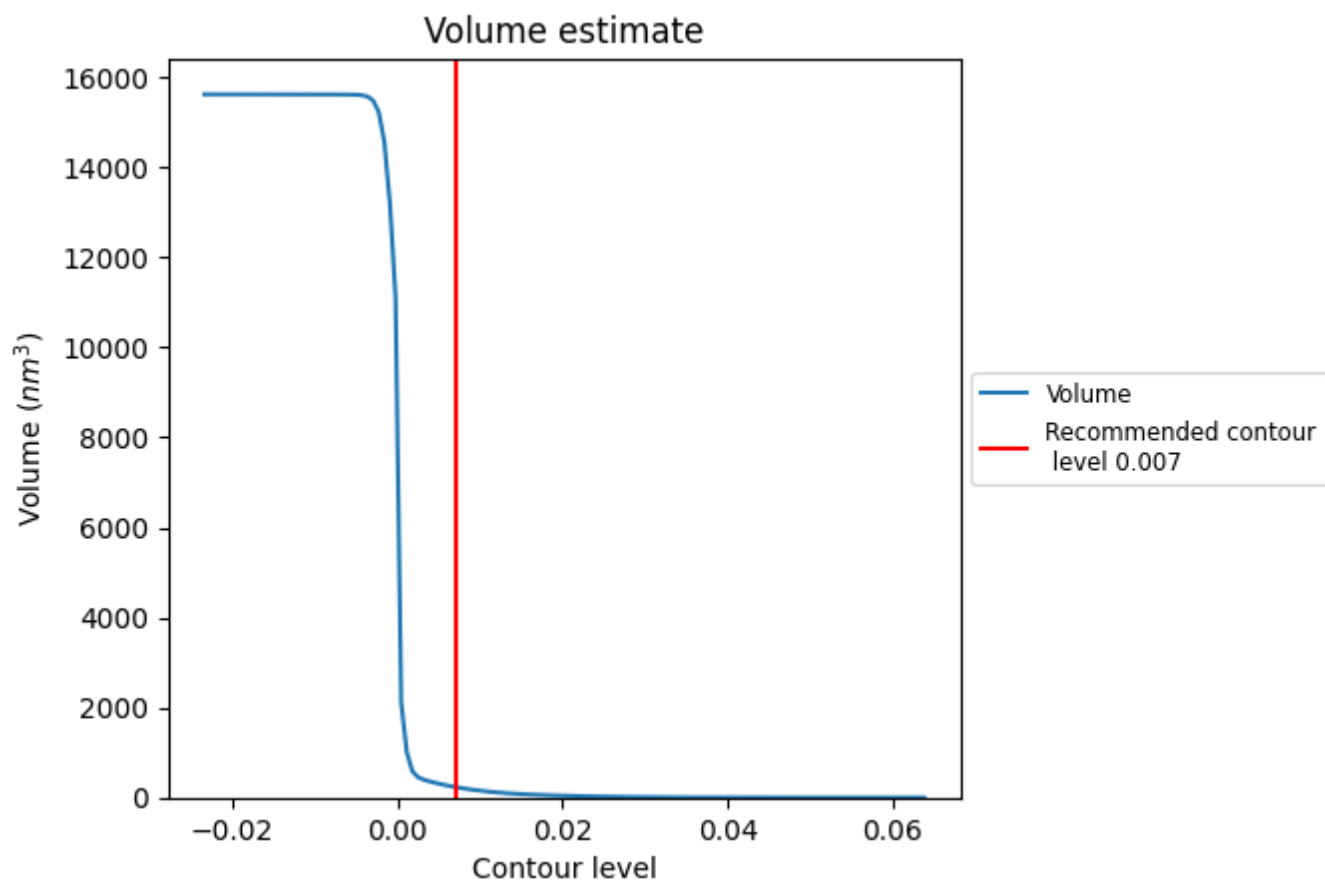
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

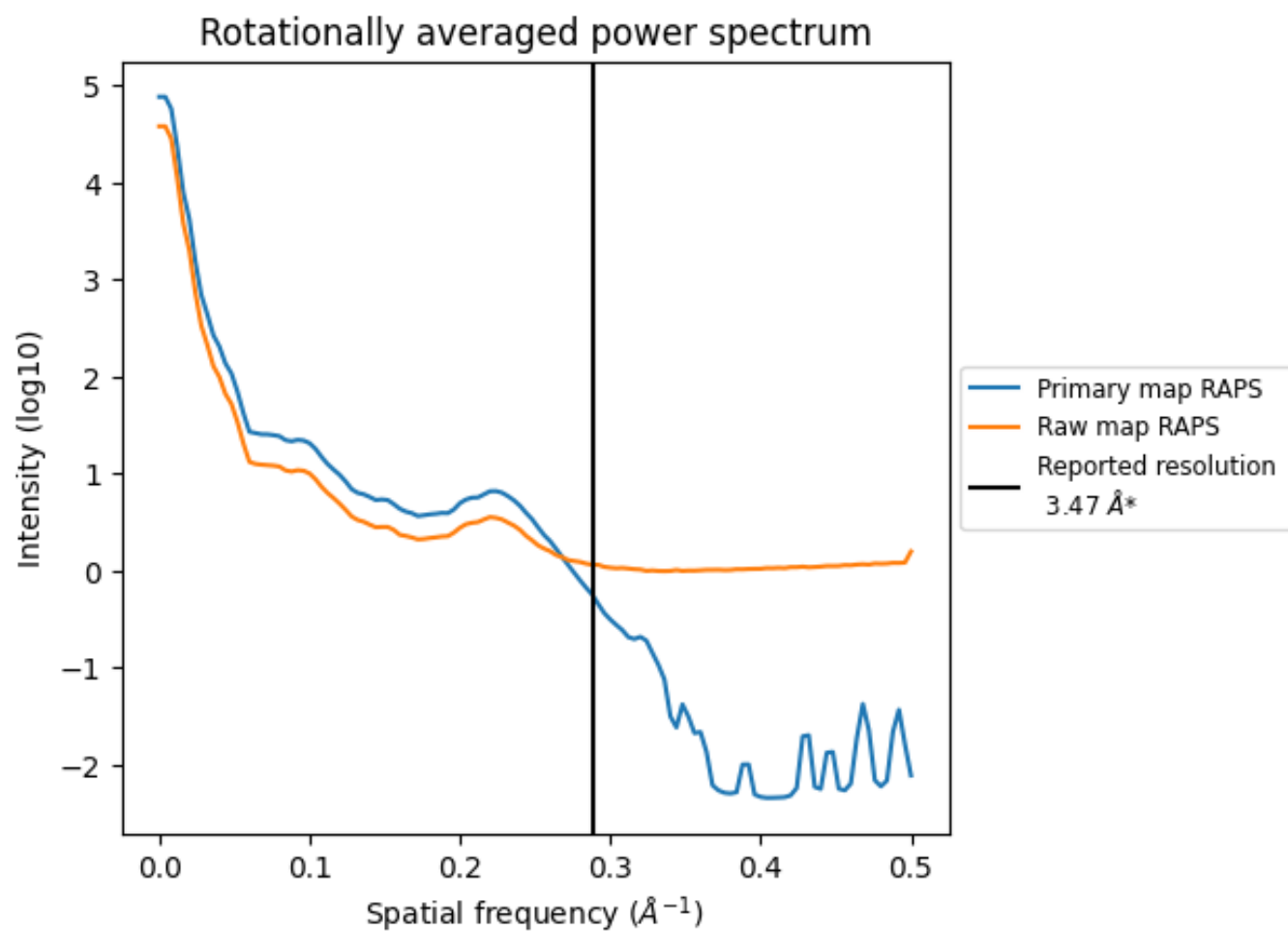
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

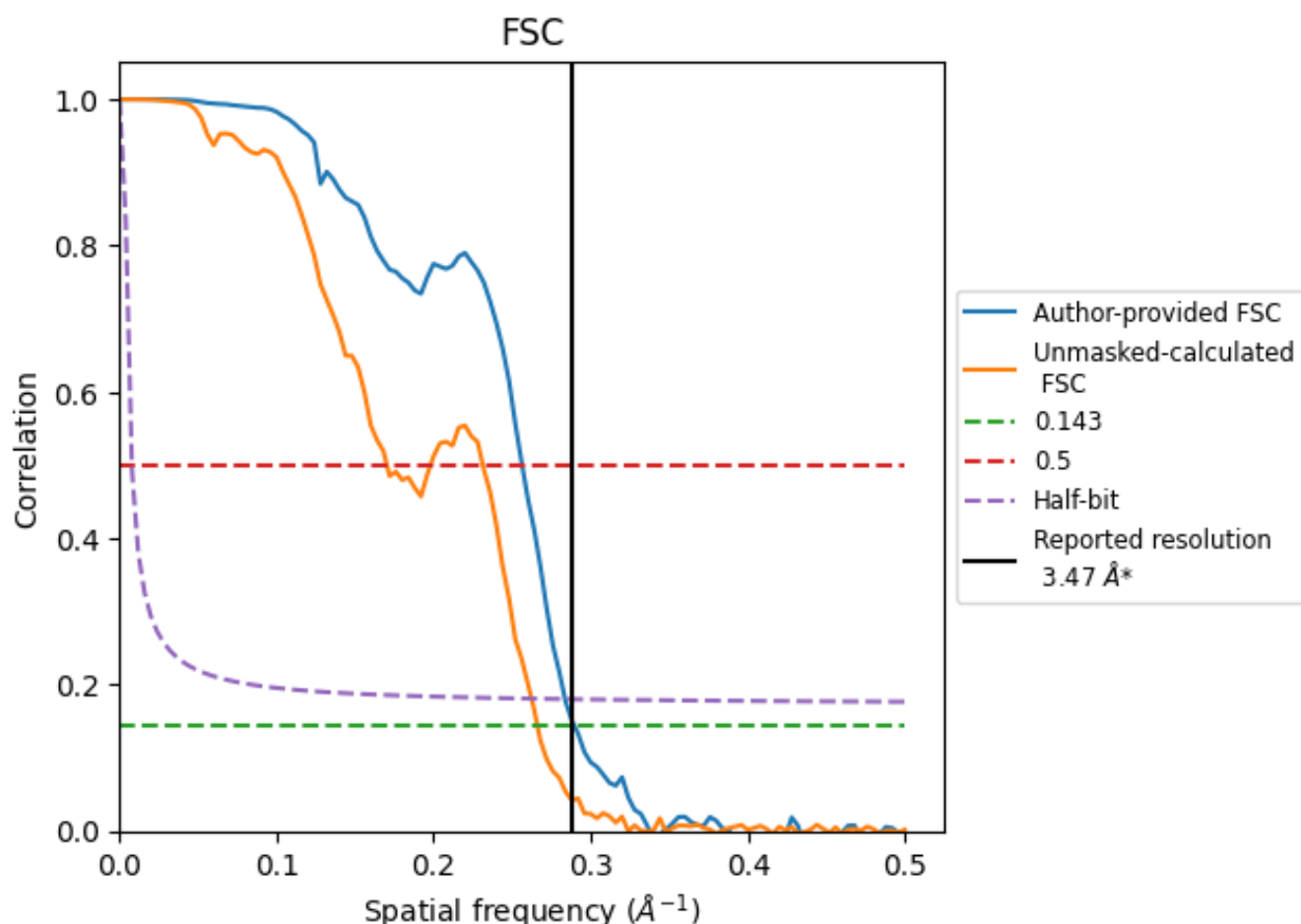


*Reported resolution corresponds to spatial frequency of 0.288 \AA^{-1}

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 0.288 Å⁻¹

8.2 Resolution estimates [i](#)

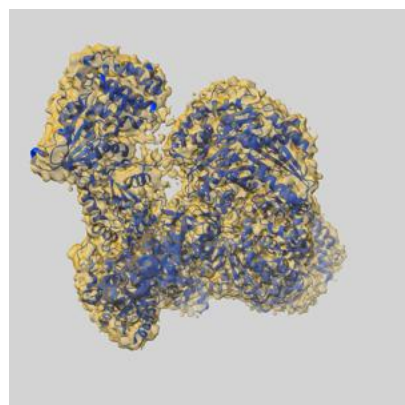
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.45	3.90	3.52
Unmasked-calculated*	3.76	5.87	3.81

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

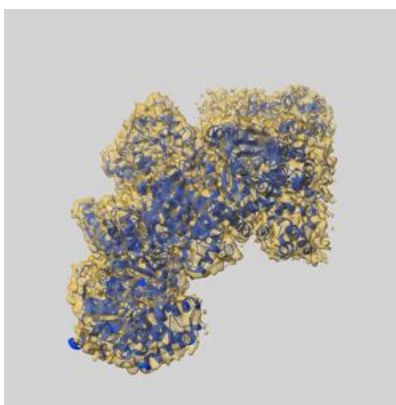
9 Map-model fit [i](#)

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](#).

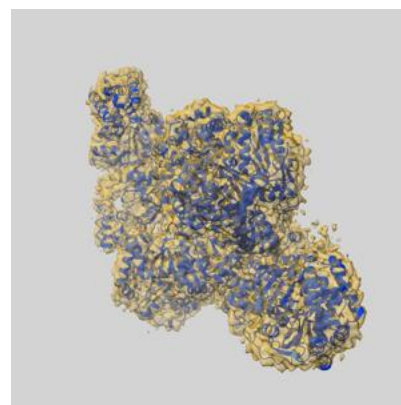
9.1 Map-model overlay [i](#)



X



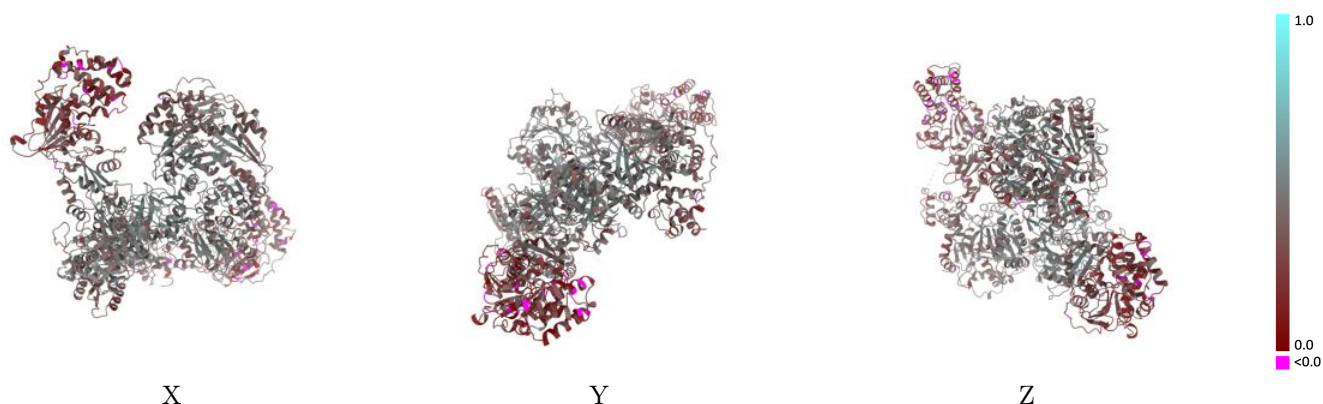
Y



Z

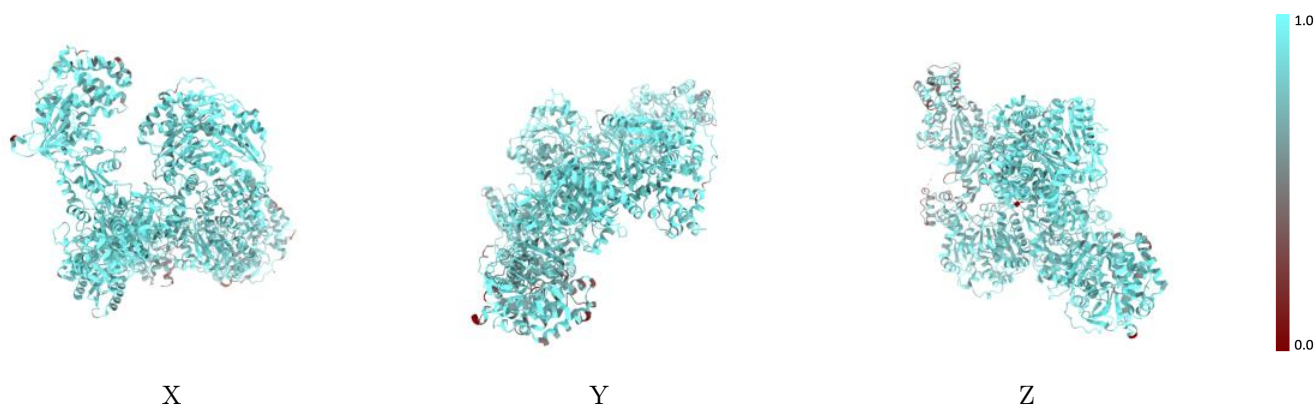
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



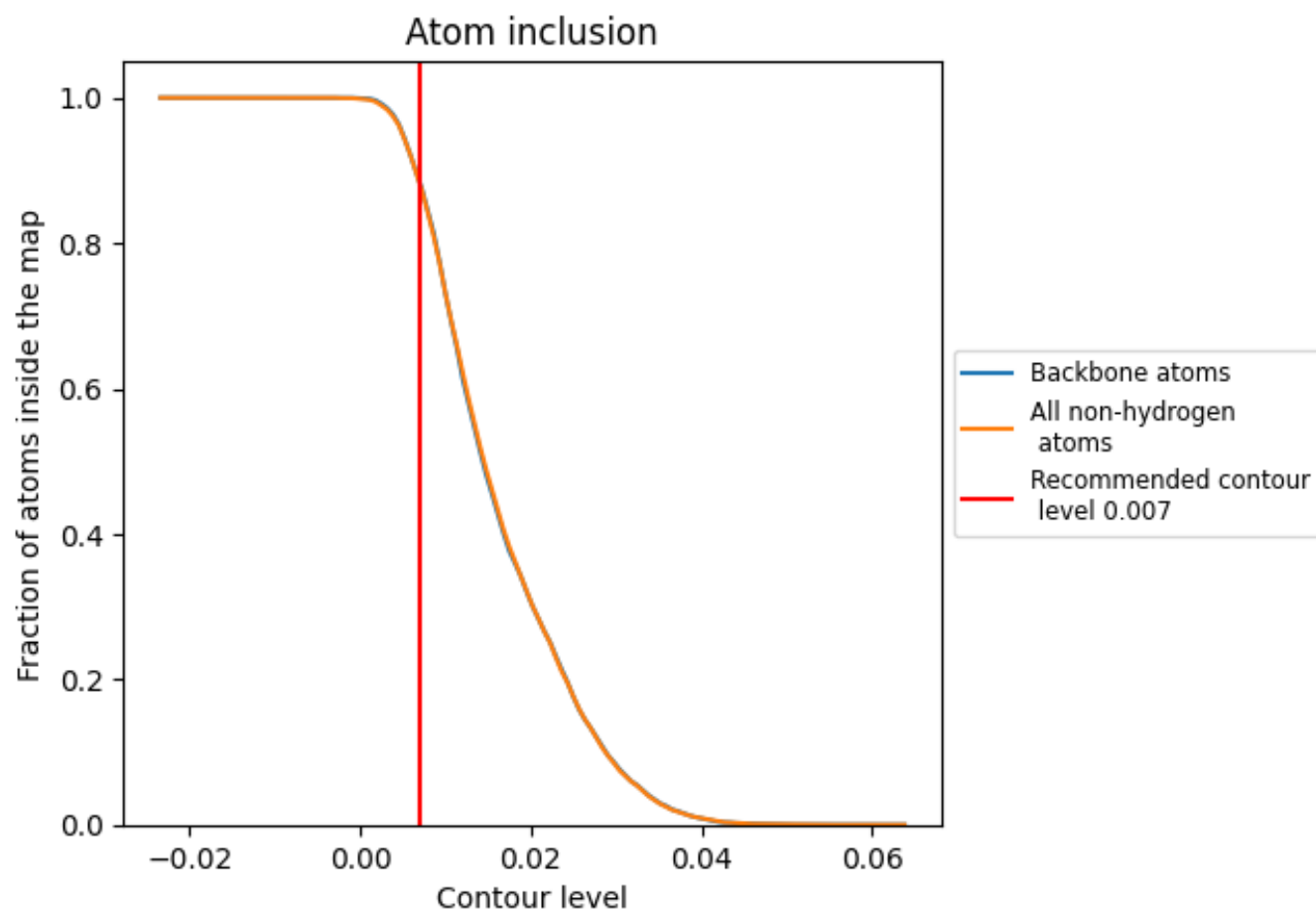
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.8824	<div></div> 0.3860
A	<div></div> 0.8628	<div></div> 0.3700
B	<div></div> 0.9226	<div></div> 0.4020

