



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:07 PM UTC

PDB ID : 3J08 / pdb_00003j08
EMDB ID : EMD-5271
Title : High resolution helical reconstruction of the bacterial p-type ATPase copper transporter CopA
Authors : Wu, C.; Allen, G.S.; Cardozo, T.; Stokes, D.L.
Deposited on : 2011-05-09
Resolution : 10.00 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
MolProbity : 4-5-2 with Phenix2.0
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

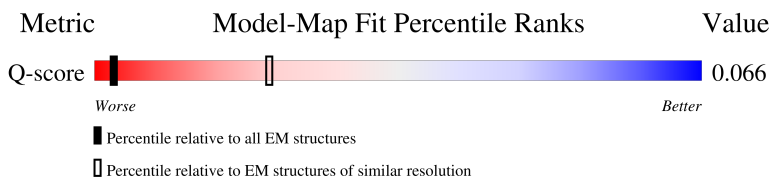
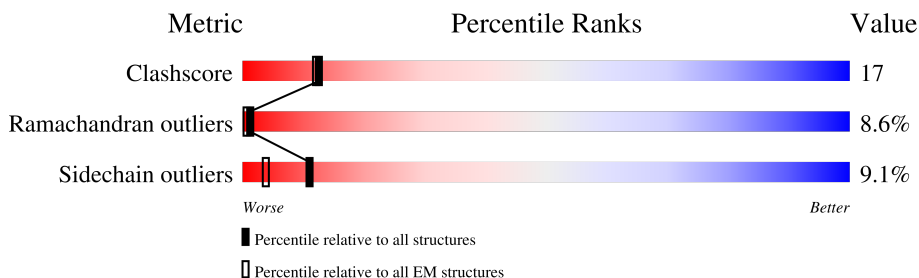
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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	147 (9.50 - 10.50)

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	645	34% 66% 23% 8% .
1	B	645	34% 66% 22% 8% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9734 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.

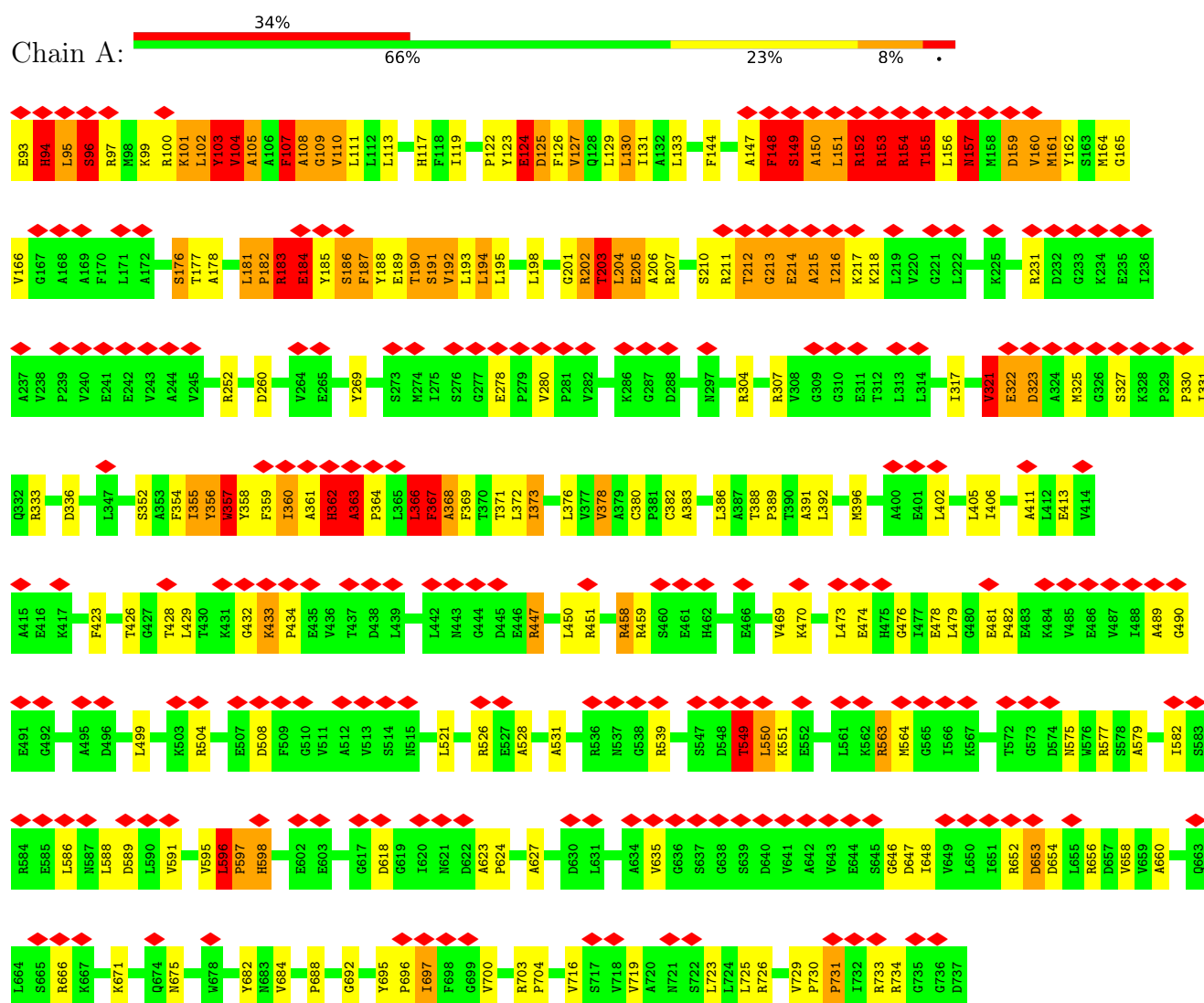
- Molecule 1 is a protein called copper-exporting P-type ATPase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	645	Total	C	N	O	S	0	0
			4867	3139	819	894	15		
1	B	645	Total	C	N	O	S	0	0
			4867	3139	819	894	15		

3 Residue-property plots

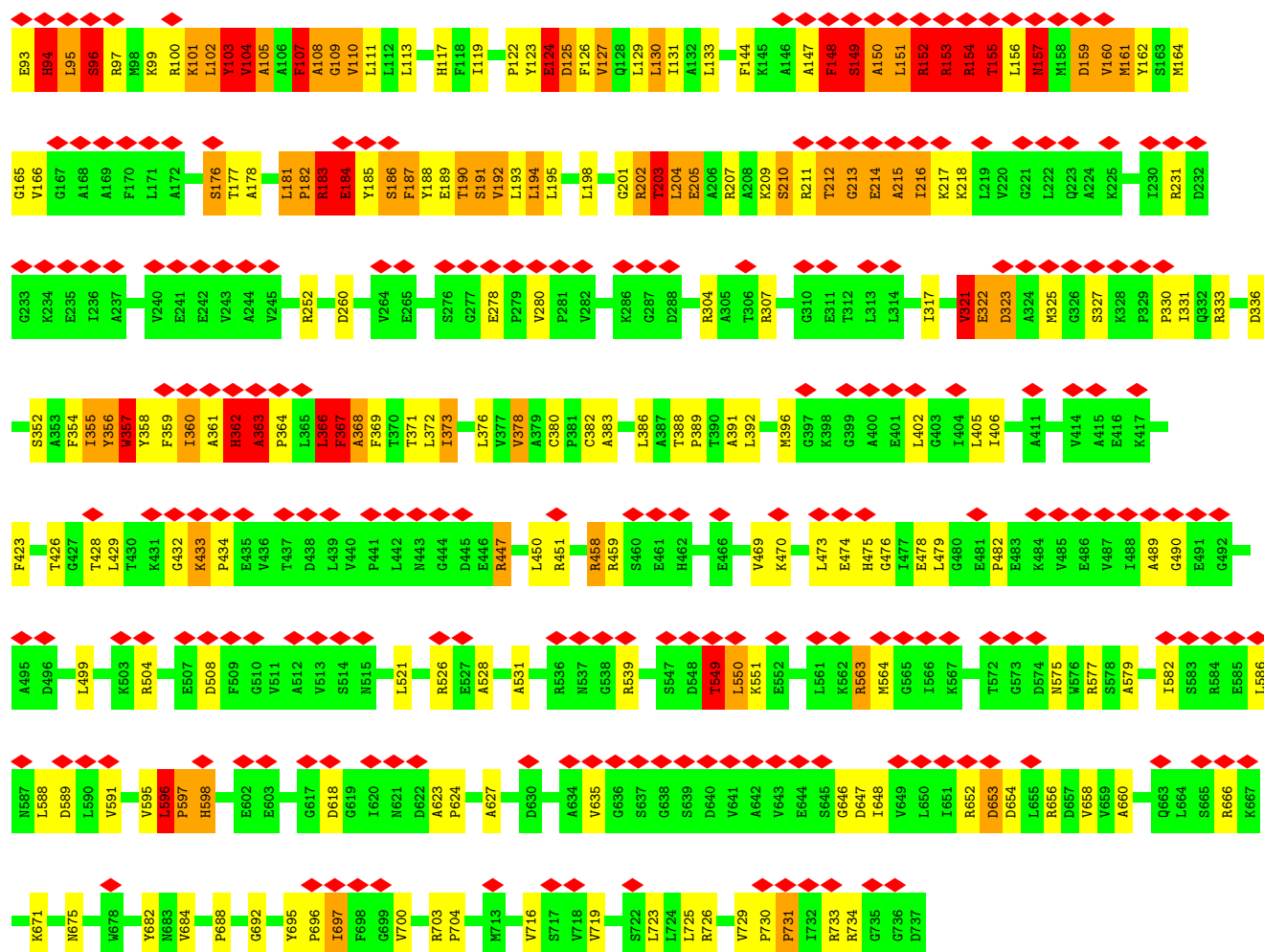
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: copper-exporting P-type ATPase A



• Molecule 1: copper-exporting P-type ATPase A





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	OTHER	Depositor
CTF correction method	each tube-crystal	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	199.593	Depositor
Minimum map value	-30.964	Depositor
Average map value	104.631	Depositor
Map value standard deviation	38.072	Depositor
Recommended contour level	130	Depositor
Map size (Å)	100, 102, 162	wwPDB
Map dimensions	50, 51, 81	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2, 2, 2	Depositor

5 Model quality

5.1 Standard geometry

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	0.91	30/4941 (0.6%)	1.27	20/6700 (0.3%)
1	B	0.91	30/4941 (0.6%)	1.27	20/6700 (0.3%)
All	All	0.91	60/9882 (0.6%)	1.27	40/13400 (0.3%)

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	30
1	B	0	30
All	All	0	60

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	ARG	NE-CZ	5.87	1.39	1.33
1	B	577	ARG	NE-CZ	5.86	1.39	1.33
1	B	451	ARG	NE-CZ	5.80	1.39	1.33
1	A	451	ARG	NE-CZ	5.80	1.39	1.33
1	A	211	ARG	NE-CZ	5.77	1.39	1.33
1	B	211	ARG	NE-CZ	5.76	1.39	1.33
1	A	703	ARG	NE-CZ	5.72	1.39	1.33
1	B	703	ARG	NE-CZ	5.71	1.39	1.33
1	B	526	ARG	NE-CZ	5.70	1.39	1.33
1	B	447	ARG	NE-CZ	5.67	1.39	1.33
1	A	526	ARG	NE-CZ	5.65	1.39	1.33
1	A	447	ARG	NE-CZ	5.65	1.39	1.33
1	A	97	ARG	NE-CZ	5.62	1.39	1.33
1	A	563	ARG	NE-CZ	5.61	1.39	1.33
1	B	563	ARG	NE-CZ	5.60	1.39	1.33
1	A	307	ARG	NE-CZ	5.57	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ARG	NE-CZ	5.57	1.39	1.33
1	B	333	ARG	NE-CZ	5.55	1.39	1.33
1	A	231	ARG	NE-CZ	5.53	1.39	1.33
1	B	97	ARG	NE-CZ	5.53	1.39	1.33
1	A	333	ARG	NE-CZ	5.53	1.39	1.33
1	B	304	ARG	NE-CZ	5.53	1.39	1.33
1	A	304	ARG	NE-CZ	5.52	1.39	1.33
1	B	504	ARG	NE-CZ	5.51	1.39	1.33
1	B	231	ARG	NE-CZ	5.51	1.39	1.33
1	B	733	ARG	NE-CZ	5.48	1.39	1.33
1	A	733	ARG	NE-CZ	5.44	1.39	1.33
1	A	504	ARG	NE-CZ	5.43	1.39	1.33
1	B	207	ARG	NE-CZ	5.41	1.39	1.33
1	A	207	ARG	NE-CZ	5.40	1.39	1.33
1	B	100	ARG	NE-CZ	5.38	1.39	1.33
1	A	100	ARG	NE-CZ	5.38	1.39	1.33
1	B	726	ARG	NE-CZ	5.37	1.39	1.33
1	B	666	ARG	NE-CZ	5.37	1.39	1.33
1	B	458	ARG	NE-CZ	5.35	1.39	1.33
1	A	726	ARG	NE-CZ	5.35	1.39	1.33
1	A	458	ARG	NE-CZ	5.33	1.39	1.33
1	A	734	ARG	NE-CZ	5.33	1.39	1.33
1	A	666	ARG	NE-CZ	5.33	1.39	1.33
1	B	734	ARG	NE-CZ	5.33	1.39	1.33
1	A	459	ARG	NE-CZ	5.30	1.38	1.33
1	A	539	ARG	NE-CZ	5.30	1.38	1.33
1	A	153	ARG	NE-CZ	5.28	1.38	1.33
1	B	539	ARG	NE-CZ	5.28	1.38	1.33
1	B	183	ARG	NE-CZ	5.25	1.38	1.33
1	A	183	ARG	NE-CZ	5.24	1.38	1.33
1	B	459	ARG	NE-CZ	5.24	1.38	1.33
1	B	252	ARG	NE-CZ	5.24	1.38	1.33
1	B	153	ARG	NE-CZ	5.22	1.38	1.33
1	A	154	ARG	NE-CZ	5.19	1.38	1.33
1	A	252	ARG	NE-CZ	5.17	1.38	1.33
1	B	154	ARG	NE-CZ	5.17	1.38	1.33
1	A	152	ARG	NE-CZ	5.13	1.38	1.33
1	A	202	ARG	NE-CZ	5.11	1.38	1.33
1	B	152	ARG	NE-CZ	5.10	1.38	1.33
1	A	656	ARG	NE-CZ	5.09	1.38	1.33
1	A	652	ARG	NE-CZ	5.07	1.38	1.33
1	B	652	ARG	NE-CZ	5.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	656	ARG	NE-CZ	5.06	1.38	1.33
1	B	202	ARG	NE-CZ	5.05	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	PHE	CA-CB-CG	8.43	122.23	113.80
1	A	187	PHE	CA-CB-CG	8.42	122.22	113.80
1	B	149	SER	O-C-N	7.24	132.22	122.59
1	A	149	SER	O-C-N	7.23	132.21	122.59
1	B	203	THR	O-C-N	6.75	131.57	122.59
1	A	203	THR	O-C-N	6.75	131.57	122.59
1	A	104	VAL	N-CA-CB	6.54	122.02	111.23
1	B	104	VAL	N-CA-CB	6.53	122.01	111.23
1	A	260	ASP	CA-CB-CG	6.44	119.04	112.60
1	B	260	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	155	THR	N-CA-CB	6.22	122.07	111.50
1	B	155	THR	N-CA-CB	6.20	122.05	111.50
1	B	96	SER	N-CA-CB	6.10	120.80	110.49
1	A	96	SER	N-CA-CB	6.08	120.77	110.49
1	B	321	VAL	O-C-N	6.01	130.08	122.57
1	A	321	VAL	O-C-N	5.99	130.05	122.57
1	B	618	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	618	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	356	TYR	O-C-N	5.86	129.17	122.25
1	B	356	TYR	O-C-N	5.85	129.16	122.25
1	B	598	HIS	N-CA-CB	5.79	120.27	110.49
1	A	598	HIS	N-CA-CB	5.78	120.26	110.49
1	B	125	ASP	CB-CA-C	5.64	120.81	110.10
1	A	125	ASP	CB-CA-C	5.62	120.77	110.10
1	A	357	TRP	CB-CA-C	5.61	121.58	110.42
1	B	357	TRP	CB-CA-C	5.60	121.56	110.42
1	A	149	SER	CA-C-O	-5.48	112.67	120.51
1	B	149	SER	CA-C-O	-5.47	112.69	120.51
1	B	94	HIS	CA-CB-CG	-5.35	108.45	113.80
1	A	94	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	215	ALA	O-C-N	5.33	125.51	120.71
1	B	215	ALA	O-C-N	5.32	125.50	120.71
1	B	589	ASP	CA-CB-CG	-5.21	107.39	112.60
1	B	192	VAL	CB-CA-C	5.20	118.54	111.88
1	A	589	ASP	CA-CB-CG	-5.20	107.40	112.60
1	A	203	THR	CA-C-O	-5.17	113.11	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	THR	CA-C-O	-5.17	113.11	120.51
1	A	192	VAL	CB-CA-C	5.16	118.48	111.88
1	A	183	ARG	O-C-N	5.01	128.35	122.34
1	B	183	ARG	O-C-N	5.00	128.34	122.34

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	LEU	Peptide
1	A	103	TYR	Peptide
1	A	107	PHE	Peptide
1	A	127	VAL	Peptide
1	A	152	ARG	Peptide
1	A	154	ARG	Peptide
1	A	182	PRO	Peptide
1	A	183	ARG	Peptide
1	A	184	GLU	Peptide
1	A	189	GLU	Peptide
1	A	190	THR	Peptide
1	A	212	THR	Peptide
1	A	213	GLY	Peptide
1	A	323	ASP	Peptide
1	A	355	ILE	Peptide
1	A	361	ALA	Peptide
1	A	362	HIS	Peptide
1	A	363	ALA	Peptide
1	A	433	LYS	Peptide
1	A	434	PRO	Peptide
1	A	549	THR	Peptide
1	A	595	VAL	Peptide
1	A	596	LEU	Peptide
1	A	597	PRO	Peptide
1	A	646	GLY	Peptide
1	A	647	ASP	Peptide
1	A	730	PRO	Peptide
1	A	731	PRO	Peptide
1	A	95	LEU	Peptide
1	A	96	SER	Peptide
1	B	102	LEU	Peptide
1	B	103	TYR	Peptide
1	B	107	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	127	VAL	Peptide
1	B	152	ARG	Peptide
1	B	154	ARG	Peptide
1	B	182	PRO	Peptide
1	B	183	ARG	Peptide
1	B	184	GLU	Peptide
1	B	189	GLU	Peptide
1	B	190	THR	Peptide
1	B	212	THR	Peptide
1	B	213	GLY	Peptide
1	B	323	ASP	Peptide
1	B	355	ILE	Peptide
1	B	361	ALA	Peptide
1	B	362	HIS	Peptide
1	B	363	ALA	Peptide
1	B	433	LYS	Peptide
1	B	434	PRO	Peptide
1	B	549	THR	Peptide
1	B	595	VAL	Peptide
1	B	596	LEU	Peptide
1	B	597	PRO	Peptide
1	B	646	GLY	Peptide
1	B	647	ASP	Peptide
1	B	730	PRO	Peptide
1	B	731	PRO	Peptide
1	B	95	LEU	Peptide
1	B	96	SER	Peptide

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	4867	0	5113	208	0
1	B	4867	0	5113	210	0
All	All	9734	0	10226	336	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 17.

All (336) 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:A:280:VAL:HG11	1:B:474:GLU:CD	1.21	1.52
1:A:458:ARG:NH1	1:B:473:LEU:HG	1.18	1.43
1:A:479:LEU:N	1:B:478:GLU:HA	1.39	1.35
1:A:458:ARG:HH12	1:B:473:LEU:CG	1.39	1.34
1:A:280:VAL:CG1	1:B:474:GLU:CD	2.01	1.29
1:A:458:ARG:NH1	1:B:473:LEU:CG	1.97	1.26
1:A:280:VAL:HG11	1:B:474:GLU:OE2	1.10	1.26
1:A:458:ARG:NH1	1:B:473:LEU:O	1.70	1.24
1:A:478:GLU:HA	1:B:479:LEU:N	1.50	1.20
1:A:280:VAL:CG1	1:B:474:GLU:OE1	1.95	1.14
1:A:478:GLU:CA	1:B:479:LEU:H	1.44	1.12
1:A:478:GLU:HB3	1:B:478:GLU:C	1.72	1.10
1:A:280:VAL:HG21	1:B:470:LYS:NZ	1.71	1.05
1:A:474:GLU:OE2	1:B:280:VAL:HG21	1.52	1.05
1:A:479:LEU:N	1:B:478:GLU:CA	2.20	1.04
1:A:473:LEU:HD11	1:B:469:VAL:CG1	1.89	1.03
1:A:479:LEU:H	1:B:478:GLU:HA	0.93	1.03
1:A:478:GLU:CA	1:B:479:LEU:N	2.02	1.01
1:A:478:GLU:CB	1:B:478:GLU:C	2.30	0.99
1:A:458:ARG:CZ	1:B:473:LEU:HG	1.93	0.99
1:A:280:VAL:HG21	1:B:470:LYS:HZ2	1.23	0.97
1:A:124:GLU:HA	1:A:125:ASP:C	1.90	0.96
1:A:473:LEU:CG	1:B:458:ARG:HH12	1.78	0.96
1:A:473:LEU:HG	1:B:458:ARG:NH1	1.81	0.96
1:A:280:VAL:CG1	1:B:474:GLU:OE2	2.04	0.95
1:A:473:LEU:HG	1:B:458:ARG:HH12	1.32	0.95
1:A:458:ARG:NH1	1:B:473:LEU:C	2.25	0.94
1:B:124:GLU:HA	1:B:125:ASP:C	1.90	0.92
1:A:447:ARG:NH2	1:B:482:PRO:HD3	1.88	0.86
1:A:402:LEU:HD13	1:A:660:ALA:HB1	1.59	0.85
1:A:458:ARG:HH12	1:B:473:LEU:CB	1.91	0.84
1:B:402:LEU:HD13	1:B:660:ALA:HB1	1.59	0.84
1:A:470:LYS:HZ2	1:B:280:VAL:HG21	1.41	0.83
1:A:470:LYS:NZ	1:B:280:VAL:HG21	1.93	0.83
1:A:280:VAL:HG11	1:B:474:GLU:OE1	1.67	0.82
1:A:474:GLU:OE2	1:B:280:VAL:CG2	2.17	0.82
1:A:458:ARG:HH12	1:B:473:LEU:HG	0.72	0.81
1:A:478:GLU:HA	1:B:479:LEU:H	0.68	0.81
1:A:478:GLU:HB3	1:B:478:GLU:HB3	1.61	0.80
1:A:473:LEU:CG	1:B:458:ARG:NH1	2.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HA	1:A:161:MET:C	2.06	0.78
1:A:362:HIS:HB3	1:A:363:ALA:HB2	1.66	0.78
1:B:362:HIS:HB3	1:B:363:ALA:HB2	1.66	0.78
1:B:160:VAL:HA	1:B:161:MET:C	2.06	0.77
1:A:458:ARG:NH1	1:B:473:LEU:CD1	2.48	0.76
1:A:473:LEU:HG	1:B:458:ARG:CZ	2.16	0.75
1:B:357:TRP:N	1:B:358:TYR:HA	2.03	0.73
1:A:469:VAL:HG13	1:B:473:LEU:HD11	1.69	0.73
1:A:473:LEU:HD11	1:B:469:VAL:HG13	1.69	0.73
1:A:478:GLU:C	1:B:478:GLU:HA	2.13	0.73
1:A:357:TRP:N	1:A:358:TYR:HA	2.03	0.72
1:A:478:GLU:HB3	1:B:478:GLU:CB	2.19	0.72
1:A:473:LEU:HG	1:B:458:ARG:NH2	2.05	0.72
1:A:478:GLU:C	1:B:478:GLU:CB	2.65	0.70
1:A:490:GLY:HA3	1:A:596:LEU:HD22	1.72	0.70
1:B:490:GLY:HA3	1:B:596:LEU:HD22	1.72	0.69
1:A:117:HIS:NE2	1:A:373:ILE:HG21	2.08	0.69
1:A:469:VAL:CG1	1:B:473:LEU:HD11	2.22	0.68
1:B:489:ALA:HB1	1:B:596:LEU:HD13	1.75	0.68
1:B:117:HIS:NE2	1:B:373:ILE:HG21	2.08	0.68
1:A:489:ALA:HB1	1:A:596:LEU:HD13	1.75	0.68
1:A:391:ALA:HB2	1:A:723:LEU:HD13	1.76	0.67
1:A:473:LEU:CD1	1:B:458:ARG:NH1	2.57	0.67
1:A:473:LEU:HD12	1:B:458:ARG:NH1	2.10	0.66
1:A:151:LEU:O	1:A:152:ARG:C	2.39	0.66
1:A:470:LYS:NZ	1:B:280:VAL:CG2	2.58	0.66
1:A:482:PRO:HD3	1:B:447:ARG:NH2	2.11	0.66
1:B:391:ALA:HB2	1:B:723:LEU:HD13	1.76	0.66
1:B:151:LEU:O	1:B:152:ARG:C	2.39	0.65
1:B:166:VAL:HG11	1:B:203:THR:HG21	1.78	0.65
1:A:280:VAL:HG13	1:B:474:GLU:OE1	1.91	0.65
1:A:479:LEU:N	1:B:478:GLU:CB	2.52	0.65
1:A:280:VAL:CG2	1:B:470:LYS:NZ	2.56	0.65
1:A:166:VAL:HG11	1:A:203:THR:HG21	1.78	0.64
1:A:473:LEU:HG	1:B:458:ARG:HH22	1.62	0.64
1:A:478:GLU:HB3	1:B:478:GLU:CA	2.27	0.64
1:A:124:GLU:CA	1:A:125:ASP:C	2.68	0.63
1:B:215:ALA:C	1:B:217:LYS:H	2.06	0.63
1:A:478:GLU:CB	1:B:478:GLU:HB3	2.29	0.62
1:A:124:GLU:HA	1:A:126:PHE:N	2.14	0.62
1:B:124:GLU:HA	1:B:126:PHE:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:O	1:A:148:PHE:C	2.43	0.62
1:A:215:ALA:C	1:A:217:LYS:H	2.06	0.62
1:A:482:PRO:HD3	1:B:447:ARG:HH21	1.64	0.62
1:A:356:TYR:O	1:A:357:TRP:C	2.42	0.62
1:B:356:TYR:O	1:B:357:TRP:C	2.42	0.62
1:A:181:LEU:HD13	1:A:182:PRO:HD2	1.82	0.61
1:B:181:LEU:HD13	1:B:182:PRO:HD2	1.82	0.61
1:A:564:MET:HE1	1:A:658:VAL:HG12	1.83	0.61
1:A:478:GLU:C	1:B:478:GLU:CA	2.70	0.61
1:B:564:MET:HE1	1:B:658:VAL:HG12	1.83	0.61
1:A:154:ARG:HA	1:A:155:THR:O	2.01	0.61
1:B:154:ARG:HA	1:B:155:THR:O	2.01	0.60
1:B:147:ALA:O	1:B:148:PHE:C	2.43	0.60
1:A:478:GLU:C	1:B:478:GLU:HB3	2.25	0.60
1:B:149:SER:O	1:B:150:ALA:C	2.45	0.60
1:A:476:GLY:HA2	1:B:458:ARG:HD3	1.83	0.59
1:A:473:LEU:HD11	1:B:469:VAL:HG11	1.81	0.59
1:A:186:SER:H	1:A:187:PHE:CA	2.15	0.59
1:A:149:SER:O	1:A:150:ALA:C	2.45	0.58
1:B:550:LEU:HD13	1:B:586:LEU:HD11	1.85	0.58
1:B:215:ALA:C	1:B:217:LYS:N	2.62	0.58
1:A:528:ALA:HB1	1:A:582:ILE:HG13	1.86	0.58
1:A:363:ALA:HB3	1:A:364:PRO:HD3	1.86	0.58
1:A:458:ARG:NH1	1:B:473:LEU:CA	2.67	0.58
1:A:107:PHE:C	1:A:109:GLY:H	2.11	0.58
1:B:186:SER:H	1:B:187:PHE:CA	2.15	0.58
1:A:321:VAL:HG22	1:A:627:ALA:CB	2.34	0.57
1:B:321:VAL:HG22	1:B:627:ALA:CB	2.34	0.57
1:A:215:ALA:C	1:A:217:LYS:N	2.62	0.57
1:B:129:LEU:HD23	1:B:129:LEU:C	2.29	0.57
1:A:550:LEU:HD13	1:A:586:LEU:HD11	1.85	0.57
1:A:129:LEU:C	1:A:129:LEU:HD23	2.29	0.57
1:A:203:THR:O	1:A:205:GLU:N	2.37	0.57
1:B:203:THR:O	1:B:205:GLU:N	2.37	0.57
1:B:107:PHE:C	1:B:109:GLY:N	2.63	0.57
1:B:107:PHE:C	1:B:109:GLY:H	2.11	0.57
1:A:203:THR:O	1:A:204:LEU:C	2.47	0.56
1:B:203:THR:O	1:B:204:LEU:C	2.47	0.56
1:B:357:TRP:H	1:B:357:TRP:CD1	2.24	0.56
1:B:363:ALA:HB3	1:B:364:PRO:HD3	1.86	0.56
1:B:528:ALA:HB1	1:B:582:ILE:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ARG:HH12	1:B:473:LEU:CA	2.18	0.56
1:B:187:PHE:CE2	1:B:188:TYR:HB2	2.41	0.56
1:B:392:LEU:O	1:B:396:MET:N	2.39	0.55
1:B:124:GLU:CA	1:B:125:ASP:C	2.68	0.55
1:A:447:ARG:HH21	1:B:482:PRO:HD3	1.69	0.55
1:A:187:PHE:CE2	1:A:188:TYR:HB2	2.41	0.55
1:A:392:LEU:O	1:A:396:MET:N	2.39	0.55
1:A:357:TRP:H	1:A:357:TRP:CD1	2.24	0.55
1:A:458:ARG:CZ	1:B:473:LEU:O	2.48	0.55
1:A:458:ARG:HH12	1:B:473:LEU:C	2.03	0.55
1:B:156:LEU:O	1:B:157:ASN:C	2.50	0.55
1:A:478:GLU:CA	1:B:478:GLU:C	2.74	0.55
1:B:186:SER:N	1:B:187:PHE:HA	2.22	0.55
1:A:107:PHE:C	1:A:109:GLY:N	2.63	0.55
1:A:684:VAL:O	1:A:688:PRO:HD2	2.07	0.55
1:A:186:SER:N	1:A:187:PHE:HA	2.22	0.54
1:A:423:PHE:CD1	1:A:428:THR:HG21	2.43	0.54
1:B:103:TYR:O	1:B:104:VAL:HG12	2.07	0.54
1:A:103:TYR:O	1:A:104:VAL:HG12	2.07	0.54
1:A:186:SER:H	1:A:187:PHE:HA	1.73	0.54
1:B:684:VAL:O	1:B:688:PRO:HD2	2.07	0.54
1:A:156:LEU:O	1:A:157:ASN:C	2.50	0.54
1:A:186:SER:CB	1:A:187:PHE:HA	2.38	0.54
1:B:423:PHE:CD1	1:B:428:THR:HG21	2.43	0.53
1:B:194:LEU:HD11	1:B:704:PRO:HB2	1.91	0.53
1:A:194:LEU:HD11	1:A:704:PRO:HB2	1.91	0.53
1:A:280:VAL:HG21	1:B:470:LYS:HZ1	1.70	0.53
1:A:317:ILE:O	1:A:321:VAL:HG23	2.09	0.53
1:B:186:SER:H	1:B:187:PHE:HA	1.73	0.53
1:B:428:THR:HA	1:B:635:VAL:HG11	1.91	0.53
1:B:317:ILE:O	1:B:321:VAL:HG23	2.09	0.52
1:B:550:LEU:HD11	1:B:582:ILE:HG23	1.92	0.52
1:B:366:LEU:O	1:B:367:PHE:C	2.52	0.52
1:A:550:LEU:HD11	1:A:582:ILE:HG23	1.92	0.52
1:B:186:SER:CB	1:B:187:PHE:HA	2.38	0.52
1:A:366:LEU:O	1:A:367:PHE:C	2.52	0.51
1:A:376:LEU:O	1:A:380:CYS:N	2.40	0.51
1:B:635:VAL:HG13	1:B:653:ASP:OD1	2.10	0.51
1:A:428:THR:HA	1:A:635:VAL:HG11	1.90	0.51
1:A:280:VAL:HG12	1:B:474:GLU:OE1	2.02	0.51
1:A:321:VAL:O	1:A:322:GLU:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:SER:N	1:B:187:PHE:CA	2.74	0.51
1:B:376:LEU:O	1:B:380:CYS:N	2.40	0.51
1:B:321:VAL:O	1:B:322:GLU:C	2.53	0.51
1:A:280:VAL:HG12	1:B:474:GLU:CD	2.23	0.51
1:A:149:SER:O	1:A:151:LEU:N	2.44	0.51
1:B:653:ASP:O	1:B:654:ASP:C	2.54	0.51
1:B:148:PHE:O	1:B:149:SER:HB3	2.11	0.51
1:A:376:LEU:C	1:A:378:VAL:N	2.68	0.50
1:B:149:SER:O	1:B:151:LEU:N	2.44	0.50
1:A:635:VAL:HG13	1:A:653:ASP:OD1	2.10	0.50
1:A:186:SER:N	1:A:187:PHE:CA	2.74	0.50
1:A:148:PHE:O	1:A:149:SER:HB3	2.11	0.50
1:B:104:VAL:O	1:B:104:VAL:HG13	2.12	0.50
1:A:653:ASP:O	1:A:654:ASP:C	2.54	0.50
1:A:152:ARG:N	1:A:153:ARG:HA	2.27	0.49
1:A:95:LEU:CB	1:A:96:SER:HB2	2.42	0.49
1:A:104:VAL:O	1:A:104:VAL:HG13	2.12	0.49
1:A:478:GLU:CA	1:B:478:GLU:CA	2.91	0.49
1:B:95:LEU:CB	1:B:96:SER:HB2	2.42	0.49
1:B:321:VAL:HG22	1:B:627:ALA:HB1	1.95	0.48
1:A:549:THR:C	1:A:550:LEU:HG	2.38	0.48
1:B:376:LEU:C	1:B:378:VAL:N	2.68	0.48
1:A:479:LEU:O	1:B:478:GLU:N	2.40	0.48
1:B:549:THR:C	1:B:550:LEU:HG	2.38	0.48
1:A:321:VAL:HG22	1:A:627:ALA:HB1	1.95	0.48
1:A:692:GLY:O	1:A:696:PRO:HD2	2.14	0.48
1:B:104:VAL:O	1:B:105:ALA:HB3	2.13	0.48
1:B:152:ARG:N	1:B:153:ARG:HA	2.27	0.47
1:A:579:ALA:HB1	1:A:591:VAL:CG2	2.44	0.47
1:B:186:SER:H	1:B:187:PHE:CB	2.27	0.47
1:B:429:LEU:O	1:B:550:LEU:C	2.57	0.47
1:B:579:ALA:HB1	1:B:591:VAL:CG2	2.44	0.47
1:A:186:SER:H	1:A:187:PHE:CB	2.27	0.47
1:B:117:HIS:CE1	1:B:373:ILE:HG12	2.50	0.47
1:A:429:LEU:O	1:A:550:LEU:C	2.57	0.47
1:A:104:VAL:O	1:A:105:ALA:HB3	2.13	0.47
1:B:204:LEU:O	1:B:205:GLU:C	2.58	0.47
1:A:117:HIS:CE1	1:A:373:ILE:HG12	2.50	0.47
1:B:489:ALA:HB1	1:B:596:LEU:CD1	2.43	0.47
1:B:692:GLY:O	1:B:696:PRO:HD2	2.14	0.47
1:A:482:PRO:HG3	1:B:476:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:TYR:C	1:B:697:ILE:H	2.22	0.46
1:A:321:VAL:O	1:A:323:ASP:N	2.48	0.46
1:B:321:VAL:O	1:B:323:ASP:N	2.48	0.46
1:A:368:ALA:O	1:A:369:PHE:CB	2.64	0.46
1:A:388:THR:N	1:A:389:PRO:HD2	2.31	0.46
1:B:105:ALA:O	1:B:107:PHE:O	2.34	0.46
1:B:635:VAL:HG13	1:B:653:ASP:CG	2.41	0.46
1:A:93:GLU:CB	1:A:150:ALA:HB2	2.47	0.45
1:A:94:HIS:O	1:A:95:LEU:C	2.58	0.45
1:A:104:VAL:O	1:A:105:ALA:CB	2.64	0.45
1:A:123:TYR:O	1:A:124:GLU:C	2.59	0.45
1:A:357:TRP:CB	1:A:358:TYR:HA	2.45	0.45
1:A:695:TYR:C	1:A:697:ILE:H	2.22	0.45
1:B:104:VAL:O	1:B:105:ALA:CB	2.64	0.45
1:A:101:LYS:O	1:A:103:TYR:N	2.49	0.45
1:A:280:VAL:HG21	1:B:470:LYS:CE	2.43	0.45
1:B:94:HIS:O	1:B:95:LEU:C	2.58	0.45
1:A:105:ALA:O	1:A:107:PHE:O	2.34	0.45
1:A:458:ARG:NH1	1:B:473:LEU:HD12	2.30	0.45
1:A:405:LEU:O	1:A:648:ILE:HG23	2.17	0.45
1:B:101:LYS:O	1:B:103:TYR:N	2.49	0.45
1:B:405:LEU:O	1:B:648:ILE:HG23	2.17	0.45
1:A:204:LEU:O	1:A:205:GLU:C	2.58	0.45
1:A:489:ALA:HB1	1:A:596:LEU:CD1	2.43	0.45
1:B:388:THR:N	1:B:389:PRO:HD2	2.31	0.45
1:B:95:LEU:HB3	1:B:96:SER:HB2	1.99	0.45
1:B:123:TYR:O	1:B:124:GLU:C	2.59	0.45
1:A:96:SER:HB3	1:A:99:LYS:HB2	1.98	0.45
1:B:117:HIS:CD2	1:B:191:SER:HA	2.52	0.44
1:B:623:ALA:N	1:B:624:PRO:CD	2.80	0.44
1:B:684:VAL:O	1:B:688:PRO:CD	2.66	0.44
1:B:176:SER:O	1:B:177:THR:C	2.60	0.44
1:B:579:ALA:HB1	1:B:591:VAL:HG21	2.00	0.44
1:A:357:TRP:N	1:A:357:TRP:CD1	2.86	0.44
1:B:93:GLU:CB	1:B:150:ALA:HB2	2.47	0.44
1:A:130:LEU:O	1:A:131:ILE:C	2.61	0.44
1:A:623:ALA:N	1:A:624:PRO:CD	2.80	0.44
1:A:635:VAL:HG13	1:A:653:ASP:CG	2.41	0.44
1:B:130:LEU:O	1:B:131:ILE:C	2.61	0.44
1:A:117:HIS:CD2	1:A:191:SER:HA	2.53	0.44
1:A:181:LEU:HD11	1:A:187:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD11	1:B:187:PHE:CE2	2.53	0.44
1:B:201:GLY:O	1:B:202:ARG:C	2.61	0.44
1:A:144:PHE:CD2	1:A:144:PHE:C	2.96	0.44
1:B:113:LEU:HD21	1:B:376:LEU:HD12	2.00	0.44
1:B:144:PHE:CD2	1:B:144:PHE:C	2.96	0.44
1:A:108:ALA:O	1:A:109:GLY:C	2.61	0.44
1:A:684:VAL:O	1:A:688:PRO:CD	2.66	0.44
1:A:113:LEU:HD21	1:A:376:LEU:HD12	2.00	0.43
1:A:164:MET:O	1:A:165:GLY:C	2.61	0.43
1:B:368:ALA:O	1:B:369:PHE:CB	2.64	0.43
1:A:579:ALA:HB1	1:A:591:VAL:HG21	2.00	0.43
1:A:352:SER:O	1:A:356:TYR:CB	2.66	0.43
1:A:426:THR:HG22	1:A:426:THR:O	2.19	0.43
1:B:388:THR:O	1:B:391:ALA:HB3	2.19	0.43
1:A:95:LEU:HB3	1:A:96:SER:HB2	1.99	0.43
1:A:176:SER:O	1:A:177:THR:C	2.60	0.43
1:A:470:LYS:HZ1	1:B:280:VAL:CG2	2.30	0.43
1:B:108:ALA:O	1:B:109:GLY:C	2.61	0.43
1:B:352:SER:O	1:B:356:TYR:CB	2.67	0.43
1:B:356:TYR:C	1:B:358:TYR:CA	2.92	0.43
1:A:117:HIS:CE1	1:A:373:ILE:HG21	2.53	0.43
1:B:96:SER:HB3	1:B:99:LYS:HB2	1.99	0.43
1:B:164:MET:O	1:B:165:GLY:C	2.61	0.43
1:A:201:GLY:O	1:A:202:ARG:C	2.61	0.42
1:A:356:TYR:C	1:A:358:TYR:CA	2.92	0.42
1:A:729:VAL:O	1:A:731:PRO:CD	2.67	0.42
1:B:95:LEU:HB2	1:B:96:SER:HB2	2.01	0.42
1:B:357:TRP:N	1:B:357:TRP:CD1	2.86	0.42
1:A:95:LEU:CB	1:A:96:SER:CB	2.97	0.42
1:A:478:GLU:CA	1:B:478:GLU:HA	2.49	0.42
1:A:478:GLU:C	1:B:478:GLU:CG	2.90	0.42
1:A:269:TYR:CE1	1:B:475:HIS:HD2	2.29	0.42
1:A:411:ALA:C	1:A:413:GLU:N	2.76	0.42
1:B:729:VAL:O	1:B:731:PRO:CD	2.67	0.42
1:A:108:ALA:O	1:A:111:LEU:N	2.52	0.42
1:A:388:THR:O	1:A:391:ALA:HB3	2.19	0.42
1:B:190:THR:O	1:B:193:LEU:N	2.53	0.42
1:A:531:ALA:O	1:A:575:ASN:ND2	2.53	0.42
1:B:108:ALA:O	1:B:111:LEU:N	2.52	0.42
1:A:129:LEU:HD23	1:A:130:LEU:N	2.35	0.42
1:A:151:LEU:C	1:A:153:ARG:HA	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:HD23	1:B:130:LEU:N	2.35	0.42
1:B:357:TRP:N	1:B:358:TYR:CA	2.79	0.42
1:B:426:THR:O	1:B:426:THR:HG22	2.19	0.42
1:A:95:LEU:HB2	1:A:96:SER:HB2	2.01	0.42
1:A:190:THR:O	1:A:193:LEU:N	2.53	0.42
1:A:371:THR:O	1:A:372:LEU:C	2.63	0.42
1:A:481:GLU:HG2	1:B:447:ARG:NH1	2.35	0.42
1:B:95:LEU:CB	1:B:96:SER:CB	2.97	0.42
1:B:354:PHE:O	1:B:355:ILE:C	2.63	0.42
1:B:382:CYS:O	1:B:383:ALA:HB3	2.20	0.42
1:A:382:CYS:O	1:A:383:ALA:HB3	2.20	0.41
1:A:458:ARG:NH2	1:B:473:LEU:HG	2.29	0.41
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.97	0.41
1:A:183:ARG:O	1:A:184:GLU:O	2.38	0.41
1:B:117:HIS:CE1	1:B:373:ILE:HG21	2.53	0.41
1:B:154:ARG:HA	1:B:155:THR:C	2.44	0.41
1:B:357:TRP:CB	1:B:358:TYR:HA	2.44	0.41
1:B:362:HIS:HA	1:B:363:ALA:HA	1.80	0.41
1:A:154:ARG:HA	1:A:155:THR:C	2.44	0.41
1:A:478:GLU:C	1:B:478:GLU:HG2	2.31	0.41
1:B:528:ALA:HB1	1:B:582:ILE:CG1	2.50	0.41
1:B:151:LEU:C	1:B:153:ARG:HA	2.45	0.41
1:B:160:VAL:HG13	1:B:161:MET:O	2.21	0.41
1:B:209:LYS:O	1:B:210:SER:C	2.64	0.41
1:A:113:LEU:HD11	1:A:376:LEU:HB2	2.03	0.41
1:A:160:VAL:HG13	1:A:161:MET:O	2.21	0.41
1:A:213:GLY:O	1:A:214:GLU:CB	2.69	0.41
1:A:357:TRP:N	1:A:358:TYR:CA	2.79	0.41
1:B:183:ARG:O	1:B:184:GLU:O	2.38	0.41
1:B:531:ALA:O	1:B:575:ASN:ND2	2.53	0.41
1:A:93:GLU:HB2	1:A:150:ALA:HB2	2.03	0.41
1:A:113:LEU:HD21	1:A:376:LEU:HB2	2.03	0.41
1:A:354:PHE:O	1:A:355:ILE:C	2.63	0.41
1:A:470:LYS:CE	1:B:280:VAL:HG21	2.51	0.41
1:B:113:LEU:HD11	1:B:376:LEU:HB2	2.03	0.41
1:B:213:GLY:O	1:B:214:GLU:CB	2.69	0.41
1:A:108:ALA:C	1:A:110:VAL:N	2.79	0.40
1:A:671:LYS:CE	1:A:725:LEU:O	2.69	0.40
1:A:729:VAL:O	1:A:731:PRO:HD3	2.21	0.40
1:B:371:THR:O	1:B:372:LEU:C	2.63	0.40
1:B:671:LYS:CE	1:B:725:LEU:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:VAL:O	1:B:731:PRO:HD3	2.21	0.40
1:A:204:LEU:C	1:A:206:ALA:N	2.80	0.40
1:B:108:ALA:C	1:B:110:VAL:N	2.79	0.40
1:B:113:LEU:HD21	1:B:376:LEU:HB2	2.03	0.40
1:B:575:ASN:OD1	1:B:575:ASN:C	2.65	0.40
1:B:635:VAL:HG22	1:B:653:ASP:OD1	2.22	0.40
1:A:130:LEU:HD23	1:A:130:LEU:HA	2.00	0.40
1:A:321:VAL:O	1:A:323:ASP:HB2	2.22	0.40
1:B:376:LEU:C	1:B:378:VAL:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	643/645 (100%)	518 (81%)	70 (11%)	55 (9%)	0	9
1	B	643/645 (100%)	518 (81%)	70 (11%)	55 (9%)	0	9
All	All	1286/1290 (100%)	1036 (81%)	140 (11%)	110 (9%)	1	9

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	101	LYS
1	A	103	TYR
1	A	104	VAL
1	A	105	ALA
1	A	107	PHE
1	A	127	VAL
1	A	130	LEU
1	A	148	PHE

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Mol	Chain	Res	Type
1	A	150	ALA
1	A	151	LEU
1	A	152	ARG
1	A	176	SER
1	A	178	ALA
1	A	185	TYR
1	A	191	SER
1	A	203	THR
1	A	204	LEU
1	A	214	GLU
1	A	322	GLU
1	A	363	ALA
1	A	433	LYS
1	A	550	LEU
1	A	598	HIS
1	A	653	ASP
1	B	96	SER
1	B	101	LYS
1	B	103	TYR
1	B	104	VAL
1	B	105	ALA
1	B	107	PHE
1	B	127	VAL
1	B	130	LEU
1	B	148	PHE
1	B	150	ALA
1	B	151	LEU
1	B	152	ARG
1	B	176	SER
1	B	178	ALA
1	B	185	TYR
1	B	191	SER
1	B	203	THR
1	B	204	LEU
1	B	214	GLU
1	B	322	GLU
1	B	363	ALA
1	B	433	LYS
1	B	550	LEU
1	B	598	HIS
1	B	653	ASP
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	109	GLY
1	A	119	ILE
1	A	124	GLU
1	A	149	SER
1	A	184	GLU
1	A	216	ILE
1	A	357	TRP
1	A	362	HIS
1	A	368	ALA
1	A	432	GLY
1	A	551	LYS
1	B	102	LEU
1	B	109	GLY
1	B	119	ILE
1	B	124	GLU
1	B	149	SER
1	B	184	GLU
1	B	216	ILE
1	B	357	TRP
1	B	362	HIS
1	B	368	ALA
1	B	432	GLY
1	B	551	LYS
1	A	155	THR
1	A	160	VAL
1	A	321	VAL
1	A	325	MET
1	A	597	PRO
1	B	155	THR
1	B	160	VAL
1	B	321	VAL
1	B	325	MET
1	B	597	PRO
1	A	108	ALA
1	A	122	PRO
1	A	157	ASN
1	A	205	GLU
1	A	210	SER
1	A	360	ILE
1	A	367	PHE
1	A	549	THR
1	B	108	ALA

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Mol	Chain	Res	Type
1	B	122	PRO
1	B	157	ASN
1	B	205	GLU
1	B	210	SER
1	B	360	ILE
1	B	367	PHE
1	B	549	THR
1	A	359	PHE
1	A	366	LEU
1	B	359	PHE
1	B	366	LEU
1	A	159	ASP
1	A	327	SER
1	B	159	ASP
1	B	327	SER
1	A	330	PRO
1	B	330	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	515/515 (100%)	468 (91%)	47 (9%)	9	27
1	B	515/515 (100%)	468 (91%)	47 (9%)	9	27
All	All	1030/1030 (100%)	936 (91%)	94 (9%)	11	27

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	104	VAL
1	A	110	VAL
1	A	124	GLU
1	A	133	LEU
1	A	148	PHE

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Mol	Chain	Res	Type
1	A	152	ARG
1	A	153	ARG
1	A	155	THR
1	A	157	ASN
1	A	159	ASP
1	A	161	MET
1	A	162	TYR
1	A	181	LEU
1	A	183	ARG
1	A	186	SER
1	A	192	VAL
1	A	194	LEU
1	A	195	LEU
1	A	198	LEU
1	A	212	THR
1	A	216	ILE
1	A	218	LYS
1	A	278	GLU
1	A	331	ILE
1	A	336	ASP
1	A	357	TRP
1	A	360	ILE
1	A	366	LEU
1	A	367	PHE
1	A	373	ILE
1	A	378	VAL
1	A	386	LEU
1	A	406	ILE
1	A	450	LEU
1	A	499	LEU
1	A	508	ASP
1	A	521	LEU
1	A	563	ARG
1	A	588	LEU
1	A	596	LEU
1	A	675	ASN
1	A	682	TYR
1	A	697	ILE
1	A	700	VAL
1	A	716	VAL
1	A	719	VAL
1	B	94	HIS

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Mol	Chain	Res	Type
1	B	104	VAL
1	B	110	VAL
1	B	124	GLU
1	B	133	LEU
1	B	148	PHE
1	B	152	ARG
1	B	153	ARG
1	B	155	THR
1	B	157	ASN
1	B	159	ASP
1	B	161	MET
1	B	162	TYR
1	B	181	LEU
1	B	183	ARG
1	B	186	SER
1	B	192	VAL
1	B	194	LEU
1	B	195	LEU
1	B	198	LEU
1	B	212	THR
1	B	216	ILE
1	B	218	LYS
1	B	278	GLU
1	B	331	ILE
1	B	336	ASP
1	B	357	TRP
1	B	360	ILE
1	B	366	LEU
1	B	367	PHE
1	B	373	ILE
1	B	378	VAL
1	B	386	LEU
1	B	406	ILE
1	B	450	LEU
1	B	499	LEU
1	B	508	ASP
1	B	521	LEU
1	B	563	ARG
1	B	588	LEU
1	B	596	LEU
1	B	675	ASN
1	B	682	TYR

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Mol	Chain	Res	Type
1	B	697	ILE
1	B	700	VAL
1	B	716	VAL
1	B	719	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	462	HIS
1	A	628	GLN
1	B	223	GLN
1	B	462	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 ⓘ

There are no ligands in this entry.

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-5271. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

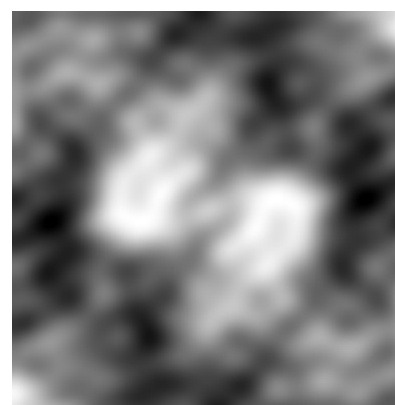
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

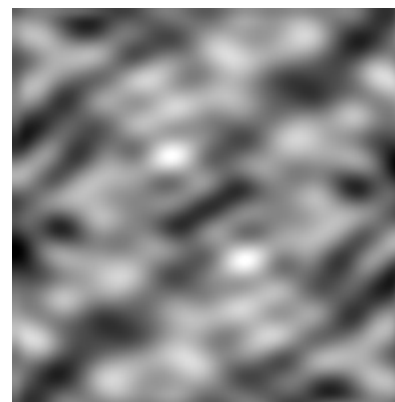
6.2.1 Primary map



X Index: 25



Y Index: 25



Z Index: 40

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

6.3 Largest variance slices [i](#)

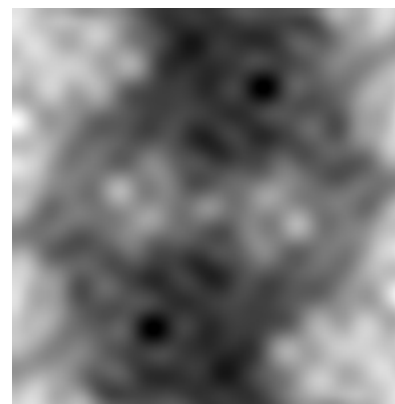
6.3.1 Primary map



X Index: 49



Y Index: 9

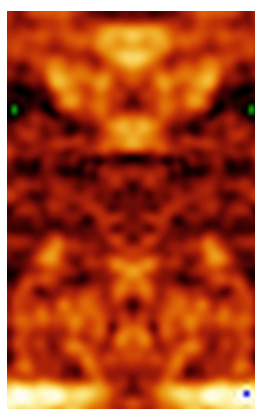


Z Index: 3

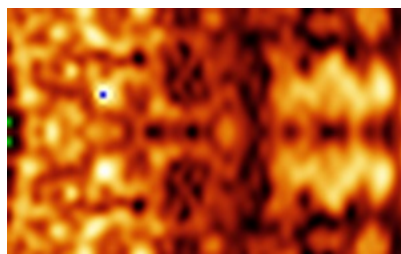
The images above show the largest variance slices of the map in three orthogonal directions.

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

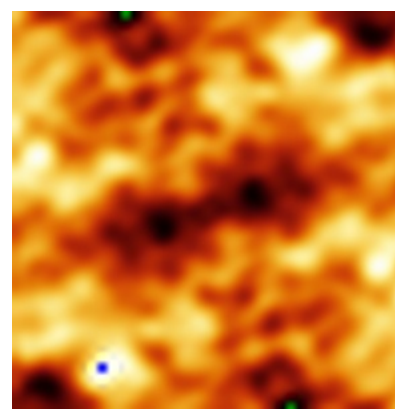
6.4.1 Primary map



X



Y

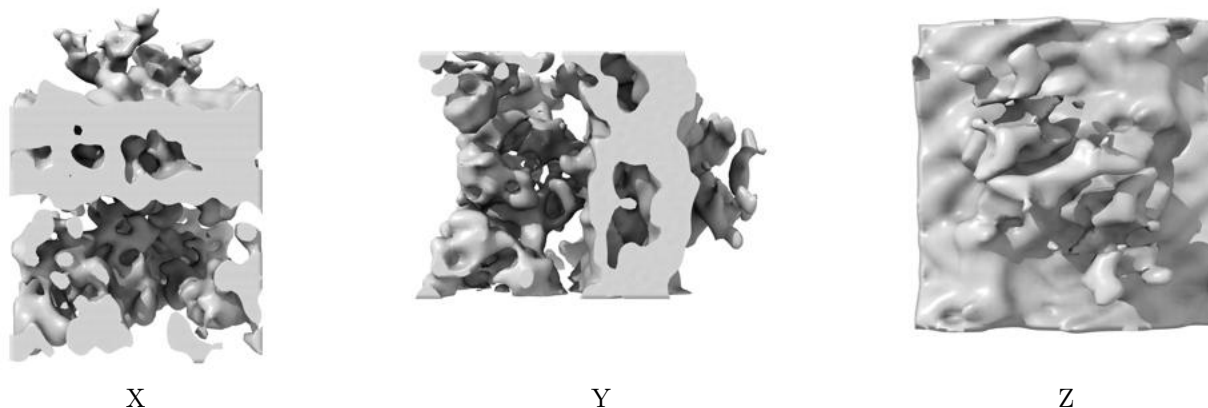


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 130.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

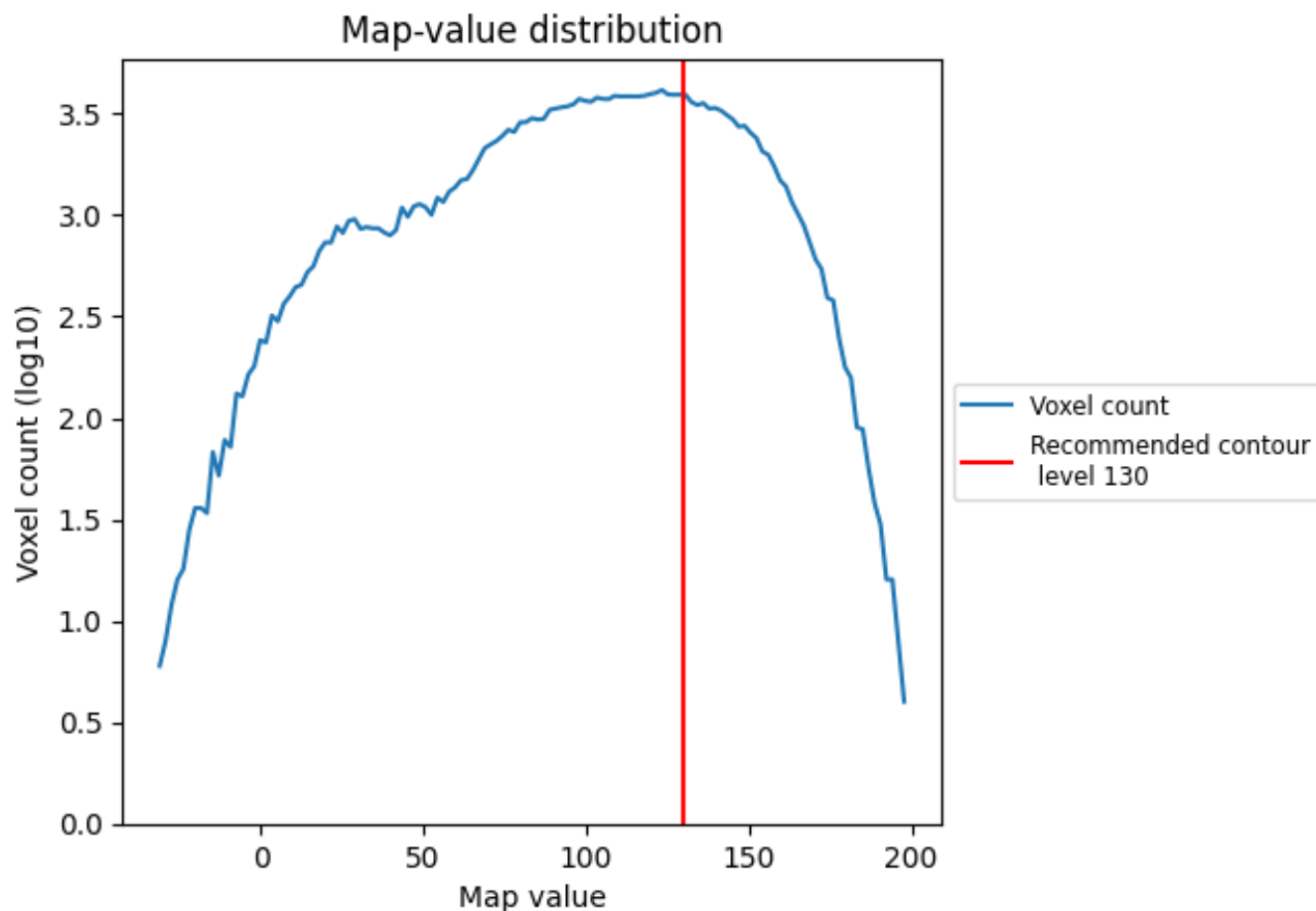
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

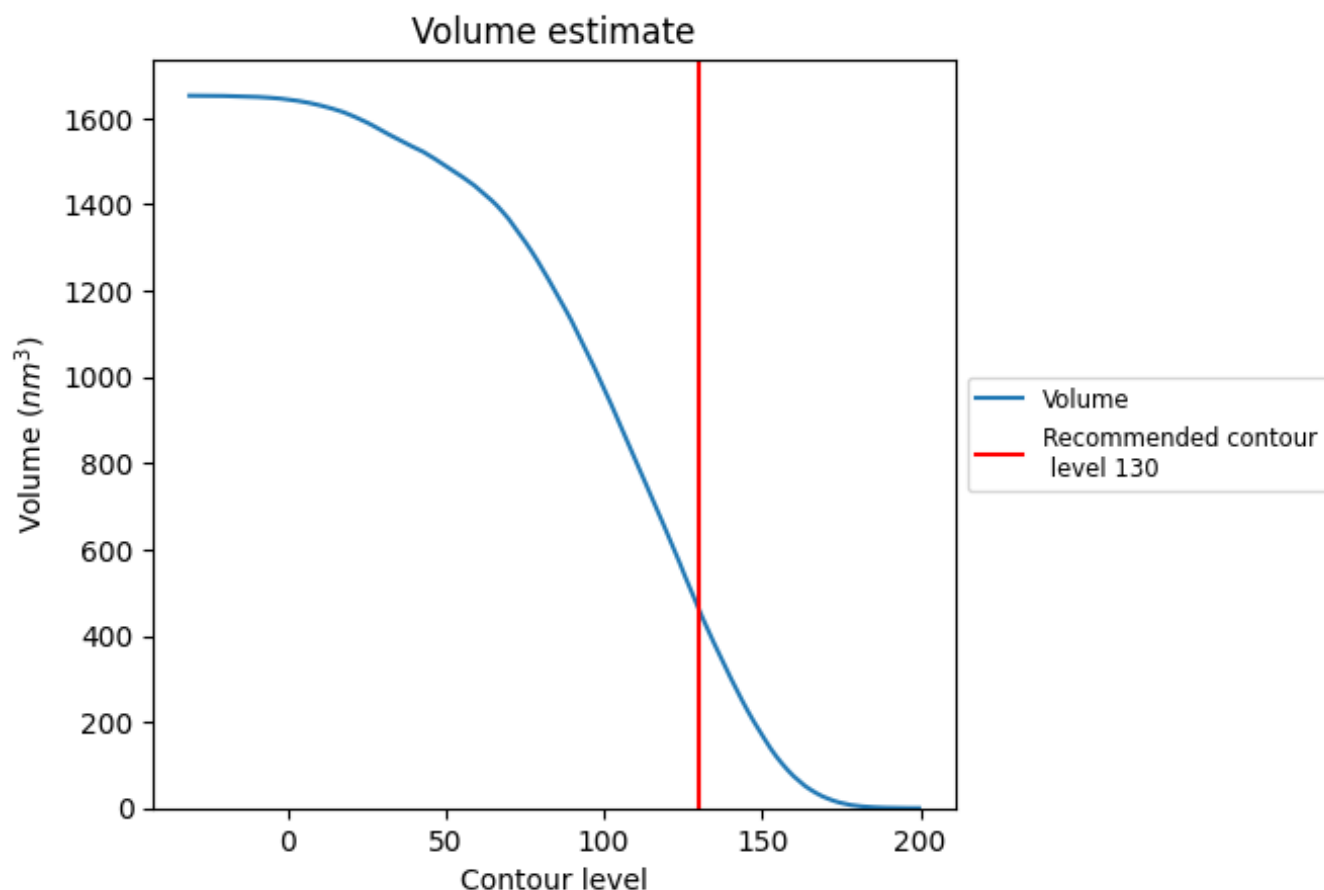
This section contains the results of statistical analysis of the map.

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 462 nm³; this corresponds to an approximate mass of 418 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

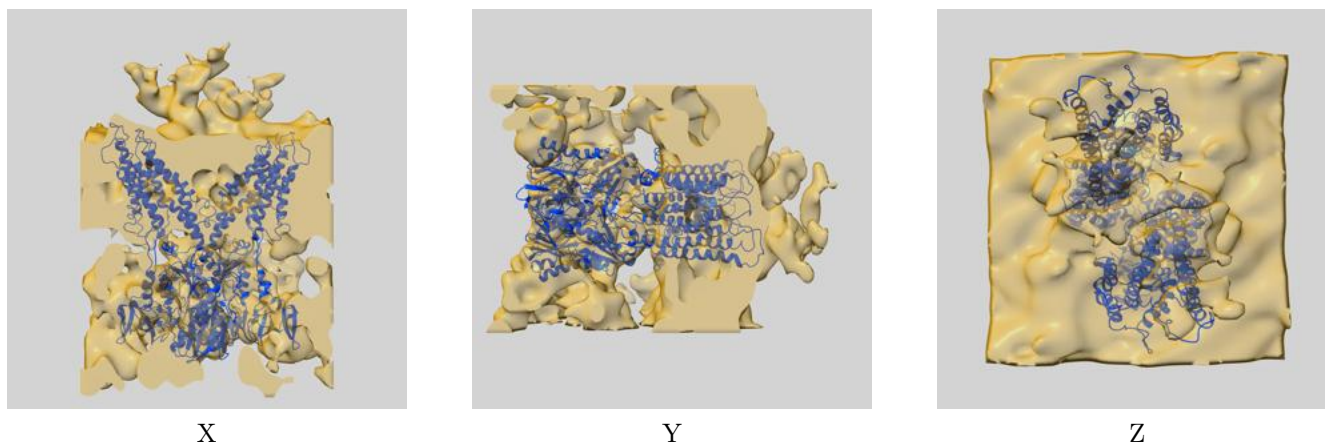
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

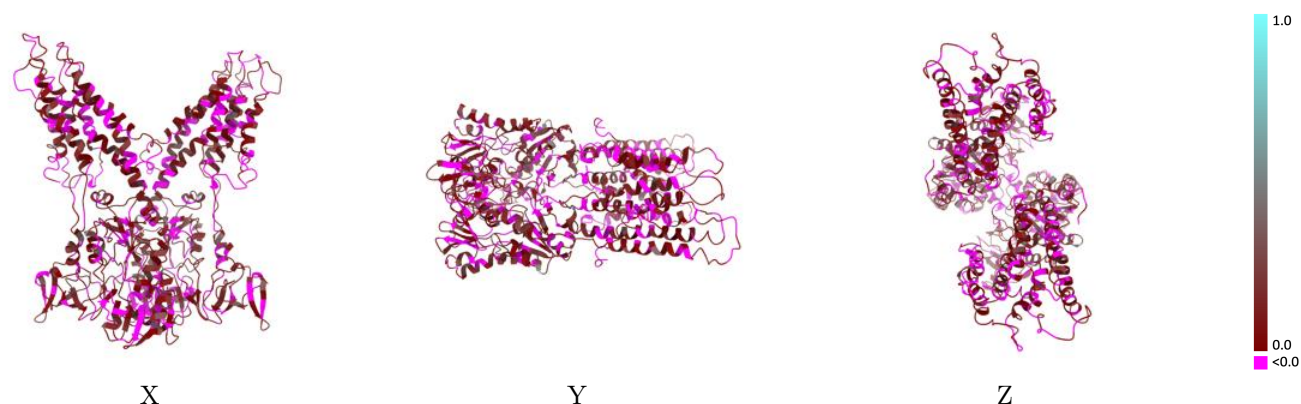
This section contains information regarding the fit between EMDB map EMD-5271 and PDB model 3J08. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



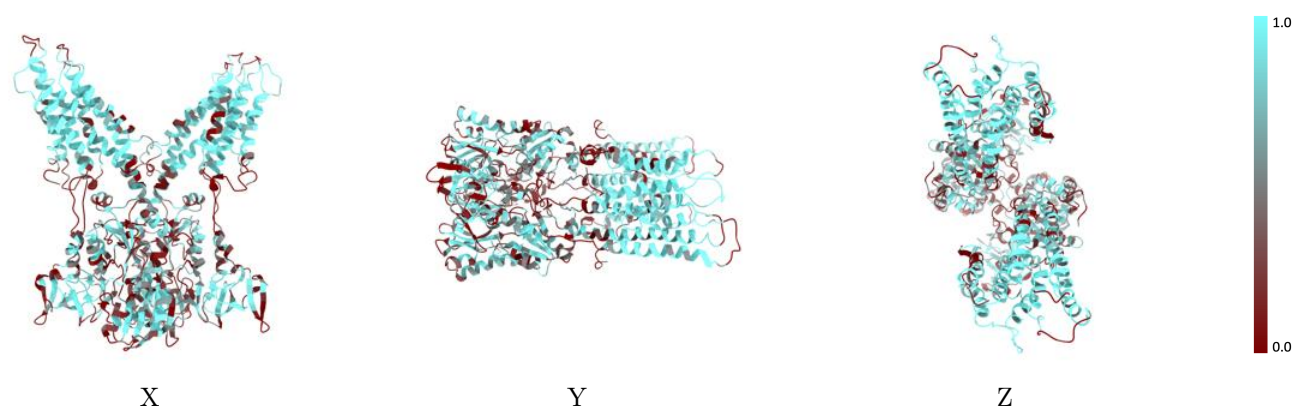
The images above show the 3D surface view of the map at the recommended contour level 130.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



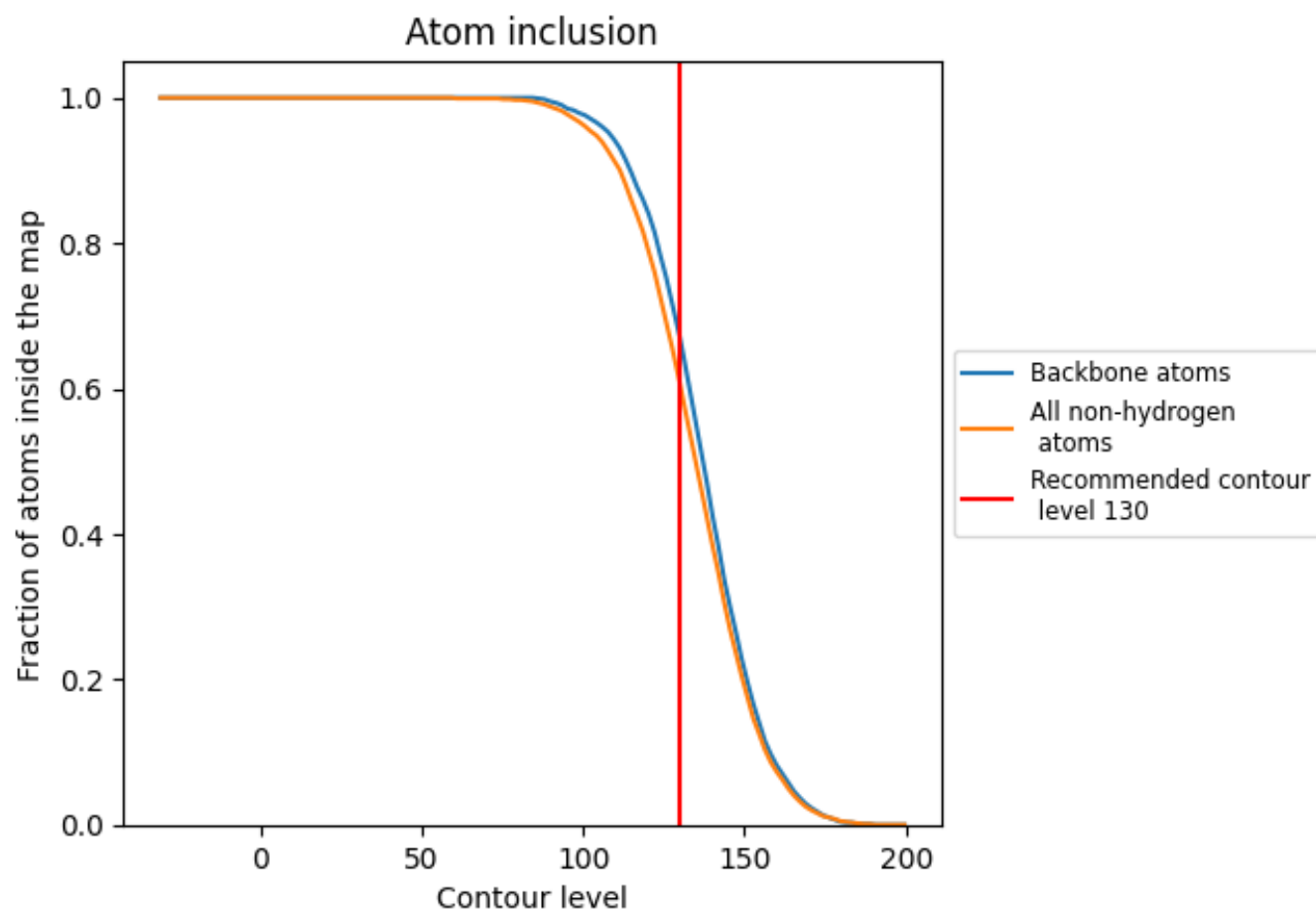
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (130).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 61% 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 (130) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6070	0.0660
A	0.6080	0.0670
B	0.6060	0.0660

