



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:21 PM UTC

PDB ID : 5LW7 / pdb_00005lw7
EMDB ID : EMD-4113
Title : S. solfataricus ABCE1 post-splitting state
Authors : Heuer, A.; Gerovac, M.; Beckmann, R.; Tampe, R.
Deposited on : 2016-09-15
Resolution : 17.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

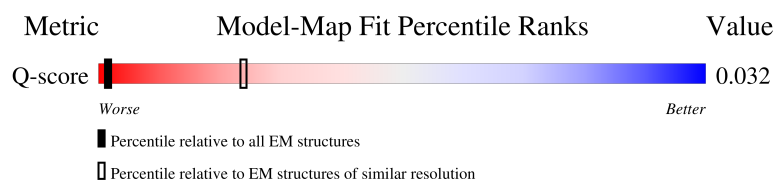
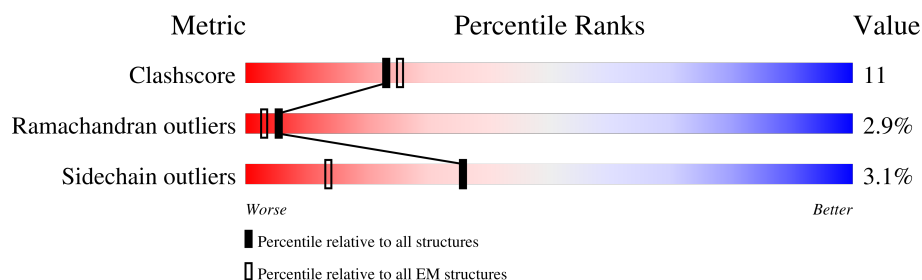
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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	38 (16.50 - 17.50)

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	B	593	40% 52% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	B	601	-	-	X	-
2	SF4	B	602	-	-	X	-

2 Entry composition [i](#)

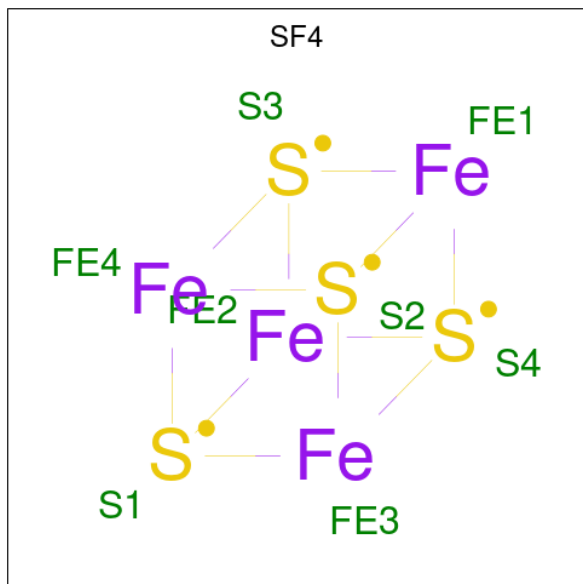
There are 2 unique types of molecules in this entry. The entry contains 4745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	593	4729	3003	826	880	20	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

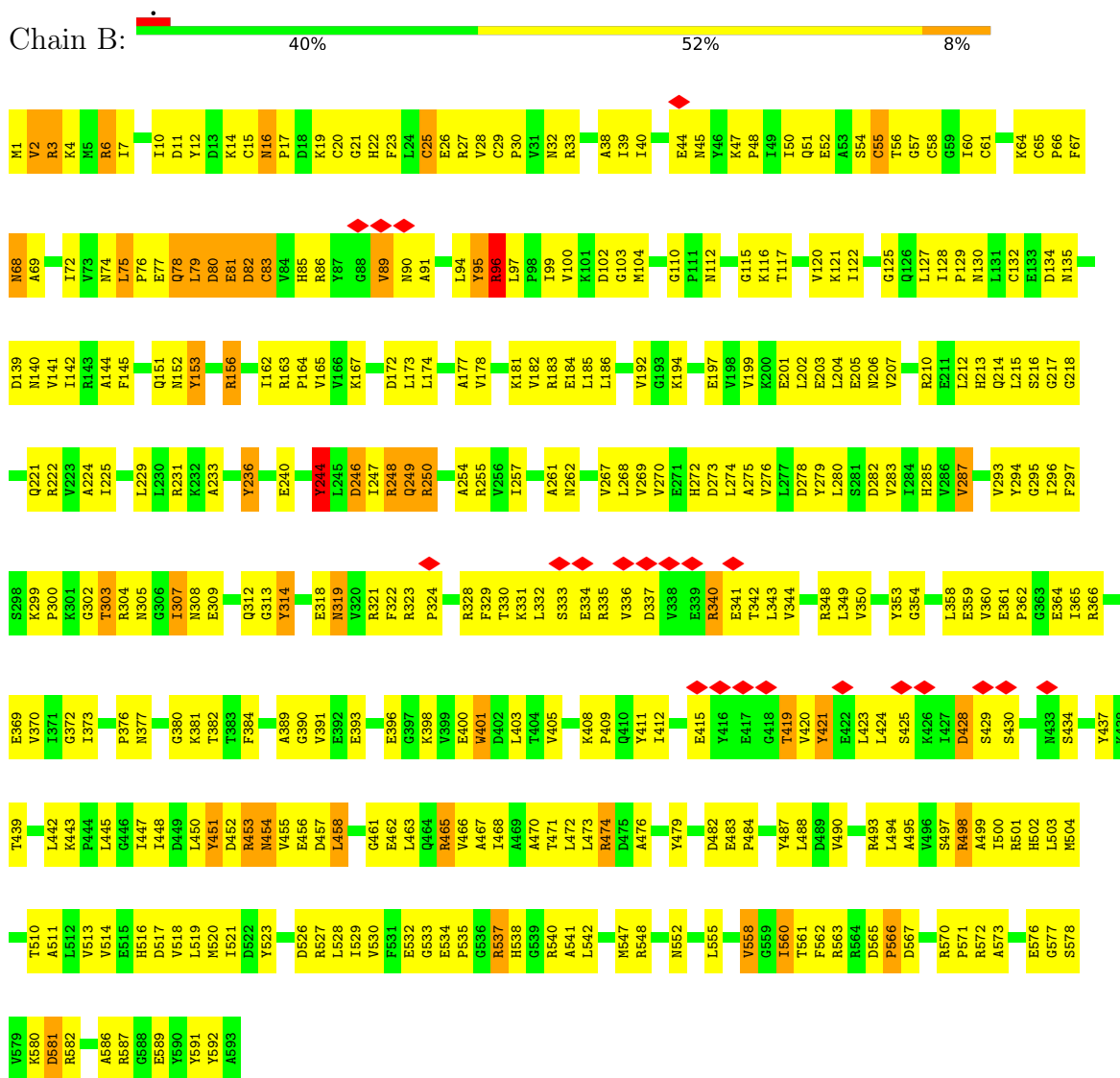


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
2	B	1	8	4	4	0
2	B	1	8	4	4	0

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: ABC transporter ATP-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19500	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	10000	Depositor
Maximum defocus (nm)	35000	Depositor
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	0.002	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.000137	Depositor
Map size ($\text{\AA}$)	509.76, 509.76, 509.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.062, 1.062, 1.062	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	2.14	165/4815 (3.4%)	2.35	295/6499 (4.5%)

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	B	0	19

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	HIS	ND1-CE1	10.37	1.43	1.32
1	B	269	VAL	CA-C	-10.01	1.40	1.52
1	B	400	GLU	CA-CB	9.76	1.65	1.52
1	B	484	PRO	CA-C	-9.37	1.40	1.52
1	B	453	ARG	NE-CZ	9.36	1.43	1.33
1	B	360	VAL	CA-CB	-9.30	1.42	1.54
1	B	95	TYR	CA-C	-8.63	1.42	1.52
1	B	563	ARG	CD-NE	8.56	1.58	1.46
1	B	233	ALA	N-CA	-8.32	1.35	1.46
1	B	540	ARG	NE-CZ	7.99	1.41	1.33
1	B	372	GLY	CA-C	-7.96	1.46	1.52
1	B	488	LEU	CA-C	-7.92	1.43	1.52
1	B	343	LEU	CA-C	-7.86	1.42	1.53
1	B	562	PHE	CA-C	-7.83	1.42	1.52
1	B	490	VAL	CA-C	-7.60	1.43	1.52
1	B	353	TYR	CA-C	-7.59	1.43	1.52
1	B	302	GLY	C-N	7.53	1.43	1.33
1	B	270	VAL	C-N	7.28	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	C-N	7.27	1.43	1.33
1	B	322	PHE	CA-C	-7.24	1.44	1.53
1	B	207	VAL	C-N	7.21	1.43	1.33
1	B	526	ASP	CA-C	-7.14	1.43	1.52
1	B	537	ARG	NE-CZ	7.07	1.40	1.33
1	B	328	ARG	NE-CZ	7.02	1.40	1.33
1	B	582	ARG	NE-CZ	7.02	1.40	1.33
1	B	483	GLU	C-N	6.97	1.40	1.34
1	B	90	ASN	CA-CB	6.89	1.63	1.53
1	B	513	VAL	CA-C	-6.88	1.43	1.52
1	B	334	GLU	CA-CB	6.87	1.62	1.53
1	B	165	VAL	CA-C	-6.86	1.43	1.52
1	B	244	TYR	C-N	6.79	1.42	1.33
1	B	297	PHE	CA-C	6.78	1.61	1.52
1	B	194	LYS	N-CA	-6.75	1.38	1.46
1	B	534	GLU	C-O	-6.74	1.18	1.25
1	B	523	TYR	CA-CB	6.56	1.63	1.53
1	B	201	GLU	C-O	-6.56	1.16	1.24
1	B	589	GLU	CA-CB	6.52	1.64	1.53
1	B	145	PHE	CA-C	-6.52	1.42	1.52
1	B	183	ARG	CA-C	-6.47	1.44	1.52
1	B	465	ARG	NE-CZ	6.47	1.40	1.33
1	B	467	ALA	C-N	6.46	1.42	1.33
1	B	358	LEU	N-CA	-6.45	1.38	1.46
1	B	537	ARG	CD-NE	6.44	1.55	1.46
1	B	502	HIS	ND1-CE1	6.39	1.39	1.32
1	B	519	LEU	CA-C	-6.39	1.44	1.52
1	B	304	ARG	NE-CZ	6.35	1.40	1.33
1	B	112	ASN	CA-C	-6.33	1.44	1.52
1	B	184	GLU	C-N	6.32	1.41	1.33
1	B	453	ARG	CZ-NH1	6.31	1.41	1.32
1	B	153	TYR	CA-CB	6.31	1.63	1.53
1	B	566	PRO	CA-C	6.29	1.61	1.52
1	B	452	ASP	CA-CB	6.29	1.64	1.53
1	B	350	VAL	N-CA	-6.28	1.38	1.46
1	B	96	ARG	C-N	6.27	1.40	1.33
1	B	91	ALA	C-N	6.24	1.41	1.33
1	B	285	HIS	CA-C	-6.23	1.45	1.52
1	B	463	LEU	CA-C	6.22	1.61	1.52
1	B	177	ALA	N-CA	-6.20	1.38	1.46
1	B	229	LEU	CB-CG	6.14	1.65	1.53
1	B	401	TRP	CA-CB	6.13	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	ARG	CD-NE	6.11	1.54	1.46
1	B	128	ILE	CA-C	-6.09	1.46	1.52
1	B	373	ILE	CA-C	-6.07	1.45	1.52
1	B	86	ARG	NE-CZ	6.04	1.39	1.33
1	B	365	ILE	CA-C	-6.02	1.45	1.52
1	B	369	GLU	C-N	6.01	1.41	1.33
1	B	349	LEU	CA-C	-6.00	1.45	1.52
1	B	500	ILE	N-CA	-5.98	1.39	1.46
1	B	313	GLY	C-N	5.96	1.42	1.33
1	B	185	LEU	CA-CB	5.96	1.62	1.53
1	B	377	ASN	C-O	-5.96	1.16	1.23
1	B	493	ARG	CD-NE	5.94	1.54	1.46
1	B	405	VAL	CA-C	-5.90	1.45	1.52
1	B	430	SER	CA-CB	5.89	1.62	1.53
1	B	272	HIS	ND1-CE1	5.86	1.38	1.32
1	B	215	LEU	CA-CB	5.84	1.63	1.53
1	B	194	LYS	CA-CB	5.83	1.61	1.53
1	B	102	ASP	CA-C	-5.83	1.45	1.52
1	B	532	GLU	C-N	5.83	1.40	1.33
1	B	229	LEU	C-N	5.82	1.42	1.33
1	B	511	ALA	N-CA	-5.81	1.38	1.45
1	B	591	TYR	CA-CB	5.81	1.63	1.53
1	B	419	THR	N-CA	-5.80	1.38	1.45
1	B	570	ARG	NE-CZ	5.80	1.39	1.33
1	B	33	ARG	CD-NE	5.77	1.54	1.46
1	B	589	GLU	CA-C	-5.76	1.45	1.52
1	B	247	ILE	CA-CB	-5.76	1.48	1.54
1	B	285	HIS	CE1-NE2	-5.74	1.26	1.32
1	B	274	LEU	CA-CB	-5.74	1.44	1.53
1	B	186	LEU	C-N	5.73	1.41	1.33
1	B	498	ARG	CA-CB	5.71	1.62	1.53
1	B	224	ALA	C-N	5.70	1.41	1.33
1	B	461	GLY	C-N	5.69	1.41	1.33
1	B	398	LYS	CA-C	-5.68	1.45	1.52
1	B	424	LEU	C-N	5.68	1.41	1.33
1	B	527	ARG	NE-CZ	5.67	1.39	1.33
1	B	240	GLU	C-N	-5.67	1.27	1.34
1	B	471	THR	CA-C	5.66	1.60	1.52
1	B	204	LEU	N-CA	-5.63	1.39	1.46
1	B	340	ARG	CZ-NH1	5.62	1.40	1.32
1	B	586	ALA	C-N	5.61	1.41	1.33
1	B	335	ARG	CZ-NH2	5.61	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	LEU	N-CA	-5.60	1.39	1.45
1	B	473	LEU	CA-C	-5.60	1.44	1.52
1	B	517	ASP	N-CA	-5.60	1.39	1.46
1	B	482	ASP	CA-C	-5.60	1.45	1.53
1	B	275	ALA	C-N	5.58	1.41	1.33
1	B	321	ARG	NE-CZ	5.57	1.39	1.33
1	B	269	VAL	C-O	-5.56	1.18	1.24
1	B	398	LYS	N-CA	-5.51	1.39	1.46
1	B	201	GLU	CA-CB	5.50	1.61	1.53
1	B	501	ARG	NE-CZ	5.49	1.39	1.33
1	B	563	ARG	NE-CZ	5.49	1.39	1.33
1	B	283	VAL	N-CA	5.46	1.52	1.46
1	B	323	ARG	CZ-NH2	5.46	1.40	1.33
1	B	100	VAL	CA-C	5.46	1.58	1.52
1	B	323	ARG	CZ-NH1	5.42	1.40	1.32
1	B	233	ALA	CA-C	-5.42	1.45	1.52
1	B	120	VAL	CA-C	-5.41	1.46	1.52
1	B	197	GLU	C-N	5.39	1.40	1.33
1	B	474	ARG	NE-CZ	5.39	1.39	1.33
1	B	541	ALA	CA-CB	-5.38	1.45	1.53
1	B	409	PRO	N-CA	5.38	1.53	1.47
1	B	222	ARG	CZ-NH1	5.38	1.40	1.32
1	B	558	VAL	CA-C	5.37	1.58	1.52
1	B	482	ASP	CA-CB	5.36	1.59	1.53
1	B	250	ARG	CD-NE	5.34	1.53	1.46
1	B	493	ARG	NE-CZ	5.34	1.39	1.33
1	B	267	VAL	CA-CB	-5.33	1.48	1.54
1	B	573	ALA	CA-C	-5.33	1.46	1.52
1	B	448	ILE	N-CA	-5.32	1.40	1.46
1	B	33	ARG	N-CA	-5.32	1.39	1.46
1	B	577	GLY	C-N	5.27	1.40	1.33
1	B	552	ASN	N-CA	5.27	1.52	1.46
1	B	309	GLU	N-CA	-5.26	1.40	1.46
1	B	96	ARG	CZ-NH1	5.25	1.40	1.32
1	B	510	THR	CA-C	-5.24	1.46	1.52
1	B	164	PRO	CA-CB	-5.22	1.46	1.53
1	B	294	TYR	CZ-OH	5.22	1.49	1.38
1	B	250	ARG	NE-CZ	5.21	1.38	1.33
1	B	272	HIS	C-O	5.21	1.31	1.24
1	B	336	VAL	N-CA	-5.19	1.40	1.46
1	B	359	GLU	C-O	-5.19	1.18	1.24
1	B	328	ARG	N-CA	-5.17	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	ARG	NE-CZ	5.16	1.38	1.33
1	B	494	LEU	C-N	5.16	1.40	1.33
1	B	174	LEU	C-N	5.15	1.41	1.33
1	B	580	LYS	CA-C	5.15	1.59	1.52
1	B	555	LEU	CA-C	-5.14	1.45	1.52
1	B	319	ASN	C-N	5.14	1.40	1.33
1	B	389	ALA	CA-C	-5.14	1.45	1.52
1	B	122	ILE	CA-CB	5.13	1.60	1.54
1	B	533	GLY	CA-C	-5.13	1.45	1.52
1	B	214	GLN	C-N	5.12	1.40	1.33
1	B	212	LEU	CB-CG	5.11	1.63	1.53
1	B	210	ARG	CD-NE	5.10	1.53	1.46
1	B	99	ILE	N-CA	-5.10	1.40	1.46
1	B	381	LYS	N-CA	-5.08	1.40	1.46
1	B	384	PHE	CA-CB	5.07	1.61	1.53
1	B	329	PHE	N-CA	5.07	1.52	1.45
1	B	295	GLY	C-N	5.06	1.40	1.33
1	B	504	MET	CA-CB	-5.05	1.45	1.53
1	B	592	TYR	CA-C	5.05	1.58	1.52
1	B	348	ARG	NE-CZ	5.03	1.38	1.33
1	B	303	THR	CA-CB	-5.00	1.45	1.53

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	GLY	N-CA-C	-12.94	98.50	111.56
1	B	565	ASP	CA-C-O	-10.79	108.94	120.70
1	B	526	ASP	N-CA-C	-9.82	101.06	113.43
1	B	425	SER	N-CA-C	9.53	122.86	111.33
1	B	362	PRO	N-CA-CB	9.50	111.61	103.25
1	B	182	VAL	N-CA-C	-9.43	101.20	110.72
1	B	381	LYS	CA-C-N	9.30	132.53	120.44
1	B	381	LYS	C-N-CA	9.30	132.53	120.44
1	B	558	VAL	N-CA-C	-9.19	104.19	113.47
1	B	442	LEU	N-CA-C	8.96	120.66	111.07
1	B	337	ASP	CA-CB-CG	-8.68	103.92	112.60
1	B	476	ALA	CA-C-N	8.64	132.55	120.29
1	B	476	ALA	C-N-CA	8.64	132.55	120.29
1	B	373	ILE	N-CA-CB	8.63	122.98	111.25
1	B	225	ILE	N-CA-CB	8.58	120.03	110.51
1	B	453	ARG	NE-CZ-NH1	-8.58	112.92	121.50
1	B	197	GLU	CA-C-N	8.52	131.35	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	GLU	C-N-CA	8.52	131.35	120.70
1	B	86	ARG	NE-CZ-NH1	-8.50	113.00	121.50
1	B	213	HIS	CG-CD2-NE2	8.50	115.70	107.20
1	B	181	LYS	CA-C-N	8.45	132.42	120.42
1	B	181	LYS	C-N-CA	8.45	132.42	120.42
1	B	462	GLU	CA-C-N	8.28	131.73	120.38
1	B	462	GLU	C-N-CA	8.28	131.73	120.38
1	B	206	ASN	N-CA-C	-8.15	103.48	113.50
1	B	257	ILE	CB-CA-C	8.04	122.56	112.02
1	B	273	ASP	CA-C-N	8.04	131.39	120.38
1	B	273	ASP	C-N-CA	8.04	131.39	120.38
1	B	412	ILE	CA-C-O	7.95	128.78	120.36
1	B	443	LYS	N-CA-CB	7.92	124.46	110.37
1	B	542	LEU	CA-C-N	7.86	128.48	120.38
1	B	542	LEU	C-N-CA	7.86	128.48	120.38
1	B	467	ALA	O-C-N	7.72	130.03	122.07
1	B	581	ASP	CA-C-N	7.71	130.93	120.44
1	B	581	ASP	C-N-CA	7.71	130.93	120.44
1	B	466	VAL	CA-C-O	-7.69	112.70	120.85
1	B	498	ARG	CA-C-N	7.68	130.89	120.44
1	B	498	ARG	C-N-CA	7.68	130.89	120.44
1	B	354	GLY	CA-C-N	7.68	133.22	120.70
1	B	354	GLY	C-N-CA	7.68	133.22	120.70
1	B	167	LYS	CA-C-N	7.41	127.42	119.78
1	B	167	LYS	C-N-CA	7.41	127.42	119.78
1	B	343	LEU	N-CA-C	-7.40	101.39	112.04
1	B	261	ALA	CA-C-N	7.38	130.04	120.44
1	B	261	ALA	C-N-CA	7.38	130.04	120.44
1	B	333	SER	CA-C-N	7.21	134.41	122.66
1	B	333	SER	C-N-CA	7.21	134.41	122.66
1	B	248	ARG	NE-CZ-NH1	-7.20	114.30	121.50
1	B	448	ILE	N-CA-C	-7.18	103.86	110.82
1	B	85	HIS	CA-C-O	-7.15	112.23	120.31
1	B	213	HIS	CA-CB-CG	7.12	120.92	113.80
1	B	255	ARG	CA-C-N	7.10	129.50	120.56
1	B	255	ARG	C-N-CA	7.10	129.50	120.56
1	B	152	ASN	CA-C-O	-7.08	112.91	120.42
1	B	110	GLY	CA-C-N	7.06	127.06	119.78
1	B	110	GLY	C-N-CA	7.06	127.06	119.78
1	B	323	ARG	CA-C-O	-7.01	110.55	120.16
1	B	254	ALA	CA-C-O	-7.01	113.12	120.55
1	B	152	ASN	N-CA-C	-6.98	103.75	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ASN	OD1-CG-ND2	6.96	129.56	122.60
1	B	530	VAL	N-CA-C	-6.96	98.34	108.71
1	B	282	ASP	N-CA-C	-6.87	105.84	114.56
1	B	552	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	B	144	ALA	CA-C-O	6.79	127.77	120.10
1	B	497	SER	CA-C-N	6.78	129.36	120.28
1	B	497	SER	C-N-CA	6.78	129.36	120.28
1	B	370	VAL	CA-C-O	6.77	126.95	120.25
1	B	361	GLU	CA-C-N	6.74	126.77	119.90
1	B	361	GLU	C-N-CA	6.74	126.77	119.90
1	B	293	VAL	N-CA-CB	-6.69	104.06	111.41
1	B	262	ASN	CA-CB-CG	-6.66	105.94	112.60
1	B	305	ASN	CA-CB-CG	-6.63	105.97	112.60
1	B	116	LYS	N-CA-CB	6.62	119.88	109.82
1	B	494	LEU	N-CA-C	6.61	118.48	111.28
1	B	341	GLU	CA-C-N	6.61	130.94	121.50
1	B	341	GLU	C-N-CA	6.61	130.94	121.50
1	B	493	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	B	314	TYR	CA-C-O	6.58	128.23	120.66
1	B	428	ASP	CA-C-N	6.58	129.40	120.38
1	B	428	ASP	C-N-CA	6.58	129.40	120.38
1	B	487	TYR	CB-CA-C	-6.56	102.11	111.95
1	B	523	TYR	N-CA-C	6.56	118.23	111.14
1	B	279	TYR	N-CA-C	6.55	118.08	111.07
1	B	142	ILE	CA-CB-CG2	6.54	121.62	110.50
1	B	451	TYR	CA-C-O	-6.53	112.88	120.20
1	B	565	ASP	O-C-N	6.53	128.71	121.53
1	B	523	TYR	O-C-N	6.52	129.13	122.09
1	B	408	LYS	CA-C-N	6.52	126.89	119.92
1	B	408	LYS	C-N-CA	6.52	126.89	119.92
1	B	429	SER	O-C-N	6.49	129.00	122.12
1	B	340	ARG	NE-CZ-NH2	6.48	125.03	119.20
1	B	581	ASP	O-C-N	-6.45	115.28	122.12
1	B	589	GLU	N-CA-C	-6.45	97.77	108.34
1	B	415	GLU	CA-C-O	6.44	125.54	118.65
1	B	571	PRO	CA-C-O	-6.43	113.39	120.92
1	B	437	TYR	N-CA-CB	6.43	120.24	110.28
1	B	547	MET	O-C-N	6.42	128.77	122.09
1	B	493	ARG	N-CA-CB	6.37	119.31	110.07
1	B	499	ALA	CA-C-O	-6.35	114.16	120.70
1	B	192	VAL	N-CA-C	-6.34	106.00	113.42
1	B	393	GLU	N-CA-C	-6.33	99.77	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	MET	N-CA-C	-6.32	104.32	111.14
1	B	548	ARG	CA-C-N	6.30	129.36	120.28
1	B	548	ARG	C-N-CA	6.30	129.36	120.28
1	B	527	ARG	N-CA-CB	6.26	121.45	111.56
1	B	548	ARG	N-CA-CB	6.26	119.15	110.07
1	B	217	GLY	O-C-N	6.22	130.79	122.70
1	B	97	LEU	O-C-N	-6.20	117.74	121.71
1	B	523	TYR	CA-C-O	-6.18	114.33	120.70
1	B	273	ASP	N-CA-C	-6.16	97.05	108.02
1	B	465	ARG	CA-C-N	6.16	129.17	120.42
1	B	465	ARG	C-N-CA	6.16	129.17	120.42
1	B	254	ALA	O-C-N	6.13	128.62	122.12
1	B	533	GLY	CA-C-N	6.12	131.73	122.42
1	B	533	GLY	C-N-CA	6.12	131.73	122.42
1	B	514	VAL	N-CA-C	-6.12	99.56	108.87
1	B	450	LEU	CA-C-N	6.12	129.31	120.38
1	B	450	LEU	C-N-CA	6.12	129.31	120.38
1	B	552	ASN	CB-CA-C	-6.10	100.47	110.85
1	B	538	HIS	CA-CB-CG	-6.10	107.70	113.80
1	B	216	SER	N-CA-C	-6.08	100.99	110.17
1	B	560	ILE	CA-C-O	6.07	126.79	120.36
1	B	365	ILE	CA-C-N	6.05	132.92	122.64
1	B	365	ILE	C-N-CA	6.05	132.92	122.64
1	B	224	ALA	CA-C-O	-6.04	114.48	120.70
1	B	116	LYS	CA-C-N	6.04	130.80	120.72
1	B	116	LYS	C-N-CA	6.04	130.80	120.72
1	B	538	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	B	555	LEU	N-CA-CB	6.01	119.48	110.22
1	B	534	GLU	CA-C-O	-6.01	113.97	119.62
1	B	307	ILE	N-CA-C	-6.00	104.66	110.72
1	B	173	LEU	N-CA-C	-5.99	104.71	112.68
1	B	128	ILE	CA-C-N	5.98	125.92	119.76
1	B	128	ILE	C-N-CA	5.98	125.92	119.76
1	B	276	VAL	CA-C-N	5.93	128.71	120.29
1	B	276	VAL	C-N-CA	5.93	128.71	120.29
1	B	194	LYS	CA-C-N	5.92	128.49	120.38
1	B	194	LYS	C-N-CA	5.92	128.49	120.38
1	B	437	TYR	N-CA-C	-5.92	104.95	111.82
1	B	97	LEU	CA-C-N	5.90	125.83	119.76
1	B	97	LEU	C-N-CA	5.90	125.83	119.76
1	B	246	ASP	CA-C-N	5.89	128.20	120.60
1	B	246	ASP	C-N-CA	5.89	128.20	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	576	GLU	CA-C-O	5.88	127.62	120.62
1	B	380	GLY	CA-C-N	5.88	128.08	120.44
1	B	380	GLY	C-N-CA	5.88	128.08	120.44
1	B	589	GLU	CA-C-O	5.87	126.46	120.24
1	B	318	GLU	CA-C-N	5.85	130.96	122.36
1	B	318	GLU	C-N-CA	5.85	130.96	122.36
1	B	86	ARG	N-CA-C	-5.84	99.14	109.06
1	B	45	ASN	N-CA-C	-5.83	106.14	113.20
1	B	129	PRO	N-CA-CB	5.83	108.50	103.31
1	B	328	ARG	CG-CD-NE	-5.83	99.18	112.00
1	B	429	SER	CA-C-N	5.82	128.00	120.44
1	B	429	SER	C-N-CA	5.82	128.00	120.44
1	B	497	SER	CB-CA-C	-5.81	101.71	110.90
1	B	365	ILE	N-CA-C	-5.80	99.98	108.11
1	B	202	LEU	CB-CA-C	-5.79	100.07	110.37
1	B	490	VAL	CA-C-N	5.78	128.50	120.29
1	B	490	VAL	C-N-CA	5.78	128.50	120.29
1	B	273	ASP	N-CA-CB	5.78	119.63	110.84
1	B	581	ASP	CA-C-O	5.77	126.67	120.55
1	B	312	GLN	OE1-CD-NE2	5.77	128.37	122.60
1	B	521	ILE	CB-CA-C	-5.75	104.38	112.14
1	B	236	TYR	N-CA-CB	5.74	119.78	110.77
1	B	308	ASN	CA-C-N	5.74	127.97	120.28
1	B	308	ASN	C-N-CA	5.74	127.97	120.28
1	B	425	SER	N-CA-CB	5.72	118.65	110.06
1	B	340	ARG	CA-C-N	5.72	132.46	121.54
1	B	340	ARG	C-N-CA	5.72	132.46	121.54
1	B	381	LYS	CB-CA-C	-5.70	101.92	110.88
1	B	359	GLU	CB-CA-C	5.70	120.01	109.70
1	B	115	GLY	O-C-N	5.69	128.34	122.54
1	B	318	GLU	N-CA-C	-5.68	106.98	114.31
1	B	587	ARG	N-CA-CB	5.68	119.54	110.73
1	B	89	VAL	CA-C-O	-5.68	115.16	121.23
1	B	163	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	B	503	LEU	CA-C-N	5.67	128.34	120.29
1	B	503	LEU	C-N-CA	5.67	128.34	120.29
1	B	128	ILE	N-CA-CB	5.67	119.14	111.21
1	B	487	TYR	N-CA-C	5.66	119.00	111.30
1	B	535	PRO	N-CA-C	5.65	120.09	111.11
1	B	434	SER	CA-C-N	5.65	128.89	120.31
1	B	434	SER	C-N-CA	5.65	128.89	120.31
1	B	529	ILE	N-CA-C	-5.64	99.43	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	MET	CA-C-O	-5.61	115.06	121.40
1	B	366	ARG	CA-C-N	5.60	130.38	122.09
1	B	366	ARG	C-N-CA	5.60	130.38	122.09
1	B	130	ASN	N-CA-CB	5.60	118.87	110.53
1	B	162	ILE	O-C-N	-5.60	117.01	123.00
1	B	213	HIS	CE1-NE2-CD2	-5.59	103.41	109.00
1	B	419	THR	N-CA-CB	5.59	118.43	110.44
1	B	382	THR	CA-C-O	-5.58	114.96	120.82
1	B	468	ILE	N-CA-CB	5.58	117.08	110.55
1	B	249	GLN	CA-C-N	5.58	127.75	120.28
1	B	249	GLN	C-N-CA	5.58	127.75	120.28
1	B	511	ALA	N-CA-C	-5.57	100.24	108.99
1	B	420	VAL	O-C-N	-5.55	116.47	121.91
1	B	409	PRO	CA-C-N	5.55	128.17	120.29
1	B	409	PRO	C-N-CA	5.55	128.17	120.29
1	B	350	VAL	CB-CA-C	-5.54	102.20	111.29
1	B	121	LYS	CA-C-N	5.54	127.65	120.56
1	B	121	LYS	C-N-CA	5.54	127.65	120.56
1	B	231	ARG	N-CA-CB	5.54	118.11	109.97
1	B	487	TYR	CB-CG-CD2	-5.52	112.52	120.80
1	B	428	ASP	N-CA-C	-5.51	99.05	110.80
1	B	21	GLY	N-CA-C	-5.50	104.68	111.45
1	B	204	LEU	N-CA-C	-5.50	105.88	112.59
1	B	139	ASP	N-CA-C	5.50	117.27	111.28
1	B	210	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	B	167	LYS	CB-CA-C	5.49	116.39	110.08
1	B	139	ASP	CB-CA-C	-5.49	101.68	110.79
1	B	324	PRO	N-CD-CG	5.49	111.43	103.20
1	B	141	VAL	CA-C-N	5.47	127.96	120.46
1	B	141	VAL	C-N-CA	5.47	127.96	120.46
1	B	278	ASP	CA-C-O	5.45	126.55	120.82
1	B	542	LEU	N-CA-C	-5.45	102.76	110.29
1	B	127	LEU	N-CA-CB	5.45	119.76	110.71
1	B	100	VAL	CB-CA-C	-5.43	104.00	111.49
1	B	330	THR	CA-C-O	-5.42	114.51	120.36
1	B	445	LEU	N-CA-C	-5.42	105.89	112.88
1	B	163	ARG	N-CA-CB	5.42	123.39	111.25
1	B	141	VAL	N-CA-CB	5.42	117.50	110.57
1	B	502	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	B	205	GLU	N-CA-C	5.40	119.50	113.01
1	B	94	LEU	CA-C-N	5.38	131.02	122.94
1	B	94	LEU	C-N-CA	5.38	131.02	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	GLN	CB-CG-CD	5.38	121.75	112.60
1	B	421	TYR	CA-C-N	5.38	127.43	120.44
1	B	421	TYR	C-N-CA	5.38	127.43	120.44
1	B	424	LEU	O-C-N	5.36	128.26	122.15
1	B	563	ARG	CA-C-N	5.35	130.46	122.86
1	B	563	ARG	C-N-CA	5.35	130.46	122.86
1	B	135	ASN	CA-C-O	5.35	127.39	121.56
1	B	430	SER	CA-C-N	5.35	127.44	120.28
1	B	430	SER	C-N-CA	5.35	127.44	120.28
1	B	456	GLU	CA-C-N	5.34	131.52	122.65
1	B	456	GLU	C-N-CA	5.34	131.52	122.65
1	B	184	GLU	CA-C-N	5.33	127.74	120.54
1	B	184	GLU	C-N-CA	5.33	127.74	120.54
1	B	16	ASN	CA-C-N	5.33	125.65	119.47
1	B	16	ASN	C-N-CA	5.33	125.65	119.47
1	B	299	LYS	CA-C-O	-5.31	114.93	120.88
1	B	578	SER	N-CA-C	-5.30	101.22	108.38
1	B	268	LEU	N-CA-C	-5.29	99.82	108.76
1	B	302	GLY	O-C-N	5.28	127.53	122.99
1	B	151	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	B	421	TYR	N-CA-C	5.26	117.76	111.71
1	B	566	PRO	N-CA-C	-5.25	101.67	112.47
1	B	376	PRO	CB-CA-C	-5.23	103.15	110.63
1	B	91	ALA	N-CA-CB	5.22	119.93	111.21
1	B	287	VAL	CB-CA-C	-5.21	103.38	110.77
1	B	472	LEU	N-CA-C	5.20	119.25	113.01
1	B	222	ARG	CA-C-N	5.20	128.83	120.30
1	B	222	ARG	C-N-CA	5.20	128.83	120.30
1	B	419	THR	CA-C-N	5.20	127.11	120.56
1	B	419	THR	C-N-CA	5.20	127.11	120.56
1	B	470	ALA	N-CA-C	5.19	116.62	111.07
1	B	178	VAL	N-CA-C	-5.18	100.06	107.78
1	B	103	GLY	O-C-N	5.17	128.74	122.32
1	B	299	LYS	CA-CB-CG	5.17	124.44	114.10
1	B	353	TYR	CB-CA-C	-5.17	102.06	110.85
1	B	221	GLN	OE1-CD-NE2	5.17	127.77	122.60
1	B	132	CYS	CB-CA-C	-5.16	104.56	111.89
1	B	518	VAL	CA-C-N	5.14	128.13	120.31
1	B	518	VAL	C-N-CA	5.14	128.13	120.31
1	B	300	PRO	CA-C-O	-5.14	115.14	121.31
1	B	391	VAL	O-C-N	5.14	126.84	122.16
1	B	495	ALA	N-CA-C	5.13	116.88	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	567	ASP	CA-CB-CG	-5.12	107.48	112.60
1	B	125	GLY	N-CA-C	-5.11	108.57	115.21
1	B	450	LEU	N-CA-CB	5.10	117.92	110.88
1	B	199	VAL	CA-C-N	5.09	129.22	120.71
1	B	199	VAL	C-N-CA	5.09	129.22	120.71
1	B	244	TYR	N-CA-C	5.09	121.64	110.80
1	B	130	ASN	CA-C-N	5.09	129.35	122.07
1	B	130	ASN	C-N-CA	5.09	129.35	122.07
1	B	296	ILE	CB-CA-C	-5.07	102.93	110.33
1	B	439	THR	CA-C-O	5.07	125.77	119.79
1	B	519	LEU	CB-CA-C	-5.06	100.95	110.67
1	B	139	ASP	CA-C-N	5.05	127.99	120.31
1	B	139	ASP	C-N-CA	5.05	127.99	120.31
1	B	390	GLY	O-C-N	5.05	128.20	122.55
1	B	194	LYS	N-CA-CB	-5.04	102.86	110.92
1	B	454	ASN	CA-CB-CG	-5.04	107.56	112.60
1	B	360	VAL	N-CA-CB	5.03	118.18	111.64
1	B	140	ASN	CA-C-N	5.02	126.99	120.56
1	B	140	ASN	C-N-CA	5.02	126.99	120.56
1	B	225	ILE	N-CA-C	-5.02	105.09	110.36
1	B	255	ARG	N-CA-CB	5.02	117.50	110.12
1	B	521	ILE	N-CA-CB	5.01	117.36	110.54
1	B	576	GLU	CB-CG-CD	-5.01	104.08	112.60
1	B	296	ILE	CB-CG1-CD1	5.00	124.31	113.80
1	B	203	GLU	CA-C-O	-5.00	115.94	122.14
1	B	396	GLU	CB-CA-C	-5.00	98.46	109.56

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	153	TYR	Sidechain
1	B	156	ARG	Sidechain
1	B	236	TYR	Sidechain
1	B	244	TYR	Sidechain
1	B	248	ARG	Sidechain
1	B	250	ARG	Sidechain
1	B	280	LEU	Peptide
1	B	314	TYR	Sidechain
1	B	340	ARG	Sidechain
1	B	411	TYR	Sidechain
1	B	421	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	451	TYR	Sidechain
1	B	465	ARG	Sidechain
1	B	474	ARG	Sidechain
1	B	479	TYR	Sidechain
1	B	498	ARG	Sidechain
1	B	537	ARG	Sidechain
1	B	572	ARG	Sidechain
1	B	95	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	B	4729	0	4783	106	0
2	B	16	0	0	17	0
All	All	4745	0	4783	106	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 11.

All (106) 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:72:ILE:HD12	2:B:601:SF4:S1	1.43	1.55
1:B:7:ILE:CG2	1:B:319:ASN:ND2	2.00	1.23
1:B:7:ILE:HG21	1:B:319:ASN:ND2	1.58	1.17
1:B:72:ILE:CD1	2:B:601:SF4:S1	2.33	1.15
1:B:58:CYS:N	2:B:601:SF4:S3	2.23	1.11
1:B:78:GLN:HG2	1:B:96:ARG:NH1	1.69	1.08
1:B:7:ILE:CG2	1:B:319:ASN:HD22	1.64	1.04
1:B:7:ILE:HG23	1:B:319:ASN:HD22	1.13	1.04
1:B:3:ARG:HB3	1:B:80:ASP:CB	1.92	1.00
1:B:48:PRO:HG3	2:B:602:SF4:S3	2.02	0.99
1:B:22:HIS:H	1:B:27:ARG:NH1	1.67	0.92
1:B:6:ARG:NH2	1:B:74:ASN:HD21	1.69	0.91
1:B:7:ILE:HG23	1:B:319:ASN:ND2	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:CG2	1:B:319:ASN:HD21	1.88	0.87
1:B:15:CYS:HG	2:B:602:SF4:FE4	0.56	0.87
1:B:3:ARG:HB3	1:B:80:ASP:HB3	1.55	0.86
1:B:77:GLU:HA	1:B:81:GLU:HB2	1.59	0.84
1:B:57:GLY:C	2:B:601:SF4:S3	2.44	0.84
1:B:72:ILE:CG2	2:B:601:SF4:S1	2.65	0.84
1:B:82:ASP:O	1:B:83:CYS:O	1.95	0.83
1:B:72:ILE:HG21	2:B:601:SF4:S1	2.19	0.82
1:B:15:CYS:SG	2:B:602:SF4:FE4	1.72	0.82
1:B:7:ILE:HG21	1:B:319:ASN:HD21	1.44	0.81
1:B:61:CYS:SG	2:B:601:SF4:S2	2.79	0.81
1:B:15:CYS:HB2	2:B:602:SF4:S2	2.20	0.80
1:B:78:GLN:HG2	1:B:96:ARG:HH11	1.44	0.79
1:B:25:CYS:SG	2:B:602:SF4:S4	2.82	0.78
1:B:2:VAL:O	1:B:3:ARG:HB2	1.84	0.75
1:B:25:CYS:HB3	1:B:39:ILE:HD13	1.68	0.75
1:B:57:GLY:HA2	2:B:601:SF4:S3	2.06	0.74
1:B:6:ARG:CZ	1:B:74:ASN:HD21	2.01	0.73
1:B:78:GLN:HG2	1:B:96:ARG:HH12	1.53	0.72
1:B:74:ASN:HB3	1:B:76:PRO:HD3	1.72	0.72
1:B:3:ARG:CB	1:B:80:ASP:CB	2.67	0.71
1:B:82:ASP:O	1:B:83:CYS:C	2.34	0.70
1:B:22:HIS:H	1:B:27:ARG:HH12	1.40	0.66
1:B:79:LEU:O	1:B:79:LEU:HD12	1.97	0.65
1:B:48:PRO:CG	2:B:602:SF4:S3	2.84	0.64
1:B:74:ASN:HB3	1:B:76:PRO:CD	2.27	0.64
1:B:7:ILE:CD1	1:B:75:LEU:HD11	2.28	0.64
1:B:74:ASN:HB3	1:B:76:PRO:HG3	1.80	0.63
1:B:67:PHE:O	1:B:68:ASN:HB2	1.99	0.62
1:B:72:ILE:HG23	2:B:601:SF4:S1	2.38	0.62
1:B:4:LYS:HG3	1:B:76:PRO:N	2.13	0.62
1:B:6:ARG:HD2	1:B:55:CYS:O	2.00	0.61
1:B:78:GLN:CG	1:B:96:ARG:NH1	2.57	0.61
1:B:54:SER:O	1:B:55:CYS:C	2.44	0.61
1:B:77:GLU:HG3	1:B:81:GLU:HG2	1.84	0.60
1:B:3:ARG:CB	1:B:80:ASP:HB3	2.31	0.59
1:B:19:LYS:HD3	1:B:67:PHE:HZ	1.66	0.59
1:B:78:GLN:O	1:B:96:ARG:NH1	2.36	0.58
1:B:10:ILE:HG23	1:B:69:ALA:O	2.04	0.57
1:B:4:LYS:HE2	1:B:74:ASN:HB3	1.85	0.57
1:B:22:HIS:H	1:B:27:ARG:HH11	1.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:HD12	1:B:75:LEU:HD11	1.88	0.55
1:B:6:ARG:CZ	1:B:74:ASN:ND2	2.70	0.55
1:B:16:ASN:C	1:B:16:ASN:HD22	2.14	0.55
1:B:6:ARG:NH2	1:B:74:ASN:ND2	2.49	0.55
1:B:72:ILE:CG1	2:B:601:SF4:S1	2.94	0.55
1:B:74:ASN:HB3	1:B:76:PRO:CG	2.37	0.54
1:B:40:ILE:HD12	1:B:51:GLN:OE1	2.06	0.54
1:B:78:GLN:CG	1:B:96:ARG:HH12	2.16	0.53
1:B:38:ALA:HA	1:B:54:SER:HB2	1.90	0.52
1:B:78:GLN:HE21	1:B:96:ARG:HH12	1.56	0.52
1:B:28:VAL:CG1	1:B:60:ILE:HG22	2.40	0.52
1:B:7:ILE:HD11	1:B:75:LEU:HD11	1.91	0.51
1:B:15:CYS:CB	2:B:602:SF4:S2	2.96	0.51
1:B:26:GLU:CG	1:B:32:ASN:HD22	2.23	0.51
1:B:82:ASP:OD2	1:B:96:ARG:HG2	2.12	0.50
1:B:453:ARG:HH21	1:B:457:ASP:HB3	1.77	0.50
1:B:58:CYS:SG	1:B:60:ILE:HG13	2.53	0.49
1:B:344:VAL:HG21	1:B:401:TRP:CE3	2.49	0.48
1:B:39:ILE:HG12	1:B:50:ILE:HG12	1.96	0.47
1:B:74:ASN:CB	1:B:76:PRO:CD	2.88	0.47
1:B:64:LYS:O	1:B:65:CYS:C	2.57	0.47
1:B:54:SER:O	1:B:55:CYS:O	2.33	0.47
1:B:20:CYS:HB3	1:B:66:PRO:HG3	1.97	0.47
1:B:423:LEU:HD22	1:B:455:VAL:HG21	1.97	0.47
1:B:558:VAL:O	1:B:560:ILE:HG12	2.15	0.47
1:B:12:TYR:C	1:B:14:LYS:H	2.23	0.46
1:B:26:GLU:HG3	1:B:32:ASN:HD22	1.80	0.46
1:B:78:GLN:HE21	1:B:96:ARG:NH1	2.14	0.46
1:B:3:ARG:NH2	1:B:80:ASP:OD1	2.46	0.45
1:B:419:THR:HA	1:B:454:ASN:HA	1.98	0.45
1:B:3:ARG:HB3	1:B:80:ASP:HB2	1.93	0.44
1:B:11:ASP:CG	1:B:14:LYS:HE2	2.43	0.44
1:B:12:TYR:C	1:B:14:LYS:N	2.74	0.43
1:B:82:ASP:C	1:B:83:CYS:O	2.58	0.43
1:B:4:LYS:CG	1:B:76:PRO:CD	2.96	0.43
1:B:28:VAL:HG11	1:B:64:LYS:HG2	2.01	0.42
1:B:79:LEU:HD12	1:B:79:LEU:C	2.44	0.42
1:B:11:ASP:OD1	1:B:14:LYS:HE2	2.19	0.42
1:B:28:VAL:HG12	1:B:60:ILE:HG22	2.01	0.42
1:B:561:THR:OG1	1:B:581:ASP:HA	2.20	0.42
1:B:17:PRO:HB3	1:B:23:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLY:CA	1:B:249:GLN:HE22	2.33	0.42
1:B:1:MET:O	1:B:2:VAL:HG13	2.20	0.41
1:B:342:THR:HG23	1:B:364:GLU:HG3	2.01	0.41
1:B:344:VAL:HG21	1:B:401:TRP:CD2	2.55	0.41
1:B:218:GLY:HA3	1:B:249:GLN:HE22	1.86	0.41
1:B:29:CYS:HB2	1:B:39:ILE:HD12	2.02	0.41
1:B:303:THR:O	1:B:307:ILE:HG13	2.20	0.41
1:B:6:ARG:NH2	1:B:56:THR:O	2.54	0.41
1:B:10:ILE:HA	1:B:69:ALA:O	2.21	0.41
1:B:16:ASN:C	1:B:16:ASN:ND2	2.78	0.41
1:B:30:PRO:HD3	1:B:60:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	591/593 (100%)	523 (88%)	51 (9%)	17 (3%)	3 23

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	ARG
1	B	55	CYS
1	B	68	ASN
1	B	75	LEU
1	B	83	CYS
1	B	134	ASP
1	B	44	GLU
1	B	428	ASP
1	B	25	CYS
1	B	96	ARG

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Mol	Chain	Res	Type
1	B	331	LYS
1	B	516	HIS
1	B	52	GLU
1	B	172	ASP
1	B	244	TYR
1	B	332	LEU
1	B	566	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	B	512/512 (100%)	496 (97%)	16 (3%)	35	56

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	VAL
1	B	6	ARG
1	B	47	LYS
1	B	78	GLN
1	B	79	LEU
1	B	80	ASP
1	B	81	GLU
1	B	82	ASP
1	B	89	VAL
1	B	117	THR
1	B	246	ASP
1	B	287	VAL
1	B	403	LEU
1	B	447	ILE
1	B	458	LEU
1	B	528	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	ASN
1	B	74	ASN
1	B	85	HIS
1	B	90	ASN
1	B	135	ASN
1	B	249	GLN
1	B	319	ASN
1	B	507	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SF4	B	601	1	0,12,12	-	-	-		
2	SF4	B	602	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	601	1	-	-	0/6/5/5
2	SF4	B	602	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	SF4	10	0
2	B	602	SF4	7	0

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-4113. 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](#)

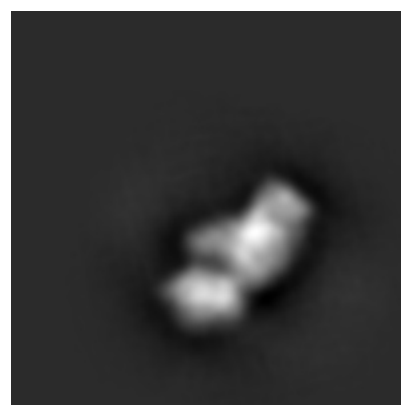
6.1.1 Primary map



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: 240



Y Index: 240

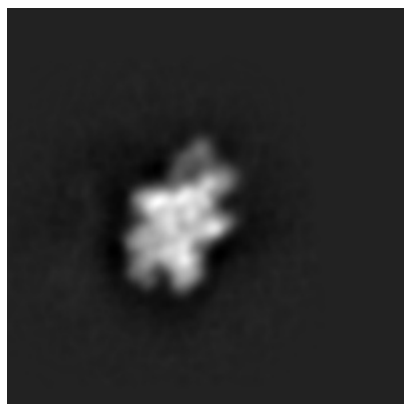


Z Index: 240

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: 298



Y Index: 208



Z Index: 213

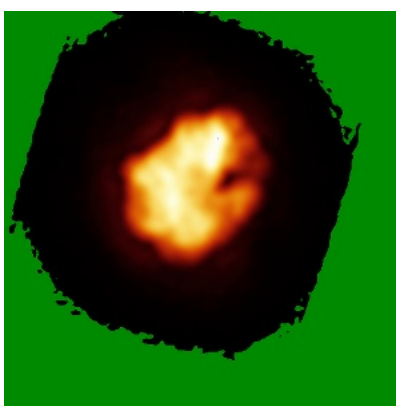
The images above show the largest variance slices of the map in three orthogonal directions.

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

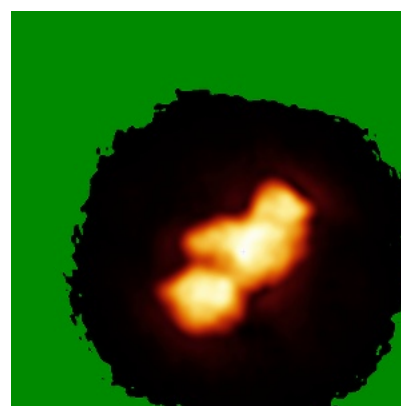
6.4.1 Primary map



X



Y

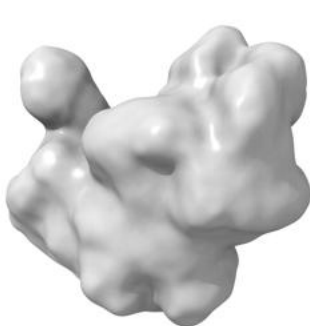


Z

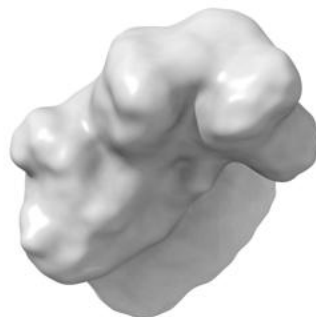
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.000137. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

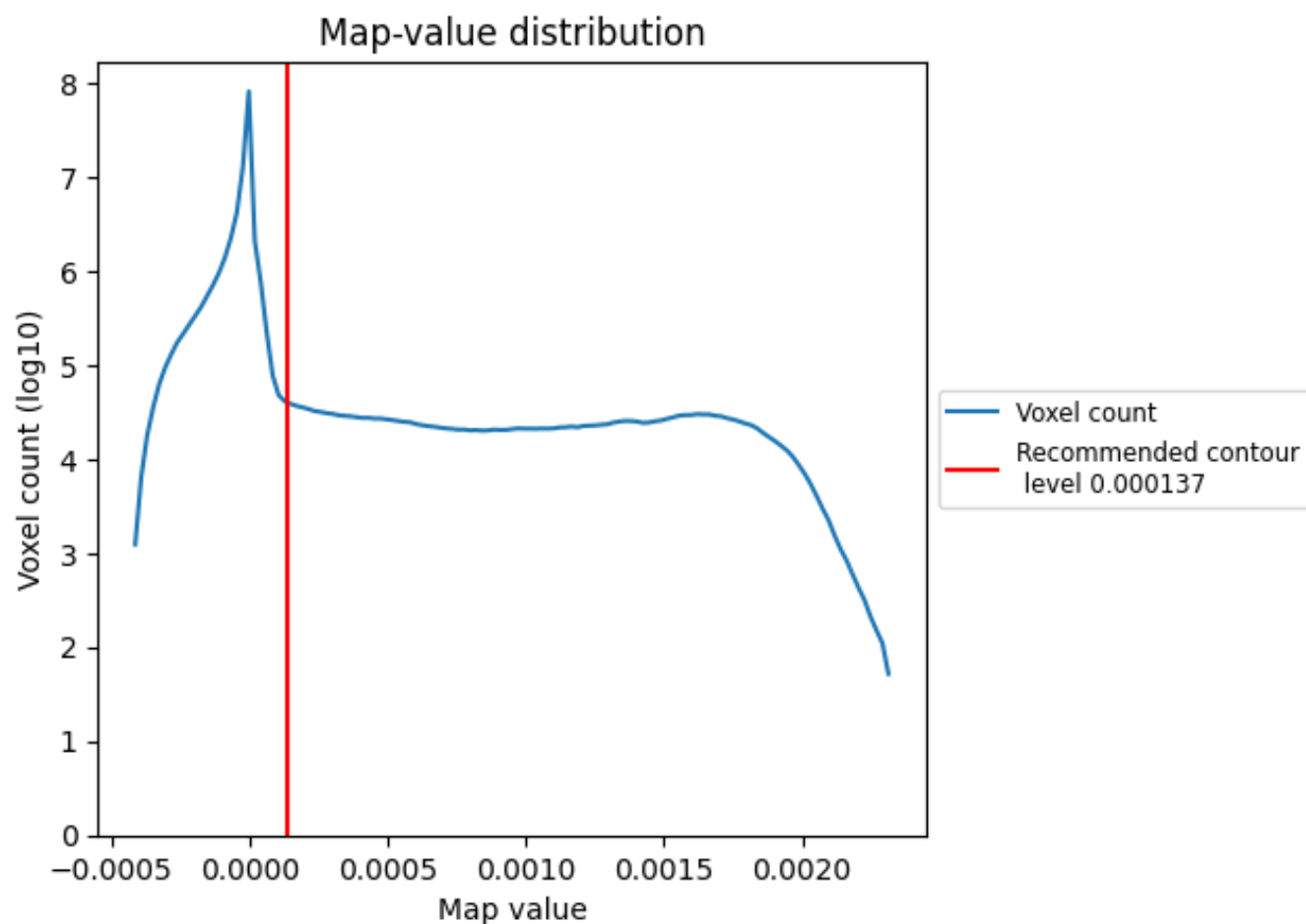
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

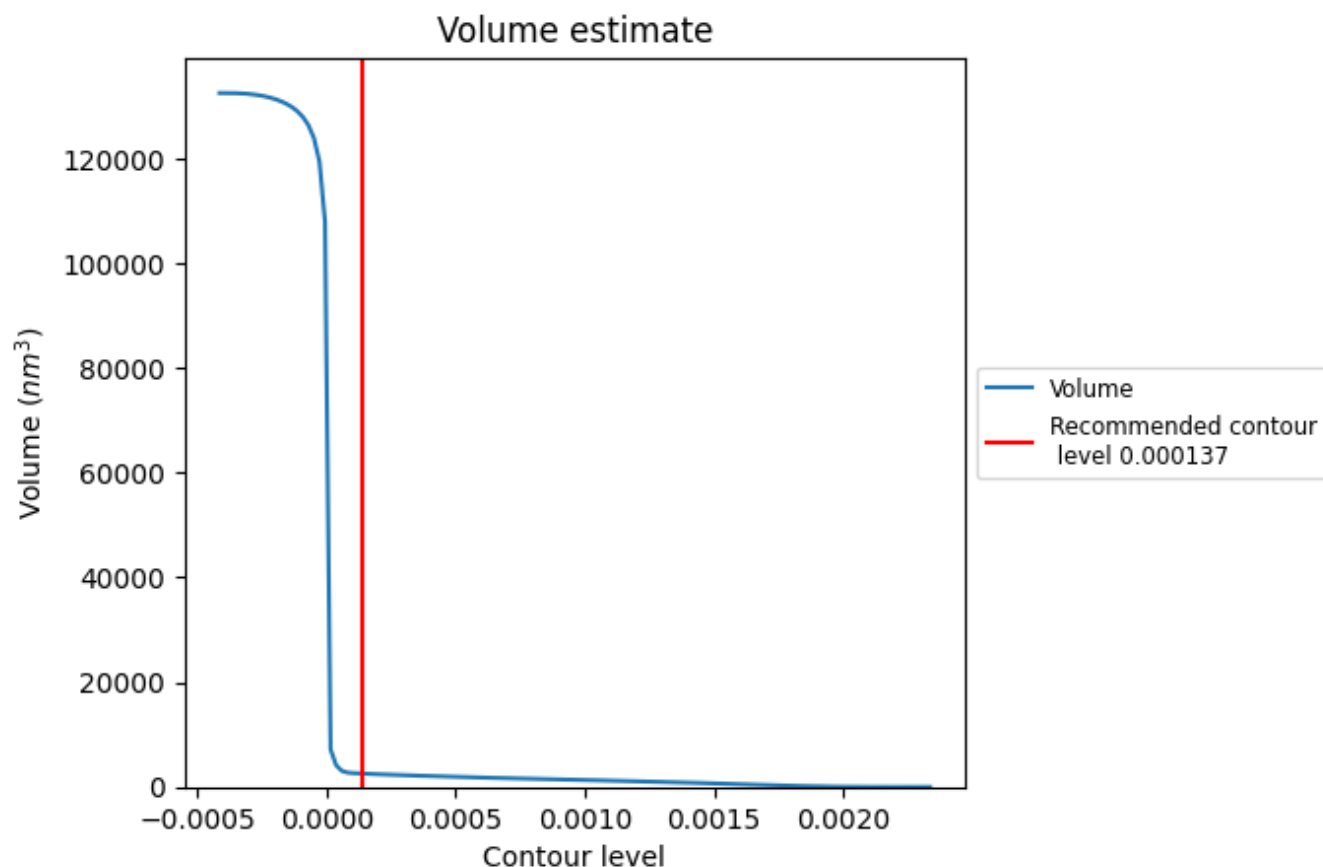
This section contains the results of statistical analysis of the map.

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.

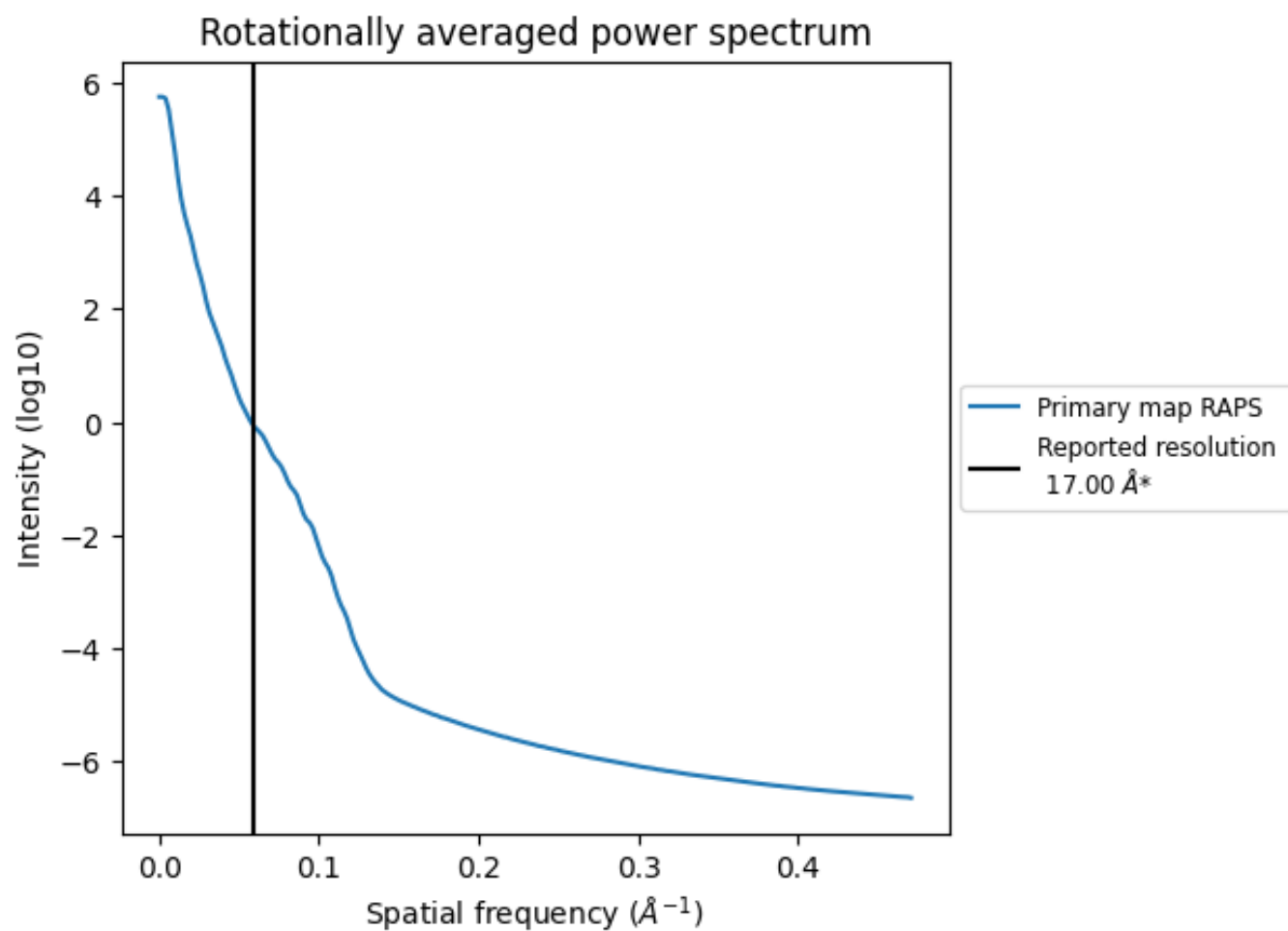
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2555 nm^3 ; this corresponds to an approximate mass of 2308 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 0.059 Å⁻¹

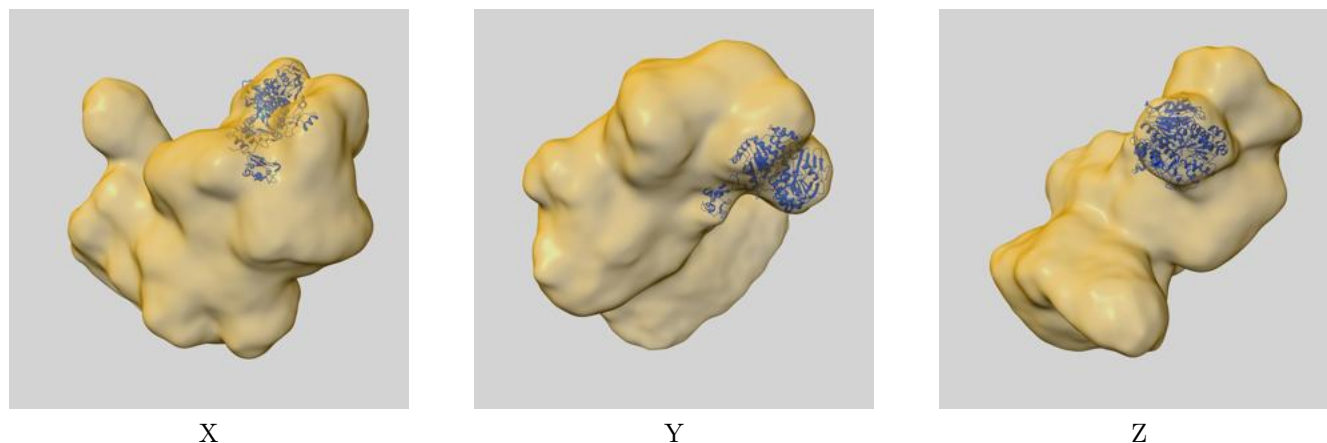
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

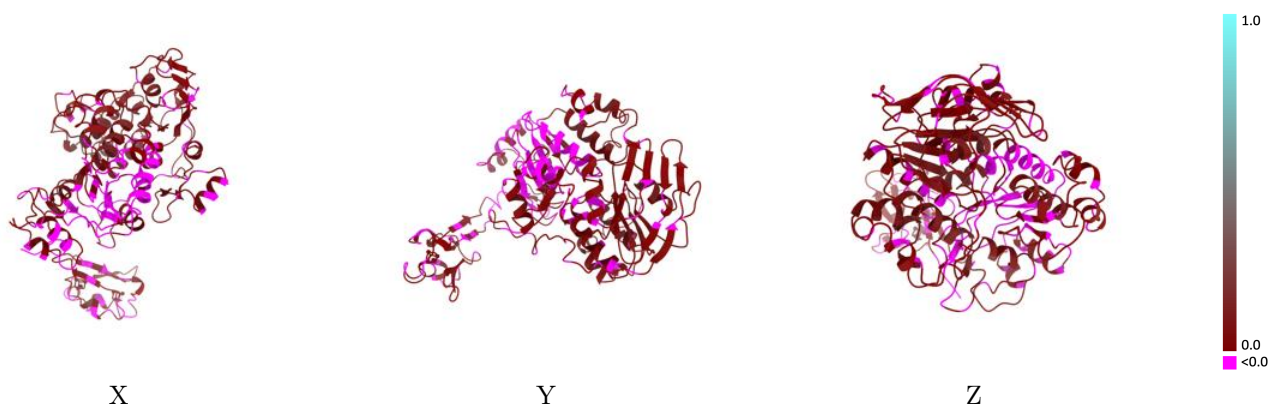
This section contains information regarding the fit between EMDB map EMD-4113 and PDB model 5LW7. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.000137 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](#)

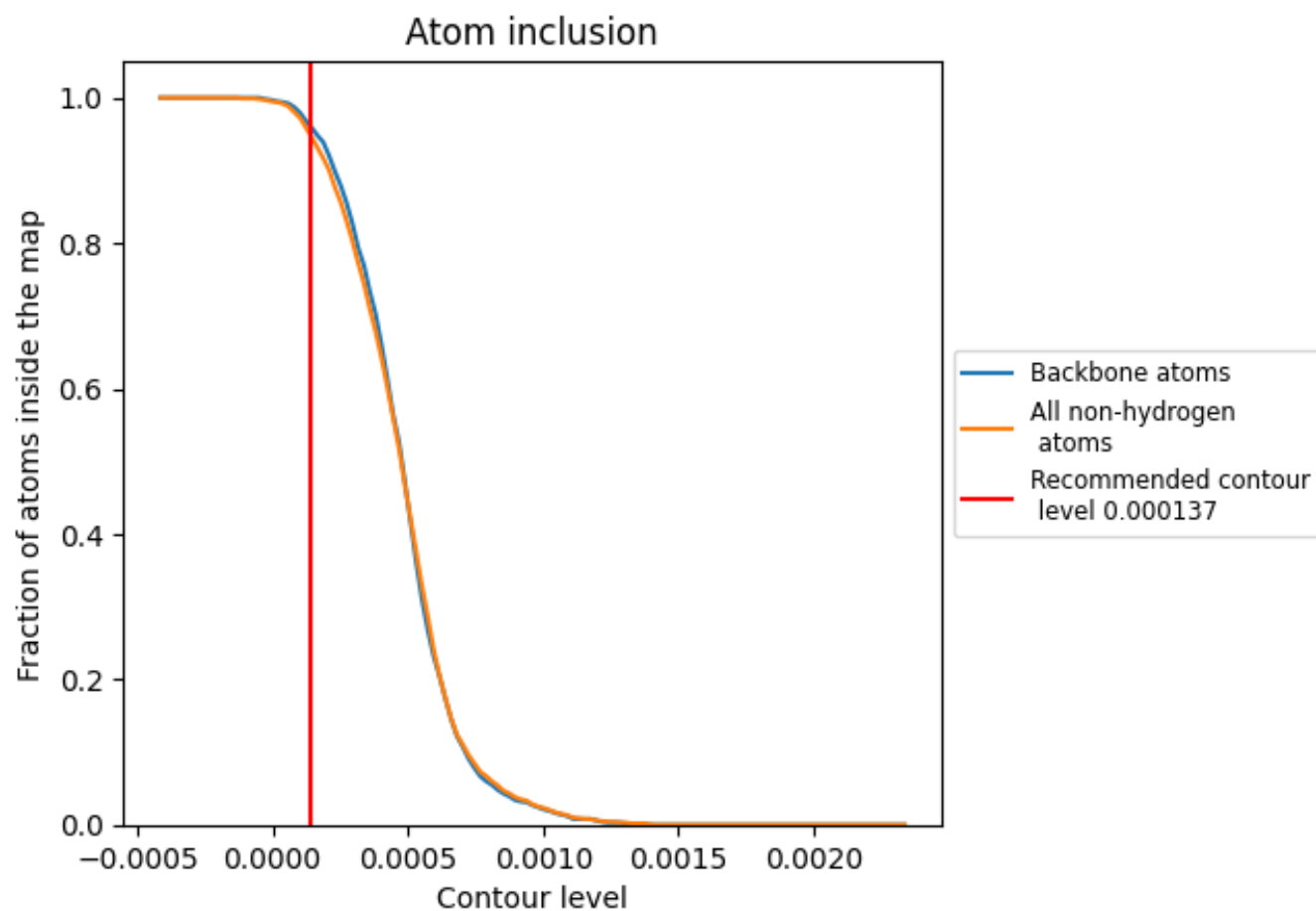


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.000137) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9500	0.0320
B	0.9500	0.0320

