



Full wwPDB EM Validation Report ⓘ

Oct 22, 2026 – 04:12 PM EDT

PDB ID : 10JE / pdb_000010je
EMDB ID : EMD-75214
Title : HIV-1 ADA.CM.755* Env (Mature VLPs)
Authors : Croft, J.T.; Lee, K.K.
Deposited on : 2026-01-22
Resolution : 8.60 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:

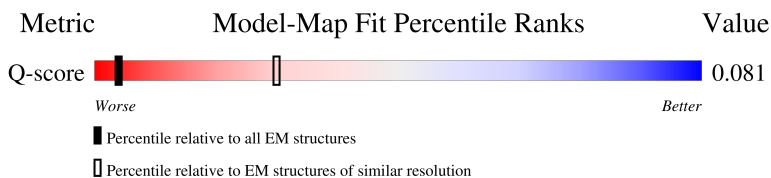
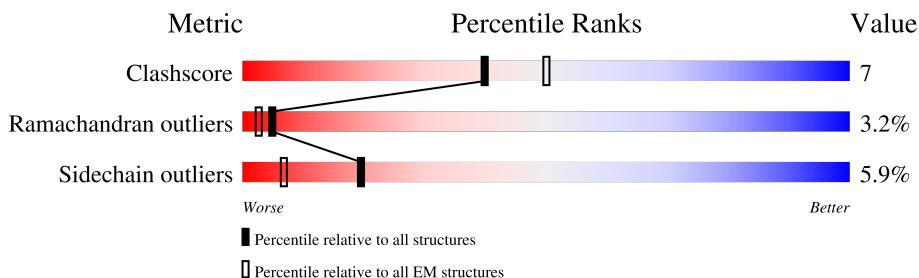
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

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 8.60 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	292 (8.10 - 9.10)

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	473	23% 72% 15% •• 11%
1	B	473	26% 74% 13% • 11%
1	C	473	22% 70% 15% • 11%
2	D	166	48% 63% 25% 6% • 5%

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Mol	Chain	Length	Quality of chain
2	E	166	43% 63% 27% 5% 5%
2	F	166	36% 66% 22% 6% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 27574 atoms, of which 13747 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 gp120.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	422	Total	C	H	N	O	S	0	0
			6613	2091	3298	575	624	25		
1	B	422	Total	C	H	N	O	S	0	0
			6612	2091	3297	575	624	25		
1	C	422	Total	C	H	N	O	S	0	0
			6612	2091	3297	575	624	25		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP Q6TAN8
A	?	-	ASN	deletion	UNP Q6TAN8
A	140	SER	ASN	conflict	UNP Q6TAN8
B	?	-	ILE	deletion	UNP Q6TAN8
B	?	-	ASN	deletion	UNP Q6TAN8
B	140	SER	ASN	conflict	UNP Q6TAN8
C	?	-	ILE	deletion	UNP Q6TAN8
C	?	-	ASN	deletion	UNP Q6TAN8
C	140	SER	ASN	conflict	UNP Q6TAN8

- Molecule 2 is a protein called gp41.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	158	Total	C	H	N	O	S	0	0
			2579	834	1285	225	229	6		
2	E	158	Total	C	H	N	O	S	0	0
			2579	834	1285	225	229	6		
2	F	158	Total	C	H	N	O	S	0	0
			2579	834	1285	225	229	6		

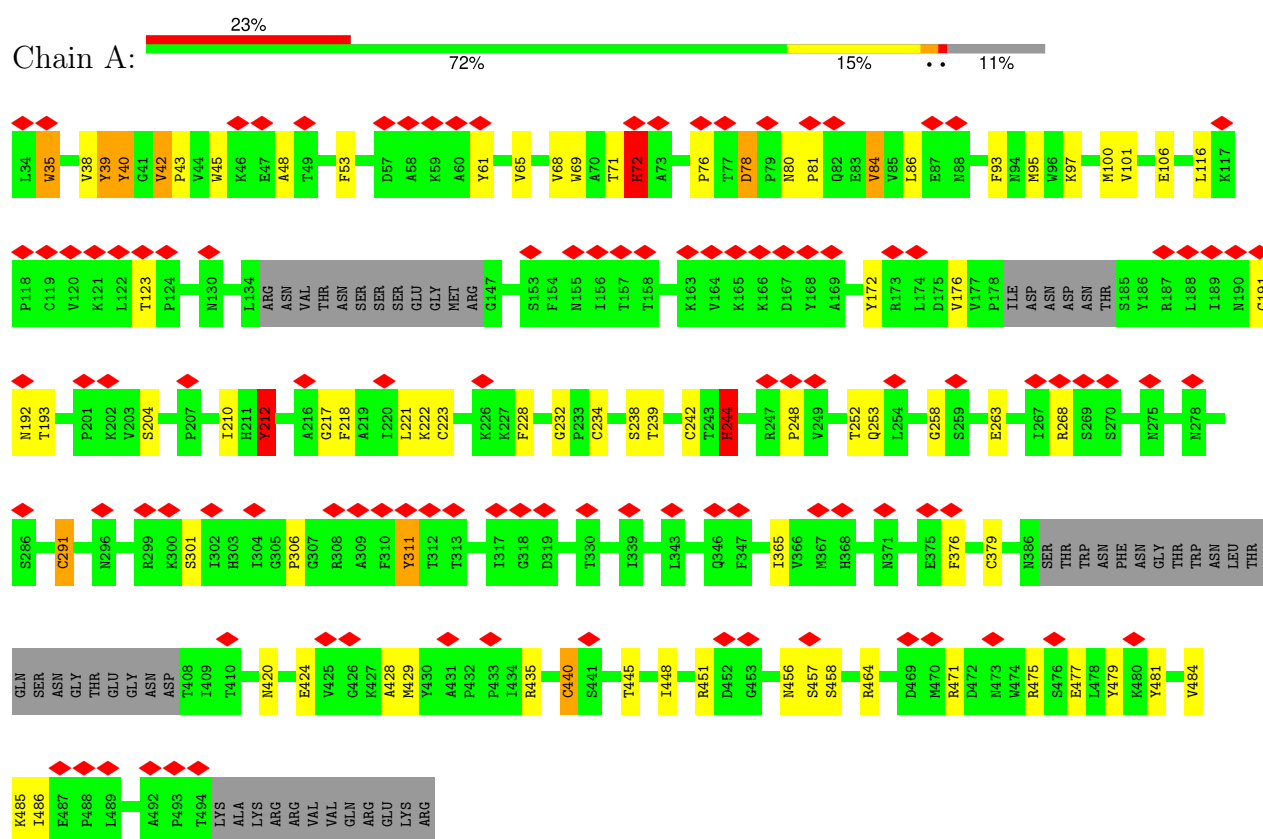
There are 12 discrepancies between the modelled and reference sequences:

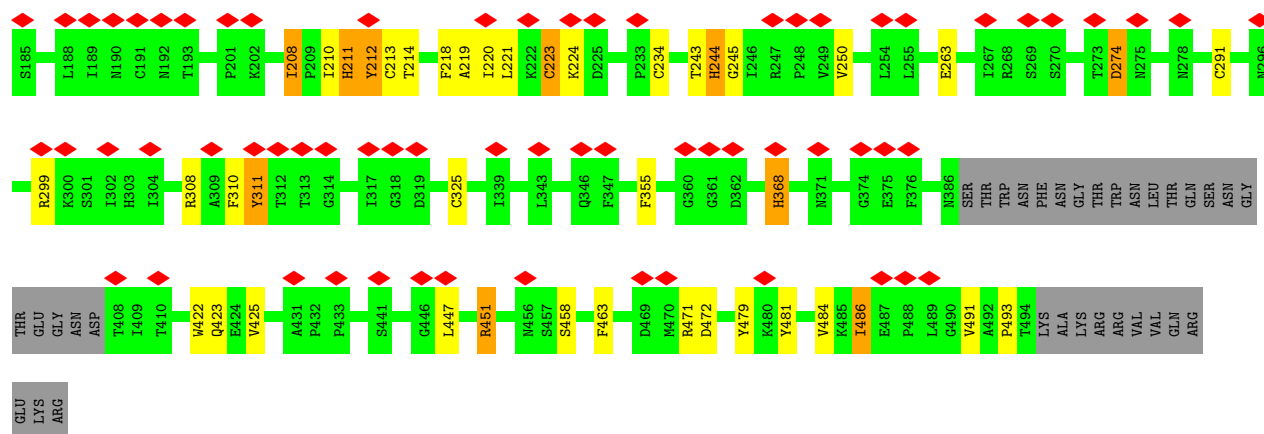
Chain	Residue	Modelled	Actual	Comment	Reference
D	535	MET	ILE	conflict	UNP A0A060L0P2
D	543	GLN	LEU	conflict	UNP A0A060L0P2
D	574	ARG	LYS	conflict	UNP A0A060L0P2
D	674	ASN	ASP	conflict	UNP A0A060L0P2
E	535	MET	ILE	conflict	UNP A0A060L0P2
E	543	GLN	LEU	conflict	UNP A0A060L0P2
E	574	ARG	LYS	conflict	UNP A0A060L0P2
E	674	ASN	ASP	conflict	UNP A0A060L0P2
F	535	MET	ILE	conflict	UNP A0A060L0P2
F	543	GLN	LEU	conflict	UNP A0A060L0P2
F	574	ARG	LYS	conflict	UNP A0A060L0P2
F	674	ASN	ASP	conflict	UNP A0A060L0P2

3 Residue-property plots

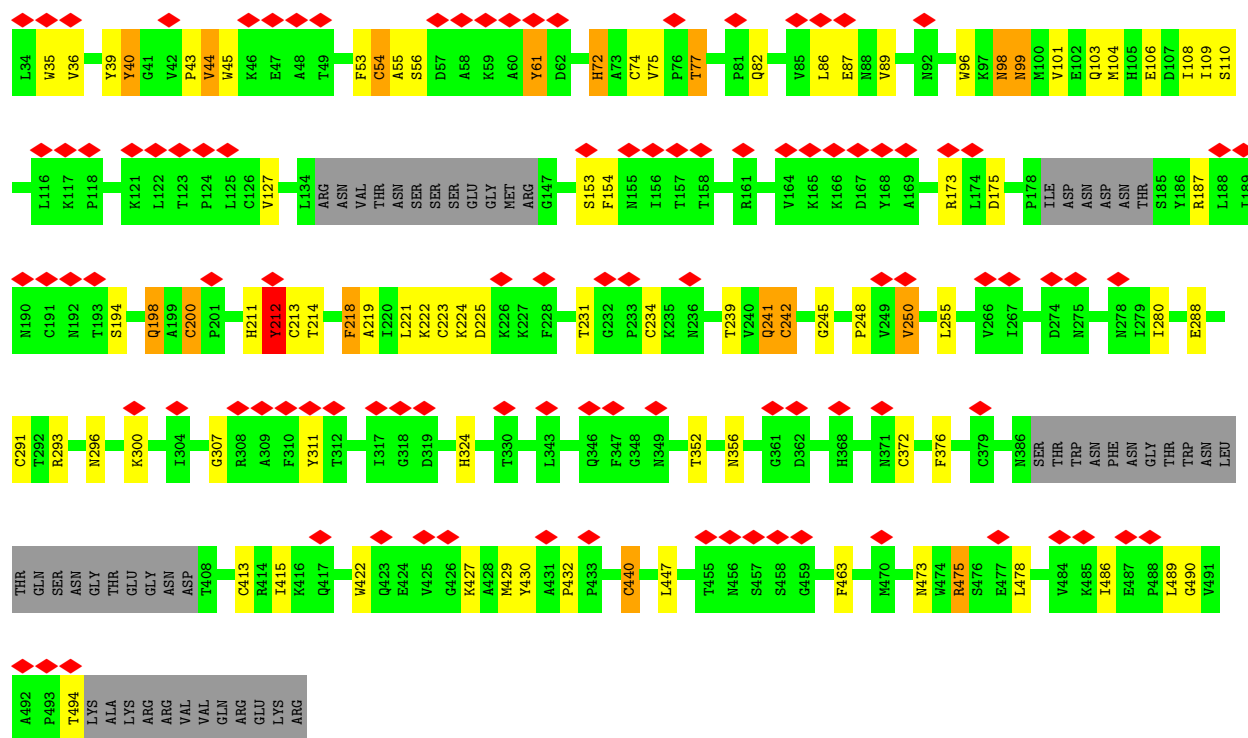
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: gp120

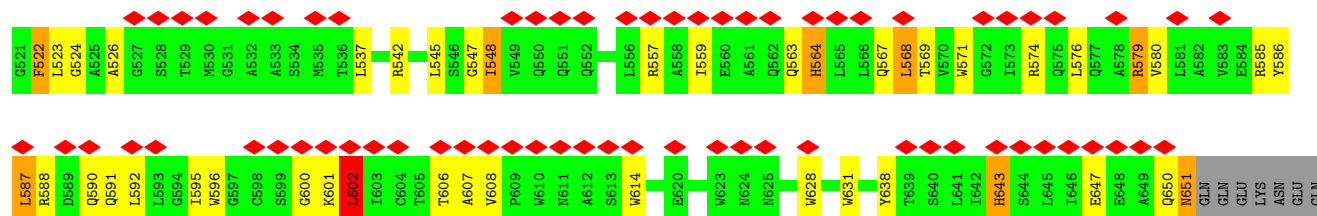


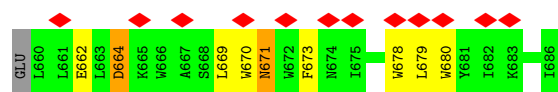


• Molecule 1: gp120

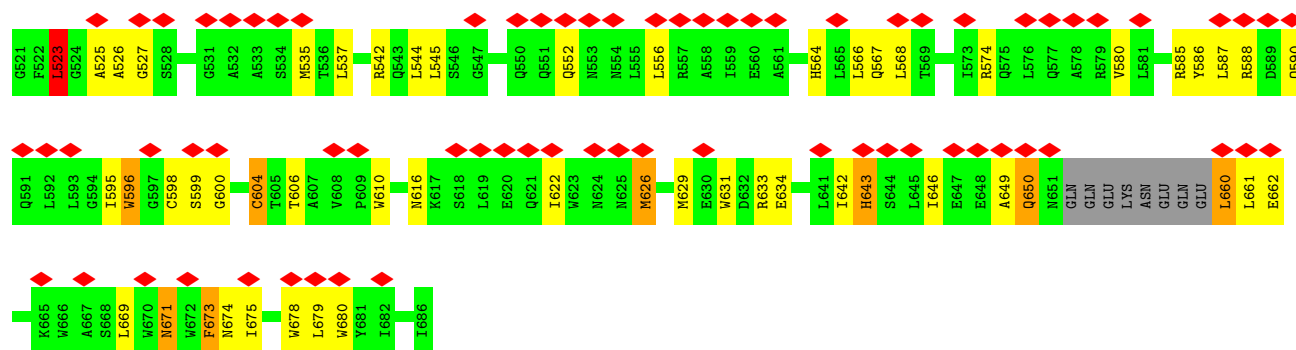
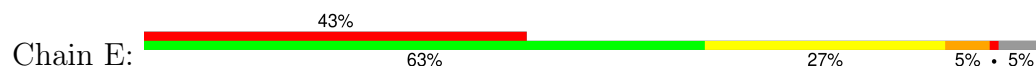


• Molecule 2: gp41

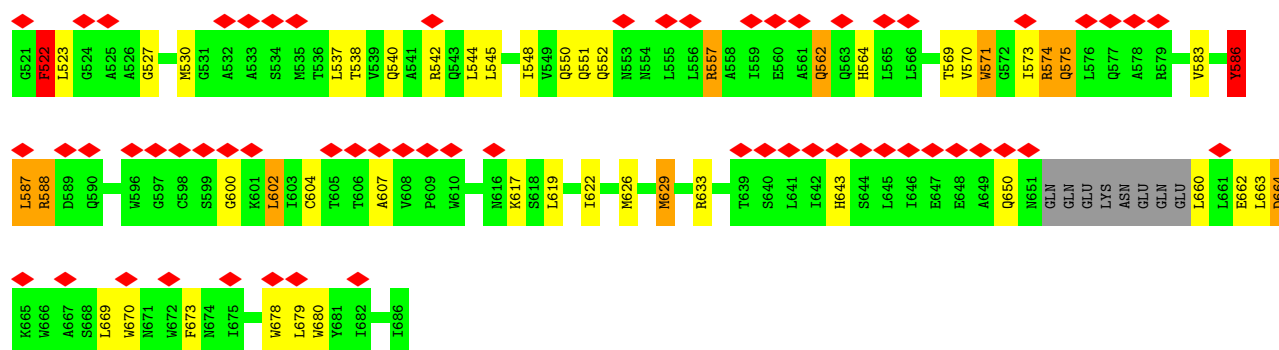




• Molecule 2: gp41



• Molecule 2: gp41



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	18619	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	18.946	Depositor
Minimum map value	-16.488	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.967	Depositor
Recommended contour level	4.6	Depositor
Map size (Å)	309.59998, 309.59998, 309.59998	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.5799997, 2.5799997, 2.5799997	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	1.72	5/3385 (0.1%)	1.55	27/4597 (0.6%)
1	B	0.89	0/3385	1.50	23/4597 (0.5%)
1	C	0.89	0/3385	1.54	23/4597 (0.5%)
2	D	1.13	2/1325 (0.2%)	1.72	18/1803 (1.0%)
2	E	2.03	3/1325 (0.2%)	1.87	25/1803 (1.4%)
2	F	0.95	1/1325 (0.1%)	1.73	17/1803 (0.9%)
All	All	1.30	11/14130 (0.1%)	1.60	133/19200 (0.7%)

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	5
1	B	0	11
1	C	0	7
2	D	0	2
2	E	0	2
2	F	0	3
All	All	0	30

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	671	ASN	CG-ND2	64.49	2.68	1.33
1	A	35	TRP	NE1-CE2	55.62	1.98	1.37
1	A	35	TRP	CG-CD2	44.18	2.23	1.43
1	A	35	TRP	CD2-CE2	34.63	2.00	1.41
1	A	35	TRP	CD1-NE1	29.63	2.00	1.37
2	D	650	GLN	C-N	-19.04	1.06	1.33
1	A	35	TRP	CG-CD1	17.88	1.81	1.36
2	F	650	GLN	C-N	-11.95	1.16	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	650	GLN	C-N	-8.04	1.22	1.33
2	E	671	ASN	CB-CG	6.21	1.67	1.52
2	D	602	LEU	CA-C	5.12	1.59	1.52

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	650	GLN	CA-C-N	18.68	155.31	121.70
2	F	650	GLN	C-N-CA	18.68	155.31	121.70
2	E	650	GLN	O-C-N	-16.23	101.01	122.59
2	E	650	GLN	CA-C-N	13.29	145.62	121.70
2	E	650	GLN	C-N-CA	13.29	145.62	121.70
2	E	671	ASN	CB-CG-OD1	-13.23	94.35	120.80
1	A	35	TRP	CG-CD2-CE3	12.38	146.28	133.90
1	C	218	PHE	CA-CB-CG	12.09	125.89	113.80
2	E	671	ASN	CB-CG-ND2	12.04	134.46	116.40
2	D	650	GLN	CA-C-N	10.97	141.45	121.70
2	D	650	GLN	C-N-CA	10.97	141.45	121.70
2	F	650	GLN	O-C-N	-10.09	109.86	122.27
1	A	35	TRP	CE2-CD2-CE3	-10.03	108.77	118.80
2	D	650	GLN	O-C-N	-9.15	110.50	122.39
2	E	671	ASN	N-CA-CB	8.61	122.47	109.98
2	E	671	ASN	OD1-CG-ND2	8.57	131.18	122.60
2	F	664	ASP	CA-CB-CG	7.93	120.53	112.60
1	B	458	SER	N-CA-C	7.62	121.67	112.38
1	A	244	HIS	CA-CB-CG	7.54	121.34	113.80
2	D	567	GLN	CA-C-N	7.50	135.86	121.54
2	D	567	GLN	C-N-CA	7.50	135.86	121.54
1	A	244	HIS	CB-CG-CD2	-7.47	121.49	131.20
2	D	662	GLU	CA-C-N	7.25	130.00	120.28
2	D	662	GLU	C-N-CA	7.25	130.00	120.28
1	A	451	ARG	NE-CZ-NH2	7.24	125.72	119.20
1	B	310	PHE	CA-CB-CG	6.95	120.75	113.80
2	E	673	PHE	CA-CB-CG	-6.93	106.87	113.80
1	A	35	TRP	CD2-CE2-CZ2	-6.88	115.52	122.40
1	B	274	ASP	CA-CB-CG	6.84	119.44	112.60
2	E	643	HIS	CA-CB-CG	-6.84	106.95	113.80
2	D	608	VAL	N-CA-CB	-6.79	103.77	110.08
1	C	72	HIS	CA-CB-CG	6.78	120.58	113.80
1	A	457	SER	N-CA-C	6.75	125.19	110.80
2	E	643	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	C	447	LEU	CA-C-N	6.51	130.25	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	447	LEU	C-N-CA	6.51	130.25	120.95
1	A	40	TYR	CB-CA-C	6.46	123.28	110.42
1	B	311	TYR	N-CA-C	6.37	119.89	109.06
2	F	633	ARG	NE-CZ-NH2	6.37	124.94	119.20
1	C	54	CYS	N-CA-CB	-6.34	99.78	110.49
1	A	80	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	228	PHE	CA-CB-CG	6.30	120.10	113.80
2	F	574	ARG	CD-NE-CZ	6.26	133.17	124.40
1	B	102	GLU	N-CA-C	-6.20	104.44	111.14
1	C	98	ASN	CA-C-N	6.20	133.38	121.54
1	C	98	ASN	C-N-CA	6.20	133.38	121.54
2	E	564	HIS	CB-CG-CD2	-6.18	123.16	131.20
1	A	172	TYR	CA-C-N	6.11	128.75	120.38
1	A	172	TYR	C-N-CA	6.11	128.75	120.38
2	E	574	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	C	475	ARG	NE-CZ-NH2	6.03	124.63	119.20
2	E	588	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	C	212	TYR	CA-CB-CG	6.00	124.71	113.90
2	F	522	PHE	CA-CB-CG	5.92	119.72	113.80
2	F	586	TYR	CB-CG-CD2	-5.89	111.96	120.80
1	A	78	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	39	TYR	CA-CB-CG	5.82	124.38	113.90
1	B	218	PHE	CA-CB-CG	5.81	119.61	113.80
2	D	579	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	C	250	VAL	N-CA-C	5.79	116.64	108.36
1	B	173	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	B	208	ILE	CA-C-N	5.76	127.04	119.84
1	B	208	ILE	C-N-CA	5.76	127.04	119.84
1	C	99	ASN	N-CA-C	5.74	123.02	110.80
1	A	456	ASN	CA-C-N	5.70	132.42	121.54
1	A	456	ASN	C-N-CA	5.70	132.42	121.54
2	D	651	ASN	CA-CB-CG	-5.68	106.92	112.60
1	A	471	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	B	368	HIS	CA-CB-CG	5.67	119.47	113.80
2	D	568	LEU	N-CA-C	5.67	122.88	110.80
1	B	451	ARG	NE-CZ-NH2	5.67	124.30	119.20
2	E	662	GLU	CA-C-N	5.66	127.87	120.28
2	E	662	GLU	C-N-CA	5.66	127.87	120.28
2	D	563	GLN	CA-CB-CG	5.63	125.37	114.10
1	A	116	LEU	CA-C-N	5.63	127.80	120.26
1	A	116	LEU	C-N-CA	5.63	127.80	120.26
1	A	72	HIS	CB-CG-CD2	-5.63	123.89	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	571	TRP	CA-CB-CG	-5.62	102.93	113.60
1	C	77	THR	CA-C-N	5.60	129.17	120.60
1	C	77	THR	C-N-CA	5.60	129.17	120.60
2	F	586	TYR	CA-CB-CG	5.60	123.99	113.90
1	C	432	PRO	N-CA-CB	5.59	106.32	103.19
2	D	671	ASN	CA-CB-CG	5.59	118.19	112.60
1	B	211	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	B	78	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	232	GLY	CA-C-N	5.48	126.69	119.84
1	A	232	GLY	C-N-CA	5.48	126.69	119.84
2	D	547	GLY	CA-C-N	5.47	131.81	121.97
2	D	547	GLY	C-N-CA	5.47	131.81	121.97
2	F	662	GLU	N-CA-C	5.46	122.42	110.80
2	F	550	GLN	OE1-CD-NE2	-5.44	117.16	122.60
2	E	596	TRP	CA-CB-CG	5.38	123.83	113.60
2	E	574	ARG	CD-NE-CZ	5.38	131.93	124.40
2	E	568	LEU	N-CA-CB	-5.38	102.83	110.46
1	A	210	ILE	N-CA-CB	-5.36	104.32	110.49
2	F	542	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	C	356	ASN	CA-C-N	5.33	129.26	121.31
1	C	356	ASN	C-N-CA	5.33	129.26	121.31
2	D	664	ASP	CA-CB-CG	5.32	117.92	112.60
2	F	562	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	C	36	VAL	N-CA-C	5.30	120.37	109.34
1	B	77	THR	N-CA-C	5.29	117.16	110.33
1	A	268	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	C	175	ASP	CA-CB-CG	-5.25	107.35	112.60
2	D	564	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	B	244	HIS	CB-CG-CD2	-5.24	124.38	131.20
1	C	153	SER	N-CA-C	5.23	117.02	109.07
1	B	223	CYS	CA-C-N	5.22	131.51	121.54
1	B	223	CYS	C-N-CA	5.22	131.51	121.54
2	E	595	ILE	CA-CB-CG2	5.22	119.37	110.50
1	B	105	HIS	CB-CG-CD2	-5.20	124.44	131.20
2	E	633	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	81	PRO	N-CA-CB	5.19	107.87	103.35
2	E	590	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	472	ASP	CA-CB-CG	5.18	117.78	112.60
2	F	575	GLN	CB-CG-CD	5.16	121.38	112.60
2	D	643	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	B	58	ALA	CA-C-N	5.14	130.29	122.11
1	B	58	ALA	C-N-CA	5.14	130.29	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	574	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	C	241	GLN	OE1-CD-NE2	-5.13	117.47	122.60
2	F	540	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	C	463	PHE	CA-CB-CG	-5.11	108.69	113.80
2	E	622	ILE	CB-CA-C	5.10	116.29	111.44
1	C	352	THR	CA-C-N	5.08	128.16	120.13
1	C	352	THR	C-N-CA	5.08	128.16	120.13
1	B	93	PHE	CA-CB-CG	-5.08	108.72	113.80
2	E	525	ALA	N-CA-C	5.06	117.69	111.82
1	B	308	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	E	604	CYS	N-CA-C	5.05	117.04	110.43
1	A	448	ILE	CB-CA-C	5.02	118.06	110.63
1	A	42	VAL	N-CA-C	-5.01	98.05	108.88
2	E	673	PHE	CA-C-O	-5.01	113.34	120.51

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	TYR	Sidechain
1	A	244	HIS	Sidechain
1	A	311	TYR	Sidechain
1	A	40	TYR	Sidechain
1	A	72	HIS	Sidechain
1	B	211	HIS	Sidechain
1	B	212	TYR	Sidechain
1	B	244	HIS	Sidechain
1	B	299	ARG	Sidechain
1	B	311	TYR	Sidechain
1	B	39	TYR	Sidechain
1	B	40	TYR	Sidechain
1	B	471	ARG	Sidechain
1	B	479	TYR	Sidechain
1	B	481	TYR	Sidechain
1	B	53	PHE	Sidechain
1	C	173	ARG	Sidechain
1	C	212	TYR	Sidechain
1	C	218	PHE	Sidechain
1	C	293	ARG	Sidechain
1	C	311	TYR	Sidechain
1	C	430	TYR	Sidechain
1	C	61	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	D	522	PHE	Sidechain
2	D	638	TYR	Sidechain
2	E	585	ARG	Sidechain
2	E	643	HIS	Sidechain
2	F	557	ARG	Sidechain
2	F	586	TYR	Sidechain
2	F	643	HIS	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3315	3298	3291	75	0
1	B	3315	3297	3291	39	0
1	C	3315	3297	3291	45	0
2	D	1294	1285	1280	41	0
2	E	1294	1285	1280	53	0
2	F	1294	1285	1280	32	0
All	All	13827	13747	13713	196	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 7.

All (196) 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:35:TRP:CG	1:A:35:TRP:CD1	1.81	1.65
1:A:35:TRP:CD2	1:A:35:TRP:CE2	2.00	1.49
1:A:35:TRP:CE2	1:A:35:TRP:NE1	1.98	1.29
1:A:35:TRP:CD1	1:A:35:TRP:NE1	2.00	1.29
1:A:35:TRP:CG	1:A:35:TRP:CD2	2.23	1.26
1:A:35:TRP:CD2	2:E:671:ASN:CG	2.15	1.24
1:A:35:TRP:CE2	2:E:671:ASN:CG	2.19	1.21
1:A:35:TRP:CG	2:E:671:ASN:CG	2.18	1.20
1:A:35:TRP:CD1	2:E:671:ASN:CG	2.20	1.19
1:A:35:TRP:CD2	2:E:671:ASN:ND2	2.14	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CG	2:E:671:ASN:ND2	2.16	1.15
1:A:35:TRP:CE2	2:E:671:ASN:ND2	2.16	1.14
1:A:35:TRP:CD1	2:E:671:ASN:ND2	2.17	1.12
1:A:35:TRP:NE1	2:E:671:ASN:CG	2.19	1.00
1:A:35:TRP:NE1	2:E:671:ASN:ND2	2.18	0.91
1:A:35:TRP:CD2	2:E:671:ASN:CB	2.58	0.87
1:A:86:LEU:HD22	2:D:526:ALA:HB3	1.60	0.83
1:A:35:TRP:CD1	2:E:671:ASN:OD1	2.40	0.74
1:A:35:TRP:CD1	2:E:671:ASN:HD21	2.06	0.69
1:A:221:LEU:CD2	2:D:523:LEU:HD21	2.22	0.68
1:A:252:THR:HG21	1:A:365:ILE:HA	1.76	0.68
1:A:35:TRP:CD2	2:E:671:ASN:HB2	2.27	0.67
1:A:239:THR:OG1	2:D:523:LEU:HD13	1.98	0.63
1:C:44:VAL:HG11	1:C:489:LEU:HD12	1.82	0.61
1:A:35:TRP:CE3	2:D:607:ALA:HA	2.36	0.60
1:A:35:TRP:CE3	2:E:671:ASN:HB2	2.36	0.60
1:B:491:VAL:HG11	2:E:642:ILE:HG23	1.84	0.59
1:B:54:CYS:SG	1:B:74:CYS:HA	2.43	0.59
1:A:221:LEU:HD22	2:D:523:LEU:HD21	1.85	0.59
1:B:221:LEU:CD1	1:B:484:VAL:HG11	2.33	0.58
2:E:545:LEU:HD22	2:F:588:ARG:HA	1.86	0.58
1:C:43:PRO:O	2:F:629:MET:HE2	2.04	0.57
1:C:494:THR:HA	2:F:619:LEU:HD12	1.85	0.56
2:D:643:HIS:CE1	2:F:551:GLN:HE22	2.23	0.56
1:A:239:THR:HB	2:D:523:LEU:HD22	1.88	0.56
1:A:218:PHE:HA	1:A:486:ILE:H	1.71	0.56
1:C:54:CYS:SG	1:C:74:CYS:HB2	2.46	0.55
1:A:239:THR:N	2:D:523:LEU:HD22	2.21	0.55
1:B:41:GLY:HA3	2:E:537:LEU:HD23	1.89	0.55
1:C:61:TYR:HA	1:C:72:HIS:CE1	2.42	0.54
1:B:221:LEU:HD12	1:B:484:VAL:HG11	1.88	0.54
1:C:72:HIS:CE1	2:F:564:HIS:CG	2.95	0.54
1:A:68:VAL:HG23	1:A:204:SER:O	2.07	0.54
1:B:101:VAL:HA	1:B:104:MET:HE2	1.90	0.53
1:B:486:ILE:HD13	2:E:523:LEU:HD21	1.90	0.53
1:C:211:HIS:HB3	1:C:242:CYS:SG	2.49	0.52
1:A:86:LEU:HD21	2:D:523:LEU:HG	1.92	0.52
1:C:39:TYR:O	1:C:39:TYR:CG	2.63	0.52
2:D:647:GLU:HG2	2:F:545:LEU:HD22	1.92	0.52
2:E:671:ASN:CG	2:E:671:ASN:ND2	2.68	0.52
2:E:552:GLN:HE22	2:E:556:LEU:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:VAL:HG21	1:C:154:PHE:CD2	2.45	0.51
1:A:35:TRP:CZ3	2:E:671:ASN:HA	2.46	0.51
1:B:53:PHE:C	1:B:53:PHE:CD1	2.85	0.51
1:C:55:ALA:HA	1:C:75:VAL:O	2.09	0.51
1:B:35:TRP:CD1	1:B:36:VAL:H	2.28	0.51
2:E:660:LEU:HD13	2:F:680:TRP:CH2	2.45	0.51
1:A:244:HIS:CD2	1:A:477:GLU:CD	2.88	0.51
1:C:96:TRP:HZ3	1:C:231:THR:HG23	1.76	0.50
1:C:54:CYS:HG	1:C:74:CYS:CB	2.23	0.50
1:B:41:GLY:HA3	2:E:537:LEU:HA	1.93	0.50
2:D:537:LEU:CB	2:D:602:LEU:HD13	2.42	0.50
1:A:35:TRP:CE2	2:E:671:ASN:HA	2.47	0.50
1:C:40:TYR:CD2	1:C:490:GLY:HA3	2.47	0.50
1:A:69:TRP:CZ3	1:A:248:PRO:HG3	2.47	0.49
2:E:626:MET:HE1	2:E:631:TRP:HB2	1.94	0.49
2:E:660:LEU:HD23	2:F:670:TRP:CE2	2.47	0.49
2:D:537:LEU:HB2	2:D:602:LEU:HD13	1.94	0.49
1:C:222:LYS:HE3	1:C:224:LYS:HE2	1.92	0.49
1:C:110:SER:HB3	2:F:570:VAL:HG22	1.95	0.49
2:F:629:MET:HE3	2:F:629:MET:H	1.78	0.49
1:B:493:PRO:HB3	2:E:610:TRP:CZ2	2.48	0.48
1:C:54:CYS:SG	1:C:74:CYS:CB	3.01	0.48
1:B:45:TRP:CZ3	1:B:221:LEU:HD13	2.48	0.48
1:B:89:VAL:HG23	2:E:527:GLY:HA2	1.95	0.48
2:F:570:VAL:HG12	2:F:574:ARG:HD3	1.96	0.48
1:A:95:MET:HE3	1:A:479:TYR:CG	2.49	0.48
1:A:97:LYS:HA	1:A:97:LYS:HE2	1.96	0.48
1:B:89:VAL:CG1	2:E:629:MET:HE1	2.43	0.48
1:C:55:ALA:HB2	1:C:213:CYS:SG	2.54	0.48
1:C:104:MET:SD	1:C:478:LEU:HD22	2.54	0.48
1:C:239:THR:HG21	2:F:523:LEU:HD23	1.95	0.48
1:A:35:TRP:CE3	2:E:671:ASN:CB	2.96	0.48
1:A:35:TRP:CZ3	2:D:607:ALA:HA	2.49	0.48
1:A:78:ASP:HB2	1:A:242:CYS:SG	2.53	0.48
1:B:208:ILE:HG22	1:B:210:ILE:HG23	1.96	0.48
1:B:45:TRP:CD2	1:B:221:LEU:HD11	2.48	0.48
1:A:35:TRP:CH2	2:E:671:ASN:HA	2.48	0.47
1:B:89:VAL:HG13	2:E:629:MET:HE1	1.95	0.47
1:C:56:SER:HB3	1:C:74:CYS:SG	2.55	0.47
1:C:250:VAL:HA	1:C:422:TRP:CH2	2.49	0.47
1:B:54:CYS:SG	1:B:74:CYS:SG	3.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ALA:HB3	1:B:486:ILE:CD1	2.45	0.47
1:B:219:ALA:HB3	1:B:486:ILE:HD11	1.96	0.47
1:A:258:GLY:O	1:A:445:THR:HG21	2.14	0.47
1:B:89:VAL:CG2	2:E:526:ALA:C	2.88	0.47
1:A:35:TRP:CE2	2:E:671:ASN:CA	2.97	0.47
1:C:53:PHE:HA	2:F:571:TRP:CZ3	2.49	0.47
2:D:670:TRP:CZ3	2:F:660:LEU:HA	2.48	0.47
1:C:55:ALA:HB1	1:C:77:THR:HB	1.96	0.47
1:C:219:ALA:HB3	1:C:486:ILE:HD11	1.97	0.47
1:A:475:ARG:HB3	1:A:479:TYR:CE1	2.49	0.46
1:C:72:HIS:CE1	2:F:564:HIS:CD2	3.03	0.46
1:C:110:SER:HB3	2:F:570:VAL:CG2	2.44	0.46
2:D:587:LEU:HD12	2:F:583:VAL:HA	1.98	0.46
1:A:42:VAL:HG11	2:D:628:TRP:CE2	2.51	0.46
1:A:223:CYS:SG	1:A:234:CYS:SG	3.11	0.46
1:A:35:TRP:CZ2	2:E:671:ASN:HA	2.50	0.46
1:C:45:TRP:CH2	1:C:86:LEU:HD21	2.50	0.46
1:C:54:CYS:HB2	2:F:571:TRP:CE3	2.51	0.46
1:A:38:VAL:CG2	2:D:596:TRP:CZ3	3.00	0.45
1:C:86:LEU:HD23	1:C:89:VAL:HG11	1.97	0.45
2:E:544:LEU:HD22	2:E:586:TYR:CD1	2.51	0.45
2:D:595:ILE:HG23	2:D:651:ASN:HB2	1.99	0.45
2:F:530:MET:H	2:F:626:MET:HB3	1.81	0.45
1:A:38:VAL:HG22	2:D:596:TRP:CZ3	2.52	0.45
1:A:42:VAL:HG23	2:D:526:ALA:HA	1.99	0.45
2:F:569:THR:HG23	2:F:571:TRP:H	1.81	0.45
1:A:217:GLY:HA3	2:D:585:ARG:HH12	1.81	0.45
1:B:109:ILE:HG12	1:B:422:TRP:CD2	2.51	0.45
1:A:212:TYR:N	1:A:212:TYR:CD1	2.85	0.45
1:B:35:TRP:CZ3	1:B:37:THR:HG21	2.52	0.45
1:B:45:TRP:CZ3	2:E:629:MET:HE1	2.52	0.45
1:C:222:LYS:HE3	1:C:224:LYS:CE	2.46	0.45
2:D:614:TRP:CH2	2:D:631:TRP:CD1	3.05	0.45
1:C:35:TRP:CD1	1:C:35:TRP:C	2.95	0.44
1:C:198:GLN:HG2	1:C:200:CYS:H	1.82	0.44
1:B:220:ILE:HD13	1:B:243:THR:HG23	1.99	0.44
1:C:55:ALA:HB3	1:C:211:HIS:O	2.17	0.44
1:A:93:PHE:CD1	1:A:223:CYS:SG	3.10	0.44
2:D:592:LEU:HD11	2:D:596:TRP:HE1	1.82	0.44
1:A:43:PRO:HG2	2:D:526:ALA:HB2	2.00	0.44
1:A:86:LEU:HD23	2:D:524:GLY:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:VAL:HG21	1:C:154:PHE:CE2	2.52	0.44
1:A:35:TRP:CE2	2:E:671:ASN:O	2.71	0.44
1:A:218:PHE:CD2	1:A:485:LYS:HA	2.52	0.44
1:C:486:ILE:HG23	2:F:522:PHE:CD2	2.53	0.44
2:D:522:PHE:CD2	2:D:523:LEU:HD12	2.53	0.44
1:A:86:LEU:HD22	2:D:526:ALA:CB	2.39	0.44
1:A:239:THR:CA	2:D:523:LEU:HD22	2.48	0.44
1:B:45:TRP:CE3	2:E:629:MET:CE	3.01	0.44
2:D:591:GLN:HB2	2:F:586:TYR:CE2	2.53	0.44
2:E:629:MET:HE3	2:E:629:MET:HB2	1.78	0.44
2:E:598:CYS:HG	2:E:604:CYS:CB	2.31	0.43
1:A:193:THR:HA	1:C:307:GLY:N	2.33	0.43
1:B:45:TRP:CZ3	2:E:629:MET:CE	3.01	0.43
1:B:72:HIS:CG	1:B:73:ALA:N	2.87	0.43
1:C:45:TRP:CZ2	1:C:86:LEU:HD21	2.52	0.43
1:A:93:PHE:CG	1:A:223:CYS:SG	3.11	0.43
1:A:45:TRP:HB2	1:A:484:VAL:HB	1.99	0.43
1:B:54:CYS:HA	1:B:212:TYR:CE2	2.54	0.43
1:C:101:VAL:HG11	1:C:475:ARG:HB2	2.01	0.43
2:D:576:LEU:O	2:D:580:VAL:HG23	2.18	0.43
1:A:53:PHE:HB3	2:D:571:TRP:CZ2	2.52	0.43
1:C:372:CYS:SG	1:C:440:CYS:HB3	2.59	0.43
2:E:587:LEU:HD21	2:F:587:LEU:HD21	2.01	0.43
2:E:596:TRP:NE1	2:E:649:ALA:HB3	2.34	0.43
1:B:223:CYS:SG	1:B:234:CYS:SG	3.16	0.43
1:B:72:HIS:CG	1:B:73:ALA:H	2.36	0.42
2:D:595:ILE:HD11	2:F:544:LEU:HB2	2.01	0.42
1:A:35:TRP:CE2	2:E:671:ASN:CB	3.01	0.42
1:A:239:THR:CB	2:D:523:LEU:HD13	2.49	0.42
1:B:45:TRP:CZ2	2:E:526:ALA:CB	3.02	0.42
1:B:212:TYR:CD1	1:B:212:TYR:N	2.87	0.42
1:B:451:ARG:HA	1:B:463:PHE:HA	2.01	0.42
2:F:571:TRP:CE3	2:F:575:GLN:HG3	2.55	0.42
1:A:86:LEU:HD21	2:D:523:LEU:CG	2.49	0.42
1:A:95:MET:HE3	1:A:479:TYR:CD2	2.54	0.42
2:D:579:ARG:HB3	2:E:580:VAL:CG1	2.49	0.42
1:C:39:TYR:CE2	2:F:538:THR:HA	2.54	0.41
2:E:566:LEU:HD21	2:F:570:VAL:HG13	2.01	0.41
2:F:617:LYS:HE2	2:F:622:ILE:HA	2.01	0.41
1:A:222:LYS:HE3	1:A:238:SER:OG	2.20	0.41
1:B:291:CYS:HB2	1:B:325:CYS:SG	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:601:LYS:C	2:D:602:LEU:HG	2.46	0.41
1:A:53:PHE:HB3	2:D:571:TRP:CE2	2.56	0.41
1:A:301:SER:HB3	1:A:311:TYR:CZ	2.56	0.41
2:E:566:LEU:HD13	2:F:573:ILE:HD12	2.03	0.41
1:C:89:VAL:HG22	2:F:527:GLY:H	1.86	0.41
1:A:86:LEU:HD21	2:D:523:LEU:HD23	2.03	0.41
1:A:291:CYS:HB2	1:A:440:CYS:SG	2.61	0.41
1:A:420:ASN:HA	1:A:428:ALA:HA	2.03	0.41
1:C:255:LEU:HD11	1:C:280:ILE:HD11	2.02	0.40
1:A:48:ALA:O	1:A:100:MET:HE2	2.20	0.40
1:C:221:LEU:HD23	1:C:239:THR:HA	2.03	0.40
1:C:324:HIS:HA	1:C:413:CYS:SG	2.61	0.40
2:D:588:ARG:CD	2:F:551:GLN:HA	2.51	0.40
2:E:673:PHE:O	2:E:675:ILE:N	2.54	0.40
1:B:89:VAL:HG13	2:E:629:MET:CE	2.51	0.40
1:B:45:TRP:CE3	2:E:629:MET:HE2	2.57	0.40
1:C:223:CYS:HA	1:C:234:CYS:SG	2.61	0.40
2:D:595:ILE:HG23	2:D:651:ASN:CG	2.46	0.40
1:A:45:TRP:HA	1:A:485:LYS:O	2.22	0.40
1:B:210:ILE:O	1:B:245:GLY:HA2	2.22	0.40
1:B:250:VAL:HG13	1:B:423:GLN:HE22	1.85	0.40
2:D:587:LEU:CD1	2:F:583:VAL:HG13	2.51	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	414/473 (88%)	362 (87%)	42 (10%)	10 (2%)	4	27
1	B	414/473 (88%)	358 (86%)	45 (11%)	11 (3%)	4	25
1	C	414/473 (88%)	361 (87%)	40 (10%)	13 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	154/166 (93%)	133 (86%)	14 (9%)	7 (4%)	2	17
2	E	154/166 (93%)	130 (84%)	15 (10%)	9 (6%)	1	14
2	F	154/166 (93%)	135 (88%)	15 (10%)	4 (3%)	4	25
All	All	1704/1917 (89%)	1479 (87%)	171 (10%)	54 (3%)	5	21

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	CYS
2	D	569	THR
2	E	599	SER
2	E	650	GLN
1	A	192	ASN
1	B	51	THR
1	B	224	LYS
1	C	99	ASN
1	C	194	SER
1	C	225	ASP
2	D	548	ILE
2	D	568	LEU
2	E	674	ASN
1	A	253	GLN
1	B	159	SER
1	B	355	PHE
1	C	198	GLN
1	C	200	CYS
1	C	242	CYS
1	C	300	LYS
2	D	545	LEU
2	D	559	ILE
2	D	673	PHE
2	E	567	GLN
2	E	616	ASN
2	E	634	GLU
2	E	661	LEU
2	F	673	PHE
1	A	71	THR
1	A	76	PRO
1	A	458	SER
1	B	158	THR
1	C	44	VAL

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Mol	Chain	Res	Type
1	C	87	GLU
2	E	523	LEU
2	F	602	LEU
2	F	607	ALA
1	A	306	PRO
1	B	73	ALA
1	B	157	THR
1	B	425	VAL
1	C	98	ASN
1	C	245	GLY
2	E	600	GLY
2	F	600	GLY
1	A	84	VAL
1	B	69	TRP
1	C	248	PRO
1	C	473	ASN
1	A	176	VAL
1	A	123	THR
1	B	76	PRO
1	B	214	THR
2	D	600	GLY

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	378/424 (89%)	359 (95%)	19 (5%)	22	43
1	B	378/424 (89%)	368 (97%)	10 (3%)	40	62
1	C	378/424 (89%)	360 (95%)	18 (5%)	23	44
2	D	136/144 (94%)	120 (88%)	16 (12%)	5	18
2	E	136/144 (94%)	125 (92%)	11 (8%)	11	31
2	F	136/144 (94%)	119 (88%)	17 (12%)	4	16
All	All	1542/1704 (90%)	1451 (94%)	91 (6%)	19	39

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	61	TYR
1	A	65	VAL
1	A	72	HIS
1	A	84	VAL
1	A	101	VAL
1	A	106	GLU
1	A	212	TYR
1	A	244	HIS
1	A	263	GLU
1	A	291	CYS
1	A	376	PHE
1	A	379	CYS
1	A	424	GLU
1	A	429	MET
1	A	435	ARG
1	A	440	CYS
1	A	464	ARG
1	A	481	TYR
1	B	75	VAL
1	B	83	GLU
1	B	101	VAL
1	B	106	GLU
1	B	213	CYS
1	B	263	GLU
1	B	274	ASP
1	B	368	HIS
1	B	447	LEU
1	B	486	ILE
1	C	40	TYR
1	C	82	GLN
1	C	103	GLN
1	C	106	GLU
1	C	108	ILE
1	C	109	ILE
1	C	187	ARG
1	C	212	TYR
1	C	214	THR
1	C	241	GLN
1	C	288	GLU
1	C	291	CYS
1	C	296	ASN

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Mol	Chain	Res	Type
1	C	376	PHE
1	C	415	ILE
1	C	427	LYS
1	C	429	MET
1	C	440	CYS
2	D	542	ARG
2	D	548	ILE
2	D	557	ARG
2	D	564	HIS
2	D	574	ARG
2	D	586	TYR
2	D	587	LEU
2	D	590	GLN
2	D	602	LEU
2	D	606	THR
2	D	664	ASP
2	D	669	LEU
2	D	671	ASN
2	D	678	TRP
2	D	679	LEU
2	D	680	TRP
2	E	523	LEU
2	E	535	MET
2	E	542	ARG
2	E	606	THR
2	E	626	MET
2	E	646	ILE
2	E	660	LEU
2	E	669	LEU
2	E	678	TRP
2	E	679	LEU
2	E	680	TRP
2	F	522	PHE
2	F	537	LEU
2	F	548	ILE
2	F	552	GLN
2	F	557	ARG
2	F	562	GLN
2	F	586	TYR
2	F	587	LEU
2	F	588	ARG
2	F	602	LEU

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Mol	Chain	Res	Type
2	F	604	CYS
2	F	629	MET
2	F	663	LEU
2	F	664	ASP
2	F	669	LEU
2	F	678	TRP
2	F	679	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	333	ASN
1	A	423	GLN
1	A	437	GLN
1	B	67	ASN
1	B	92	ASN
1	B	103	GLN
1	B	130	ASN
1	B	278	ASN
1	B	423	GLN
1	C	72	HIS
1	C	82	GLN
1	C	92	ASN
1	C	94	ASN
1	C	278	ASN
2	D	621	GLN
2	D	625	ASN
2	D	671	ASN
2	E	540	GLN
2	E	552	GLN
2	E	590	GLN
2	E	624	ASN
2	E	650	GLN
2	E	671	ASN
2	F	543	GLN
2	F	551	GLN
2	F	552	GLN
2	F	591	GLN
2	F	611	ASN
2	F	616	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	650:GLN	C	651:ASN	N	1.16
1	D	650:GLN	C	651:ASN	N	1.06

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75214. These allow visual inspection of the internal detail of the map and identification of artifacts.

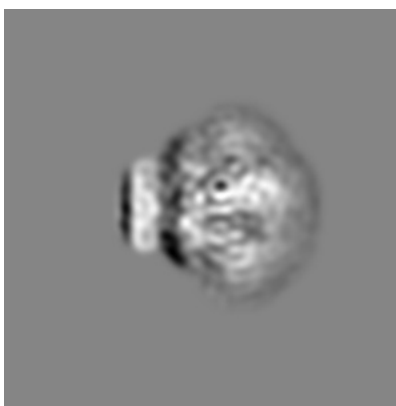
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

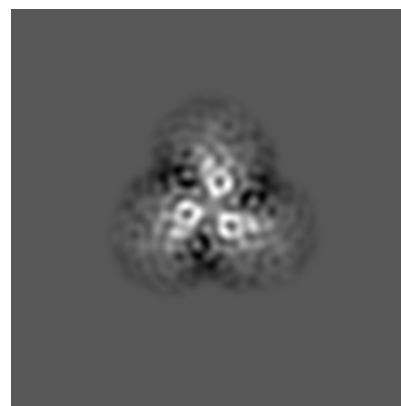
6.1.1 Primary map



X

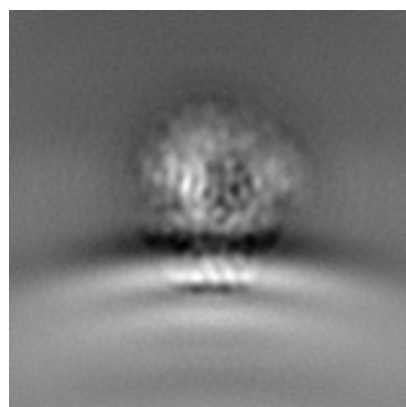


Y

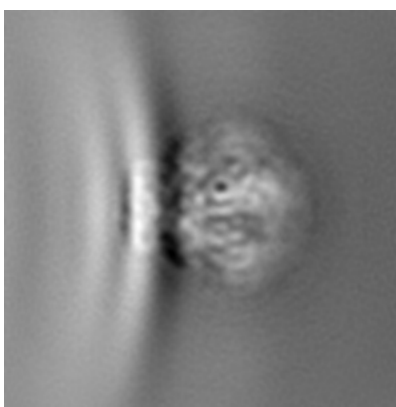


Z

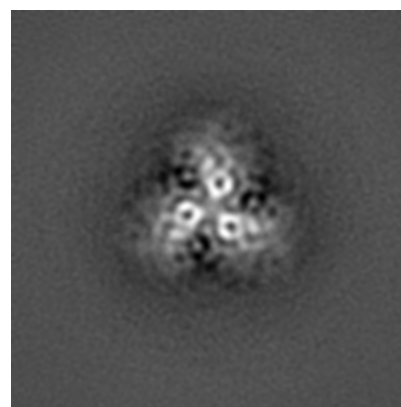
6.1.2 Raw map



X



Y



Z

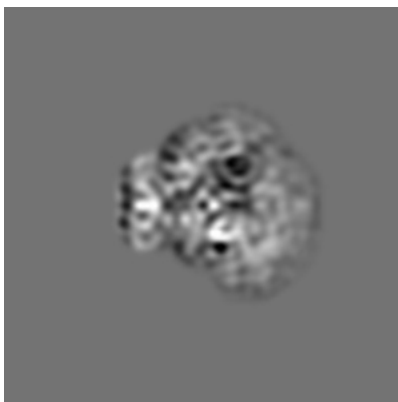
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

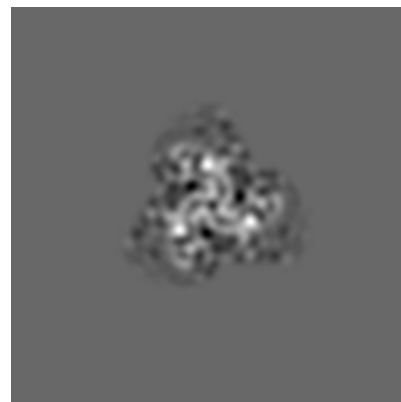
6.2.1 Primary map



X Index: 60

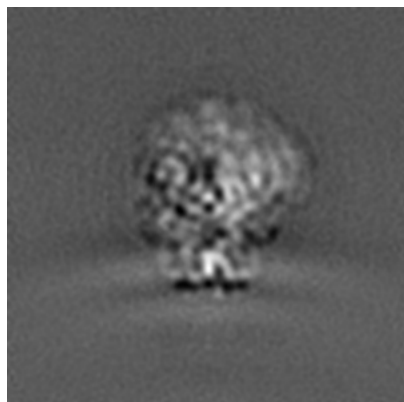


Y Index: 60

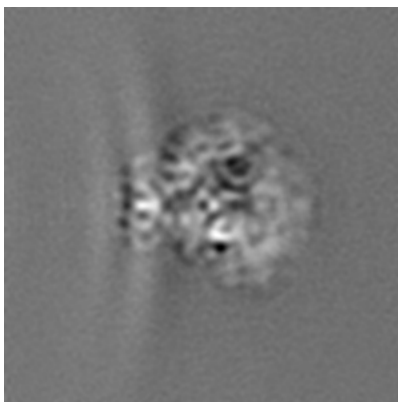


Z Index: 60

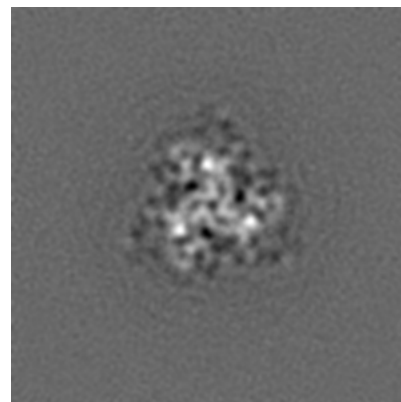
6.2.2 Raw map



X Index: 60



Y Index: 60



Z Index: 60

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

6.3 Largest variance slices [i](#)

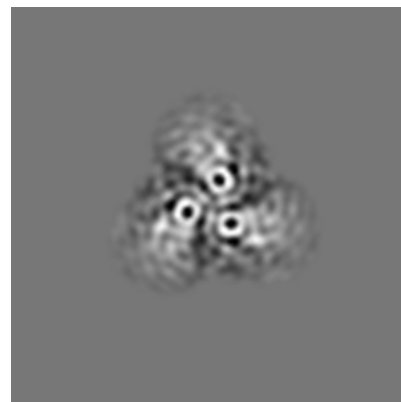
6.3.1 Primary map



X Index: 64

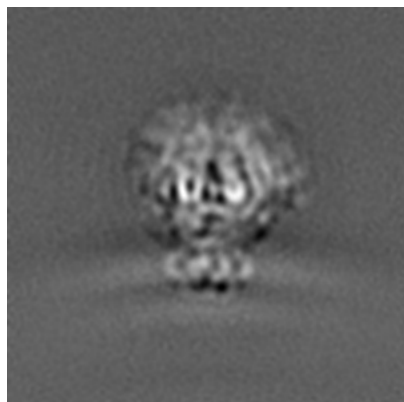


Y Index: 57

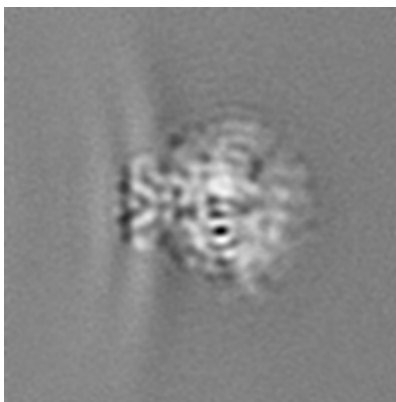


Z Index: 65

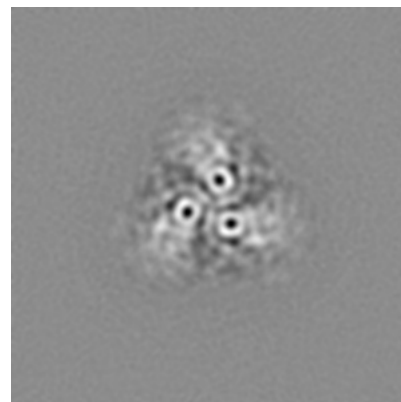
6.3.2 Raw map



X Index: 64



Y Index: 57



Z Index: 65

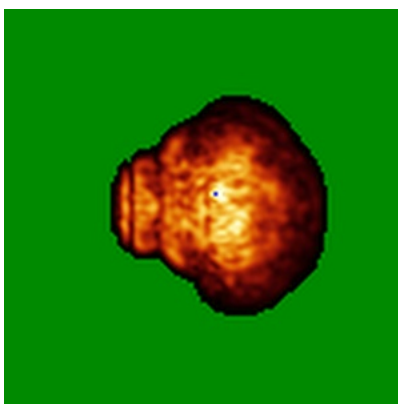
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

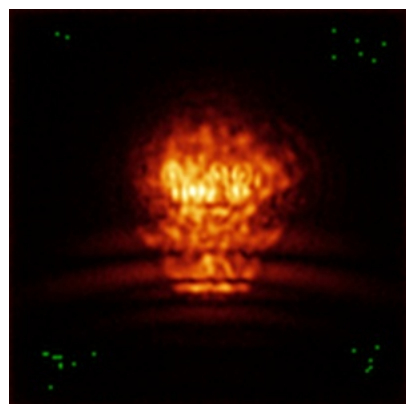


Y

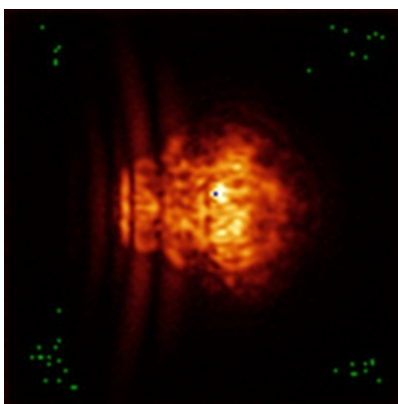


Z

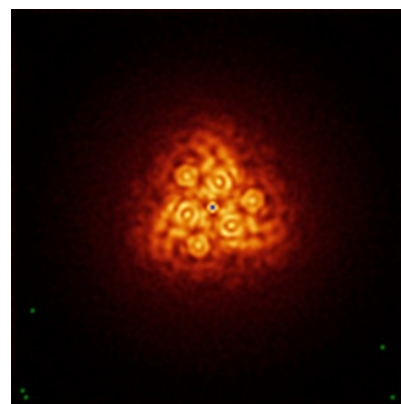
6.4.2 Raw map



X



Y

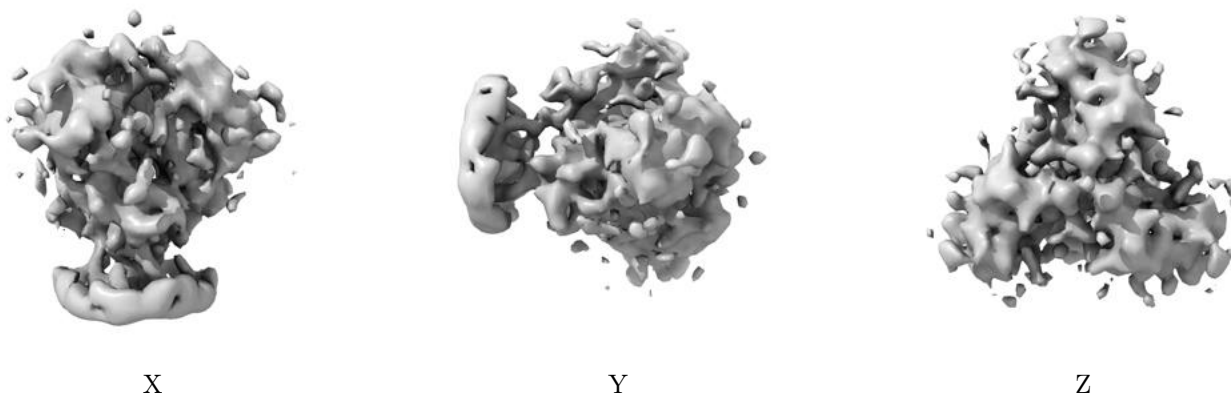


Z

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

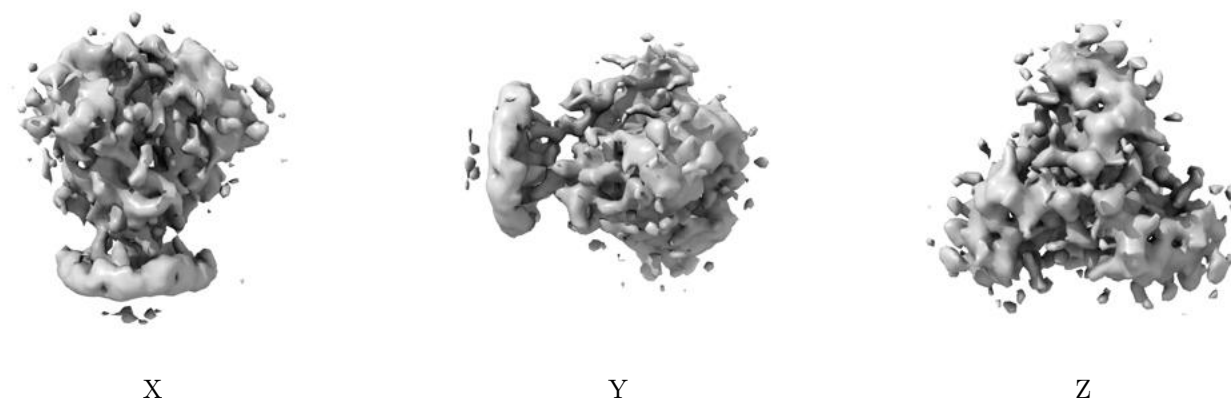
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

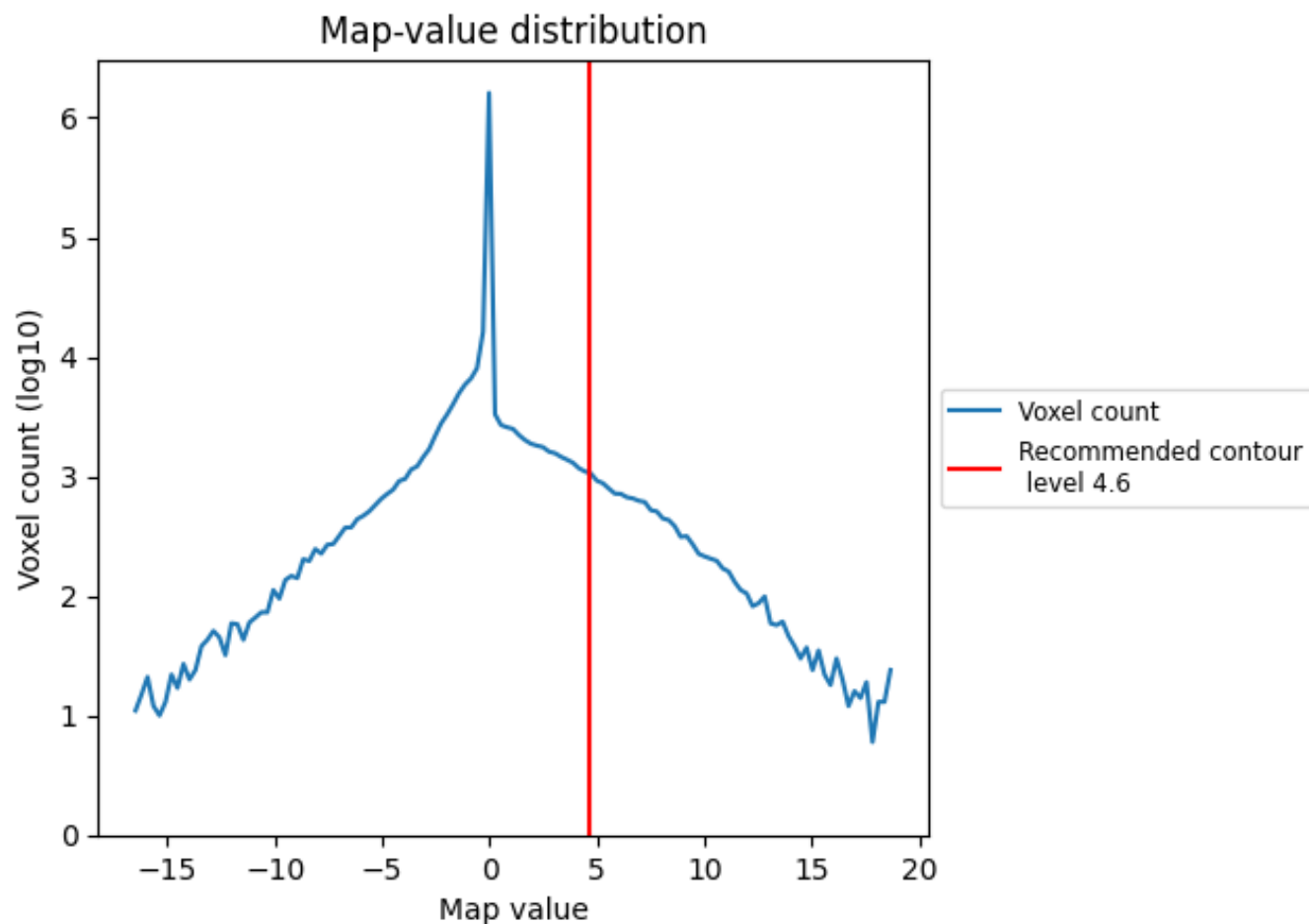
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

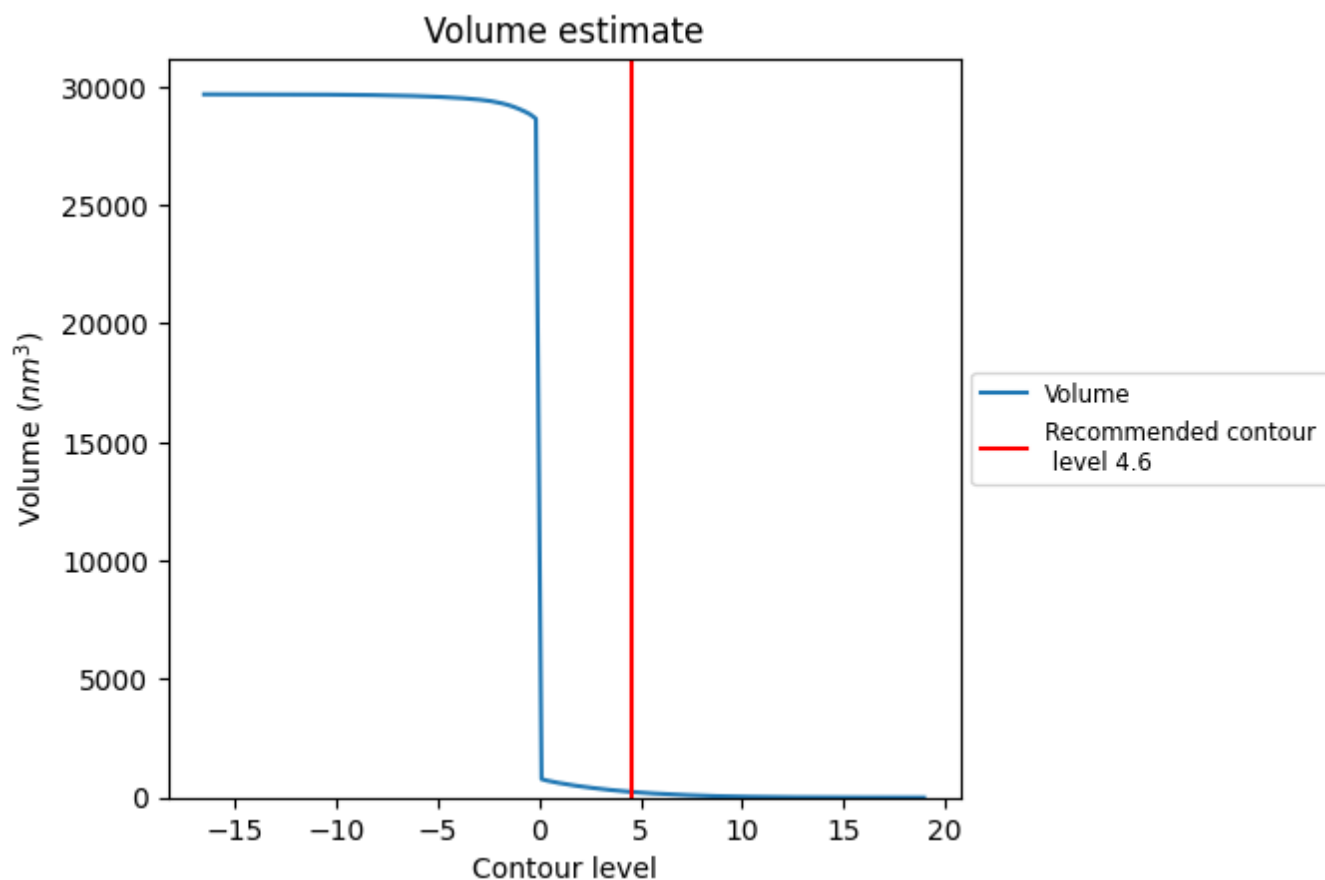
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

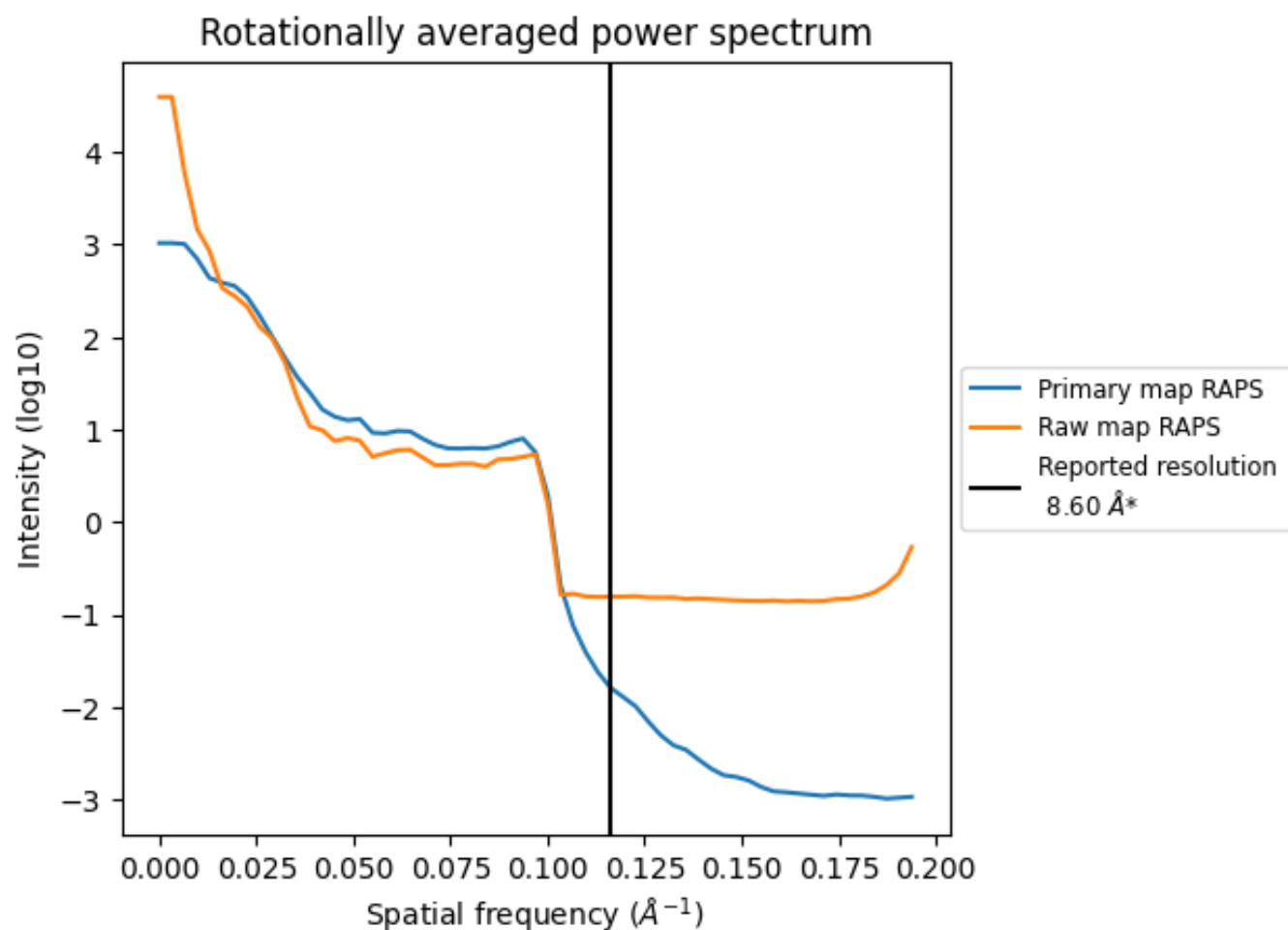
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm³; 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 ⓘ

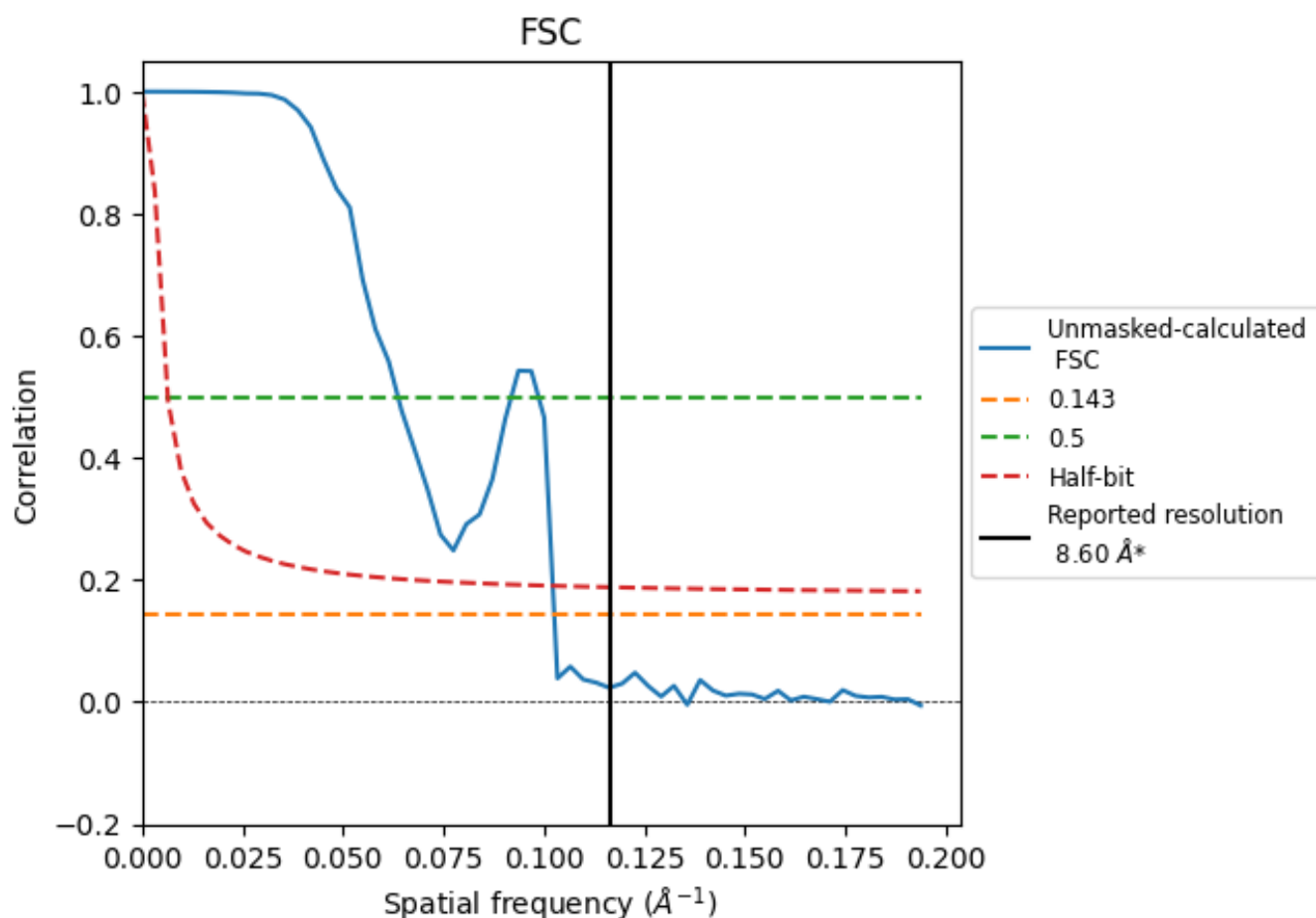


*Reported resolution corresponds to spatial frequency of 0.116 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.116 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

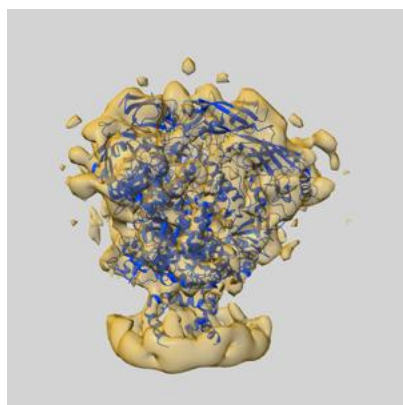
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.75	15.70	9.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.75 differs from the reported value 8.6 by more than 10 %

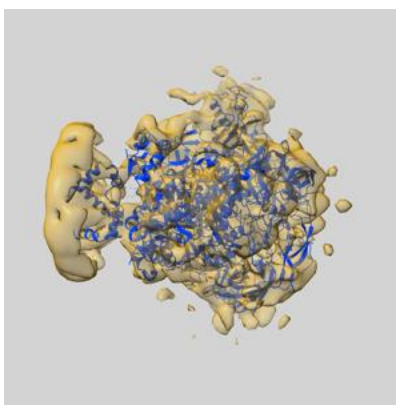
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75214 and PDB model 10JE. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

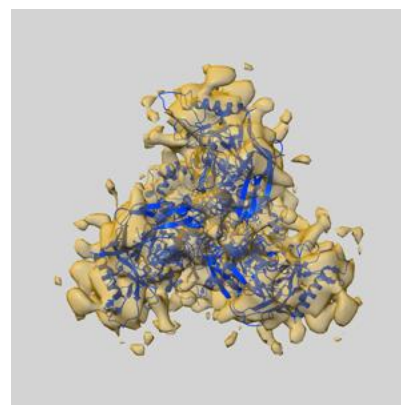
9.1 Map-model overlay [i](#)



X



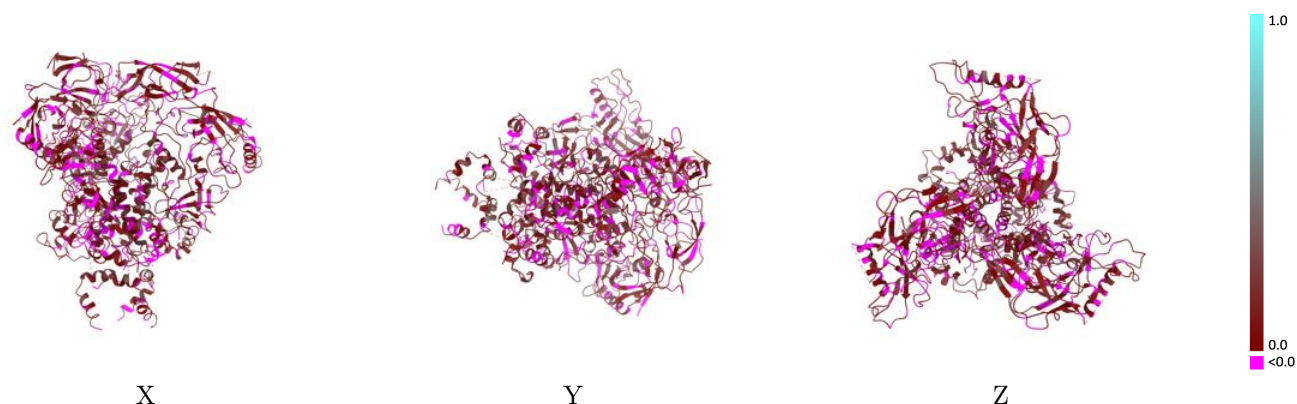
Y



Z

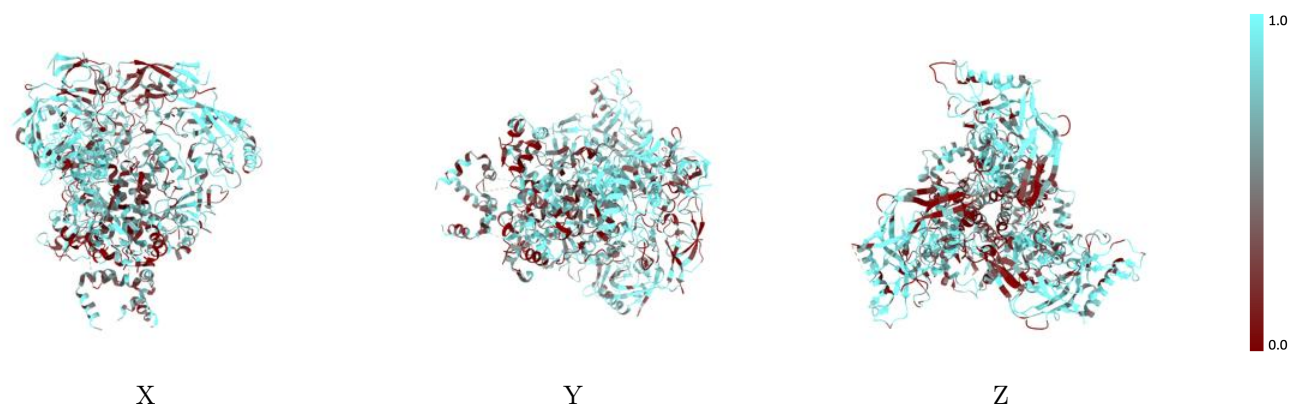
The images above show the 3D surface view of the map at the recommended contour level 4.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



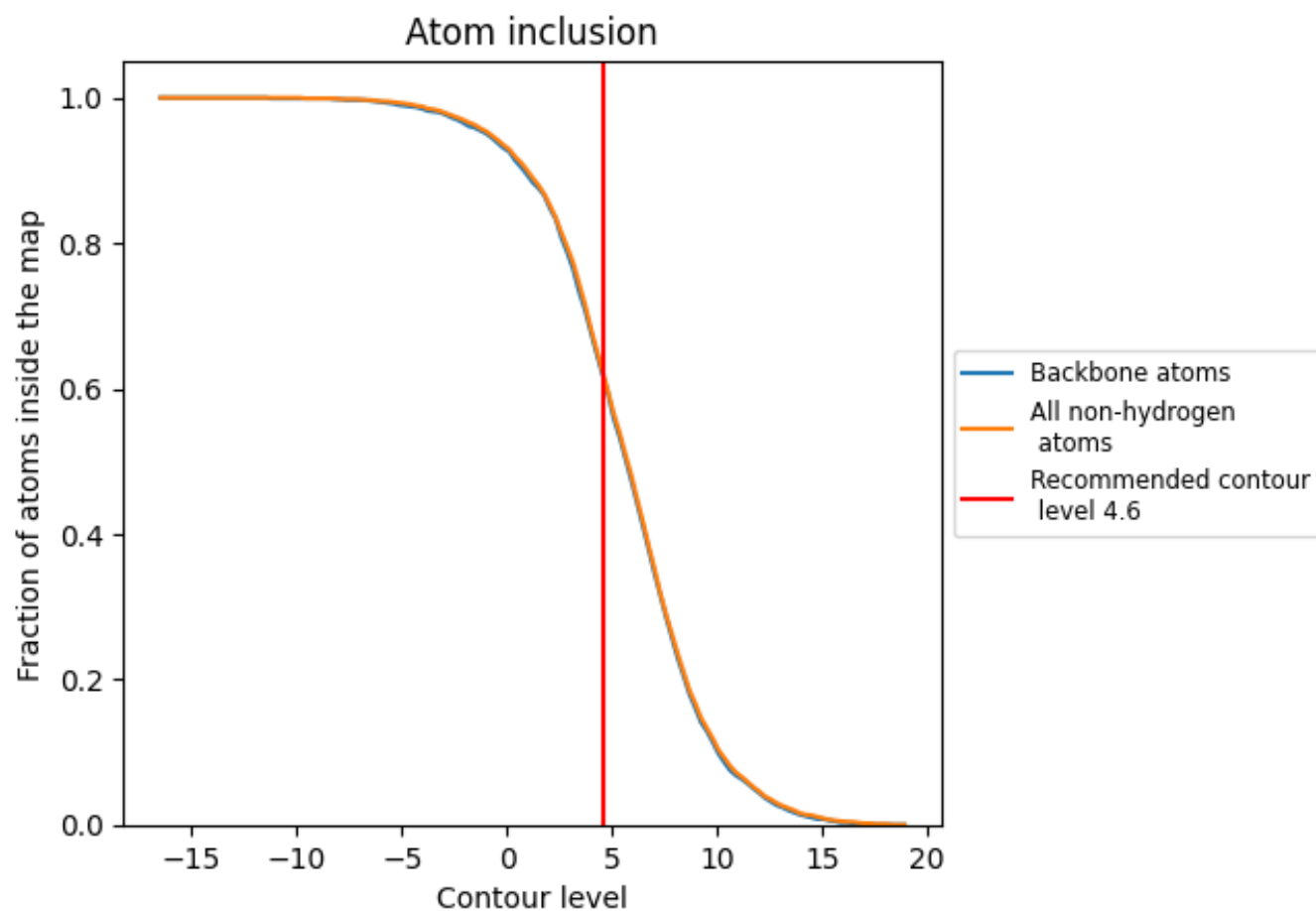
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 62% 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 (4.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.0810
A	0.6720	0.0780
B	0.6620	0.0680
C	0.6840	0.0810
D	0.4730	0.0810
E	0.4920	0.0900
F	0.5260	0.1160

1.0

0.0

<0.0