



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:15 PM UTC

PDB ID : 8GHL / pdb_00008ghl
EMDB ID : EMD-40006
Title : the Hir complex core
Authors : Kim, H.J.; Murakami, K.
Deposited on : 2023-03-10
Resolution : 2.96 Å(reported)
Based on initial model : .

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

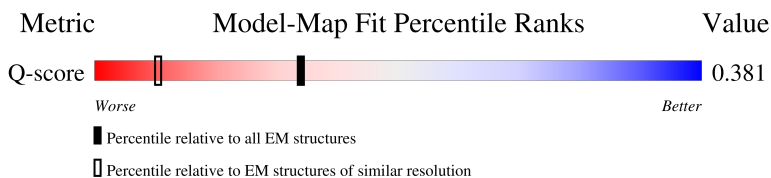
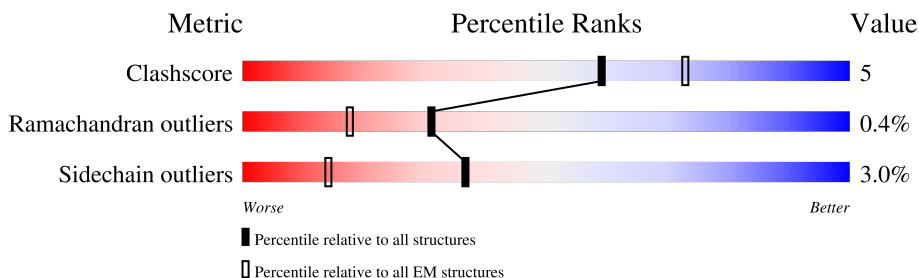
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	13155 (2.46 - 3.46)

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	840	
1	G	840	
2	D	1648	
2	J	1648	

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Mol	Chain	Length	Quality of chain
3	B	875	41%6%52%
3	C	875	34%7%57%
3	H	875	42%6%52%
3	I	875	37%5%57%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30648 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 Protein HIR1.

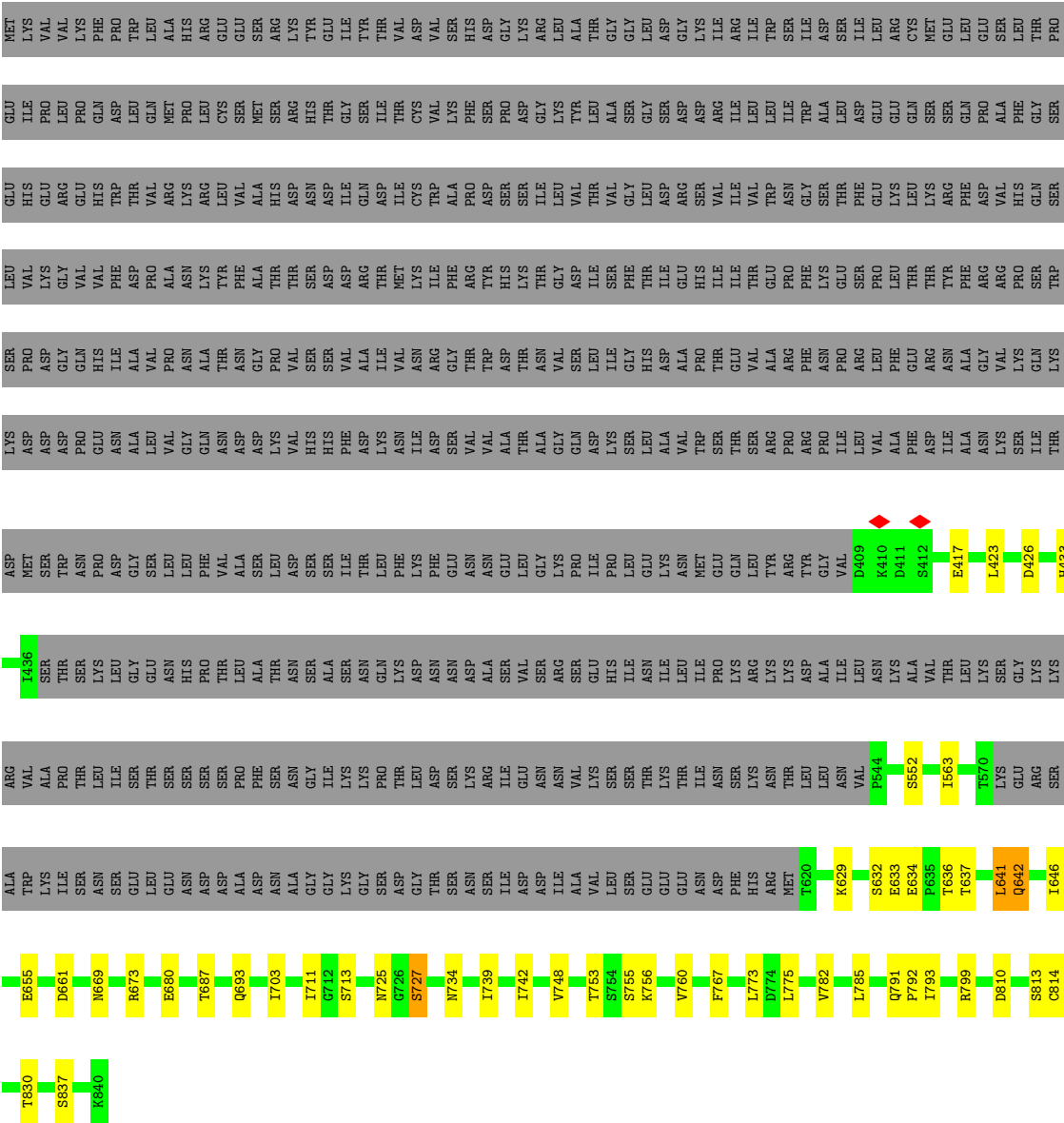
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	276	Total	C	N	O	S	0	0
			2169	1390	365	403	11		
1	G	276	Total	C	N	O	S	0	0
			2169	1390	365	403	11		

- Molecule 2 is a protein called Histone transcription regulator 3.

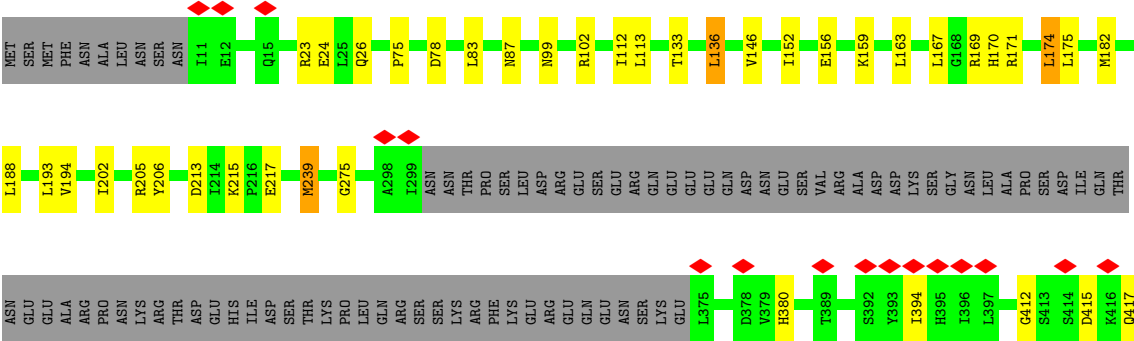
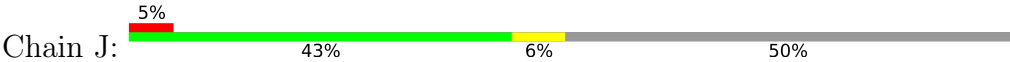
Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	818	Total	C	N	O	S	0	0
			6781	4349	1127	1284	21		
2	D	818	Total	C	N	O	S	0	0
			6781	4349	1127	1284	21		

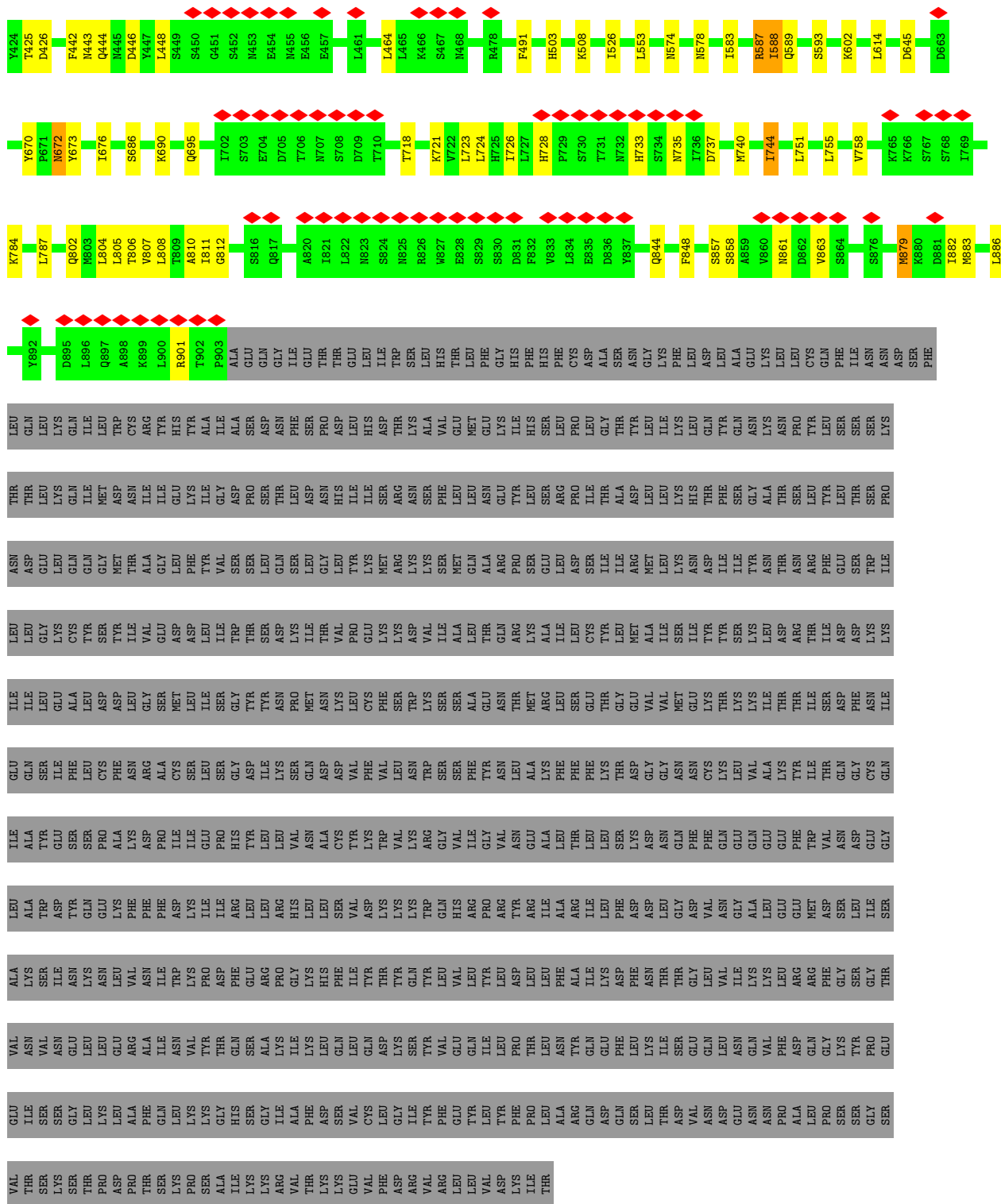
- Molecule 3 is a protein called Protein HIR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	419	Total	C	N	O	S	0	0
			3351	2132	556	645	18		
3	C	377	Total	C	N	O	S	0	0
			3023	1936	498	572	17		
3	H	419	Total	C	N	O	S	0	0
			3351	2132	556	645	18		
3	I	377	Total	C	N	O	S	0	0
			3023	1936	498	572	17		



• Molecule 2: Histone transcription regulator 3

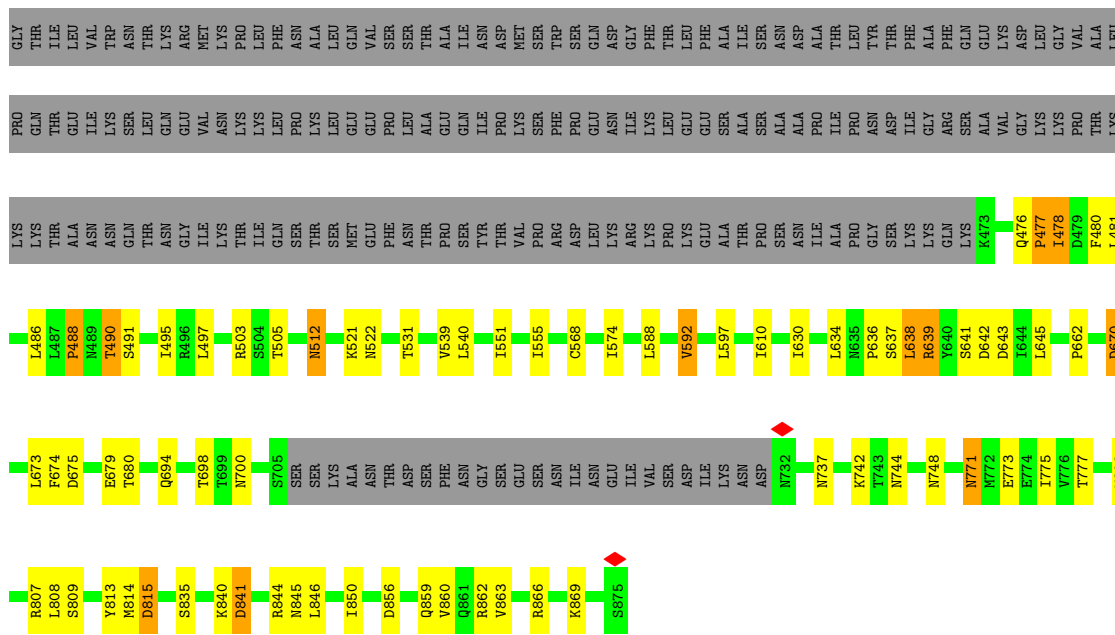




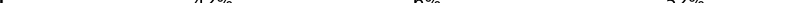
- Molecule 2: Histone transcription regulator 3

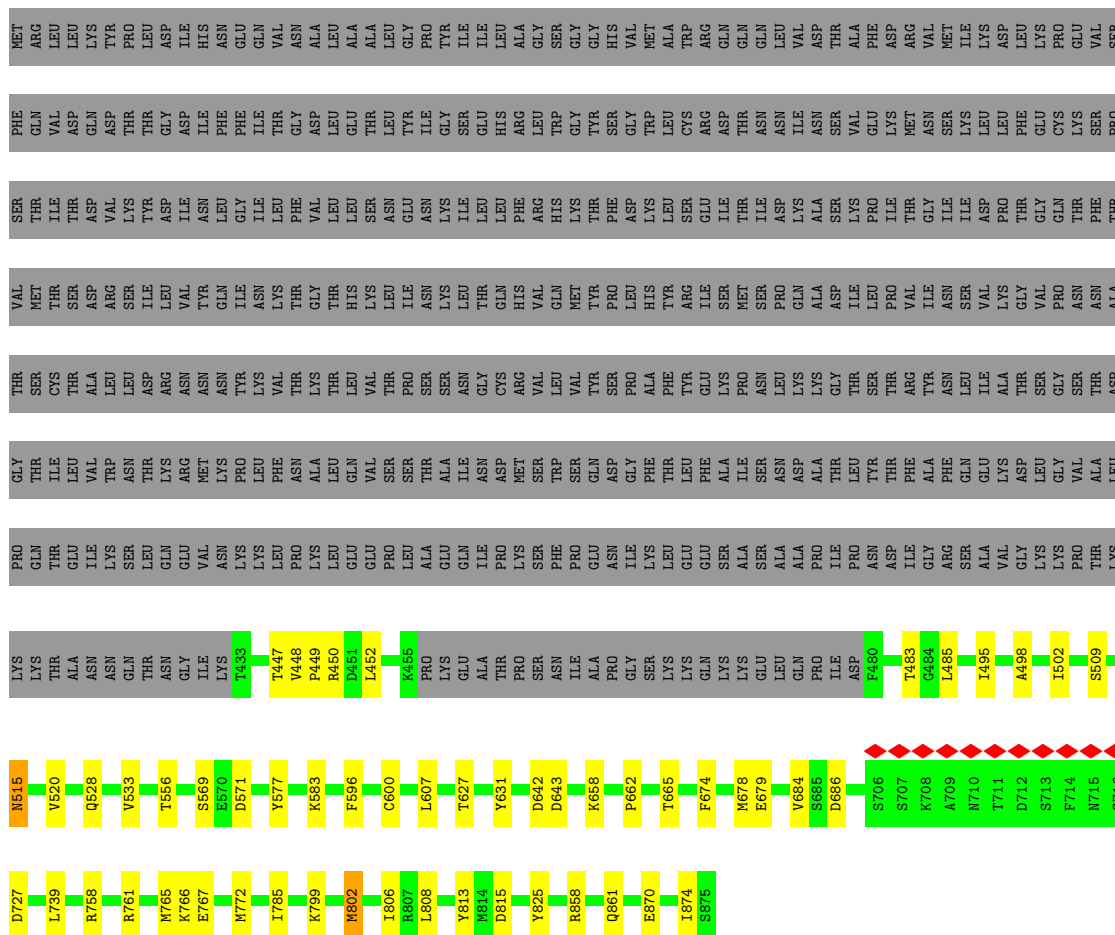






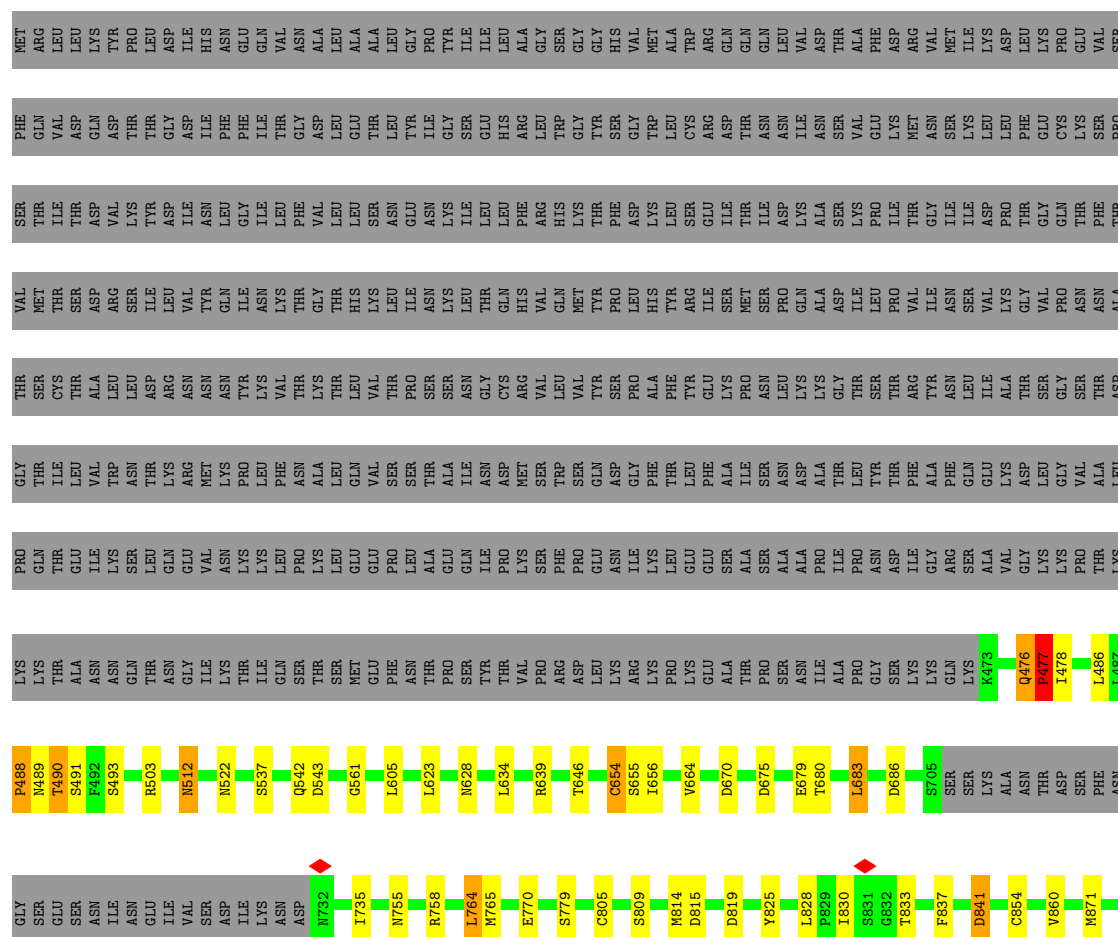
- Molecule 3: Protein HIR2

Chain H:  42% 6% 52%



- Molecule 3: Protein HIR2

Response	Percentage
Yes	37%
No	5%
Don't know	57%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	495250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.172	Depositor
Minimum map value	-0.643	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.315	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	0.27	0/2207	0.63	0/2982
1	G	0.29	0/2207	0.67	4/2982 (0.1%)
2	D	0.24	0/6927	0.65	8/9358 (0.1%)
2	J	0.23	1/6927 (0.0%)	0.58	6/9358 (0.1%)
3	B	0.24	0/3413	0.58	0/4618
3	C	0.27	0/3081	0.66	3/4171 (0.1%)
3	H	0.24	0/3413	0.58	3/4618 (0.1%)
3	I	0.29	0/3081	0.71	5/4171 (0.1%)
All	All	0.25	1/31256 (0.0%)	0.63	29/42258 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2
2	J	0	2
3	C	0	2
3	I	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	194	VAL	C-N	5.05	1.40	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	588	ILE	N-CA-C	-9.78	103.15	112.83
1	G	642	GLN	CA-CB-CG	9.00	132.09	114.10
3	I	871	MET	N-CA-C	-8.65	102.74	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	791	GLN	CA-CB-CG	7.93	129.97	114.10
2	D	446	ASP	N-CA-C	7.19	117.47	108.19
2	J	588	ILE	N-CA-C	-7.10	103.35	113.07
2	D	214	ILE	N-CA-C	6.74	113.42	106.21
2	J	193	LEU	CA-C-N	6.60	124.40	120.24
2	J	193	LEU	C-N-CA	6.60	124.40	120.24
2	J	446	ASP	N-CA-C	6.12	116.09	108.19
2	D	814	LEU	CA-CB-CG	5.99	137.27	116.30
3	I	871	MET	CA-CB-CG	5.83	125.75	114.10
3	H	767	GLU	CA-CB-CG	5.79	125.69	114.10
3	C	481	LEU	CA-CB-CG	5.76	136.47	116.30
3	I	476	GLN	CA-CB-CG	5.74	125.59	114.10
1	G	641	LEU	CA-C-N	5.61	132.26	121.54
1	G	641	LEU	C-N-CA	5.61	132.26	121.54
3	C	814	MET	CB-CG-SD	5.57	129.40	112.70
2	J	446	ASP	CA-C-N	5.33	135.59	126.32
2	J	446	ASP	C-N-CA	5.33	135.59	126.32
2	D	239	MET	CB-CG-SD	5.24	128.43	112.70
2	D	197	LEU	CA-CB-CG	5.16	134.37	116.30
2	D	214	ILE	CB-CG1-CD1	5.16	124.63	113.80
3	H	766	LYS	CA-C-N	5.08	131.24	121.54
3	H	766	LYS	C-N-CA	5.08	131.24	121.54
3	I	871	MET	CG-SD-CE	5.08	112.06	100.90
2	D	456	GLU	CA-CB-CG	5.07	124.23	114.10
3	C	540	LEU	CA-CB-CG	5.06	134.01	116.30
3	I	764	LEU	CA-CB-CG	5.01	133.84	116.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	476	GLN	Peptide
3	C	636	PRO	Peptide
2	D	444	GLN	Peptide
2	D	445	ASN	Peptide
3	I	477	PRO	Peptide
2	J	444	GLN	Peptide
2	J	587	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2169	0	2236	27	0
1	G	2169	0	2236	25	0
2	D	6781	0	6706	62	0
2	J	6781	0	6706	60	0
3	B	3351	0	3366	34	0
3	C	3023	0	3048	44	0
3	H	3351	0	3366	33	0
3	I	3023	0	3048	31	0
All	All	30648	0	30712	285	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 5.

All (285) 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)
2:D:23:ARG:HH22	2:D:72:ASN:HD21	1.41	0.69
2:J:744:ILE:HG12	2:J:755:LEU:HD11	1.76	0.67
2:D:697:ILE:HG13	2:D:715:HIS:HE1	1.60	0.67
1:A:669:ASN:HA	1:A:687:THR:HG22	1.79	0.63
3:C:866:ARG:HA	3:C:869:LYS:HE2	1.80	0.63
1:G:552:SER:HB3	3:H:600:CYS:HB2	1.81	0.63
2:J:202:ILE:HA	2:J:205:ARG:HB3	1.82	0.61
3:I:477:PRO:HD2	3:I:478:ILE:HD12	1.82	0.61
2:J:670:TYR:HB3	2:J:673:TYR:HB2	1.84	0.60
2:D:708:SER:HB2	2:D:712:SER:HB3	1.83	0.60
2:D:69:MET:SD	2:D:69:MET:N	2.75	0.60
3:H:520:VAL:HG22	3:H:533:VAL:HG22	1.83	0.59
2:J:133:THR:HG21	2:J:156:GLU:HB2	1.84	0.59
2:D:133:THR:HG21	2:D:156:GLU:HB2	1.85	0.59
3:C:840:LYS:HE3	3:C:844:ARG:HD3	1.85	0.59
2:J:526:ILE:O	2:J:672:ASN:ND2	2.36	0.59
1:G:629:LYS:O	1:G:633:GLU:HB3	2.00	0.59
3:I:814:MET:HE1	3:I:860:VAL:HG12	1.84	0.59
3:B:815:ASP:OD1	3:B:815:ASP:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:490:THR:O	3:B:496:ARG:NH1	2.35	0.58
1:G:669:ASN:HA	1:G:687:THR:HG22	1.84	0.58
2:D:811:ILE:HA	2:D:814:LEU:HD23	1.85	0.58
3:B:480:PHE:N	3:B:502:ILE:O	2.36	0.58
1:G:792:PRO:HB2	3:H:485:LEU:HD23	1.86	0.58
2:D:445:ASN:H	2:D:588:ILE:HG22	1.70	0.57
2:D:456:GLU:HG2	2:D:588:ILE:HD13	1.85	0.57
3:C:859:GLN:O	3:C:862:ARG:NH2	2.38	0.57
2:D:230:GLU:OE1	2:D:234:GLN:NE2	2.38	0.57
1:G:725:ASN:O	3:I:639:ARG:NH2	2.38	0.56
1:A:646:ILE:O	1:A:673:ARG:NH2	2.38	0.56
3:B:520:VAL:HG22	3:B:533:VAL:HG22	1.86	0.56
3:I:764:LEU:HD12	3:I:765:MET:HB3	1.87	0.56
2:D:74:SER:HB3	2:D:77:LEU:HG	1.87	0.56
3:C:698:THR:HA	3:C:744:ASN:HD21	1.69	0.56
1:G:767:PHE:HB2	1:G:782:VAL:HB	1.87	0.56
3:I:488:PRO:HD2	3:I:491:SER:HB3	1.87	0.56
3:I:755:ASN:OD1	3:I:758:ARG:NH1	2.38	0.56
2:J:442:PHE:HA	2:J:805:LEU:HD13	1.86	0.56
1:A:725:ASN:O	3:C:639:ARG:NH2	2.39	0.56
1:G:755:SER:OG	1:G:756:LYS:N	2.37	0.55
2:D:645:ASP:O	2:D:695:GLN:NE2	2.38	0.55
2:J:175:LEU:HD11	3:B:870:GLU:HG3	1.87	0.55
3:I:654:CYS:HB2	3:I:664:VAL:HG22	1.89	0.55
3:C:637:SER:OG	3:C:638:LEU:N	2.36	0.55
2:D:272:SER:HB3	2:D:276:ARG:HH21	1.72	0.55
3:B:515:ASN:OD1	3:B:515:ASN:N	2.40	0.54
3:H:515:ASN:OD1	3:H:515:ASN:N	2.39	0.54
2:D:524:ARG:HD3	2:D:563:TYR:HB3	1.88	0.54
1:A:655:GLU:HB2	1:A:662:ILE:HD11	1.90	0.54
1:A:755:SER:OG	1:A:756:LYS:N	2.38	0.54
3:H:815:ASP:OD1	3:H:815:ASP:N	2.39	0.54
3:C:694:GLN:NE2	3:C:773:GLU:OE1	2.41	0.54
2:J:673:TYR:HB3	2:J:676:ILE:HD12	1.90	0.53
3:H:758:ARG:HA	3:H:761:ARG:HD2	1.90	0.53
3:H:642:ASP:OD1	3:H:642:ASP:N	2.40	0.53
2:D:83:LEU:O	2:D:87:ASN:ND2	2.42	0.53
3:B:642:ASP:OD1	3:B:642:ASP:N	2.41	0.53
2:D:443:ASN:HB3	2:D:589:GLN:HA	1.91	0.53
3:I:561:GLY:O	2:D:169:ARG:NH2	2.42	0.53
2:D:478:ARG:NH1	2:D:482:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:HG	3:B:645:LEU:HD12	1.91	0.52
2:J:879:MET:HA	2:J:882:ILE:HG22	1.91	0.52
2:J:737:ASP:HB3	2:J:740:MET:HG3	1.91	0.52
3:C:634:LEU:O	3:C:639:ARG:NH1	2.42	0.52
2:D:394:ILE:O	2:D:901:ARG:NH1	2.39	0.52
2:D:156:GLU:HG2	2:D:181:MET:HE1	1.92	0.52
2:D:431:LEU:HD11	2:D:852:VAL:HG22	1.92	0.52
1:A:552:SER:HB3	3:B:600:CYS:HB2	1.92	0.52
3:I:634:LEU:O	3:I:639:ARG:NH1	2.43	0.52
3:C:856:ASP:OD1	3:C:856:ASP:N	2.41	0.52
2:D:208:LEU:HD11	2:D:214:ILE:HG21	1.91	0.52
3:B:677:ASN:HD22	3:B:790:ARG:HH22	1.58	0.51
3:C:841:ASP:OD1	3:C:841:ASP:N	2.42	0.51
3:H:569:SER:OG	3:H:571:ASP:OD1	2.28	0.51
2:J:75:PRO:HA	2:J:78:ASP:HB2	1.93	0.51
2:D:710:THR:HA	2:D:713:GLU:HB2	1.91	0.51
3:H:684:VAL:HG11	3:H:739:LEU:HD13	1.93	0.51
2:D:442:PHE:HA	2:D:805:LEU:HD13	1.93	0.51
1:A:777:LEU:HD22	3:C:679:GLU:HG3	1.93	0.50
2:J:503:HIS:NE2	1:G:655:GLU:OE2	2.37	0.50
1:G:563:ILE:HG23	3:H:498:ALA:HB3	1.93	0.50
3:I:655:SER:OG	3:I:656:ILE:N	2.44	0.50
2:J:587:ARG:HG3	2:J:593:SER:HB3	1.91	0.50
1:A:660:ASP:OD2	1:A:660:ASP:N	2.36	0.50
2:J:812:GLY:HA3	2:J:882:ILE:HD11	1.94	0.50
1:A:646:ILE:HG23	1:A:652:VAL:HG21	1.93	0.50
2:J:464:LEU:HD13	2:J:751:LEU:HD13	1.92	0.50
2:J:645:ASP:O	2:J:695:GLN:NE2	2.45	0.50
2:D:804:LEU:HD11	2:D:848:PHE:HZ	1.77	0.50
3:I:815:ASP:N	3:I:815:ASP:OD2	2.45	0.49
1:A:425:GLU:OE2	3:B:858:ARG:NH1	2.45	0.49
3:C:773:GLU:O	3:C:777:THR:OG1	2.29	0.49
3:B:489:ASN:ND2	3:B:591:GLY:O	2.45	0.49
1:G:417:GLU:OE2	3:H:858:ARG:NH1	2.45	0.49
3:C:670:ASP:N	3:C:670:ASP:OD1	2.43	0.49
1:G:423:LEU:HB2	3:H:874:ILE:HD11	1.94	0.49
3:H:727:ASP:OD1	3:H:799:LYS:NZ	2.44	0.49
2:D:450:SER:O	2:D:817:GLN:NE2	2.44	0.49
3:H:452:LEU:HD22	3:H:643:ASP:HB3	1.94	0.49
2:J:804:LEU:HD11	2:J:848:PHE:HZ	1.77	0.49
2:D:67:TRP:HB2	2:D:69:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:133:THR:HG23	2:J:152:ILE:HG13	1.94	0.49
1:G:646:ILE:O	1:G:673:ARG:NH2	2.45	0.49
1:G:661:ASP:OD2	1:G:693:GLN:NE2	2.45	0.49
3:I:490:THR:O	3:I:490:THR:OG1	2.30	0.49
3:B:502:ILE:HG12	3:B:556:THR:HG22	1.93	0.49
2:J:215:LYS:HG3	2:J:217:GLU:HG2	1.95	0.49
2:J:415:ASP:HA	2:J:417:GLN:HE21	1.77	0.49
1:G:810:ASP:O	1:G:814:CYS:HA	2.13	0.49
1:A:767:PHE:HB2	1:A:782:VAL:HB	1.94	0.48
2:J:723:LEU:HD23	2:J:726:ILE:HD12	1.94	0.48
1:G:734:ASN:ND2	3:I:819:ASP:OD2	2.46	0.48
2:J:443:ASN:HB3	2:J:589:GLN:HG2	1.93	0.48
3:C:675:ASP:O	3:C:679:GLU:N	2.46	0.48
1:A:568:MET:HE2	3:B:643:ASP:HA	1.94	0.48
1:A:622:ASN:HB2	3:C:642:ASP:HB3	1.94	0.48
3:C:551:ILE:HD11	3:C:555:ILE:HD11	1.96	0.48
2:D:524:ARG:NH1	2:D:567:SER:OG	2.47	0.48
2:J:721:LYS:O	2:J:733:HIS:NE2	2.47	0.48
2:J:412:GLY:HA3	2:J:425:THR:HG21	1.95	0.48
1:A:661:ASP:OD2	1:A:693:GLN:NE2	2.47	0.47
1:A:687:THR:OG1	1:A:703:ILE:O	2.31	0.47
1:G:739:ILE:HD13	1:G:775:LEU:HD13	1.96	0.47
3:C:477:PRO:HB2	3:C:478:ILE:H	1.44	0.47
3:C:490:THR:O	3:C:490:THR:OG1	2.31	0.47
2:J:686:SER:OG	2:J:690:LYS:NZ	2.48	0.47
3:I:512:ASN:OD1	3:I:512:ASN:N	2.40	0.47
2:J:159:LYS:O	2:J:163:LEU:N	2.46	0.47
1:G:426:ASP:OD2	2:D:42:LYS:NZ	2.46	0.47
3:H:662:PRO:HD2	3:H:674:PHE:HB3	1.95	0.47
2:D:259:LYS:HE3	2:D:534:GLN:HG2	1.97	0.47
2:J:171:ARG:HH22	3:B:822:GLN:HB3	1.80	0.47
1:G:687:THR:OG1	1:G:703:ILE:O	2.32	0.47
2:D:847:PHE:HA	2:D:850:TYR:HB3	1.96	0.47
3:B:495:ILE:HD11	3:B:631:TYR:HB2	1.95	0.47
3:C:488:PRO:HD2	3:C:491:SER:HB3	1.97	0.47
1:A:420:ASN:HA	1:A:423:LEU:HD12	1.97	0.46
2:D:448:LEU:HB2	2:D:810:ALA:HB1	1.97	0.46
3:H:502:ILE:HG12	3:H:556:THR:HG22	1.96	0.46
2:D:50:ASP:OD1	2:D:88:ARG:NH2	2.48	0.46
3:C:662:PRO:HD2	3:C:674:PHE:HB3	1.98	0.46
3:C:505:THR:HG22	3:C:521:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:883:MET:HA	2:J:886:LEU:HD12	1.97	0.46
3:B:662:PRO:HD2	3:B:674:PHE:HB3	1.97	0.46
1:A:785:LEU:HD23	3:C:486:LEU:HD12	1.97	0.46
3:H:577:TYR:OH	3:H:583:LYS:NZ	2.49	0.46
2:J:167:LEU:HD12	2:J:206:TYR:HE2	1.80	0.46
2:J:721:LYS:HA	2:J:724:LEU:HB2	1.98	0.46
2:J:239:MET:HE1	3:I:770:GLU:HB2	1.98	0.46
2:J:394:ILE:O	2:J:901:ARG:NH1	2.45	0.46
2:J:718:THR:OG1	2:J:735:ASN:ND2	2.48	0.46
2:J:146:VAL:HG13	2:J:188:LEU:HD11	1.97	0.46
2:J:448:LEU:HB2	2:J:810:ALA:HB1	1.98	0.46
2:D:414:SER:O	2:D:417:GLN:NE2	2.49	0.46
2:D:858:SER:O	2:D:862:ASP:N	2.49	0.46
2:J:380:HIS:NE2	2:J:857:SER:OG	2.39	0.45
3:H:448:VAL:HG23	3:I:476:GLN:HE21	1.81	0.45
3:B:641:SER:HB2	3:B:644:ILE:HG23	1.98	0.45
3:C:771:ASN:OD1	3:C:771:ASN:N	2.50	0.45
3:I:830:ILE:HB	3:I:837:PHE:HB3	1.99	0.45
1:A:806:CYS:O	1:A:819:GLU:HB3	2.16	0.45
2:J:787:LEU:HD11	2:J:807:VAL:HG11	1.98	0.45
2:J:152:ILE:HD12	2:J:152:ILE:HA	1.90	0.45
3:B:670:ASP:OD1	3:B:670:ASP:N	2.49	0.45
1:A:813:SER:OG	1:A:815:ASP:OD2	2.34	0.45
3:C:637:SER:O	3:C:639:ARG:N	2.49	0.45
3:H:772:MET:HE2	3:H:772:MET:HB3	1.85	0.45
2:D:446:ASP:HB3	2:D:447:TYR:H	1.55	0.45
2:J:574:ASN:O	2:J:578:ASN:ND2	2.43	0.45
3:B:517:ILE:HG23	3:B:536:THR:HB	1.98	0.45
2:D:723:LEU:HA	2:D:726:ILE:HD12	1.98	0.45
3:B:727:ASP:OD2	3:B:799:LYS:NZ	2.42	0.45
3:B:771:ASN:OD1	3:B:771:ASN:N	2.39	0.45
2:D:518:ASP:OD2	2:D:521:ASN:N	2.49	0.45
1:A:662:ILE:HG23	2:D:504:GLN:HG2	1.99	0.45
3:C:748:ASN:OD1	3:C:748:ASN:N	2.47	0.45
1:G:727:SER:HA	1:G:742:ILE:O	2.17	0.45
3:C:574:ILE:HB	3:C:588:LEU:HB2	1.98	0.45
3:C:700:ASN:ND2	3:C:737:ASN:OD1	2.49	0.45
3:H:858:ARG:O	3:H:861:GLN:NE2	2.50	0.45
3:I:841:ASP:OD1	3:I:841:ASP:N	2.49	0.45
3:C:846:LEU:O	3:C:850:ILE:HD12	2.16	0.45
2:J:491:PHE:HE1	2:J:508:LYS:HG2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:879:MET:O	2:J:883:MET:HG3	2.16	0.44
3:B:750:LYS:O	3:B:750:LYS:NZ	2.40	0.44
3:B:507:LYS:HD3	3:B:517:ILE:HD11	1.99	0.44
3:C:512:ASN:OD1	3:C:512:ASN:N	2.38	0.44
3:H:596:PHE:HB2	3:H:607:LEU:HB3	2.00	0.44
2:J:113:LEU:HD22	3:I:764:LEU:HB2	1.99	0.44
3:C:802:MET:HE2	3:C:802:MET:HB2	1.77	0.44
2:D:459:PHE:HB2	2:D:462:ASN:HB3	1.99	0.44
2:J:23:ARG:NH2	2:J:26:GLN:OE1	2.50	0.44
3:H:450:ARG:NH1	3:I:477:PRO:O	2.50	0.44
3:B:493:SER:OG	3:B:495:ILE:O	2.33	0.44
3:H:658:LYS:HB3	3:H:658:LYS:HE2	1.64	0.44
1:G:680:GLU:OE1	3:I:758:ARG:NH2	2.51	0.44
1:G:748:VAL:HG13	1:G:760:VAL:HG13	1.99	0.44
2:D:112:ILE:HD13	2:D:112:ILE:HA	1.92	0.44
1:A:764:ARG:HA	1:A:764:ARG:HD3	1.81	0.44
3:H:452:LEU:HD23	3:H:452:LEU:HA	1.89	0.44
2:D:862:ASP:HB3	2:D:865:ASN:HD22	1.83	0.44
2:J:99:ASN:OD1	2:J:102:ARG:NH1	2.51	0.43
2:J:112:ILE:HD13	2:J:112:ILE:HA	1.91	0.43
2:J:755:LEU:HA	2:J:758:VAL:HG22	1.99	0.43
3:B:569:SER:OG	3:B:571:ASP:OD1	2.34	0.43
1:G:785:LEU:HD13	3:I:486:LEU:HD23	2.00	0.43
3:C:592:VAL:HG11	3:C:610:ILE:HG23	2.00	0.43
2:D:582:GLU:O	2:D:586:LYS:HB2	2.18	0.43
3:C:522:ASN:HA	3:C:531:THR:HG23	1.99	0.43
3:I:683:LEU:HD11	3:I:686:ASP:HB3	2.00	0.43
2:D:464:LEU:HD22	2:D:751:LEU:HD22	2.01	0.43
2:D:485:SER:HB2	2:D:489:ARG:HH22	1.83	0.43
2:D:722:VAL:HA	2:D:725:HIS:HB3	2.01	0.43
2:D:706:THR:HA	2:D:766:LYS:HA	2.00	0.43
3:C:841:ASP:O	3:C:845:ASN:ND2	2.42	0.43
1:A:777:LEU:HD21	1:A:780:ARG:HB2	2.01	0.43
2:J:275:GLY:O	2:J:602:LYS:NZ	2.43	0.43
3:I:543:ASP:N	3:I:543:ASP:OD1	2.50	0.43
2:D:686:SER:OG	2:D:690:LYS:NZ	2.52	0.43
3:B:505:THR:HA	3:B:520:VAL:O	2.19	0.43
3:C:815:ASP:OD2	3:C:815:ASP:N	2.51	0.43
3:C:844:ARG:HA	3:C:844:ARG:HD2	1.85	0.43
2:D:727:LEU:HD11	2:D:785:GLY:HA3	2.01	0.43
1:G:629:LYS:O	1:G:633:GLU:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:813:SER:O	1:G:813:SER:OG	2.36	0.43
2:J:83:LEU:O	2:J:87:ASN:ND2	2.52	0.42
3:B:596:PHE:HB2	3:B:607:LEU:HB3	2.00	0.42
2:D:278:MET:SD	2:D:278:MET:N	2.91	0.42
3:I:805:CYS:O	3:I:809:SER:OG	2.36	0.42
2:J:583:ILE:O	2:J:588:ILE:N	2.51	0.42
3:B:758:ARG:O	3:B:762:THR:OG1	2.31	0.42
2:J:858:SER:HA	2:J:861:ASN:HB2	2.01	0.42
3:B:577:TYR:OH	3:B:583:LYS:NZ	2.52	0.42
3:C:742:LYS:HD3	3:C:742:LYS:HA	1.81	0.42
3:I:670:ASP:OD1	3:I:670:ASP:N	2.52	0.42
2:D:408:LYS:HA	2:D:411:ILE:HG12	2.01	0.42
2:D:697:ILE:O	2:D:715:HIS:ND1	2.51	0.42
2:J:724:LEU:O	2:J:728:HIS:N	2.42	0.42
3:H:765:MET:SD	3:H:765:MET:N	2.93	0.42
3:H:825:TYR:OH	3:H:870:GLU:OE1	2.32	0.42
2:D:448:LEU:HD21	2:D:783:MET:HE3	2.02	0.42
2:D:715:HIS:CD2	2:D:718:THR:HB	2.54	0.42
2:D:721:LYS:O	2:D:733:HIS:NE2	2.53	0.42
3:B:781:LEU:HD23	3:B:781:LEU:HA	1.92	0.42
3:I:675:ASP:O	3:I:679:GLU:N	2.52	0.42
1:G:799:ARG:HA	1:G:799:ARG:HD3	1.92	0.42
2:J:614:LEU:HD23	2:J:614:LEU:HA	1.91	0.42
2:J:721:LYS:HG2	2:J:724:LEU:HD12	2.02	0.42
2:J:808:LEU:HA	2:J:811:ILE:HD12	2.02	0.42
2:D:602:LYS:HA	2:D:605:LYS:HD2	2.01	0.42
2:J:202:ILE:HG23	2:J:205:ARG:HH21	1.85	0.42
2:J:802:GLN:O	2:J:806:THR:HG23	2.20	0.42
3:C:639:ARG:H	3:C:639:ARG:HG2	1.59	0.42
3:H:802:MET:HE2	3:H:802:MET:HB2	1.86	0.42
3:C:641:SER:OG	3:C:643:ASP:OD2	2.33	0.41
1:A:798:VAL:HB	3:C:480:PHE:HA	2.01	0.41
3:C:694:GLN:OE1	3:C:807:ARG:NH2	2.53	0.41
3:H:679:GLU:HG2	3:I:623:LEU:HD12	2.01	0.41
1:A:646:ILE:HG13	1:A:652:VAL:HG11	2.01	0.41
3:B:524:SER:HB3	3:B:529:ARG:HE	1.84	0.41
2:J:423:PRO:HA	2:J:426:ASP:HB2	2.02	0.41
3:H:686:ASP:OD1	3:H:686:ASP:N	2.53	0.41
2:D:124:GLN:H	2:D:124:GLN:HG2	1.66	0.41
1:A:749:ILE:HG22	1:A:750:LYS:HB3	2.02	0.41
3:C:568:CYS:HB3	3:C:597:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LYS:HE3	2:J:24:GLU:HB3	2.02	0.41
3:H:447:THR:HB	3:I:478:ILE:HD13	2.03	0.41
3:I:830:ILE:O	3:I:833:THR:OG1	2.30	0.41
2:J:136:LEU:HD12	2:J:136:LEU:HA	1.88	0.41
3:B:686:ASP:OD1	3:B:686:ASP:N	2.53	0.41
3:I:503:ARG:O	3:I:522:ASN:ND2	2.48	0.41
3:H:528:GLN:H	3:H:528:GLN:HG3	1.73	0.41
2:D:136:LEU:HD23	2:D:136:LEU:HA	1.92	0.41
3:C:808:LEU:HD22	3:C:813:TYR:HB2	2.03	0.41
2:D:517:TYR:N	2:D:523:ARG:O	2.53	0.41
3:C:809:SER:HA	3:C:860:VAL:HG11	2.02	0.40
2:D:378:ASP:HA	2:D:381:LYS:HD2	2.03	0.40
2:D:119:LEU:HD22	2:D:132:VAL:HG13	2.04	0.40
3:C:503:ARG:O	3:C:522:ASN:ND2	2.51	0.40
2:D:693:ILE:O	2:D:697:ILE:HG12	2.21	0.40
2:J:784:LYS:NZ	2:J:844:GLN:OE1	2.41	0.40
3:B:802:MET:HB2	3:B:802:MET:HE2	1.82	0.40
3:H:495:ILE:HD11	3:H:631:TYR:HB2	2.04	0.40
3:H:808:LEU:HD22	3:H:813:TYR:HB2	2.03	0.40
2:D:510:LEU:HD23	2:D:510:LEU:HA	1.94	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	270/840 (32%)	254 (94%)	15 (6%)	1 (0%)	30	53
1	G	270/840 (32%)	247 (92%)	22 (8%)	1 (0%)	30	53
2	D	814/1648 (49%)	774 (95%)	37 (4%)	3 (0%)	30	53
2	J	814/1648 (49%)	787 (97%)	24 (3%)	3 (0%)	30	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	415/875 (47%)	403 (97%)	12 (3%)	0	100	100
3	C	373/875 (43%)	353 (95%)	15 (4%)	5 (1%)	9	26
3	H	415/875 (47%)	399 (96%)	15 (4%)	1 (0%)	43	66
3	I	373/875 (43%)	357 (96%)	14 (4%)	2 (0%)	24	49
All	All	3744/8476 (44%)	3574 (96%)	154 (4%)	16 (0%)	31	53

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	477	PRO
3	C	478	ILE
3	C	488	PRO
3	I	488	PRO
1	A	642	GLN
2	J	169	ARG
2	J	174	LEU
3	C	835	SER
3	H	449	PRO
2	D	173	PHE
2	D	486	ASP
2	J	170	HIS
3	C	638	LEU
2	D	266	PRO
3	I	477	PRO
1	G	634	GLU

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	248/753 (33%)	234 (94%)	14 (6%)	19	43
1	G	248/753 (33%)	234 (94%)	14 (6%)	19	43
2	D	769/1528 (50%)	761 (99%)	8 (1%)	68	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	769/1528 (50%)	759 (99%)	10 (1%)	61	78
3	B	384/790 (49%)	371 (97%)	13 (3%)	32	58
3	C	343/790 (43%)	326 (95%)	17 (5%)	22	47
3	H	384/790 (49%)	375 (98%)	9 (2%)	44	67
3	I	343/790 (43%)	325 (95%)	18 (5%)	21	46
All	All	3488/7722 (45%)	3385 (97%)	103 (3%)	37	60

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	LEU
1	A	636	THR
1	A	637	THR
1	A	645	VAL
1	A	646	ILE
1	A	649	THR
1	A	653	VAL
1	A	703	ILE
1	A	711	ILE
1	A	759	LEU
1	A	773	LEU
1	A	777	LEU
1	A	784	ILE
1	A	830	THR
2	J	136	LEU
2	J	174	LEU
2	J	182	MET
2	J	213	ASP
2	J	239	MET
2	J	553	LEU
2	J	672	ASN
2	J	744	ILE
2	J	863	VAL
2	J	879	MET
3	B	439	MET
3	B	505	THR
3	B	515	ASN
3	B	517	ILE
3	B	546	LEU
3	B	628	ASN

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Mol	Chain	Res	Type
3	B	629	THR
3	B	661	VAL
3	B	665	THR
3	B	673	LEU
3	B	741	CYS
3	B	771	ASN
3	B	874	ILE
3	C	490	THR
3	C	495	ILE
3	C	497	LEU
3	C	512	ASN
3	C	539	VAL
3	C	592	VAL
3	C	630	ILE
3	C	639	ARG
3	C	645	LEU
3	C	670	ASP
3	C	673	LEU
3	C	680	THR
3	C	771	ASN
3	C	775	ILE
3	C	815	ASP
3	C	841	ASP
3	C	863	VAL
1	G	433	HIS
1	G	632	SER
1	G	636	THR
1	G	637	THR
1	G	641	LEU
1	G	642	GLN
1	G	711	ILE
1	G	713	SER
1	G	727	SER
1	G	753	THR
1	G	773	LEU
1	G	793	ILE
1	G	830	THR
1	G	837	SER
3	H	483	THR
3	H	509	SER
3	H	515	ASN
3	H	627	THR

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Mol	Chain	Res	Type
3	H	665	THR
3	H	678	MET
3	H	785	ILE
3	H	802	MET
3	H	806	ILE
3	I	489	ASN
3	I	490	THR
3	I	493	SER
3	I	512	ASN
3	I	537	SER
3	I	542	GLN
3	I	605	LEU
3	I	628	ASN
3	I	646	THR
3	I	654	CYS
3	I	680	THR
3	I	683	LEU
3	I	735	ILE
3	I	779	SER
3	I	825	TYR
3	I	828	LEU
3	I	841	ASP
3	I	854	CYS
2	D	88	ARG
2	D	100	TYR
2	D	134	ASP
2	D	211	TYR
2	D	249	LEU
2	D	486	ASP
2	D	615	GLU
2	D	691	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	GLN
1	A	642	GLN
1	A	746	HIS
2	J	15	GLN
2	J	43	ASN
2	J	79	ASN
2	J	87	ASN

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Mol	Chain	Res	Type
2	J	118	ASN
2	J	124	GLN
2	J	125	HIS
2	J	160	GLN
2	J	162	ASN
2	J	246	ASN
2	J	277	ASN
2	J	417	GLN
2	J	443	ASN
2	J	589	GLN
2	J	687	GLN
2	J	695	GLN
2	J	707	ASN
2	J	735	ASN
3	B	677	ASN
3	C	548	GLN
3	C	822	GLN
1	G	746	HIS
1	G	801	ASN
3	H	818	ASN
3	H	822	GLN
3	H	861	GLN
3	I	542	GLN
3	I	628	ASN
3	I	737	ASN
3	I	783	ASN
3	I	861	GLN
2	D	72	ASN
2	D	118	ASN
2	D	184	ASN
2	D	200	ASN
2	D	246	ASN
2	D	481	ASN
2	D	549	ASN
2	D	628	HIS
2	D	728	HIS
2	D	735	ASN
2	D	802	GLN
2	D	865	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](#)

There are no chain breaks in this entry.

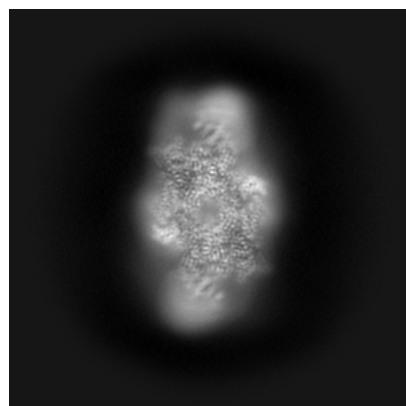
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40006. These allow visual inspection of the internal detail of the map and identification of artifacts.

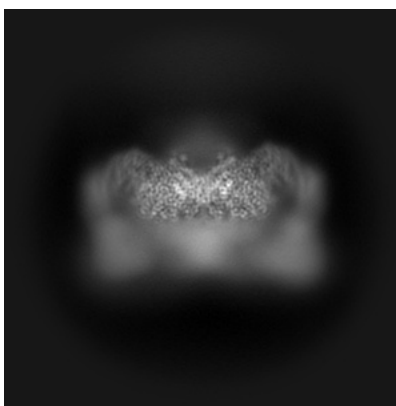
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

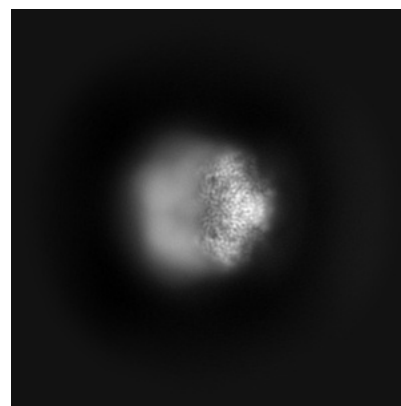
6.1.1 Primary map



X

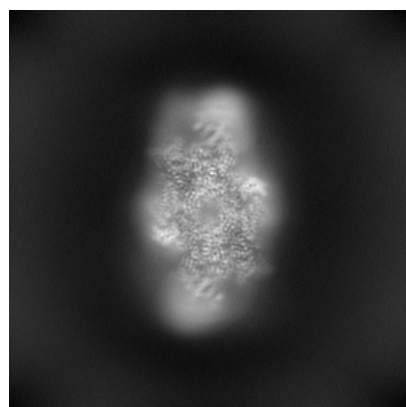


Y

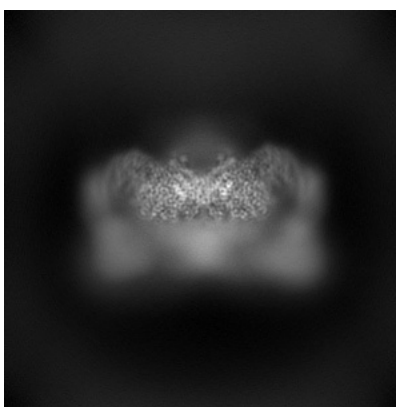


Z

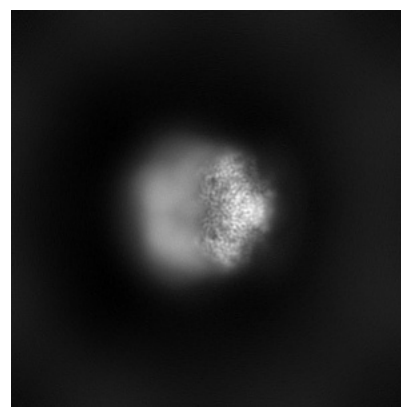
6.1.2 Raw map



X



Y

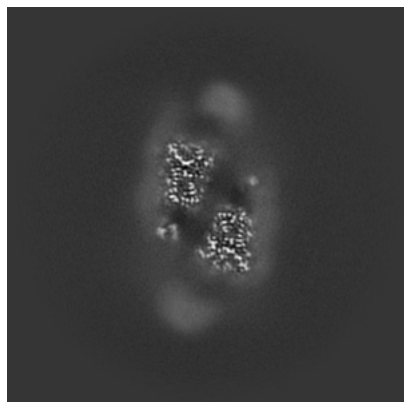


Z

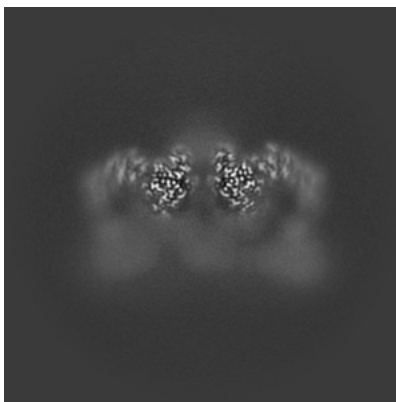
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

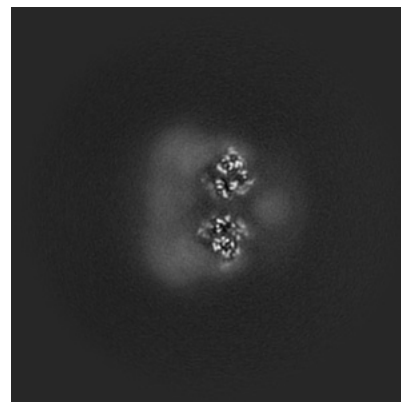
6.2.1 Primary map



X Index: 150

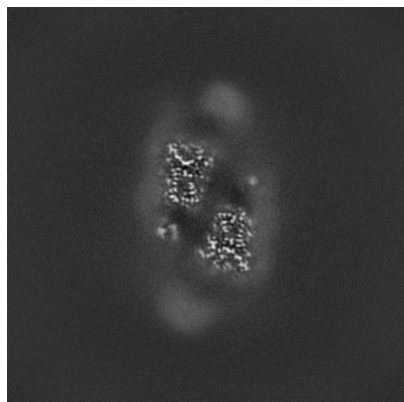


Y Index: 150

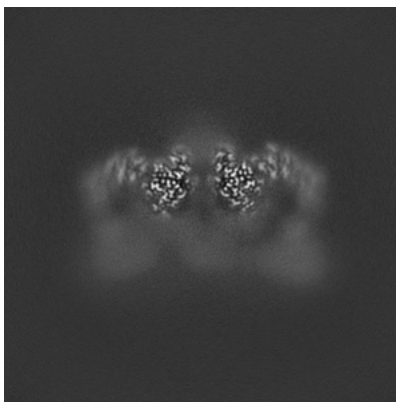


Z Index: 150

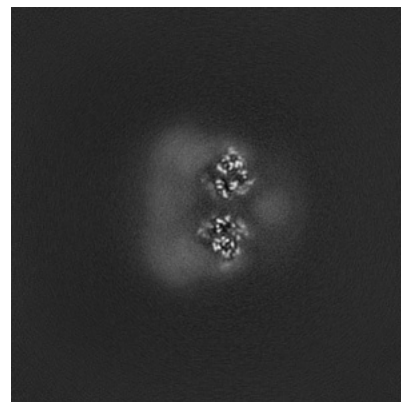
6.2.2 Raw map



X Index: 150



Y Index: 150

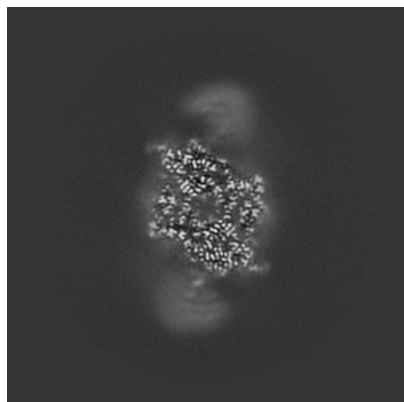


Z Index: 150

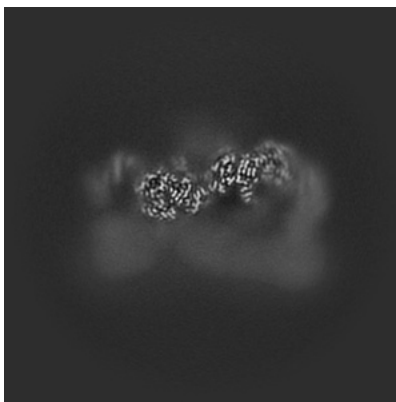
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

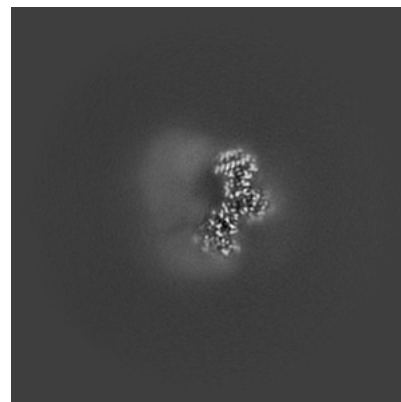
6.3.1 Primary map



X Index: 165

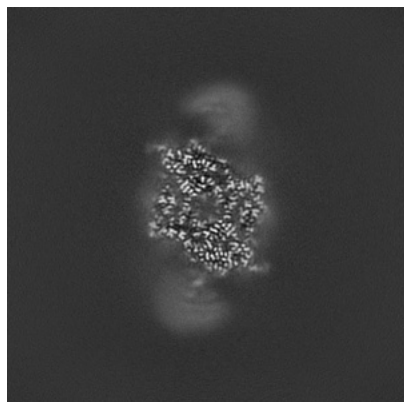


Y Index: 159

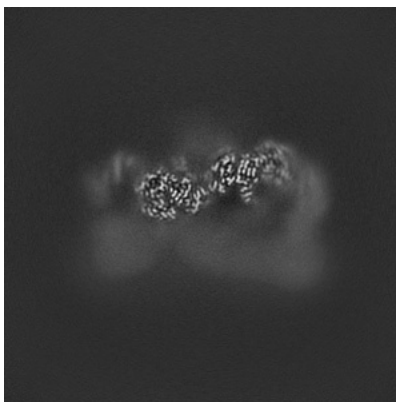


Z Index: 164

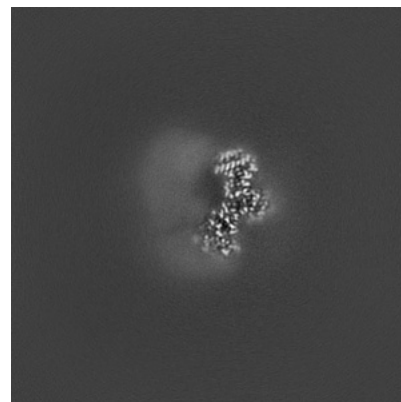
6.3.2 Raw map



X Index: 165



Y Index: 159

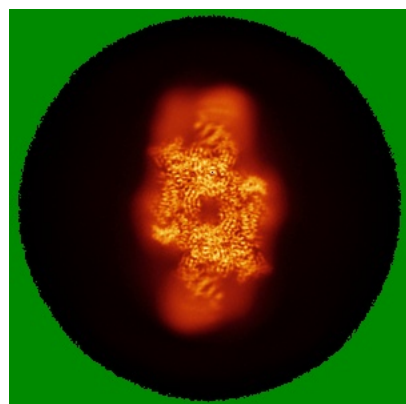


Z Index: 164

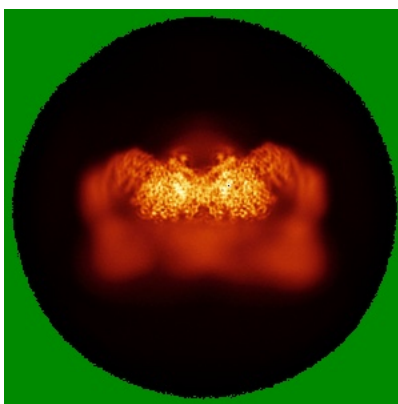
The images above show the largest variance slices of the map in three orthogonal directions.

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

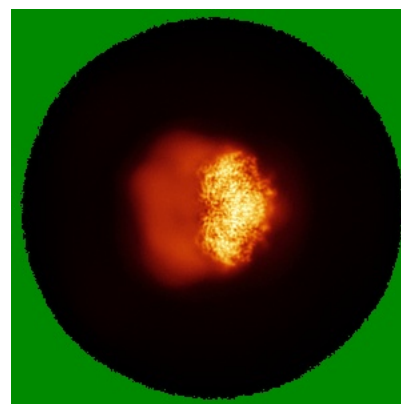
6.4.1 Primary map



X

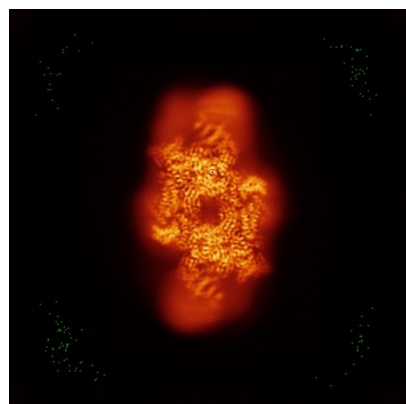


Y

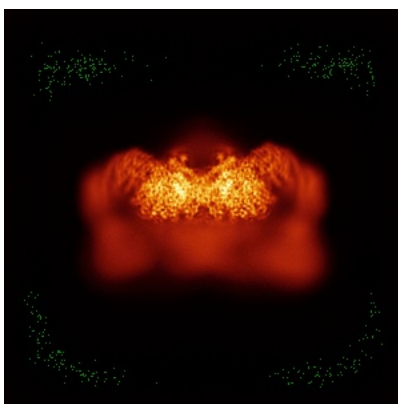


Z

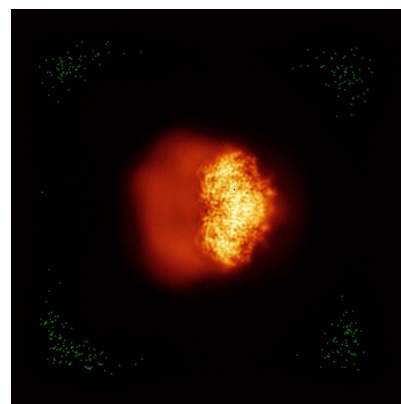
6.4.2 Raw map



X



Y

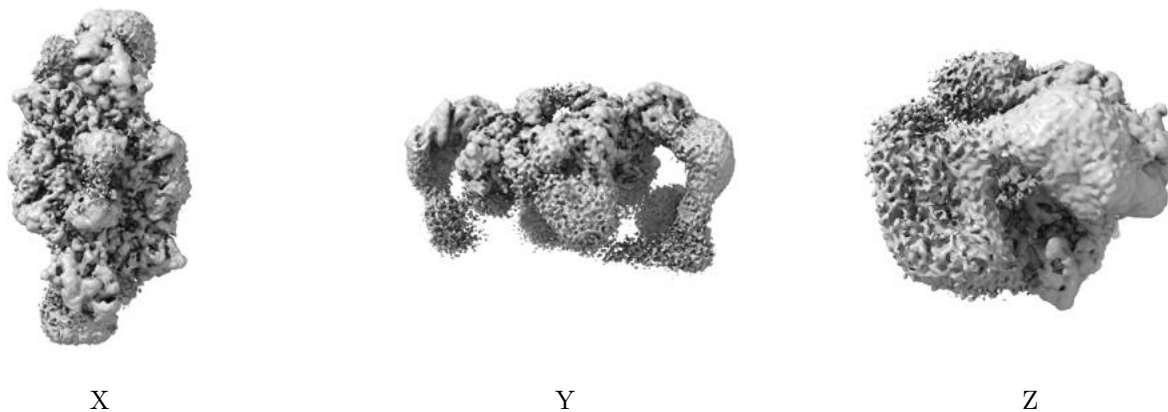


Z

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

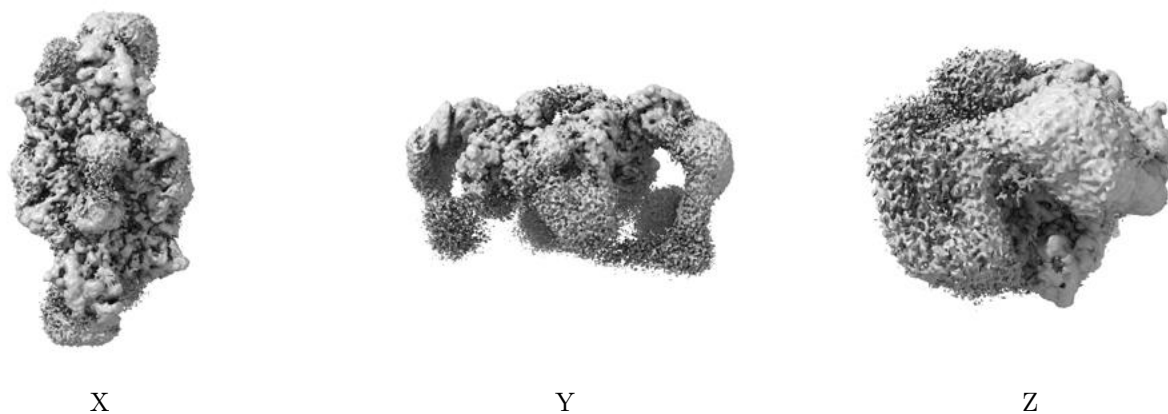
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.315. 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.

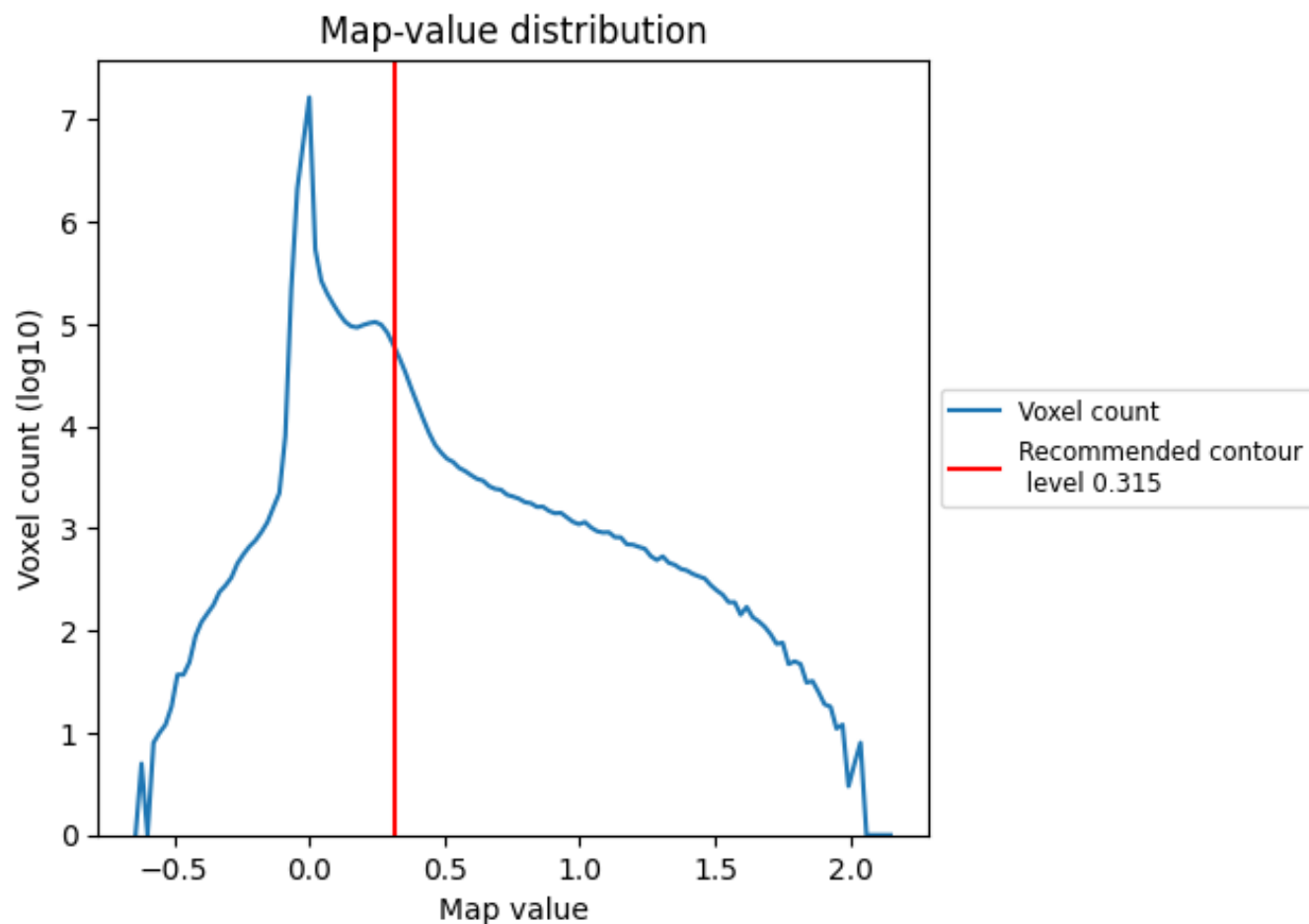
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

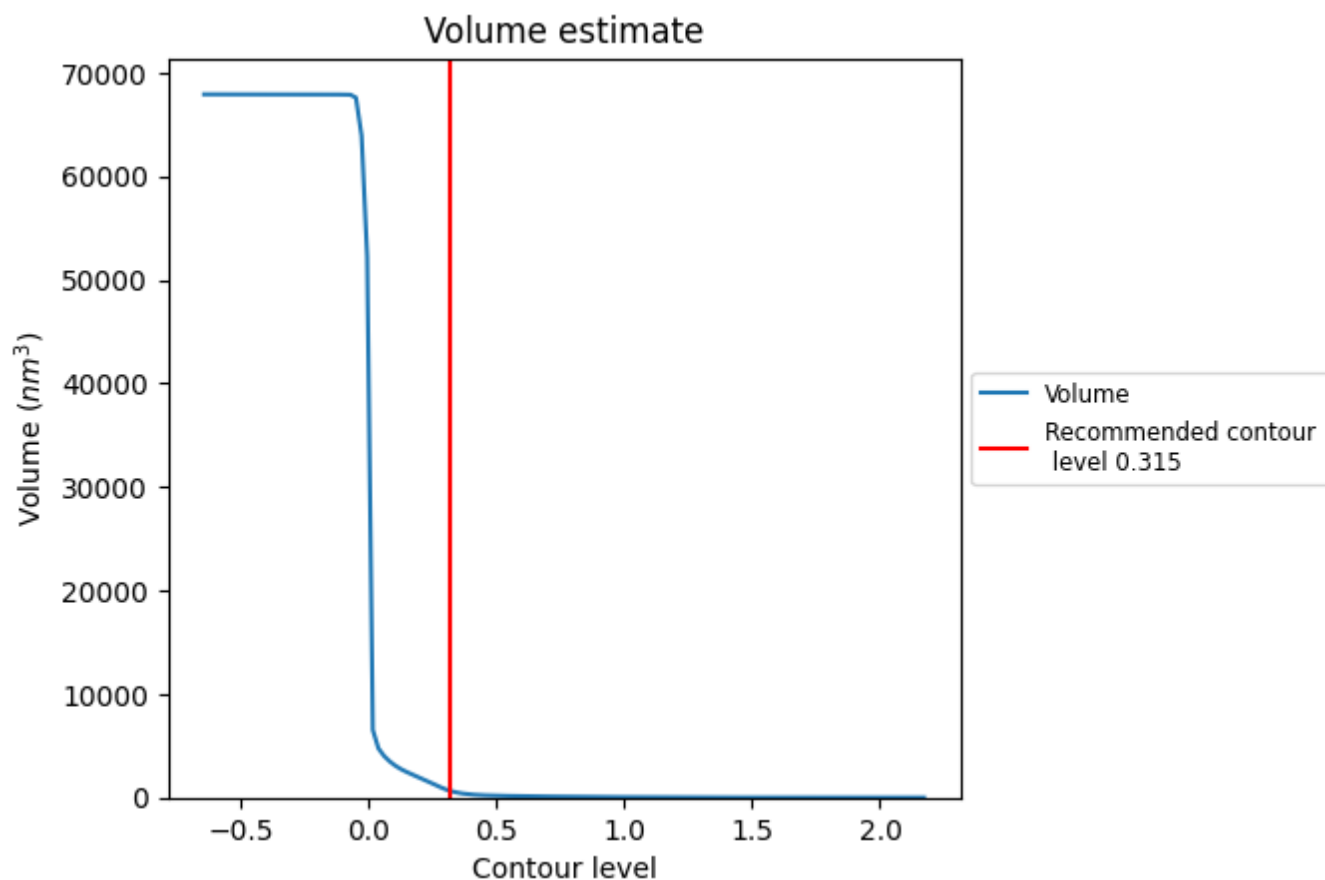
This section contains the results of statistical analysis of the map.

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.

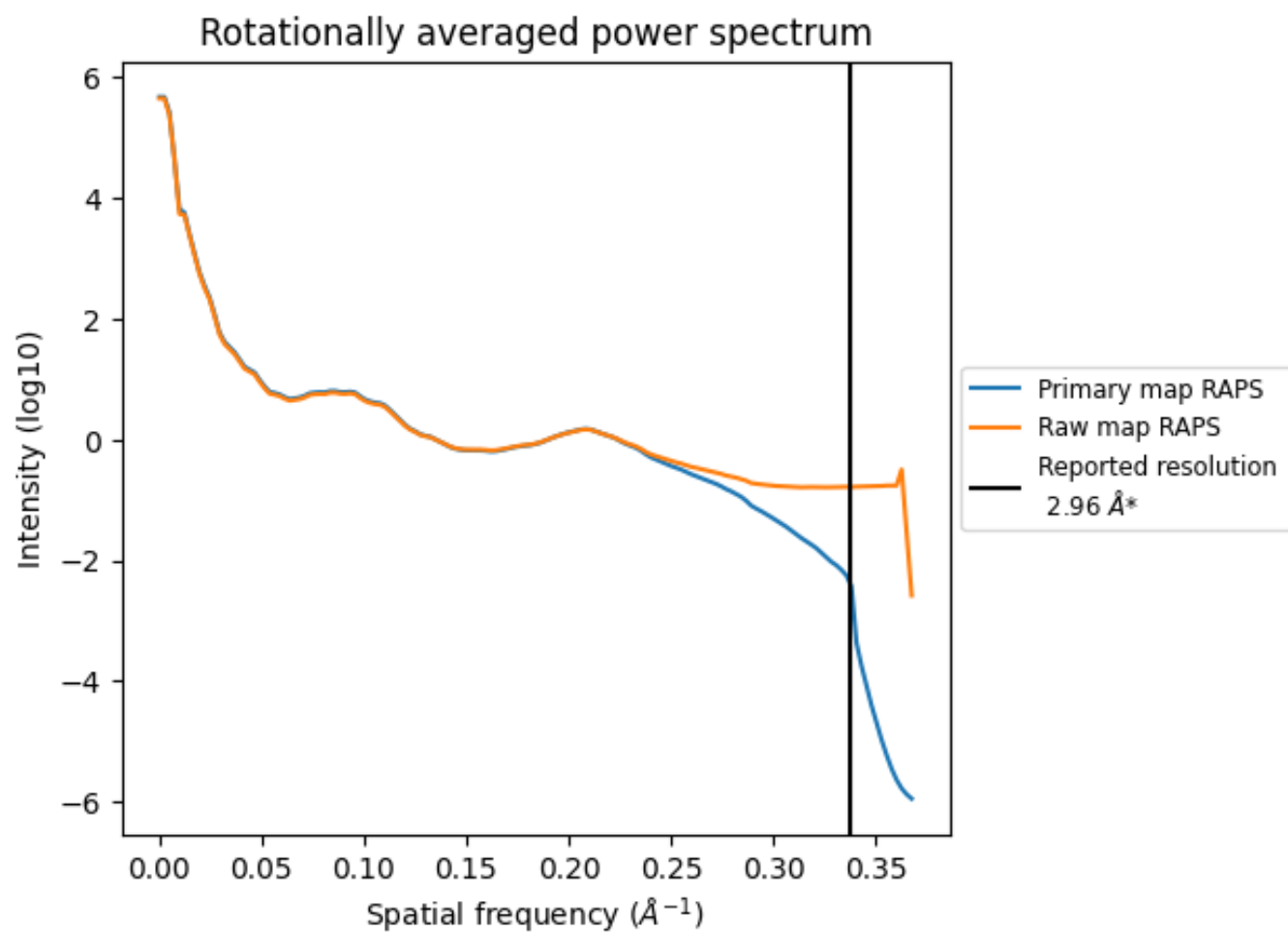
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 687 nm^3 ; this corresponds to an approximate mass of 620 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 ⓘ

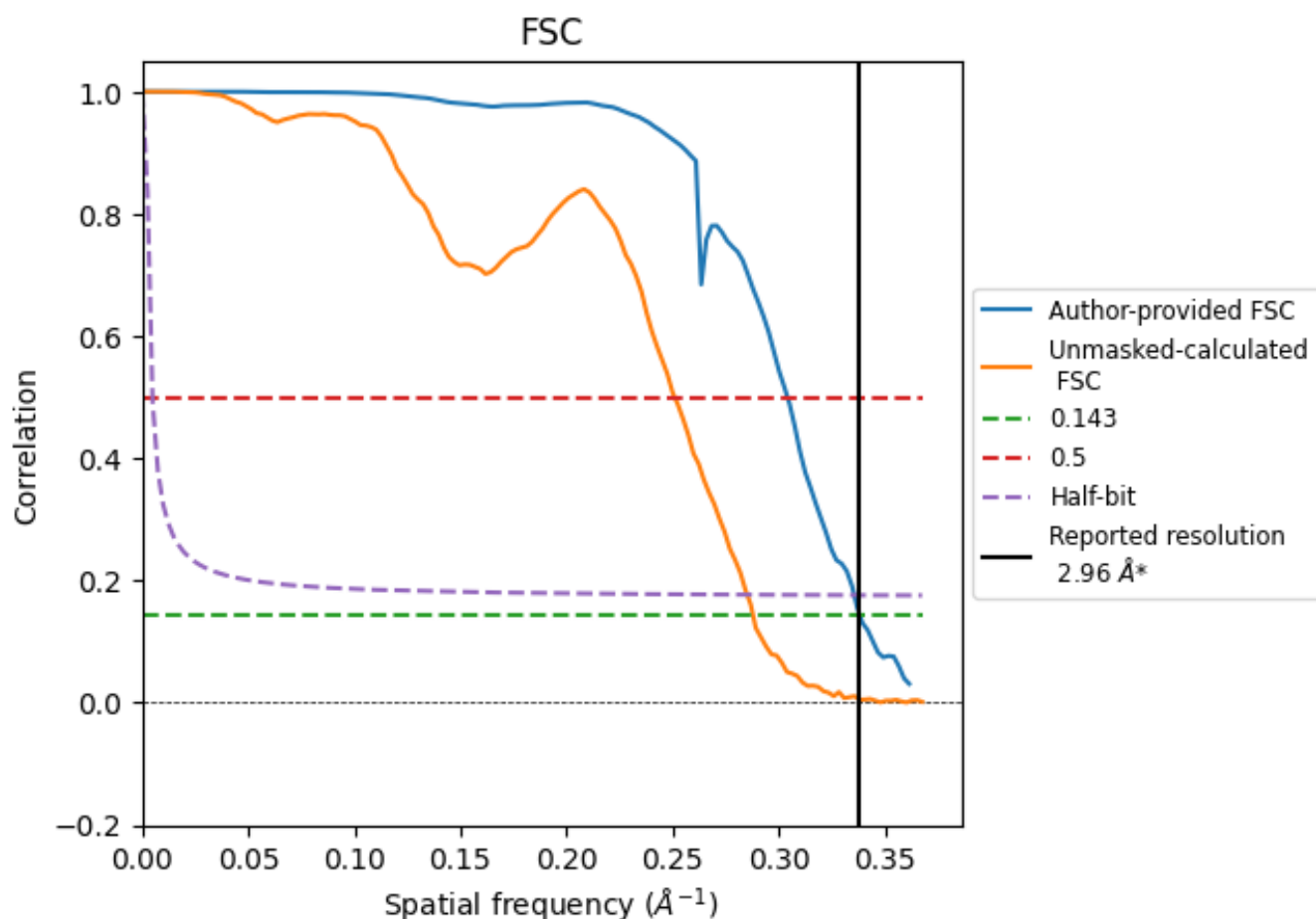


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

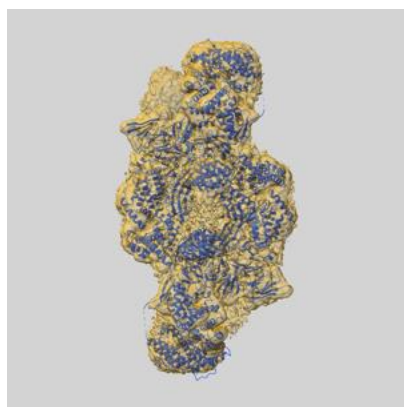
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.29	2.98
Unmasked-calculated*	3.47	3.99	3.51

*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 3.47 differs from the reported value 2.96 by more than 10 %

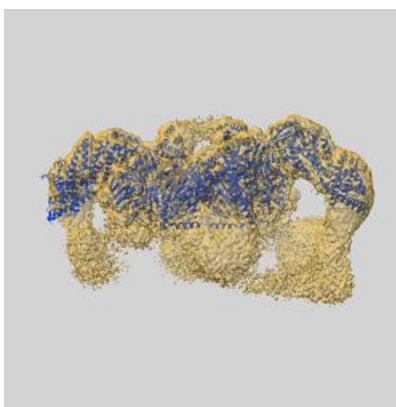
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40006 and PDB model 8GHL. Per-residue inclusion information can be found in section [3](#) on page [5](#).

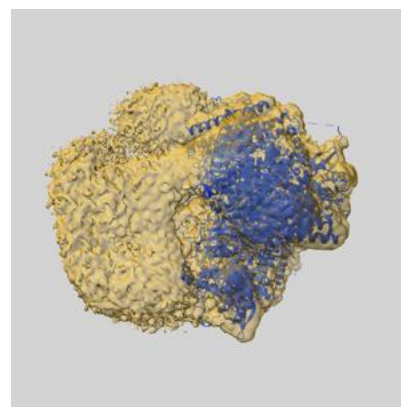
9.1 Map-model overlay [i](#)



X



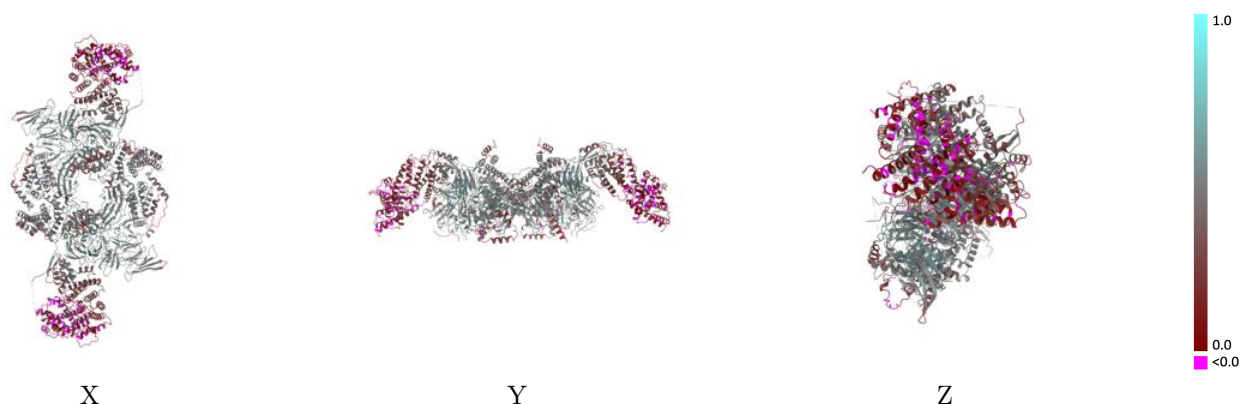
Y



Z

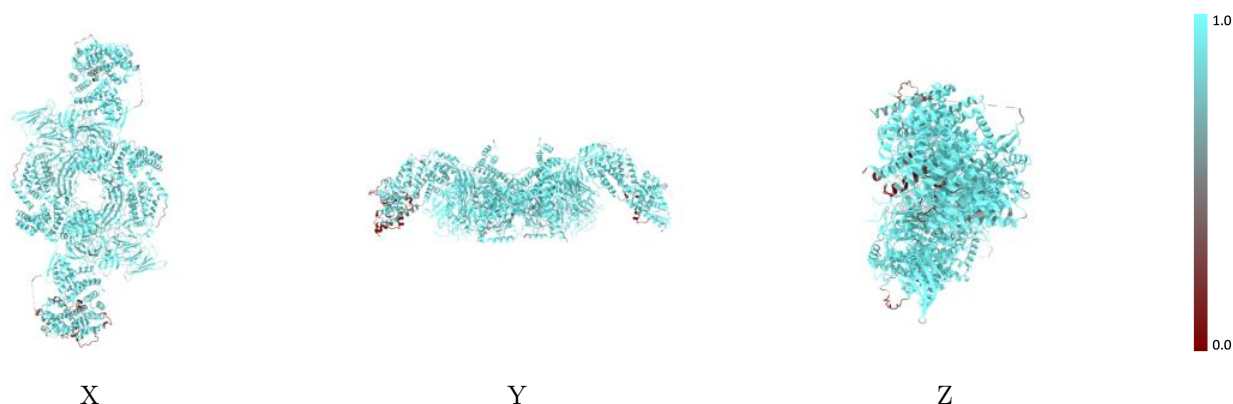
The images above show the 3D surface view of the map at the recommended contour level 0.315 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



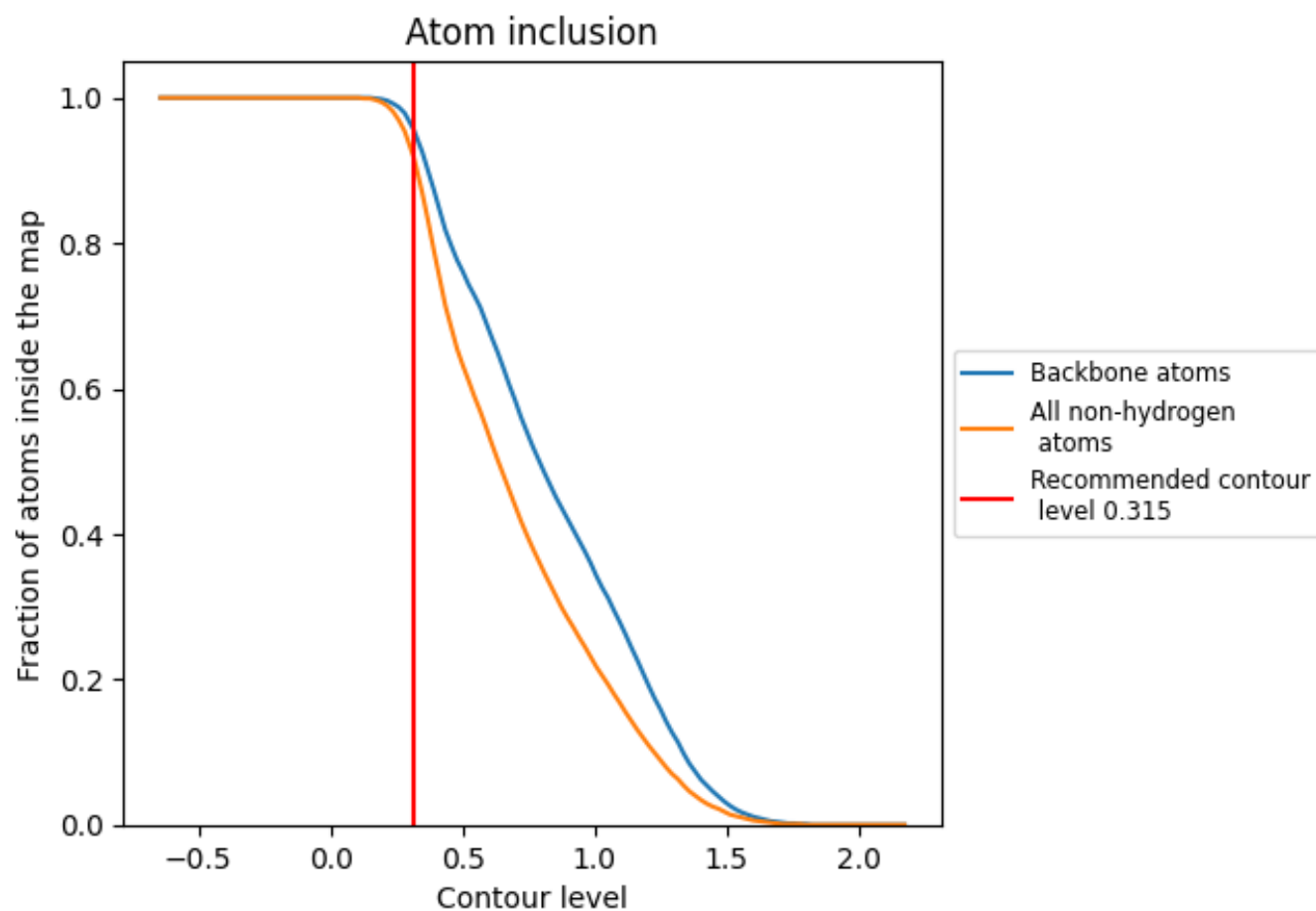
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.315).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.315) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.3810
A	0.9640	0.5000
B	0.9410	0.4660
C	0.9540	0.4930
D	0.9090	0.2540
G	0.9730	0.5000
H	0.9510	0.4660
I	0.9490	0.4960
J	0.8350	0.2460

