Full wwPDB EM Validation Report

May 26, 2026 – 10:09 AM JST

PDB ID	:	9VAX / pdb_00009vax
EMDB ID	:	EMD-64908
Title	:	Cryo-EM structure of human Neurotensin Receptor 1 (hNTSR1)-Gi1 complex in nucleotide-free C state 1
Authors	:	Kobayashi, K.; Matsui, T.E.; Fukuda, M.; Kawakami, K.; Yamashita, K.; Kato, H.E.
Deposited on	:	2025-06-04
Resolution	:	3.46 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 (i) 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 (i)) were used in the production of this report:

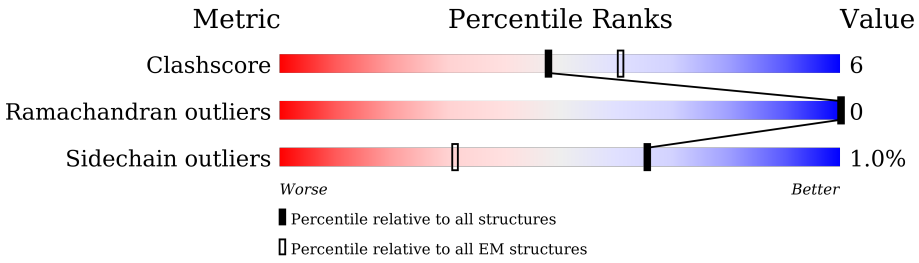
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

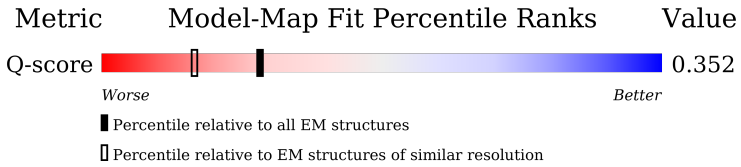
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 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	13788 (2.96 - 3.96)

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 <=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	354	18% 55% 6% • 38%
2	B	358	9% 81% 12% • 6%
3	C	71	24% 75% 25%
4	D	259	29% 75% 14% 11%

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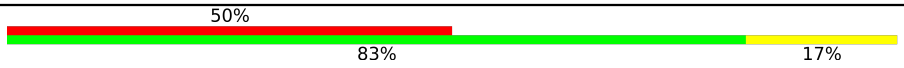
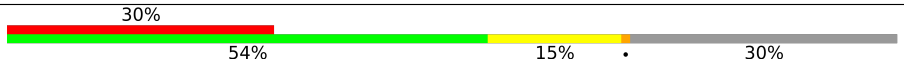
Mol	Chain	Length	Quality of chain
5	L	6	
6	R	436	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8936 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	218	1747	1112	292	331	12	0	0

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	338	2584	1595	462	506	21	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	53	Total	C	N	O	S	0	0
			404	256	70	75	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	231	Total	C	N	O	S	0	0
			1762	1121	294	337	10		

- Molecule 5 is a protein called JMV449.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	6	Total	C	N	O	0	0
			53	38	8	7		

- Molecule 6 is a protein called Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	306	Total	C	N	O	S	0	0
			2386	1565	396	410	15		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-11	MET	-	initiating methionine	UNP P30989
R	-10	GLY	-	expression tag	UNP P30989
R	-9	GLN	-	expression tag	UNP P30989
R	-8	PRO	-	expression tag	UNP P30989
R	-7	GLY	-	expression tag	UNP P30989
R	-6	ASN	-	expression tag	UNP P30989
R	-5	GLY	-	expression tag	UNP P30989
R	-4	SER	-	expression tag	UNP P30989
R	-3	ALA	-	expression tag	UNP P30989
R	-2	PHE	-	expression tag	UNP P30989
R	-1	LEU	-	expression tag	UNP P30989
R	0	LEU	-	expression tag	UNP P30989
R	1	ALA	-	expression tag	UNP P30989
R	2	PRO	-	expression tag	UNP P30989
R	3	ASN	-	expression tag	UNP P30989
R	4	ARG	-	expression tag	UNP P30989

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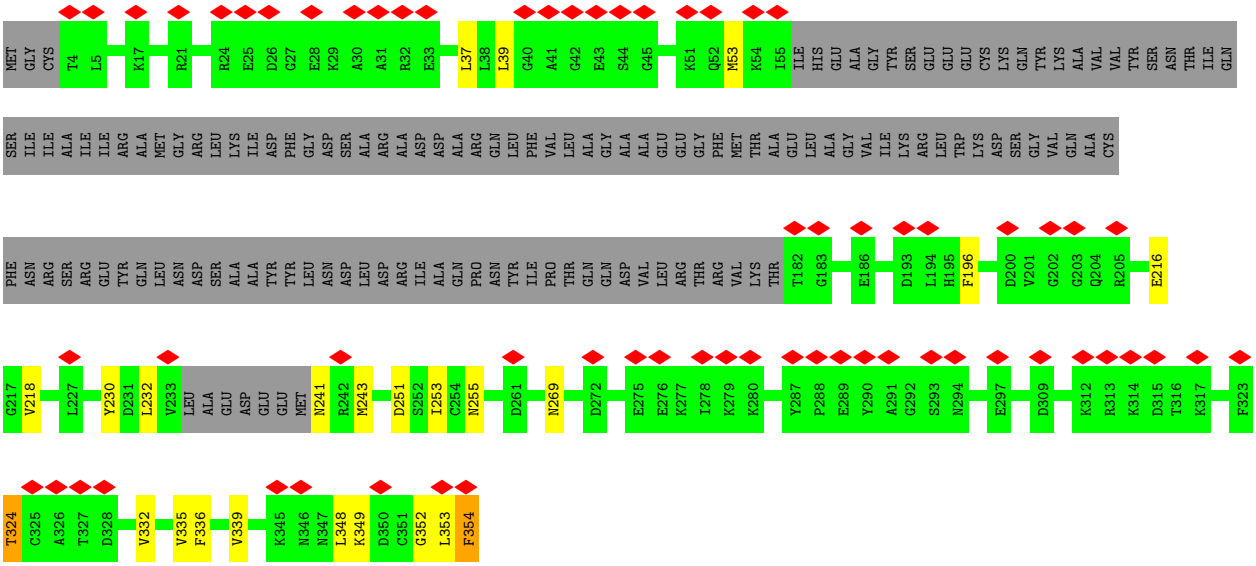
Chain	Residue	Modelled	Actual	Comment	Reference
R	5	SER	-	expression tag	UNP P30989
R	6	HIS	-	expression tag	UNP P30989
R	7	ALA	-	expression tag	UNP P30989
R	8	PRO	-	expression tag	UNP P30989
R	9	ASP	-	expression tag	UNP P30989
R	10	HIS	-	expression tag	UNP P30989
R	11	ASP	-	expression tag	UNP P30989
R	12	VAL	-	expression tag	UNP P30989
R	13	GLU	-	expression tag	UNP P30989
R	14	ASN	-	expression tag	UNP P30989
R	15	LEU	-	expression tag	UNP P30989
R	16	TYR	-	expression tag	UNP P30989
R	17	PHE	-	expression tag	UNP P30989
R	18	GLN	-	expression tag	UNP P30989
R	19	GLY	-	expression tag	UNP P30989
R	85	LEU	ALA	engineered mutation	UNP P30989
R	419	LEU	-	expression tag	UNP P30989
R	420	GLU	-	expression tag	UNP P30989
R	421	VAL	-	expression tag	UNP P30989
R	422	LEU	-	expression tag	UNP P30989
R	423	PHE	-	expression tag	UNP P30989
R	424	GLN	-	expression tag	UNP P30989

3 Residue-property plots (i)

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

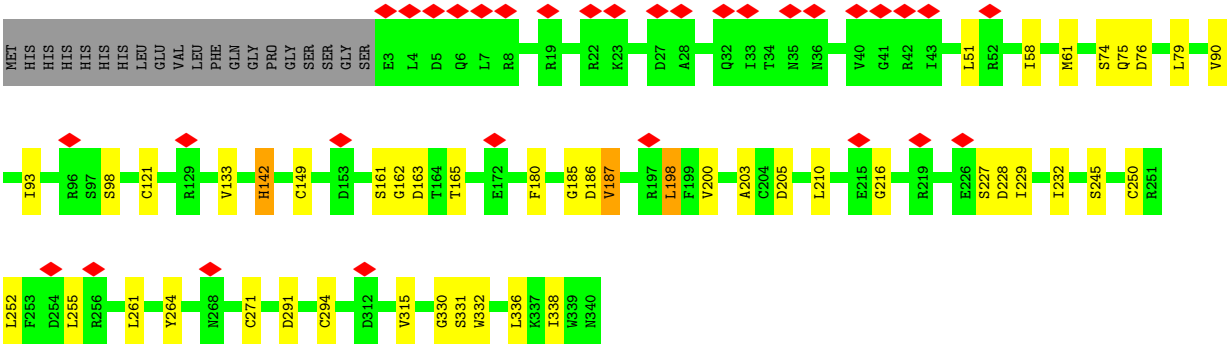
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



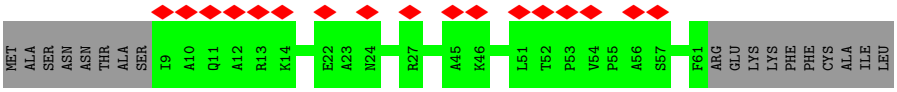
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



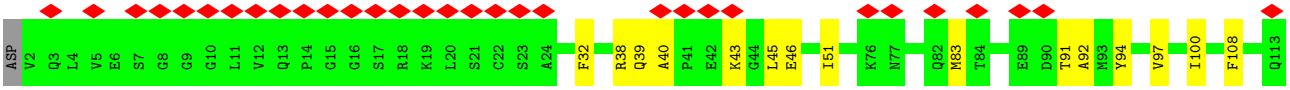
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

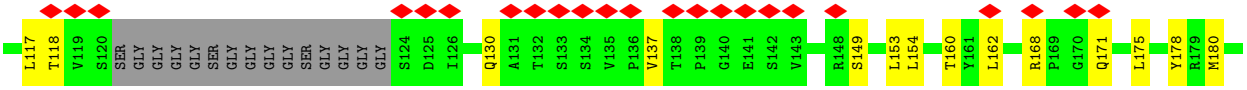
Chain C:

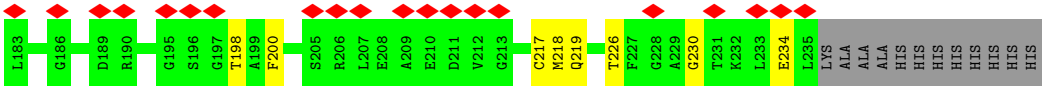


• Molecule 4: scFv16

Chain D:

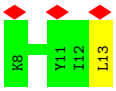






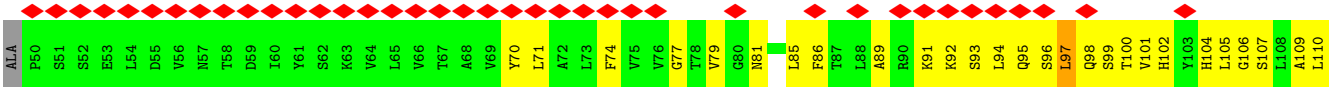
• Molecule 5: JMV449

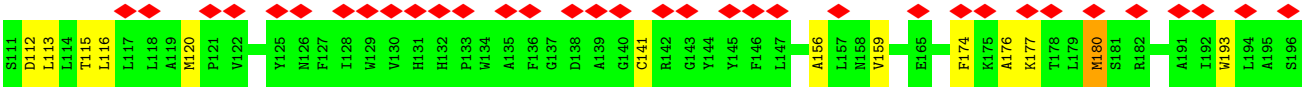
Chain L:

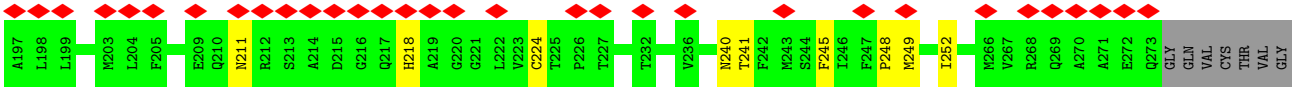


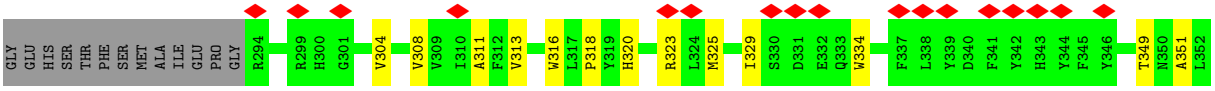
• Molecule 6: Neurotensin receptor type 1

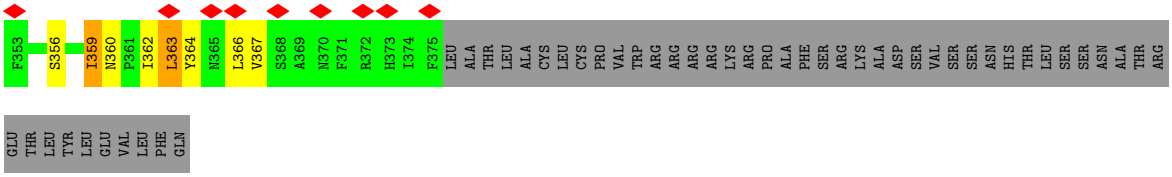
Chain R:










F353
S356
I359
N360
P361
I362
L363
Y364
N365
L366
V367
S368
A369
N370
F371
R372
H373
I374
F375
LEU ALA THR LEU ALA CYS LEU CYS PRO VAL TRP ARG ARG ARG ARG LYS ARG PRO ALA PHE SER ARG LYS ALA ASP SER VAL SER SER ASN HIS THR LEU SER SER ASN ALA THR ARG
GLU THR LEU TYR LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58597	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.164	Depositor
Minimum map value	-0.603	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.308	Depositor
Map size (Å)	160.46666, 160.46666, 160.46666	wwPDB
Map dimensions	116, 116, 116	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3833333, 1.3833333, 1.3833333	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	0.53	0/1776	1.09	4/2382 (0.2%)
2	B	0.58	0/2631	0.95	0/3569
3	C	0.53	0/410	0.99	0/554
4	D	0.59	0/1806	0.96	0/2450
5	L	0.60	0/54	0.70	0/69
6	R	0.61	3/2447 (0.1%)	1.21	9/3343 (0.3%)
All	All	0.58	3/9124 (0.0%)	1.06	13/12367 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	174	PHE	CG-CD1	7.56	1.54	1.38
6	R	174	PHE	CG-CD2	-5.64	1.27	1.38
6	R	180	MET	CB-CG	-5.28	1.36	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	97	LEU	N-CA-C	-10.63	99.69	111.07
6	R	95	GLN	N-CA-C	-9.87	99.56	111.69
1	A	352	GLY	N-CA-C	-8.29	103.74	115.43
6	R	104	HIS	N-CA-C	-7.37	103.25	111.28
6	R	180	MET	CA-CB-CG	6.80	127.70	114.10
6	R	79	VAL	N-CA-CB	6.19	117.12	110.62
1	A	354	PHE	CA-CB-CG	6.07	119.87	113.80
6	R	367	VAL	N-CA-CB	5.93	117.09	110.51
6	R	174	PHE	CB-CG-CD2	5.63	130.27	120.70
6	R	180	MET	CB-CA-C	-5.61	102.08	110.16
1	A	216	GLU	N-CA-CB	5.48	118.02	109.97
6	R	174	PHE	CB-CG-CD1	-5.46	111.42	120.70
1	A	324	THR	CA-CB-OG1	-5.17	101.84	109.60

There are no chirality outliers.

There are no planarity outliers.

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	1747	0	1731	12	0
2	B	2584	0	2475	28	0
3	C	404	0	416	0	0
4	D	1762	0	1696	20	0
5	L	53	0	63	0	0
6	R	2386	0	2393	42	0
All	All	8936	0	8774	102	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 6.

All (102) 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:B:121:CYS:HG	2:B:149:CYS:HG	0.82	0.80
2:B:142:HIS:CD2	2:B:161:SER:HB2	2.23	0.73
6:R:177:LYS:HD3	6:R:180:MET:SD	2.29	0.72
6:R:176:ALA:O	6:R:180:MET:HG3	1.92	0.69
1:A:332:VAL:HG22	1:A:336:PHE:CE2	2.31	0.66
4:D:40:ALA:HB3	4:D:43:LYS:HB2	1.76	0.66
4:D:175:LEU:HD21	4:D:178:TYR:HB3	1.78	0.64
1:A:39:LEU:HD13	1:A:253:ILE:HD13	1.80	0.62
6:R:116:LEU:O	6:R:120:MET:HB3	2.00	0.62
2:B:180:PHE:HE1	2:B:216:GLY:HA2	1.63	0.62
6:R:159:VAL:HG12	6:R:252:ILE:HD11	1.81	0.61
2:B:58:ILE:HD11	2:B:330:GLY:HA3	1.84	0.59
6:R:101:VAL:O	6:R:102:HIS:C	2.45	0.59
4:D:91:THR:HG23	4:D:118:THR:HA	1.87	0.57
6:R:107:SER:OG	6:R:193:TRP:NE1	2.37	0.57
6:R:86:PHE:O	6:R:89:ALA:HB3	2.04	0.56
1:A:37:LEU:HD22	1:A:39:LEU:HG	1.87	0.56
2:B:142:HIS:NE2	2:B:161:SER:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.39	0.54
4:D:39:GLN:HB2	4:D:45:LEU:HD23	1.88	0.54
6:R:245:PHE:HB2	6:R:320:HIS:ND1	2.22	0.54
2:B:74:SER:OG	2:B:76:ASP:OD1	2.25	0.53
2:B:163:ASP:OD1	2:B:165:THR:HG22	2.08	0.53
6:R:74:PHE:HA	6:R:116:LEU:HD21	1.91	0.53
2:B:79:LEU:HD11	2:B:93:ILE:HD12	1.91	0.52
6:R:112:ASP:O	6:R:115:THR:OG1	2.21	0.52
2:B:198:LEU:HD13	2:B:210:LEU:HD11	1.92	0.52
1:A:53:MET:HE1	1:A:335:VAL:HG21	1.91	0.52
1:A:230:TYR:HA	1:A:243:MET:HB2	1.92	0.52
6:R:211:ASN:HD21	6:R:218:HIS:H	1.57	0.52
4:D:162:LEU:HD11	4:D:217:CYS:HB2	1.93	0.51
4:D:83:MET:HE1	4:D:117:LEU:HD13	1.91	0.51
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.93	0.51
6:R:308:VAL:HA	6:R:363:LEU:HD21	1.94	0.50
6:R:99:SER:HA	6:R:102:HIS:CD2	2.46	0.50
6:R:110:LEU:HD12	6:R:113:LEU:HD23	1.94	0.50
4:D:149:SER:HB3	4:D:198:THR:HA	1.92	0.50
4:D:219:GLN:HE21	4:D:226:THR:H	1.60	0.50
6:R:70:TYR:HE1	6:R:351:ALA:HA	1.76	0.50
6:R:329:ILE:O	6:R:334:TRP:NE1	2.44	0.49
2:B:51:LEU:HD11	2:B:338:ILE:HD11	1.93	0.49
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.95	0.49
6:R:362:ILE:HA	6:R:366:LEU:HB3	1.95	0.49
2:B:75:GLN:O	2:B:98:SER:OG	2.29	0.49
2:B:93:ILE:HG12	2:B:133:VAL:HG21	1.93	0.49
4:D:130:GLN:HG3	4:D:230:GLY:H	1.77	0.49
6:R:311:ALA:HB1	6:R:359:ILE:HD12	1.95	0.49
6:R:96:SER:HA	6:R:99:SER:H	1.77	0.49
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.94	0.48
1:A:37:LEU:HB2	1:A:218:VAL:HG11	1.96	0.47
4:D:162:LEU:HD12	4:D:218:MET:O	2.14	0.47
1:A:349:LYS:HA	1:A:354:PHE:CD1	2.49	0.47
2:B:200:VAL:HG12	2:B:232:ILE:HD13	1.97	0.47
6:R:70:TYR:HB3	6:R:120:MET:HE1	1.96	0.47
2:B:229:ILE:HG22	2:B:245:SER:HB3	1.97	0.46
2:B:294:CYS:SG	2:B:315:VAL:HG11	2.55	0.46
4:D:137:VAL:N	4:D:234:GLU:O	2.48	0.46
6:R:98:GLN:O	6:R:102:HIS:N	2.28	0.46
2:B:271:CYS:SG	2:B:291:ASP:HB2	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:ALA:HB3	4:D:94:TYR:HE1	1.81	0.46
2:B:229:ILE:HA	2:B:245:SER:HA	1.98	0.46
1:A:269:ASN:HA	1:A:324:THR:HG22	1.97	0.45
2:B:227:SER:OG	2:B:228:ASP:N	2.45	0.45
6:R:156:ALA:HB2	6:R:316:TRP:HZ3	1.82	0.45
6:R:141:CYS:CB	6:R:224:CYS:HG	2.30	0.45
6:R:159:VAL:HG12	6:R:252:ILE:CD1	2.45	0.45
4:D:153:LEU:HD12	4:D:200:PHE:CZ	2.52	0.45
6:R:85:LEU:HD21	6:R:109:ALA:HB3	1.99	0.45
6:R:101:VAL:HG13	6:R:105:LEU:HD13	1.99	0.45
4:D:162:LEU:HD22	4:D:200:PHE:CG	2.52	0.44
2:B:161:SER:OG	2:B:162:GLY:N	2.50	0.44
6:R:325:MET:HG2	6:R:329:ILE:HD12	2.00	0.43
4:D:38:ARG:O	4:D:46:GLU:N	2.46	0.43
6:R:106:GLY:O	6:R:107:SER:C	2.61	0.43
6:R:97:LEU:O	6:R:100:THR:OG1	2.36	0.43
2:B:187:VAL:HG12	2:B:203:ALA:HB2	2.00	0.43
6:R:106:GLY:O	6:R:109:ALA:N	2.52	0.43
1:A:196:PHE:HE1	1:A:339:VAL:HG11	1.82	0.43
1:A:232:LEU:O	1:A:241:ASN:N	2.53	0.42
6:R:318:PRO:CB	6:R:349:THR:HG22	2.50	0.42
2:B:252:LEU:HD11	2:B:261:LEU:HD23	2.01	0.42
6:R:112:ASP:O	6:R:113:LEU:C	2.62	0.42
6:R:240:ASN:OD1	6:R:323:ARG:NH1	2.52	0.42
4:D:154:LEU:HA	4:D:160:THR:HG22	2.00	0.42
6:R:92:LYS:C	6:R:94:LEU:H	2.28	0.42
6:R:249:MET:SD	6:R:313:VAL:HG22	2.59	0.42
2:B:331:SER:OG	2:B:332:TRP:N	2.52	0.42
4:D:168:ARG:HB2	4:D:171:GLN:HB2	2.00	0.42
2:B:61:MET:HB3	2:B:61:MET:HE3	1.87	0.41
2:B:185:GLY:N	2:B:205:ASP:OD1	2.51	0.41
4:D:32:PHE:CD1	4:D:100:ILE:HB	2.55	0.41
6:R:77:GLY:O	6:R:81:ASN:ND2	2.52	0.41
6:R:71:LEU:HD13	6:R:71:LEU:HA	1.88	0.41
6:R:360:ASN:O	6:R:364:TYR:HB2	2.21	0.41
4:D:180:MET:HB2	4:D:180:MET:HE3	1.63	0.41
1:A:348:LEU:HG	1:A:353:LEU:HD23	2.02	0.41
6:R:241:THR:HG23	6:R:320:HIS:HB3	2.03	0.41
6:R:91:LYS:NZ	6:R:93:SER:HA	2.36	0.41
6:R:156:ALA:HB1	6:R:248:PRO:HG3	2.02	0.41
2:B:162:GLY:HA2	2:B:186:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:362:ILE:HA	6:R:366:LEU:CB	2.51	0.40
4:D:97:VAL:HG11	4:D:108:PHE:HD1	1.86	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	212/354 (60%)	212 (100%)	0	0	100	100
2	B	336/358 (94%)	328 (98%)	8 (2%)	0	100	100
3	C	51/71 (72%)	51 (100%)	0	0	100	100
4	D	227/259 (88%)	224 (99%)	3 (1%)	0	100	100
5	L	4/6 (67%)	4 (100%)	0	0	100	100
6	R	302/436 (69%)	290 (96%)	12 (4%)	0	100	100
All	All	1132/1484 (76%)	1109 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	191/305 (63%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	277/298 (93%)	273 (99%)	4 (1%)	59 72
3	C	42/58 (72%)	42 (100%)	0	100 100
4	D	191/209 (91%)	190 (100%)	1 (0%)	81 81
5	L	6/6 (100%)	5 (83%)	1 (17%)	2 13
6	R	255/368 (69%)	251 (98%)	4 (2%)	55 71
All	All	962/1244 (77%)	952 (99%)	10 (1%)	65 76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	90	VAL
2	B	142	HIS
2	B	187	VAL
2	B	198	LEU
4	D	51	ILE
5	L	13	LEU
6	R	304	VAL
6	R	356	SER
6	R	359	ILE
6	R	363	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
2	B	75	GLN
2	B	91	HIS
2	B	176	GLN
2	B	259	GLN
2	B	311	HIS
2	B	340	ASN
4	D	130	GLN
4	D	171	GLN
4	D	219	GLN
6	R	81	ASN
6	R	211	ASN
6	R	269	GLN
6	R	365	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

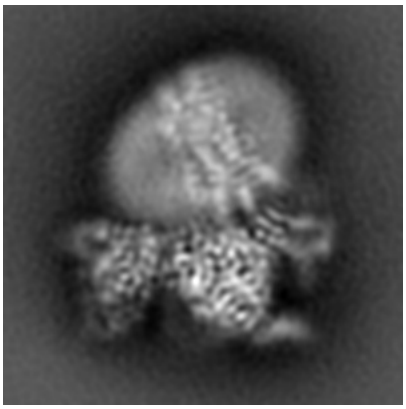
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64908. These allow visual inspection of the internal detail of the map and identification of artifacts.

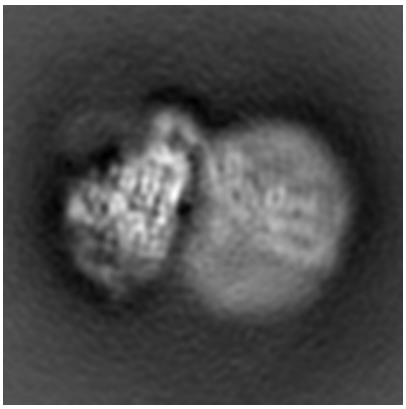
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

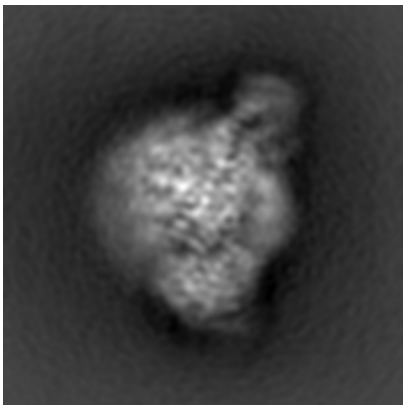
6.1.1 Primary map



X

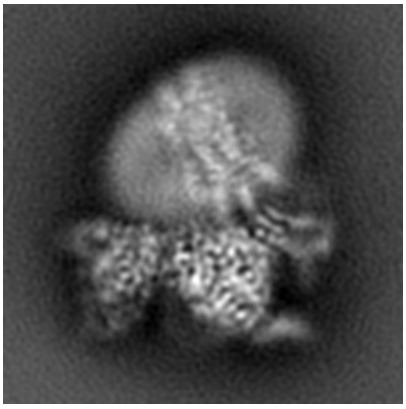


Y

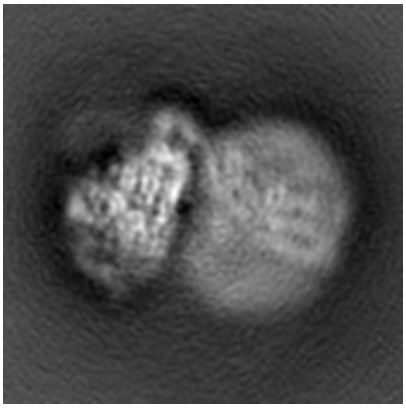


Z

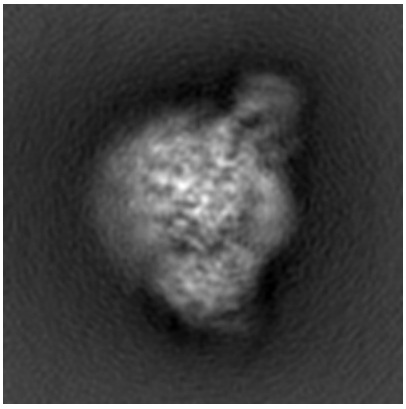
6.1.2 Raw map



X



Y

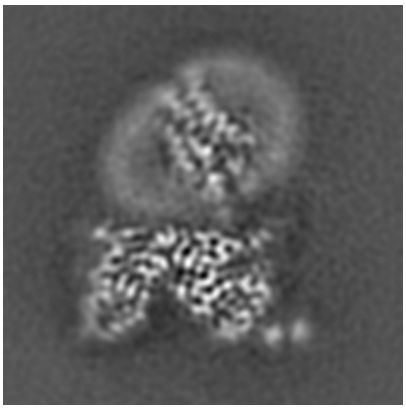


Z

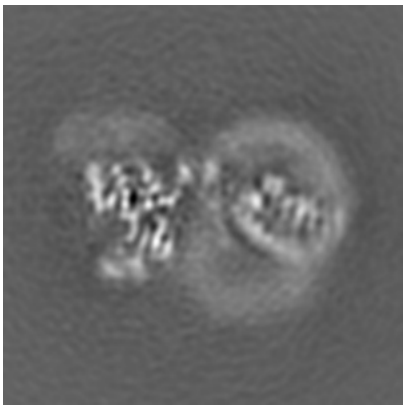
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

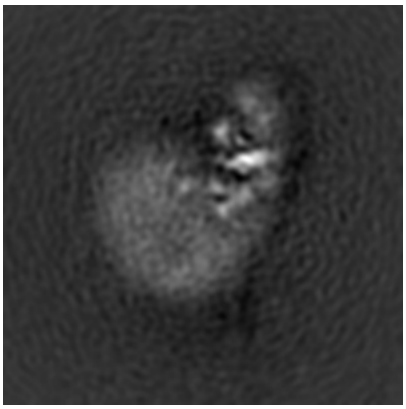
6.2.1 Primary map



X Index: 58

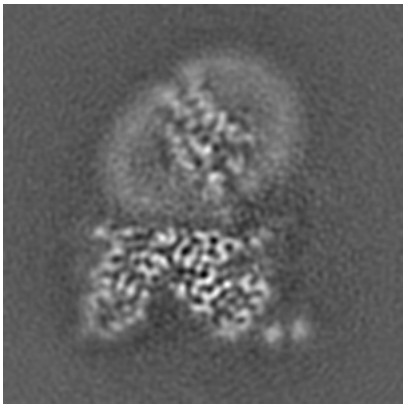


Y Index: 58

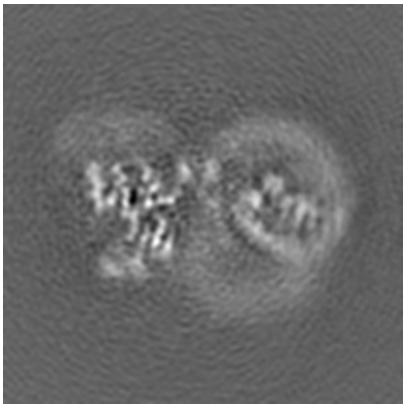


Z Index: 58

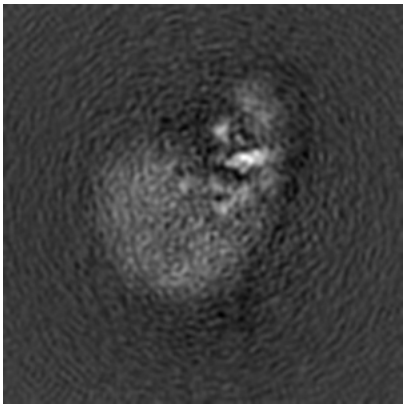
6.2.2 Raw map



X Index: 58



Y Index: 58

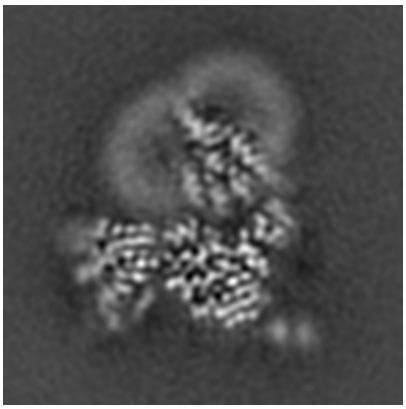


Z Index: 58

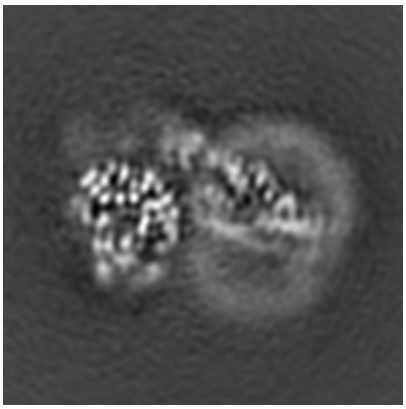
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

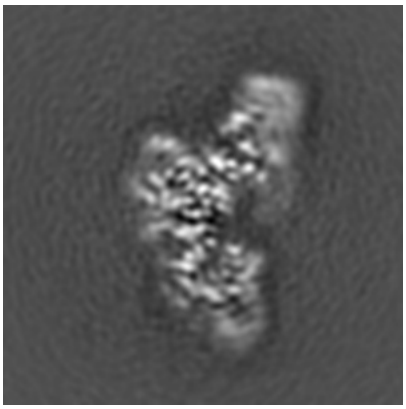
6.3.1 Primary map



X Index: 62

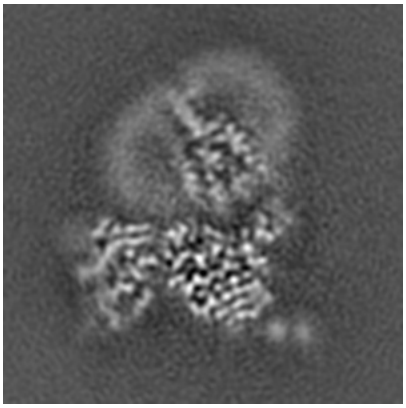


Y Index: 63

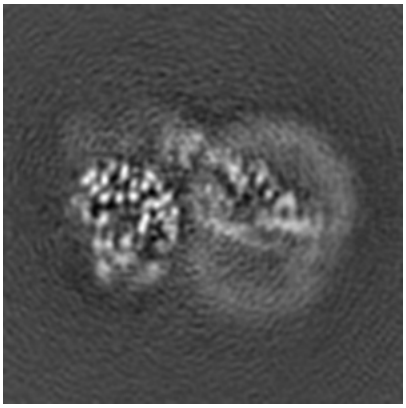


Z Index: 45

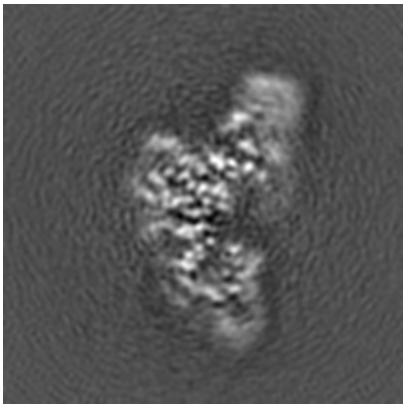
6.3.2 Raw map



X Index: 61



Y Index: 63

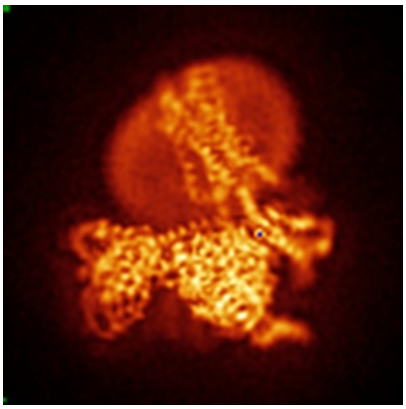


Z Index: 45

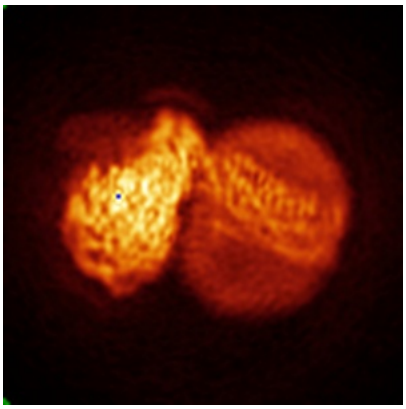
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

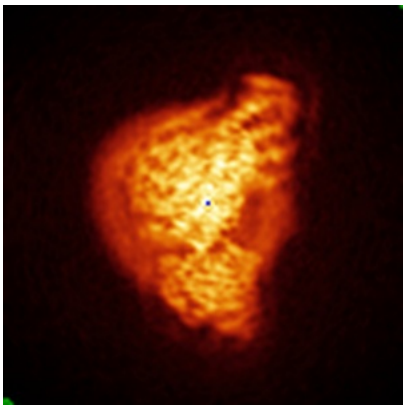
6.4.1 Primary map



X

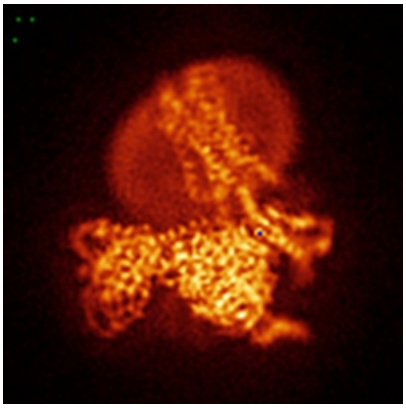


Y

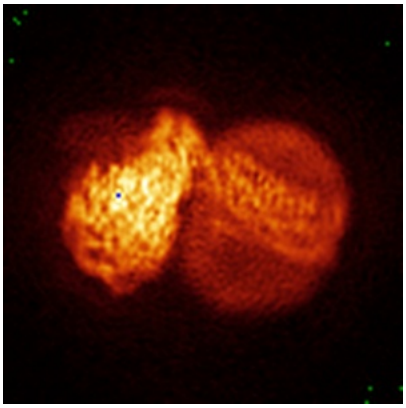


Z

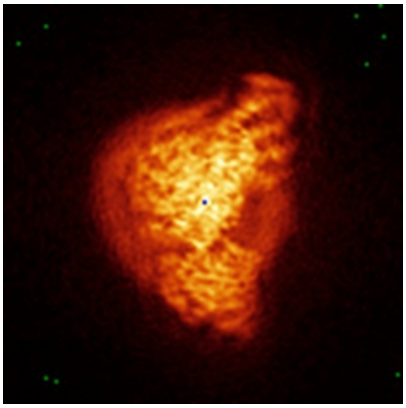
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.308. 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

X Y Z

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.

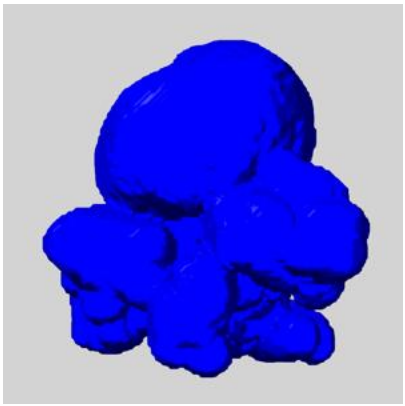
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

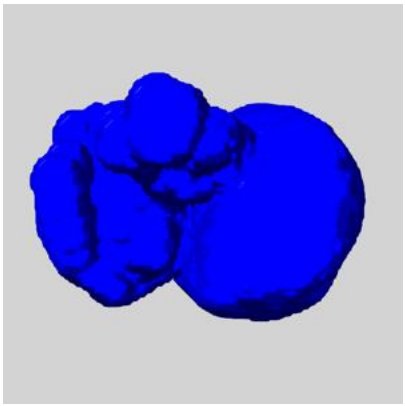
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

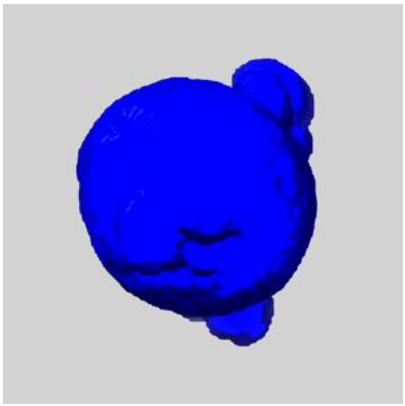
6.6.1 emd_64908_msk_1.map (i)



X



Y

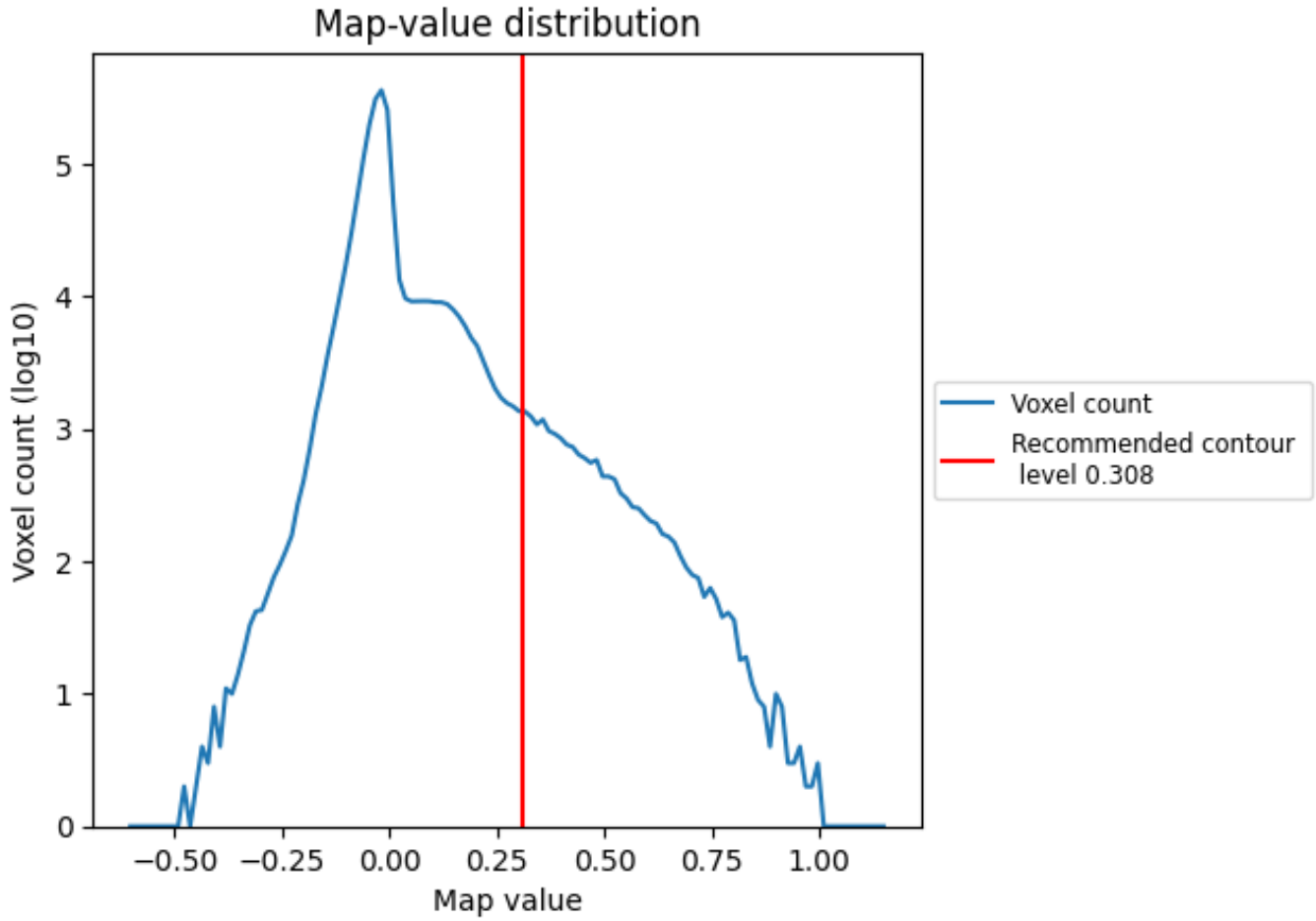


Z

7 Map analysis

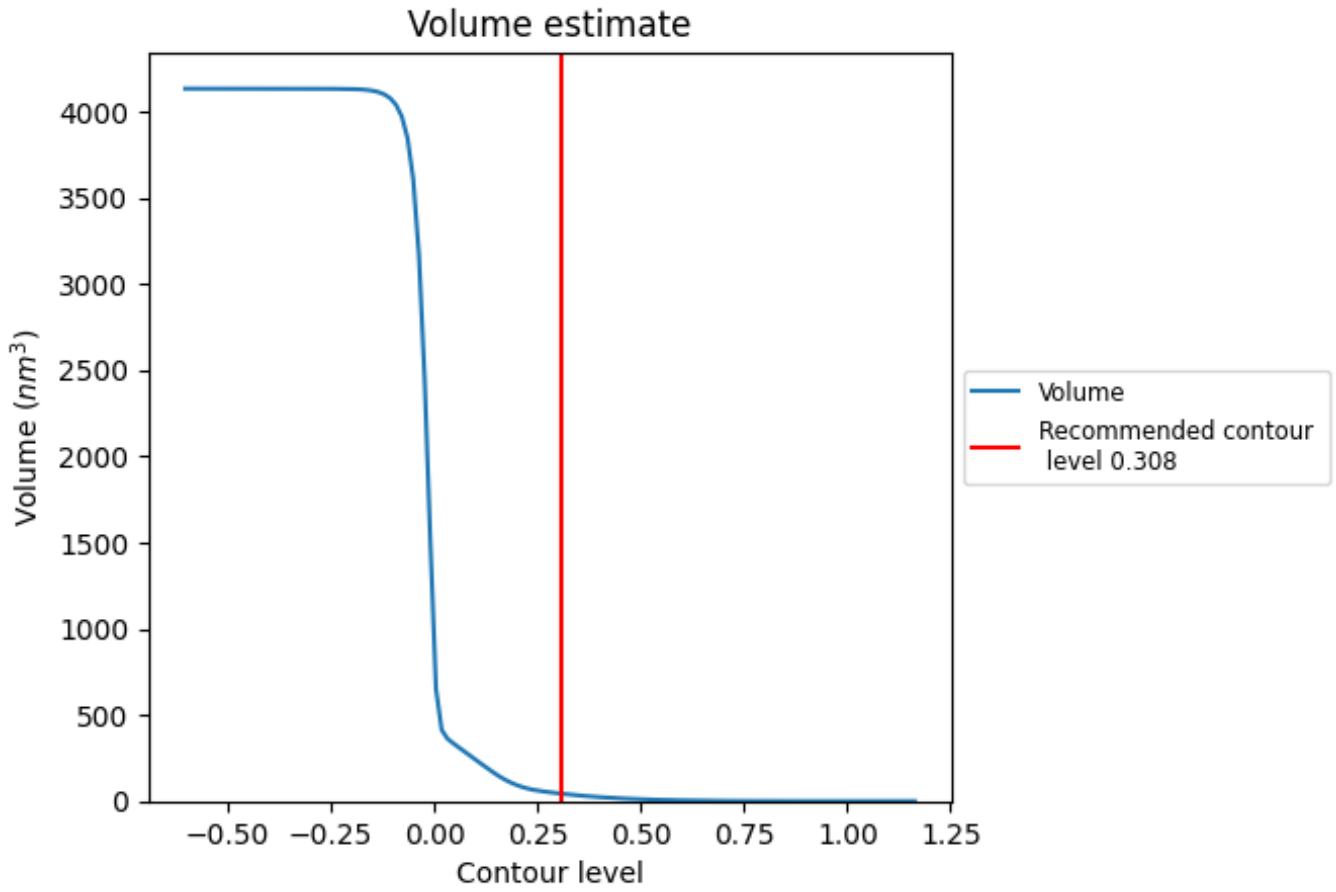
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

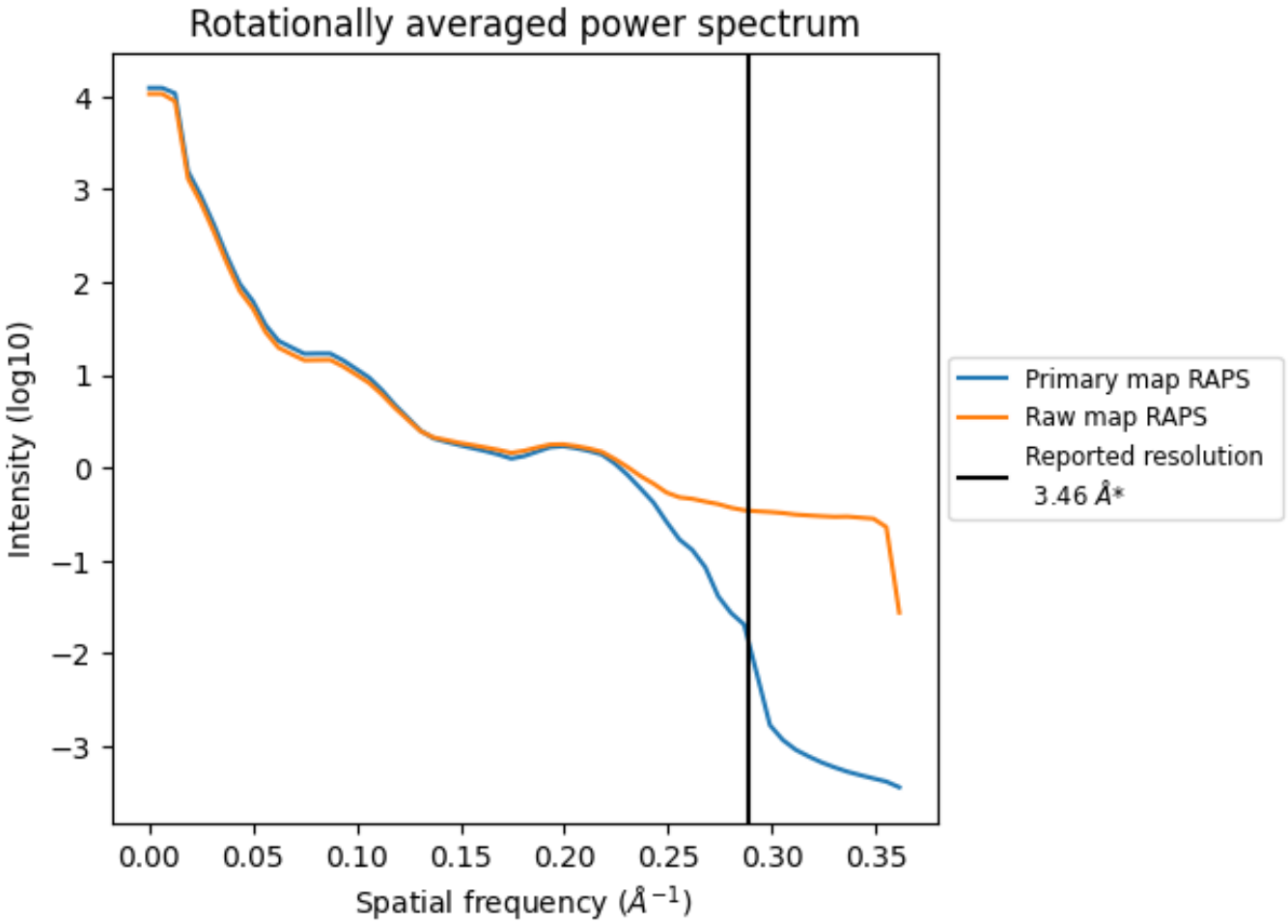
7.2 Volume estimate (i)



The volume at the recommended contour level is 43 nm^3; this corresponds to an approximate mass of 39 kDa.

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

7.3 Rotationally averaged power spectrum (i)

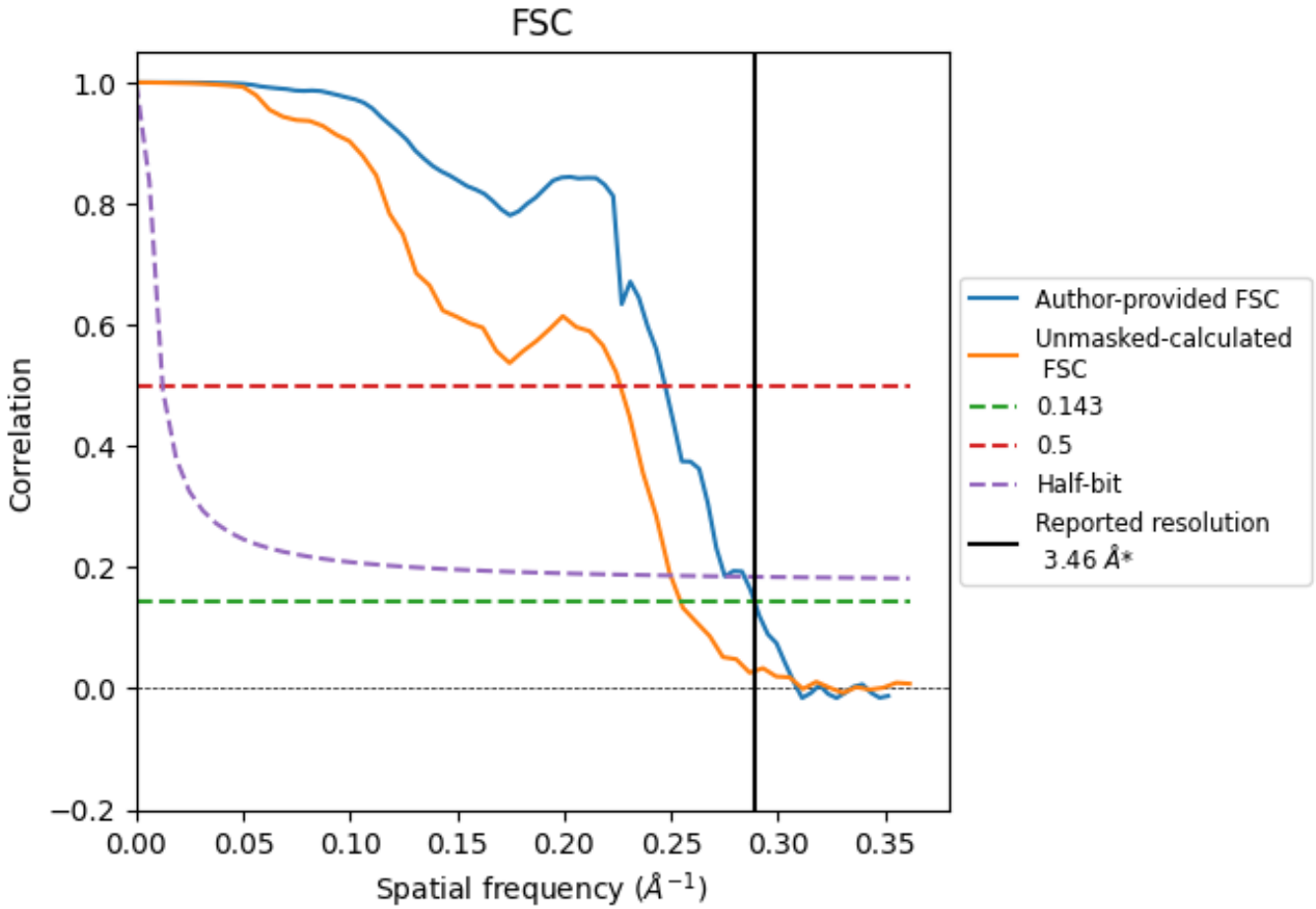


*Reported resolution corresponds to spatial frequency of 0.289 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.289 Å^{-1}

8.2 Resolution estimates (i)

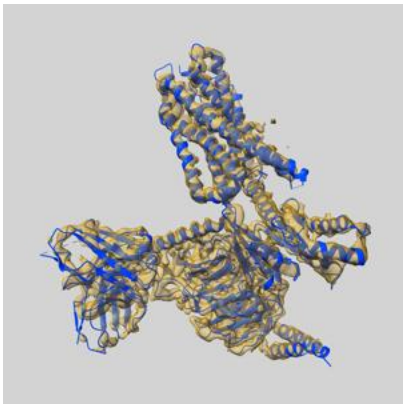
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	4.05	3.51
Unmasked-calculated*	3.93	4.42	4.00

*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 3.93 differs from the reported value 3.46 by more than 10 %

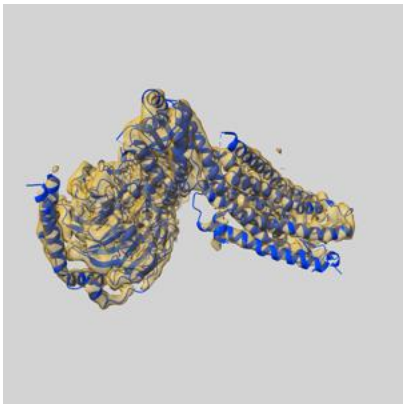
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64908 and PDB model 9VAX. Per-residue inclusion information can be found in section 3 on page 7.

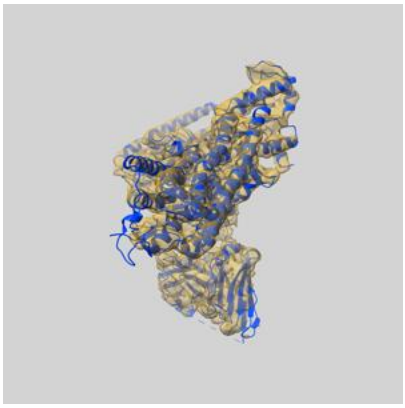
9.1 Map-model overlay



X



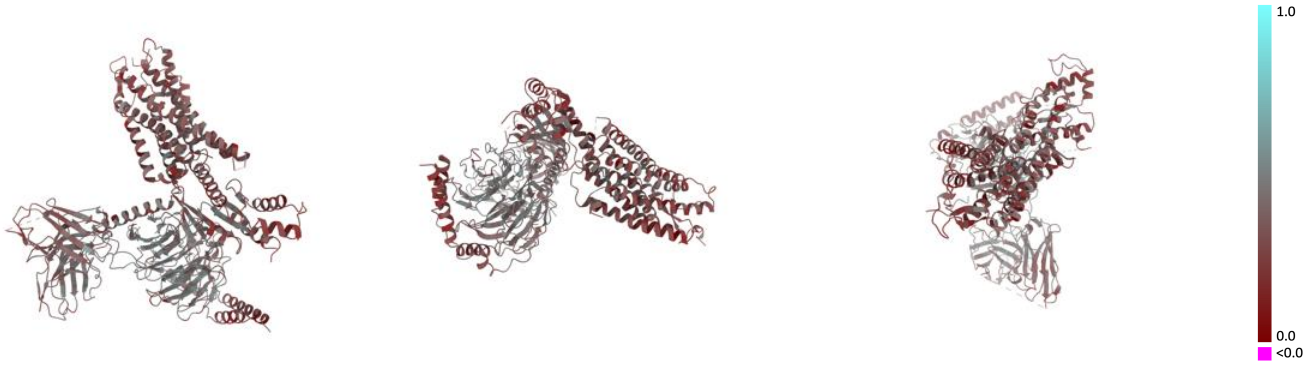
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.308 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.

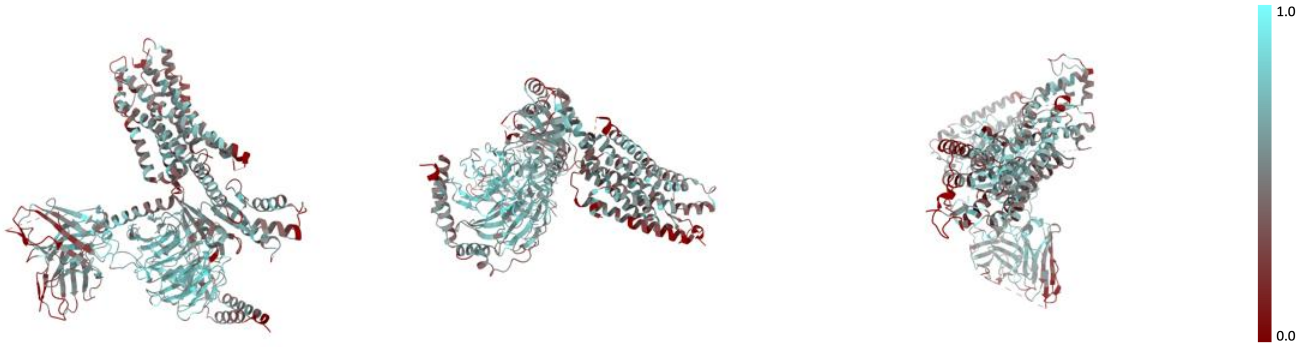
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

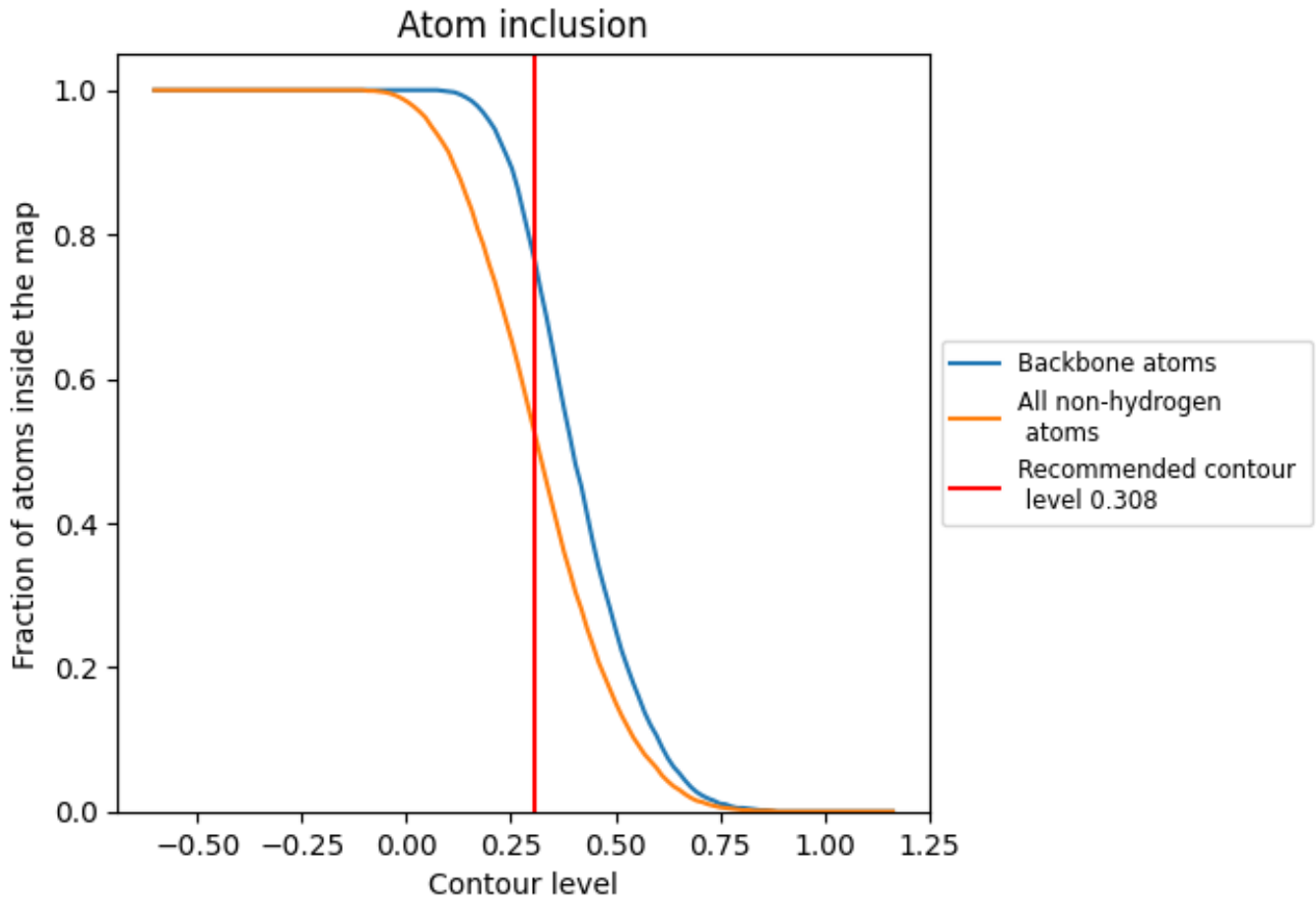
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.308).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 52% 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 (0.308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5210	0.3520
A	0.4930	0.3320
B	0.6590	0.4140
C	0.4810	0.2910
D	0.4980	0.3840
L	0.3080	0.3450
R	0.4210	0.2860