



Full wwPDB EM Validation Report ⓘ

May 27, 2026 – 07:09 PM JST

PDB ID : 9W3Z / pdb_00009w3z
EMDB ID : EMD-65613
Title : Cryo-EM structure of the 4:4 LacI-Lip1 complex
Authors : Xie, T.; Gong, X.
Deposited on : 2025-07-30
Resolution : 3.36 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

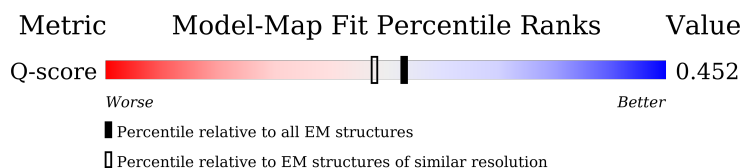
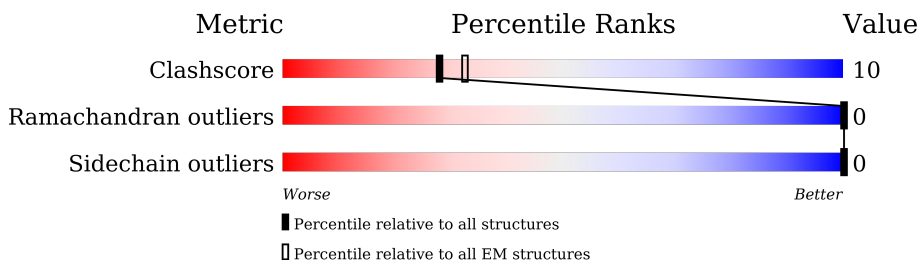
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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	14332 (2.86 - 3.86)

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	428	
1	C	428	
1	E	428	
1	G	428	

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Mol	Chain	Length	Quality of chain
2	B	150	 61%27%12%
2	D	150	 61%29%10%
2	F	150	 62%26%12%
2	H	150	 64%26%10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29422 atoms, of which 14568 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 Ceramide synthase LAC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	0
			5098	1731	2531	407	416	13		
1	C	321	Total	C	H	N	O	S	0	0
			5323	1802	2650	427	431	13		
1	E	312	Total	C	H	N	O	S	0	0
			5098	1731	2531	407	416	13		
1	G	321	Total	C	H	N	O	S	0	0
			5323	1802	2650	427	431	13		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P28496
A	420	GLU	-	expression tag	UNP P28496
A	421	ASP	-	expression tag	UNP P28496
A	422	TYR	-	expression tag	UNP P28496
A	423	LYS	-	expression tag	UNP P28496
A	424	ASP	-	expression tag	UNP P28496
A	425	ASP	-	expression tag	UNP P28496
A	426	ASP	-	expression tag	UNP P28496
A	427	ASP	-	expression tag	UNP P28496
A	428	LYS	-	expression tag	UNP P28496
C	419	LEU	-	expression tag	UNP P28496
C	420	GLU	-	expression tag	UNP P28496
C	421	ASP	-	expression tag	UNP P28496
C	422	TYR	-	expression tag	UNP P28496
C	423	LYS	-	expression tag	UNP P28496
C	424	ASP	-	expression tag	UNP P28496
C	425	ASP	-	expression tag	UNP P28496
C	426	ASP	-	expression tag	UNP P28496
C	427	ASP	-	expression tag	UNP P28496
C	428	LYS	-	expression tag	UNP P28496
E	419	LEU	-	expression tag	UNP P28496
E	420	GLU	-	expression tag	UNP P28496

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Chain	Residue	Modelled	Actual	Comment	Reference
E	421	ASP	-	expression tag	UNP P28496
E	422	TYR	-	expression tag	UNP P28496
E	423	LYS	-	expression tag	UNP P28496
E	424	ASP	-	expression tag	UNP P28496
E	425	ASP	-	expression tag	UNP P28496
E	426	ASP	-	expression tag	UNP P28496
E	427	ASP	-	expression tag	UNP P28496
E	428	LYS	-	expression tag	UNP P28496
G	419	LEU	-	expression tag	UNP P28496
G	420	GLU	-	expression tag	UNP P28496
G	421	ASP	-	expression tag	UNP P28496
G	422	TYR	-	expression tag	UNP P28496
G	423	LYS	-	expression tag	UNP P28496
G	424	ASP	-	expression tag	UNP P28496
G	425	ASP	-	expression tag	UNP P28496
G	426	ASP	-	expression tag	UNP P28496
G	427	ASP	-	expression tag	UNP P28496
G	428	LYS	-	expression tag	UNP P28496

- Molecule 2 is a protein called Ceramide synthase subunit LIP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	132	Total	C	H	N	O	S	0	0
			2120	698	1038	177	201	6		
2	D	135	Total	C	H	N	O	S	0	0
			2170	714	1065	181	204	6		
2	F	132	Total	C	H	N	O	S	0	0
			2120	698	1038	177	201	6		
2	H	135	Total	C	H	N	O	S	0	0
			2170	714	1065	181	204	6		

THR
ASP
SER
THR
THR
PRO
PRO
THR
LYS
LYS
ASP
ASP
ILE
LEU
GLU
ASP
TYR
LYS
LYS
ASP
ASP
ASP
LYS

• Molecule 1: Ceramide synthase LAC1

Chain E: 

MET
SER
THR
THR
ILE
LYS
LYS
PRO
SER
PRO
SER
ASN
ASN
ASN
LEU
LEU
LYS
VAL
ARG
SER
ARG
PRO
ARG
ARG
LYS
SER
SER
SER
ILE
GLY
LYS
LYS
ILE
ASP
LEU
GLY
THR
VAL
PRO
SER
LEU
GLY
MET
PHE
GLU
THR
LYS
GLU
SER
LYS
THR
ALA
ALA
LYS
ARG
MET
GLN
ARG
LEU
SER
GLU
ALA

THR
LYS
ASN
ASP
SER
ASP
LEU
VAL
LYS
LYS
171
W72
F73
S74
F75
R76
S79
H82
A83
W84
I85
P87
I88
M89
I90
L91
Y94
Y95
S96
A97
Y98
G102
N103
T104
N108
Y118
G121
D122
N131
D132
L133
F137
Y138
I141
F142
F143
T144
F145
L146

F149
L150
M151
I155
A159
I160
R161
L162
HIS
VAL
THR
S166
K167
H168
R169
I170
K171
R172
I173
M174
E175
D176
M177
Y178
A179
I180
F181
Y182
T183
G184
Y185
S186
G187
I191
L199
F202
N203
T204
R205
A206
M207
Y208
R209
T210
T211
P212
D213
N216
L219
F220
K221
V222

L226
Q227
V239
L240
Q241
L242
E243
K244
P245
R246
K247
D248
H249
N250
E251
L252
H256
L260
T272
K273
L276
P277
L278
D286
F287
T294
L302
A303
F304
F305
S306
F307
A308
I309
F310
V311
V312
I315
Y316
H319
L323
K324
I325
L326
W327
V329

L330
T331
Q332
V340
T345
S353
L354
P355
I356
V357
F358
I361
L366
L369
Y370
W371
L372
F373
L374
I375
F376
R377
V378
L379
Y380
R381
I382
L383
W384
R385
ILE
LEU
LYS
ASP
ASP
SER
SER
ASP
GLU
SER
ASP
GLU
SER
SER
THR
THR
PRO
THR

ASP
SER
THR
PRO
THR
LYS
LYS
ASP
ILE
GLU
GLU
ASP
TYR
LYS
ASP
ASP
ASP
LYS

• Molecule 1: Ceramide synthase LAC1

Chain G: 

MET
SER
THR
THR
ILE
LYS
LYS
PRO
SER
PRO
SER
ASN
ASN
ASN
LEU
LEU
LYS
VAL
ARG
SER
ARG
PRO
ARG
ARG
LYS
SER
SER
SER
ILE
GLY
LYS
LYS
ILE
ASP
LEU
GLY
THR
MET
PHE
GLU
THR
LYS
GLU
SER
LYS
THR
ALA
ALA
LYS
ARG
MET
GLN
ARG
LEU
SER
GLU
ALA

THR
LYS
ASN
ASP
SER
ASP
VAL
LYS
LYS
171
W72
F73
S74
A86
P87
I120
T123
L133
F142
F145
V153
V154
I155
L162
S166
R169
I170
M174
A179
Y182
T183
M194
L199
W200
F201
F202
Y208
R209
T210
Y211
P212
D213

L219
F220
K221
Y222
F223
Y224
F230
Q233
C236
L240
Q241
L242
T272
K273
H274
G275
L276
D283
L288
L289
L298
D299
S300
G301
L302
A313
I325
S328
V340
C350
W351
D391
ARG
SER
ASP
SER
GLU
SER
GLU
GLU
SER
ASP
GLU
SER
GLU
SER
GLU
SER
SER

THR
THR
PRO
THR
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ASP
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ILE
LEU
GLU
ASP
TYR
LYS
ASP
ASP
ASP
ASP
LYS

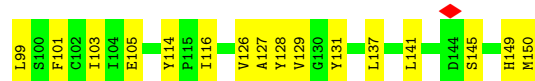
• Molecule 2: Ceramide synthase subunit LIP1

Chain B: 

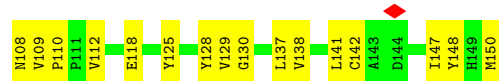
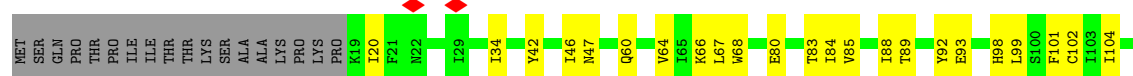
MET
SER
GLN
PRO
PRO
THR
THR
ILE
ILE
THR
THR
LYS
LYS
SER
SER
ALA
ALA
LYS
PRO
LYS
PRO
K19
I20
F21
H22
I29
I34
Y42
I46
N47
Q60
V64
I65
K66
L67
W68
A69
E80
T83
I84
V85
T88
T89
Y92
E93
H98
L99
S100
F101
C102
I103
I104



- Molecule 2: Ceramide synthase subunit LIP1



- Molecule 2: Ceramide synthase subunit LIP1



- Molecule 2: Ceramide synthase subunit LIP1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219798	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.868	Depositor
Minimum map value	-2.888	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.072, 1.072, 1.072	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.14	0/2650	0.38	1/3607 (0.0%)
1	C	0.19	0/2762	0.40	0/3758
1	E	0.14	0/2650	0.38	1/3607 (0.0%)
1	G	0.19	0/2762	0.40	0/3758
2	B	0.18	0/1114	0.38	0/1512
2	D	0.18	0/1139	0.35	0/1546
2	F	0.18	0/1114	0.37	0/1512
2	H	0.18	0/1139	0.35	0/1546
All	All	0.17	0/15330	0.38	2/20846 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	VAL	N-CA-C	-5.10	107.86	112.96
1	E	185	VAL	N-CA-C	-5.08	107.88	112.96

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	2567	2531	2529	49	0
1	C	2673	2650	2649	35	0
1	E	2567	2531	2529	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2673	2650	2649	35	0
2	B	1082	1038	1037	35	0
2	D	1105	1065	1065	29	0
2	F	1082	1038	1037	34	0
2	H	1105	1065	1065	27	0
All	All	14854	14568	14560	283	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 10.

All (283) 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:E:118:TYR:OH	1:E:131:ASN:OD1	1.87	0.92
1:A:118:TYR:OH	1:A:131:ASN:OD1	1.87	0.91
1:G:224:TYR:OH	1:G:272:THR:O	1.90	0.89
1:C:224:TYR:OH	1:C:272:THR:O	1.94	0.86
1:E:137:PHE:CE2	1:E:141:ILE:HD11	2.18	0.79
2:F:64:VAL:HG21	2:F:137:LEU:HD22	1.65	0.78
2:B:64:VAL:HG21	2:B:137:LEU:HD22	1.65	0.78
1:A:146:LEU:HD12	1:A:149:PHE:HE1	1.55	0.72
2:H:88:ILE:HG23	2:H:129:VAL:HG21	1.73	0.71
2:F:60:GLN:OE1	2:F:64:VAL:HG23	1.90	0.71
2:B:60:GLN:OE1	2:B:64:VAL:HG23	1.90	0.71
1:E:146:LEU:HD12	1:E:149:PHE:HE1	1.55	0.71
2:D:88:ILE:HG23	2:D:129:VAL:HG21	1.73	0.70
1:C:86:ALA:HB3	1:C:87:PRO:HD3	1.74	0.70
1:E:216:ASN:OD1	1:E:272:THR:HG21	1.92	0.70
1:A:216:ASN:OD1	1:A:272:THR:HG21	1.92	0.69
2:H:101:PHE:HB3	2:H:129:VAL:HG23	1.74	0.69
2:D:101:PHE:HB3	2:D:129:VAL:HG23	1.74	0.68
1:G:86:ALA:HB3	1:G:87:PRO:HD3	1.74	0.68
1:A:216:ASN:ND2	1:A:272:THR:OG1	2.26	0.68
1:E:216:ASN:ND2	1:E:272:THR:OG1	2.26	0.68
2:B:89:THR:O	2:D:78:ARG:NH2	2.27	0.67
2:F:89:THR:O	2:H:78:ARG:NH2	2.27	0.67
2:D:81:TYR:HE1	2:D:103:ILE:HD13	1.61	0.65
2:B:67:LEU:HB3	2:B:84:ILE:HD12	1.79	0.65
2:H:58:GLU:OE2	2:H:68:TRP:NE1	2.30	0.65
2:F:67:LEU:HB3	2:F:84:ILE:HD12	1.78	0.64
2:D:58:GLU:OE2	2:D:68:TRP:NE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:TYR:HE1	2:H:103:ILE:HD13	1.61	0.64
2:H:69:ALA:O	2:H:114:TYR:OH	2.10	0.64
2:D:69:ALA:O	2:D:114:TYR:OH	2.10	0.63
2:F:125:TYR:OH	2:H:149:HIS:O	2.18	0.62
2:B:125:TYR:OH	2:D:149:HIS:O	2.18	0.61
1:E:210:THR:HG23	1:E:210:THR:O	2.00	0.61
1:E:302:LEU:O	1:E:306:SER:N	2.33	0.60
1:A:210:THR:O	1:A:210:THR:HG23	2.00	0.60
1:G:162:LEU:HD21	1:G:298:LEU:HD13	1.84	0.59
1:A:353:SER:O	1:A:357:VAL:HG23	2.02	0.59
2:F:85:VAL:HG11	2:H:85:VAL:HG11	1.84	0.59
1:C:133:LEU:HD11	2:D:34:ILE:HG21	1.85	0.59
2:B:85:VAL:HG11	2:D:85:VAL:HG11	1.85	0.58
1:E:353:SER:O	1:E:357:VAL:HG23	2.02	0.58
1:G:133:LEU:HD11	2:H:34:ILE:HG21	1.85	0.58
1:A:302:LEU:O	1:A:306:SER:N	2.36	0.58
2:D:103:ILE:O	2:D:145:SER:OG	2.12	0.58
2:F:20:ILE:O	2:F:20:ILE:HG22	2.03	0.58
1:E:187:GLY:O	1:E:191:ILE:HD12	2.04	0.57
1:C:162:LEU:HD21	1:C:298:LEU:HD13	1.85	0.57
1:A:187:GLY:O	1:A:191:ILE:HD12	2.04	0.57
1:A:202:PHE:O	1:A:204:THR:HG23	2.05	0.57
2:D:29:ILE:O	2:D:33:LEU:HD23	2.05	0.56
2:B:20:ILE:HG22	2:B:20:ILE:O	2.03	0.56
1:E:202:PHE:O	1:E:204:THR:HG23	2.05	0.56
2:H:29:ILE:O	2:H:33:LEU:HD23	2.05	0.56
1:E:252:LEU:O	1:E:256:HIS:ND1	2.36	0.55
2:D:99:LEU:HD23	2:D:150:MET:HB2	1.89	0.55
1:E:325:ILE:O	1:E:329:VAL:HG13	2.06	0.55
1:G:220:PHE:HE1	1:G:276:LEU:HD22	1.71	0.55
1:A:256:HIS:O	1:A:260:LEU:HD23	2.06	0.55
1:A:325:ILE:O	1:A:329:VAL:HG13	2.06	0.55
2:B:150:MET:HE2	2:D:78:ARG:HA	1.89	0.55
1:G:210:THR:HG23	1:G:210:THR:O	2.07	0.54
1:C:210:THR:HG23	1:C:210:THR:O	2.08	0.54
1:E:256:HIS:O	1:E:260:LEU:HD23	2.07	0.54
2:D:93:GLU:HG2	2:D:93:GLU:O	2.07	0.54
2:H:65:ILE:HD11	2:H:67:LEU:HD11	1.89	0.54
1:G:302:LEU:HD12	1:G:302:LEU:O	2.08	0.54
1:G:170:ILE:HG22	1:G:174:MET:HE2	1.90	0.54
1:A:239:VAL:HG12	1:A:239:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ILE:HD11	2:D:67:LEU:HD11	1.89	0.54
1:A:252:LEU:O	1:A:256:HIS:ND1	2.35	0.53
1:E:82:HIS:HD1	1:E:84:TRP:HZ3	1.56	0.53
1:G:208:TYR:HE1	1:G:274:MET:HE2	1.74	0.53
2:F:150:MET:HE2	2:H:78:ARG:HA	1.89	0.53
1:C:302:LEU:HD12	1:C:302:LEU:O	2.08	0.53
1:E:239:VAL:HG12	1:E:239:VAL:O	2.08	0.53
2:H:99:LEU:HD23	2:H:150:MET:HB2	1.89	0.53
2:D:65:ILE:CD1	2:D:67:LEU:HD11	2.38	0.53
2:H:93:GLU:O	2:H:93:GLU:HG2	2.07	0.53
2:B:64:VAL:HG21	2:B:137:LEU:CD2	2.38	0.53
2:H:65:ILE:CD1	2:H:67:LEU:HD11	2.38	0.53
1:C:216:ASN:HD21	1:C:272:THR:HG21	1.74	0.52
1:C:153:VAL:HG12	1:C:153:VAL:O	2.09	0.52
2:D:79:GLY:O	2:D:83:THR:HG22	2.10	0.52
2:H:79:GLY:O	2:H:83:THR:HG22	2.10	0.52
1:A:137:PHE:CE2	1:A:141:ILE:HD11	2.45	0.52
2:B:68:TRP:C	2:B:84:ILE:HD11	2.35	0.52
2:H:126:VAL:HG12	2:H:127:ALA:N	2.25	0.52
2:F:68:TRP:C	2:F:84:ILE:HD11	2.34	0.51
1:G:153:VAL:HG12	1:G:153:VAL:O	2.09	0.51
2:D:126:VAL:HG12	2:D:127:ALA:N	2.25	0.51
2:B:67:LEU:HD22	2:B:88:ILE:HG13	1.93	0.51
2:F:67:LEU:HD22	2:F:88:ILE:HG13	1.92	0.51
1:E:309:ILE:HA	1:E:312:VAL:HG22	1.92	0.51
2:F:64:VAL:HG21	2:F:137:LEU:CD2	2.38	0.51
1:C:220:PHE:HE1	1:C:276:LEU:HD22	1.74	0.51
1:E:203:ASN:OD1	1:E:206:ALA:N	2.42	0.51
1:E:227:GLN:HA	1:E:227:GLN:OE1	2.11	0.51
1:G:142:PHE:O	1:G:145:PHE:HB3	2.11	0.50
1:G:350:CYS:HG	1:G:351:TRP:CD1	2.29	0.50
1:A:227:GLN:HA	1:A:227:GLN:OE1	2.11	0.50
1:C:350:CYS:HG	1:C:351:TRP:CD1	2.30	0.50
2:D:77:LYS:NZ	2:D:105:GLU:OE2	2.28	0.50
1:G:154:VAL:HG23	1:G:155:ILE:N	2.27	0.50
1:A:331:THR:HG23	1:A:332:GLN:N	2.27	0.50
1:A:85:ILE:O	1:A:89:MET:HG3	2.12	0.50
2:B:118:GLU:OE1	2:B:118:GLU:N	2.45	0.50
2:F:92:TYR:HE2	2:F:129:VAL:HG13	1.77	0.50
1:A:309:ILE:HA	1:A:312:VAL:HG22	1.92	0.50
2:B:101:PHE:HB2	2:B:128:TYR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:THR:HG23	1:E:332:GLN:N	2.27	0.49
2:F:101:PHE:HB2	2:F:128:TYR:O	2.12	0.49
2:F:60:GLN:NE2	2:F:66:LYS:HB3	2.27	0.49
2:B:92:TYR:HE2	2:B:129:VAL:HG13	1.77	0.49
1:C:154:VAL:HG23	1:C:155:ILE:N	2.27	0.49
1:G:350:CYS:SG	1:G:351:TRP:N	2.84	0.49
2:F:118:GLU:OE2	2:F:118:GLU:N	2.45	0.49
1:C:350:CYS:SG	1:C:351:TRP:N	2.84	0.49
1:A:219:LEU:HA	1:A:222:VAL:HG12	1.94	0.49
2:B:60:GLN:NE2	2:B:66:LYS:HB3	2.28	0.49
1:C:120:ILE:O	1:C:123:THR:HG22	2.13	0.49
1:C:142:PHE:O	1:C:145:PHE:HB3	2.11	0.49
1:G:240:LEU:O	1:G:240:LEU:HG	2.13	0.49
1:E:179:ALA:HA	1:E:182:TYR:CE1	2.48	0.48
1:E:326:LEU:HD11	1:E:358:PHE:CD2	2.48	0.48
1:G:120:ILE:O	1:G:123:THR:HG22	2.13	0.48
2:F:80:GLU:HA	2:F:83:THR:HG22	1.95	0.48
2:B:64:VAL:HG12	2:B:130:GLY:HA3	1.94	0.48
1:A:179:ALA:HA	1:A:182:TYR:CE1	2.48	0.48
2:D:28:PHE:O	2:D:32:LEU:HD13	2.14	0.48
1:C:240:LEU:HG	1:C:240:LEU:O	2.13	0.48
2:B:80:GLU:HA	2:B:83:THR:HG22	1.95	0.48
1:E:85:ILE:O	1:E:89:MET:HG3	2.13	0.48
2:H:28:PHE:O	2:H:32:LEU:HD13	2.13	0.48
1:E:219:LEU:HA	1:E:222:VAL:HG12	1.95	0.48
2:F:64:VAL:HG12	2:F:130:GLY:HA3	1.94	0.47
2:B:98:HIS:ND1	2:B:150:MET:O	2.48	0.47
1:E:340:VAL:HG23	1:E:340:VAL:O	2.14	0.47
2:F:98:HIS:ND1	2:F:150:MET:O	2.48	0.47
2:B:102:CYS:SG	2:B:104:ILE:HD11	2.54	0.47
2:F:102:CYS:SG	2:F:104:ILE:HD11	2.54	0.47
2:D:58:GLU:O	2:D:66:LYS:N	2.47	0.47
1:A:206:ALA:O	1:A:273:LYS:NZ	2.41	0.47
1:A:340:VAL:HG23	1:A:340:VAL:O	2.14	0.47
1:A:326:LEU:HD11	1:A:358:PHE:CD2	2.49	0.47
1:C:325:ILE:O	1:C:328:SER:OG	2.23	0.46
2:B:137:LEU:HD21	2:B:141:LEU:CD1	2.45	0.46
2:H:103:ILE:O	2:H:145:SER:OG	2.12	0.46
1:A:203:ASN:OD1	1:A:206:ALA:N	2.42	0.46
1:A:278:ILE:HD12	1:A:278:ILE:H	1.80	0.46
2:F:137:LEU:HD21	2:F:141:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:58:GLU:O	2:H:66:LYS:N	2.47	0.46
2:B:108:ASN:C	2:B:109:VAL:HG23	2.41	0.46
1:G:155:ILE:HG22	1:G:174:MET:HG2	1.98	0.46
2:F:108:ASN:C	2:F:109:VAL:HG23	2.41	0.46
1:A:183:THR:HG22	1:A:287:PHE:HB2	1.97	0.46
1:C:179:ALA:HA	1:C:182:TYR:CE1	2.51	0.45
1:C:288:LEU:HD12	1:C:313:ALA:HB3	1.99	0.45
2:H:98:HIS:O	2:H:132:ASP:HB2	2.16	0.45
1:E:183:THR:HG22	1:E:287:PHE:HB2	1.98	0.45
1:E:278:ILE:H	1:E:278:ILE:HD12	1.80	0.45
1:G:179:ALA:HA	1:G:182:TYR:CE1	2.51	0.45
2:F:137:LEU:HD23	2:F:137:LEU:O	2.17	0.45
2:B:112:VAL:O	2:B:112:VAL:HG13	2.16	0.45
1:E:138:TYR:HA	1:E:141:ILE:HD12	1.97	0.45
2:H:137:LEU:O	2:H:141:LEU:HD23	2.16	0.45
1:E:166:SER:N	1:E:169:ARG:HE	2.14	0.45
1:G:220:PHE:CE1	1:G:276:LEU:HD22	2.51	0.45
1:C:236:CYS:O	1:C:240:LEU:HD23	2.17	0.45
2:D:116:ILE:HD12	2:D:116:ILE:H	1.80	0.45
1:E:103:ASN:O	1:E:108:ASN:ND2	2.48	0.45
2:H:116:ILE:HD12	2:H:116:ILE:H	1.80	0.45
2:F:99:LEU:CD2	2:F:150:MET:HB2	2.46	0.45
1:A:166:SER:N	1:A:169:ARG:HE	2.15	0.45
1:A:221:LYS:O	1:A:225:LEU:HD23	2.17	0.45
2:B:137:LEU:HD23	2:B:137:LEU:O	2.17	0.45
1:E:327:TRP:O	1:E:331:THR:HG22	2.17	0.45
1:A:199:LEU:HD13	1:A:207:MET:HG3	1.99	0.45
1:E:331:THR:HG23	1:E:332:GLN:HG2	1.99	0.45
1:G:236:CYS:O	1:G:240:LEU:HD23	2.17	0.45
1:E:206:ALA:O	1:E:273:LYS:NZ	2.41	0.45
2:B:101:PHE:CE2	2:B:148:TYR:HD1	2.35	0.44
2:D:137:LEU:O	2:D:141:LEU:HD23	2.17	0.44
1:A:91:LEU:HD21	1:A:142:PHE:HD1	1.81	0.44
2:B:99:LEU:CD2	2:B:150:MET:HB2	2.46	0.44
1:E:199:LEU:HD13	1:E:207:MET:HG3	1.99	0.44
1:E:221:LYS:O	1:E:225:LEU:HD23	2.17	0.44
1:A:331:THR:HG23	1:A:332:GLN:HG2	1.99	0.44
1:C:300:SER:O	1:C:301:GLY:C	2.61	0.44
1:G:288:LEU:HD12	1:G:313:ALA:HB3	1.99	0.44
1:G:300:SER:O	1:G:301:GLY:C	2.61	0.44
1:A:220:PHE:CE2	1:A:276:LEU:HD22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASN:ND2	1:C:272:THR:HG21	2.32	0.44
2:F:112:VAL:HG13	2:F:112:VAL:O	2.16	0.44
1:E:94:VAL:HG11	1:E:138:TYR:CE1	2.53	0.44
1:G:340:VAL:HG23	1:G:340:VAL:O	2.18	0.44
1:A:94:VAL:HG11	1:A:138:TYR:CE1	2.52	0.44
1:C:183:THR:CG2	1:C:283:ASP:O	2.66	0.44
1:A:327:TRP:O	1:A:331:THR:HG22	2.18	0.43
1:E:91:LEU:HD21	1:E:142:PHE:HD1	1.83	0.43
1:E:173:ILE:O	1:E:177:MET:HG2	2.18	0.43
2:F:101:PHE:CE2	2:F:148:TYR:HD1	2.35	0.43
1:A:103:ASN:O	1:A:108:ASN:ND2	2.49	0.43
1:E:212:PRO:O	1:E:213:ASP:C	2.61	0.43
1:A:212:PRO:O	1:A:213:ASP:C	2.61	0.43
1:C:289:LEU:HD12	1:C:289:LEU:O	2.18	0.43
2:D:42:TYR:CZ	2:D:46:ILE:HG21	2.54	0.43
2:F:138:VAL:O	2:F:142:CYS:SG	2.77	0.43
1:E:146:LEU:HD11	1:E:181:PHE:HE2	1.83	0.43
1:G:183:THR:CG2	1:G:283:ASP:O	2.66	0.43
1:G:325:ILE:O	1:G:328:SER:OG	2.24	0.43
2:F:42:TYR:CE1	2:F:46:ILE:HG21	2.53	0.43
1:A:173:ILE:O	1:A:177:MET:HG2	2.18	0.43
2:B:42:TYR:CE1	2:B:46:ILE:HG21	2.53	0.43
1:E:220:PHE:CE2	1:E:276:LEU:HD22	2.53	0.43
1:G:219:LEU:HA	1:G:222:VAL:HG12	2.01	0.43
1:G:289:LEU:O	1:G:289:LEU:HD12	2.19	0.43
1:C:166:SER:OG	1:C:169:ARG:HB2	2.18	0.43
2:B:138:VAL:O	2:B:142:CYS:SG	2.77	0.43
1:G:166:SER:OG	1:G:169:ARG:HB2	2.19	0.43
1:G:199:LEU:O	1:G:200:TRP:C	2.61	0.43
1:C:219:LEU:HA	1:C:222:VAL:HG12	2.00	0.43
2:B:147:ILE:HG22	2:B:148:TYR:N	2.34	0.43
1:C:199:LEU:O	1:C:200:TRP:C	2.61	0.42
1:C:153:VAL:O	1:C:153:VAL:CG1	2.67	0.42
1:C:340:VAL:O	1:C:340:VAL:HG23	2.18	0.42
2:H:42:TYR:CZ	2:H:46:ILE:HG21	2.54	0.42
1:A:91:LEU:HD21	1:A:142:PHE:CD1	2.53	0.42
2:B:69:ALA:O	2:B:114:TYR:OH	2.27	0.42
1:A:345:THR:O	1:A:345:THR:HG22	2.19	0.42
1:G:153:VAL:O	1:G:153:VAL:CG1	2.67	0.42
1:E:345:THR:HG22	1:E:345:THR:O	2.19	0.42
1:C:230:PHE:O	1:C:233:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ASP:OD1	2:D:76:ASP:N	2.49	0.42
1:E:208:TYR:O	1:E:209:ARG:C	2.62	0.42
2:F:147:ILE:HG22	2:F:148:TYR:N	2.34	0.42
1:E:91:LEU:HD21	1:E:142:PHE:CD1	2.54	0.42
1:G:212:PRO:O	1:G:213:ASP:C	2.63	0.42
1:C:220:PHE:CE1	1:C:276:LEU:HD22	2.54	0.42
2:D:48:TYR:O	2:D:51:PHE:N	2.43	0.42
1:A:210:THR:O	1:A:210:THR:CG2	2.67	0.41
1:A:308:ALA:O	1:A:312:VAL:HG13	2.20	0.41
2:B:109:VAL:HG12	2:B:110:PRO:O	2.20	0.41
1:C:194:MET:HE2	1:C:202:PHE:H	1.85	0.41
2:F:109:VAL:HG12	2:F:110:PRO:O	2.20	0.41
2:H:101:PHE:HB2	2:H:128:TYR:O	2.20	0.41
2:B:20:ILE:O	2:B:20:ILE:CG2	2.69	0.41
2:B:68:TRP:CA	2:B:84:ILE:HD11	2.51	0.41
2:B:93:GLU:N	2:B:93:GLU:OE2	2.54	0.41
2:F:20:ILE:O	2:F:20:ILE:CG2	2.68	0.41
1:A:203:ASN:C	1:A:204:THR:HG23	2.46	0.41
1:C:208:TYR:HE1	1:C:274:MET:HE2	1.85	0.41
1:G:194:MET:HE2	1:G:202:PHE:H	1.86	0.41
1:A:141:ILE:O	1:A:144:THR:HG22	2.20	0.41
2:D:97:GLU:HB2	2:D:131:TYR:CD1	2.56	0.41
1:E:203:ASN:C	1:E:204:THR:HG23	2.46	0.41
1:G:230:PHE:O	1:G:233:GLN:HG3	2.20	0.41
1:C:240:LEU:O	1:C:242:LEU:HD12	2.21	0.41
1:E:366:LEU:O	1:E:369:LEU:N	2.53	0.41
2:B:47:ASN:OD1	2:B:47:ASN:O	2.38	0.41
2:D:101:PHE:HB2	2:D:128:TYR:O	2.20	0.41
1:G:220:PHE:HE2	1:G:272:THR:OG1	2.04	0.41
2:F:93:GLU:OE2	2:F:93:GLU:N	2.54	0.41
1:A:146:LEU:HD11	1:A:181:PHE:HE2	1.84	0.41
2:D:61:SER:O	2:D:62:GLY:C	2.64	0.41
1:E:141:ILE:O	1:E:144:THR:HG22	2.21	0.41
1:E:308:ALA:O	1:E:312:VAL:HG13	2.20	0.41
1:G:240:LEU:O	1:G:242:LEU:HD12	2.21	0.41
2:F:92:TYR:CE2	2:F:129:VAL:HG13	2.55	0.41
1:A:354:LEU:HB3	1:A:355:PRO:HD3	2.03	0.40
1:C:220:PHE:HE2	1:C:272:THR:OG1	2.04	0.40
1:E:354:LEU:HB3	1:E:355:PRO:HD3	2.03	0.40
1:A:98:TYR:OH	1:A:104:THR:HG23	2.21	0.40
1:A:199:LEU:HD21	1:A:277:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:ASN:OD1	2:F:47:ASN:O	2.38	0.40
2:H:76:ASP:N	2:H:76:ASP:OD1	2.49	0.40
1:A:208:TYR:O	1:A:209:ARG:C	2.62	0.40
1:C:88:LEU:HB2	1:C:145:PHE:CE1	2.56	0.40
1:E:199:LEU:HD21	1:E:277:PRO:CG	2.51	0.40
1:E:98:TYR:OH	1:E:104:THR:HG23	2.21	0.40
1:E:133:LEU:HD11	2:F:34:ILE:HG21	2.04	0.40
2:H:97:GLU:HB2	2:H:131:TYR:CD1	2.55	0.40
1:A:133:LEU:HD11	2:B:34:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	308/428 (72%)	291 (94%)	17 (6%)	0	100	100
1	C	319/428 (74%)	293 (92%)	26 (8%)	0	100	100
1	E	308/428 (72%)	291 (94%)	17 (6%)	0	100	100
1	G	319/428 (74%)	293 (92%)	26 (8%)	0	100	100
2	B	130/150 (87%)	118 (91%)	12 (9%)	0	100	100
2	D	133/150 (89%)	125 (94%)	8 (6%)	0	100	100
2	F	130/150 (87%)	118 (91%)	12 (9%)	0	100	100
2	H	133/150 (89%)	124 (93%)	9 (7%)	0	100	100
All	All	1780/2312 (77%)	1653 (93%)	127 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	266/391 (68%)	266 (100%)	0	100	100
1	C	280/391 (72%)	280 (100%)	0	100	100
1	E	266/391 (68%)	266 (100%)	0	100	100
1	G	280/391 (72%)	280 (100%)	0	100	100
2	B	119/135 (88%)	119 (100%)	0	100	100
2	D	122/135 (90%)	122 (100%)	0	100	100
2	F	119/135 (88%)	119 (100%)	0	100	100
2	H	122/135 (90%)	122 (100%)	0	100	100
All	All	1574/2104 (75%)	1574 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	249	HIS
1	A	342	ASN
1	C	216	ASN
1	C	234	GLN
2	B	106	ASN
2	B	113	HIS
2	D	117	HIS
2	D	149	HIS
1	E	216	ASN
1	E	342	ASN
1	G	234	GLN
1	G	322	ASN
1	G	365	GLN
2	F	106	ASN
2	H	117	HIS
2	H	149	HIS

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.

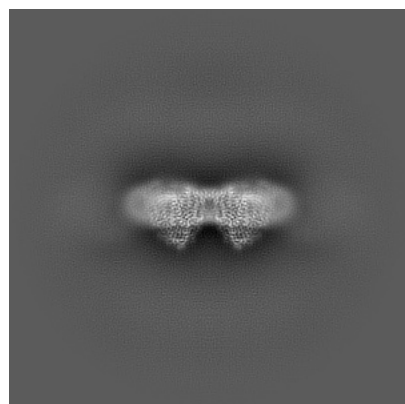
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65613. These allow visual inspection of the internal detail of the map and identification of artifacts.

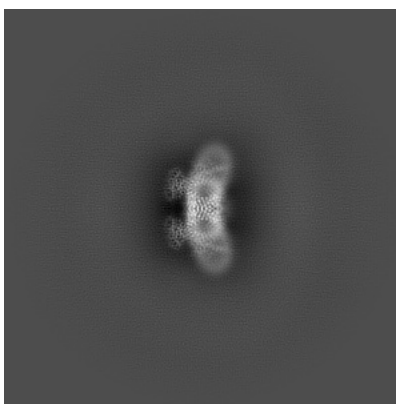
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

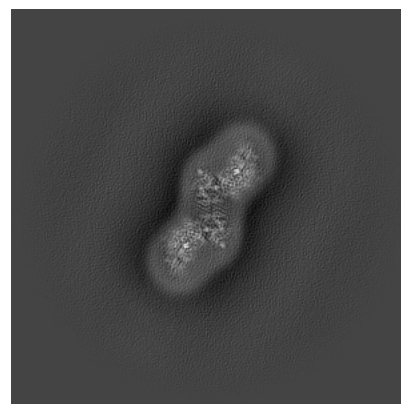
6.1.1 Primary map



X

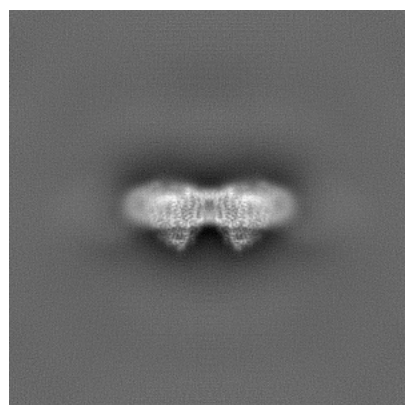


Y

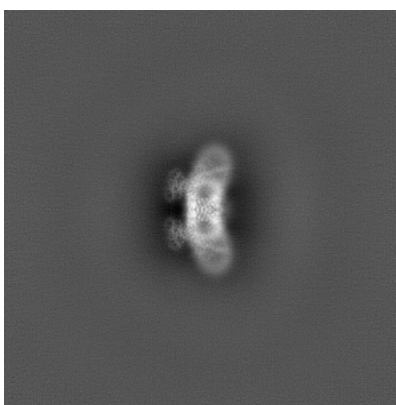


Z

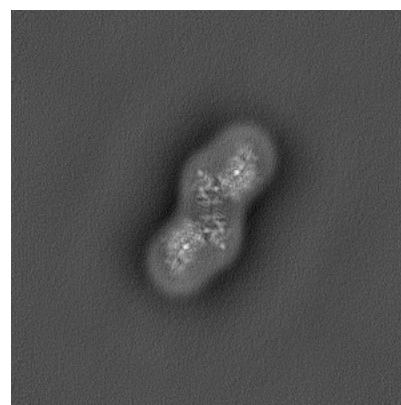
6.1.2 Raw map



X



Y

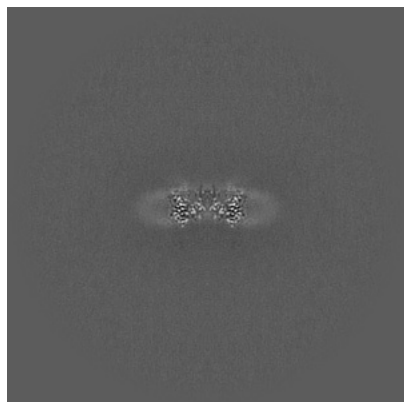


Z

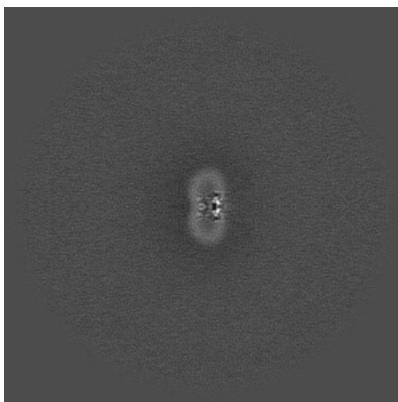
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

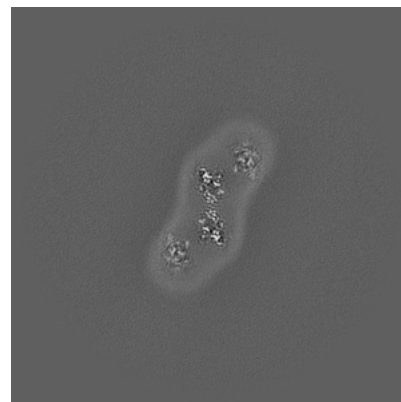
6.2.1 Primary map



X Index: 240

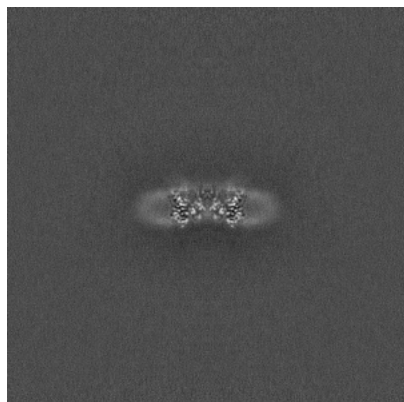


Y Index: 240

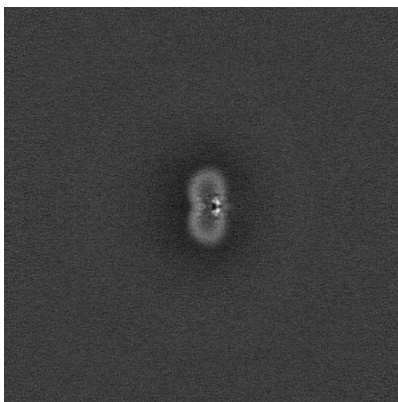


Z Index: 240

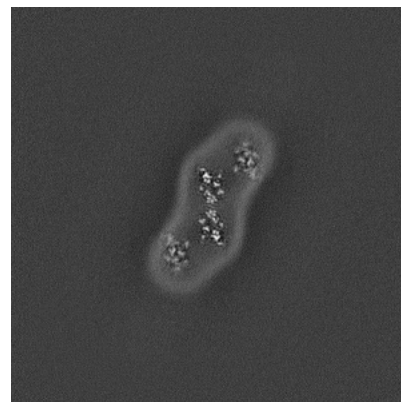
6.2.2 Raw map



X Index: 240



Y Index: 240

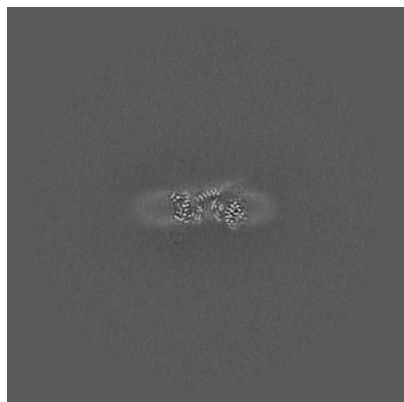


Z Index: 240

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

6.3 Largest variance slices [i](#)

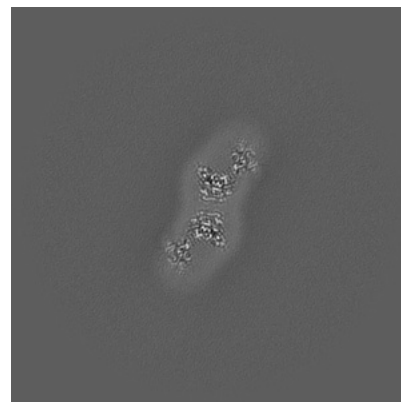
6.3.1 Primary map



X Index: 236

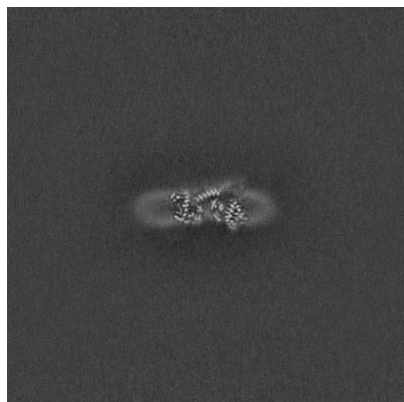


Y Index: 275

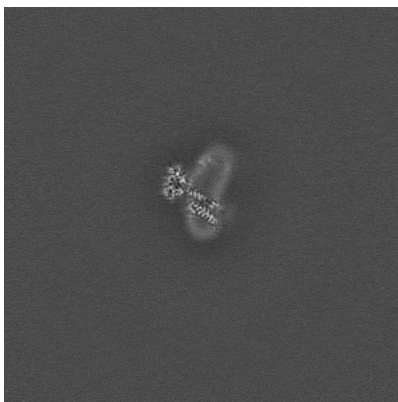


Z Index: 229

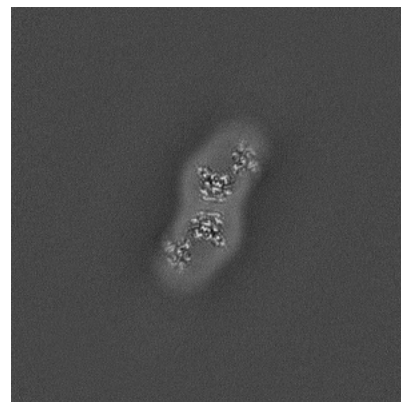
6.3.2 Raw map



X Index: 236



Y Index: 275



Z Index: 229

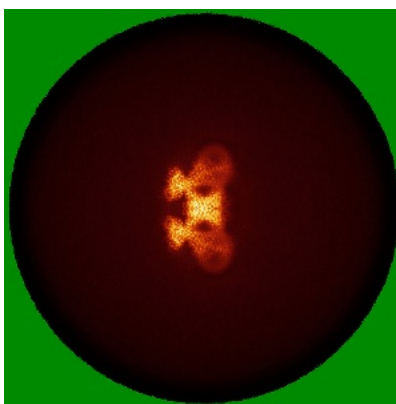
The images above show the largest variance slices of the map in three orthogonal directions.

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

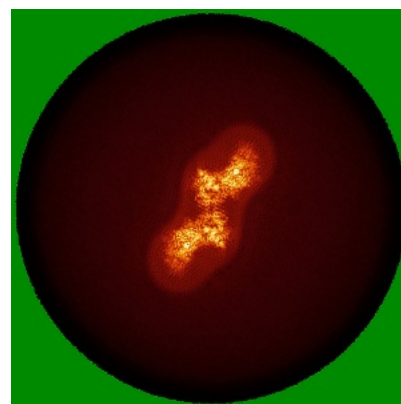
6.4.1 Primary map



X

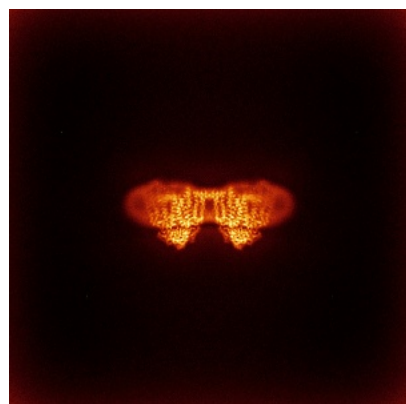


Y

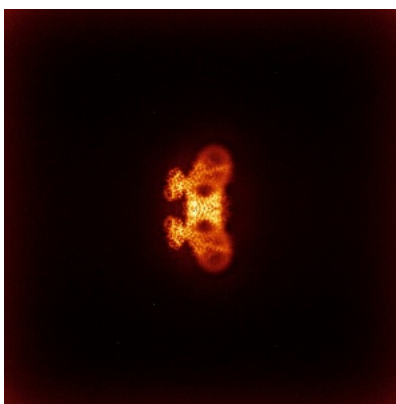


Z

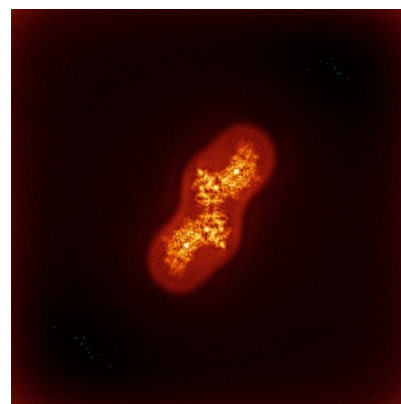
6.4.2 Raw map



X



Y

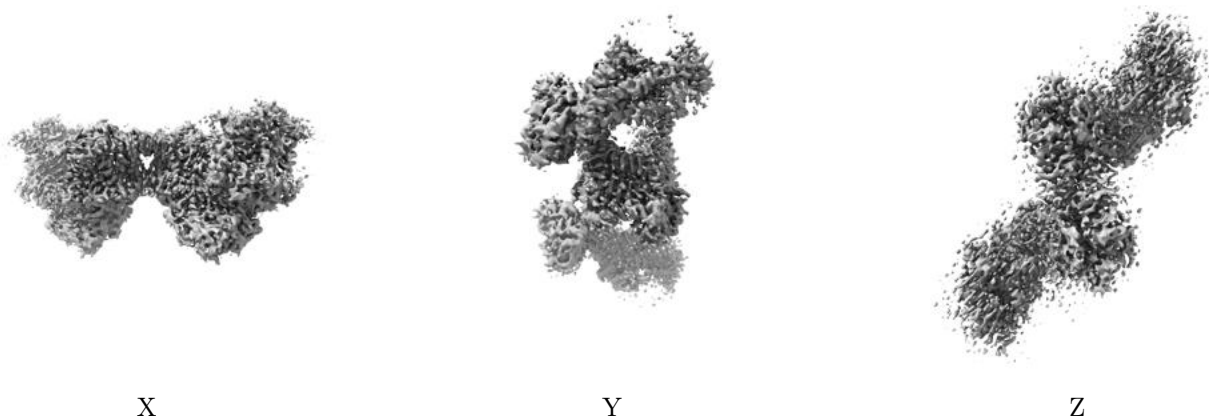


Z

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 0.4. 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.

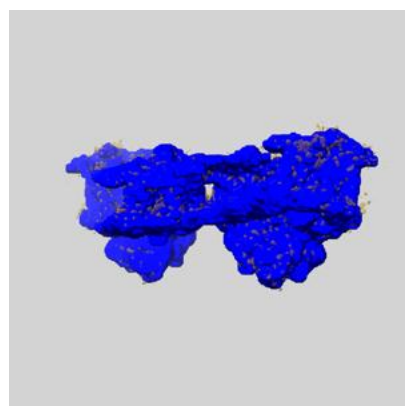
6.6 Mask visualisation [i](#)

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

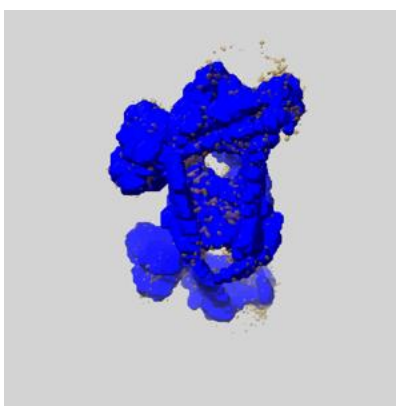
A mask typically either:

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

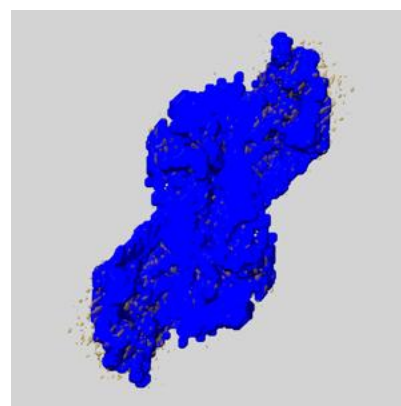
6.6.1 emd_65613_msk_2.map [i](#)



X



Y

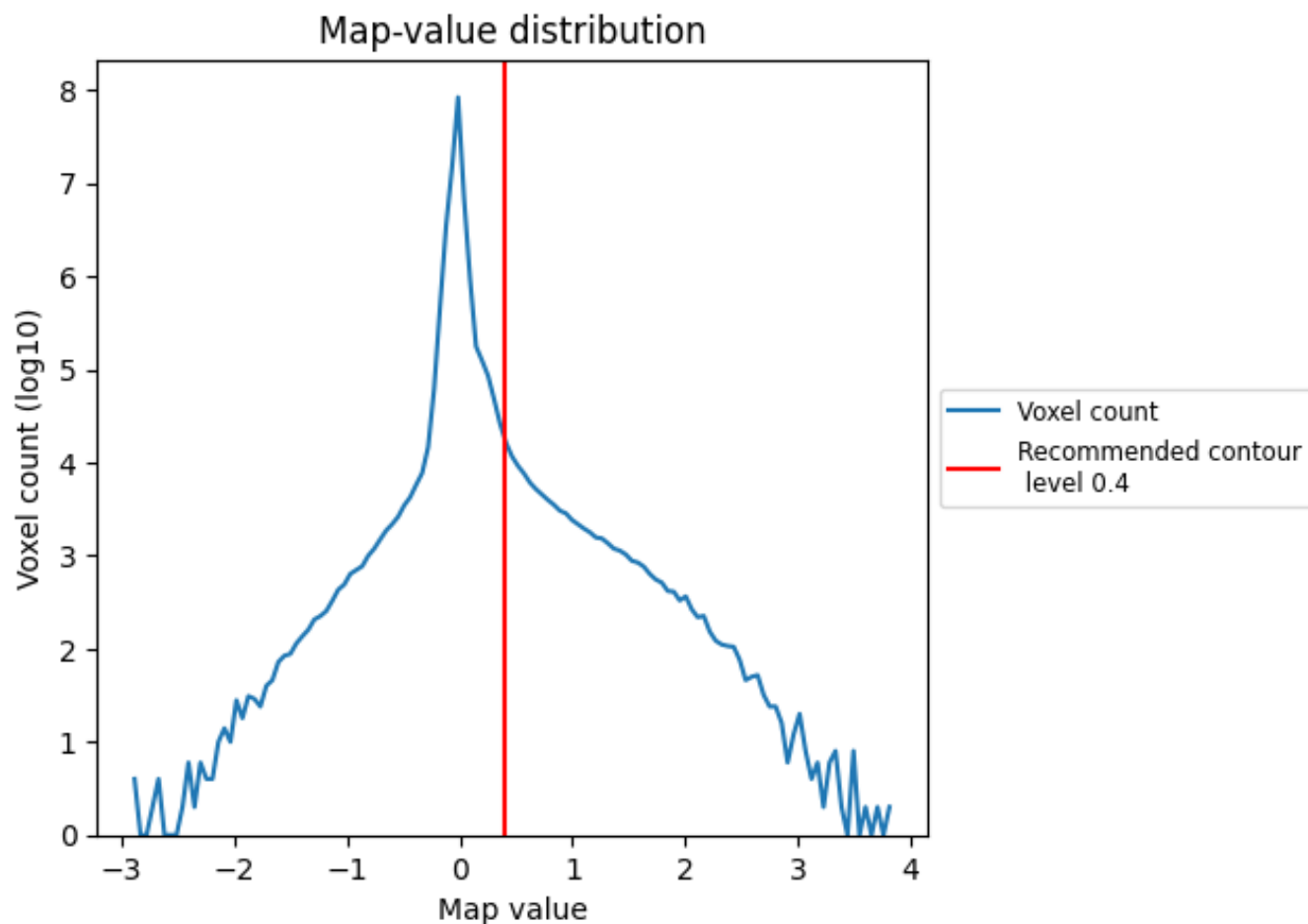


Z

7 Map analysis [i](#)

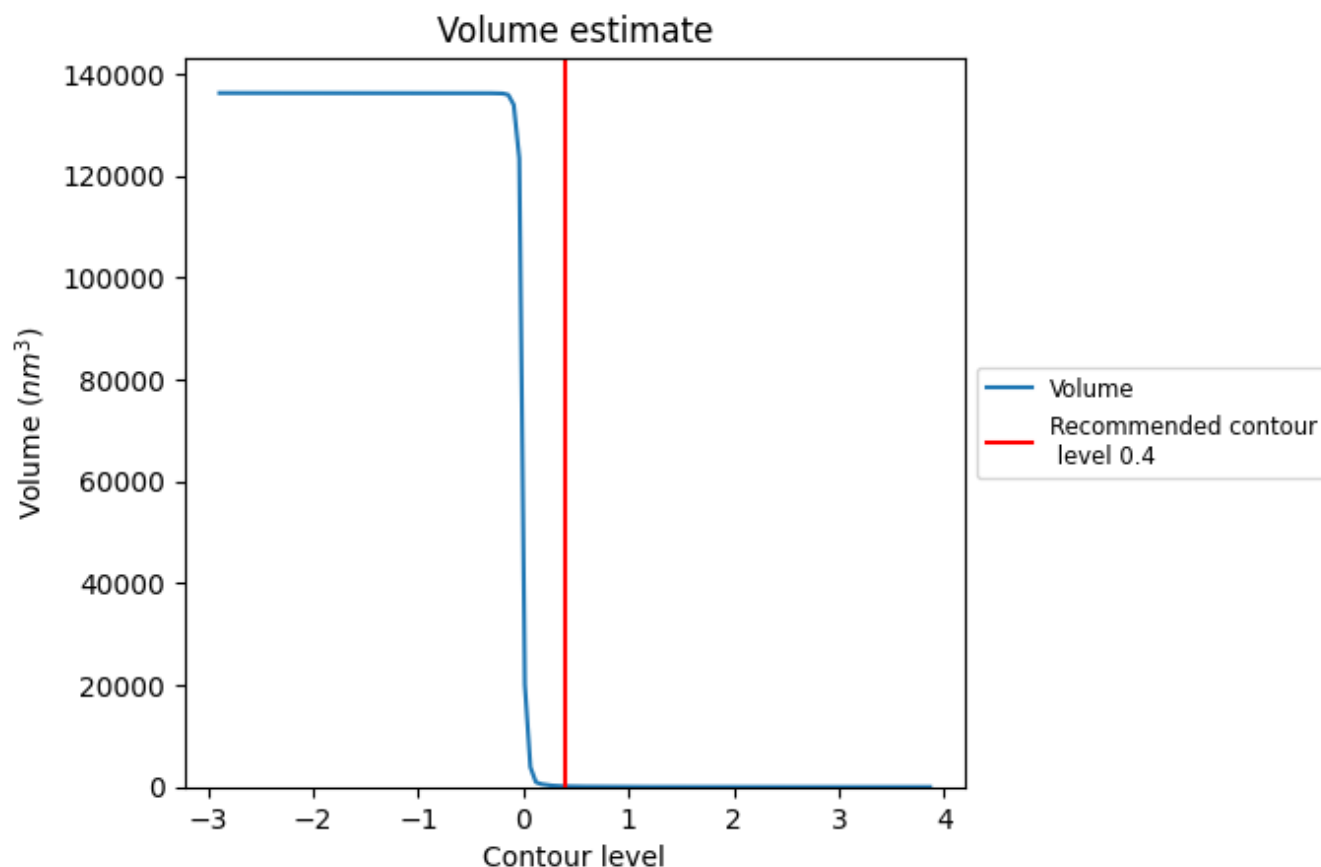
This section contains the results of statistical analysis of the map.

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.

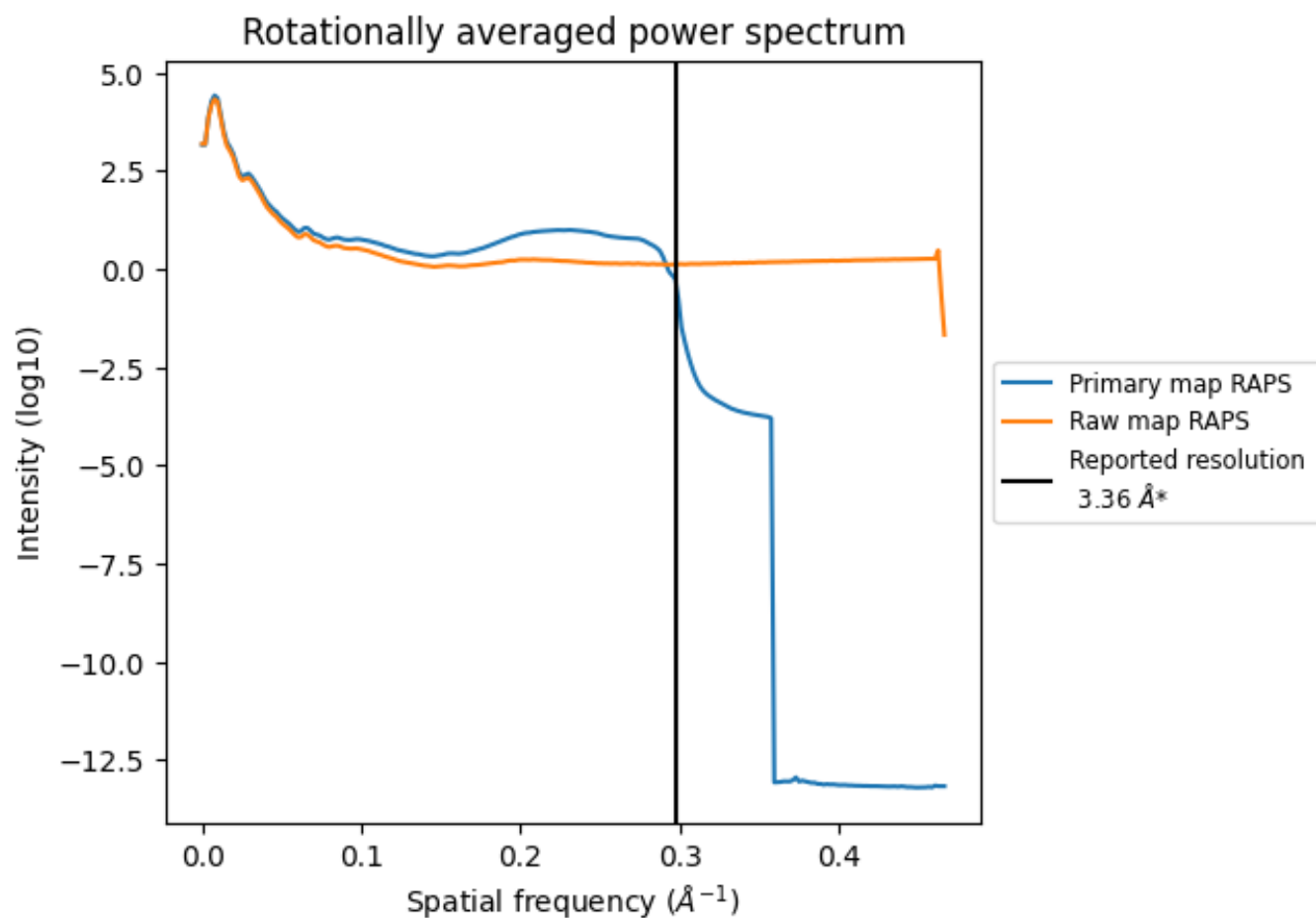
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 126 nm³; this corresponds to an approximate mass of 114 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 ⓘ

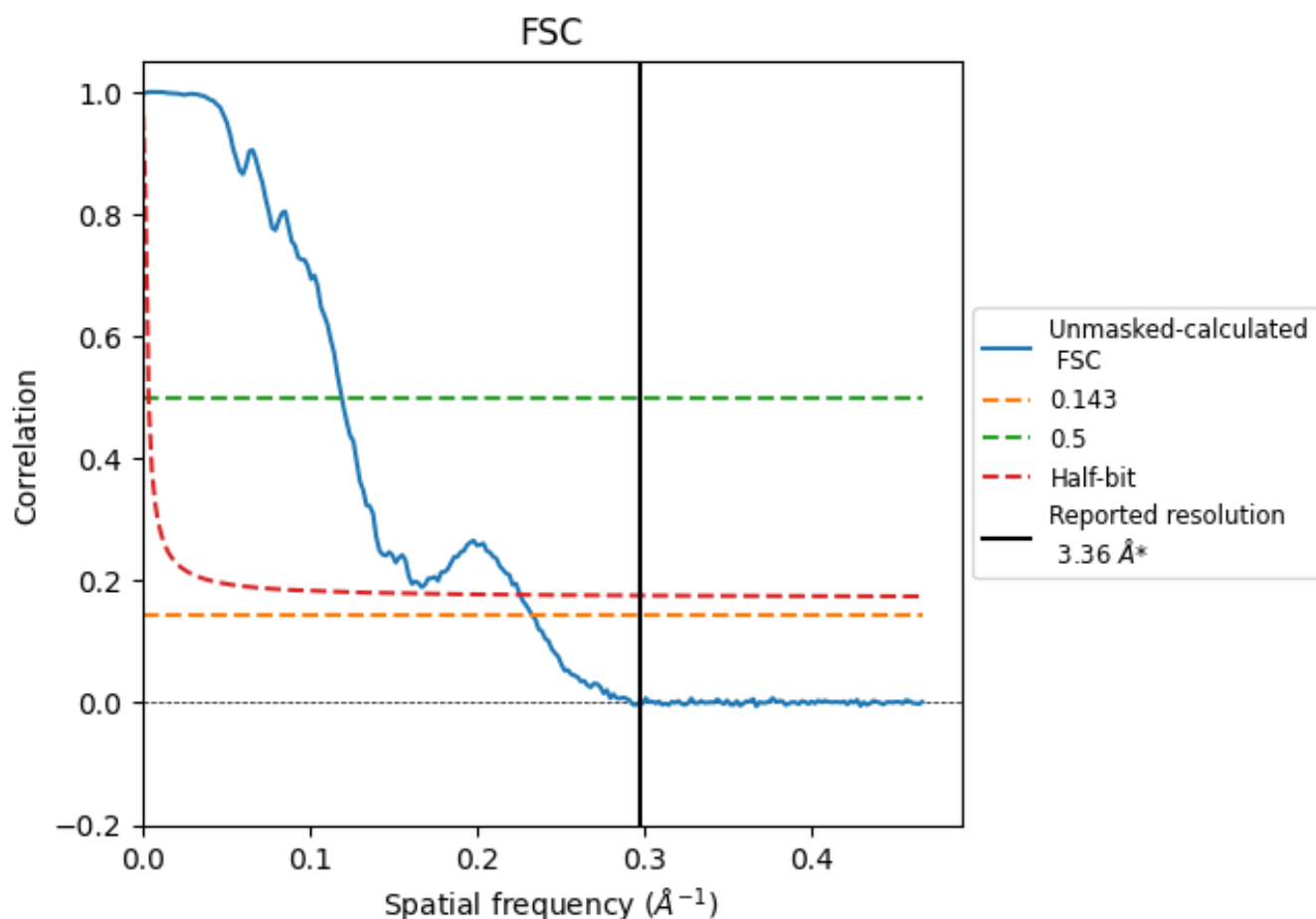


*Reported resolution corresponds to spatial frequency of 0.298 Å⁻¹

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 0.298 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

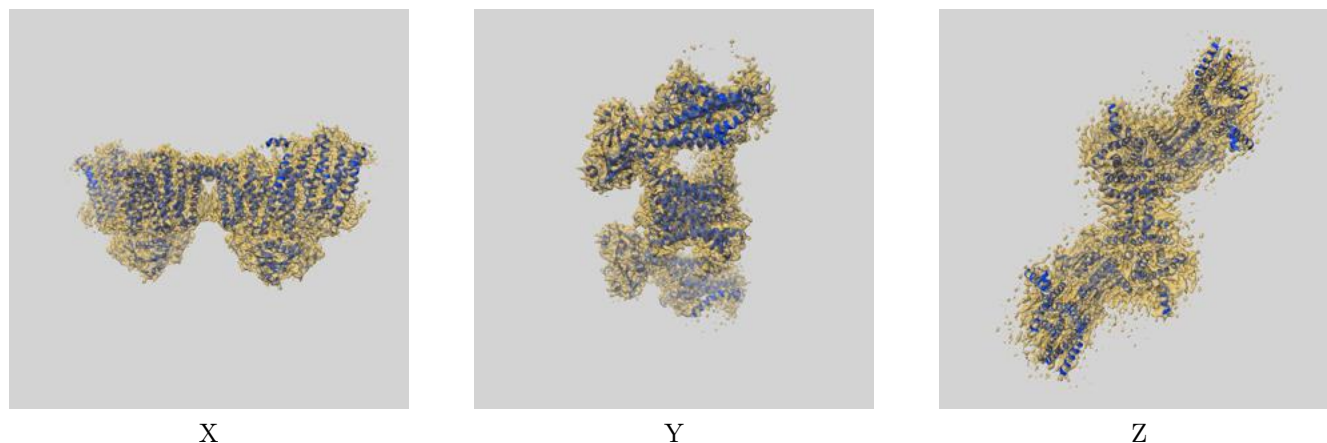
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.29	8.38	4.42

*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 4.29 differs from the reported value 3.36 by more than 10 %

9 Map-model fit [i](#)

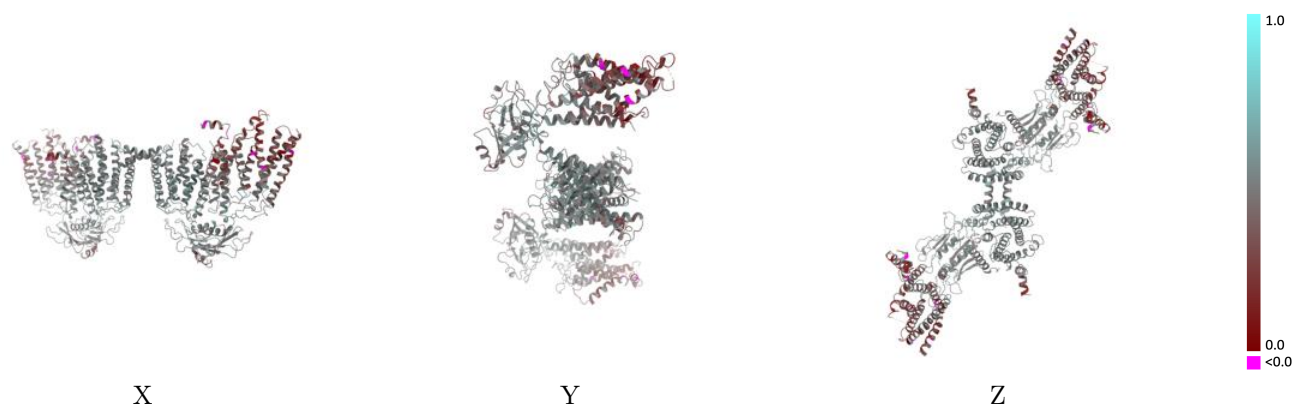
This section contains information regarding the fit between EMDB map EMD-65613 and PDB model 9W3Z. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



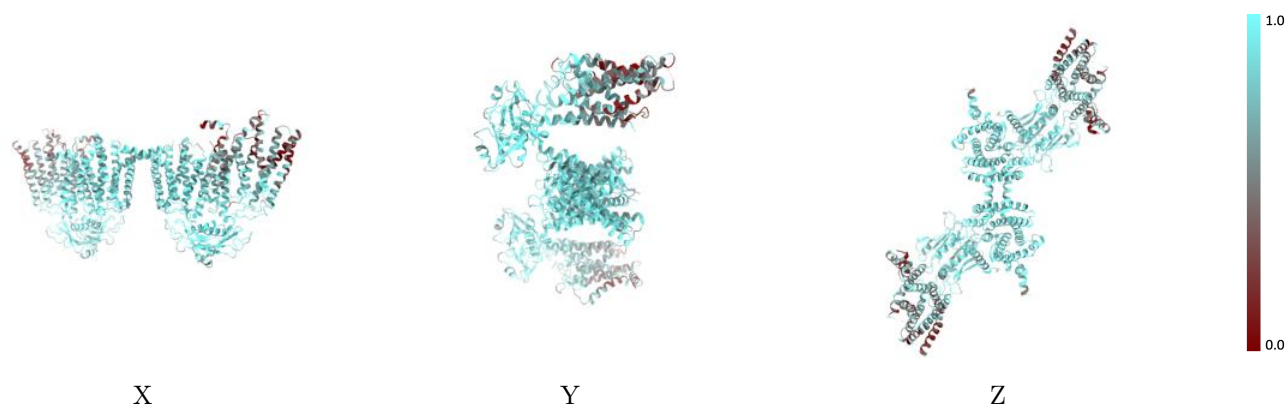
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



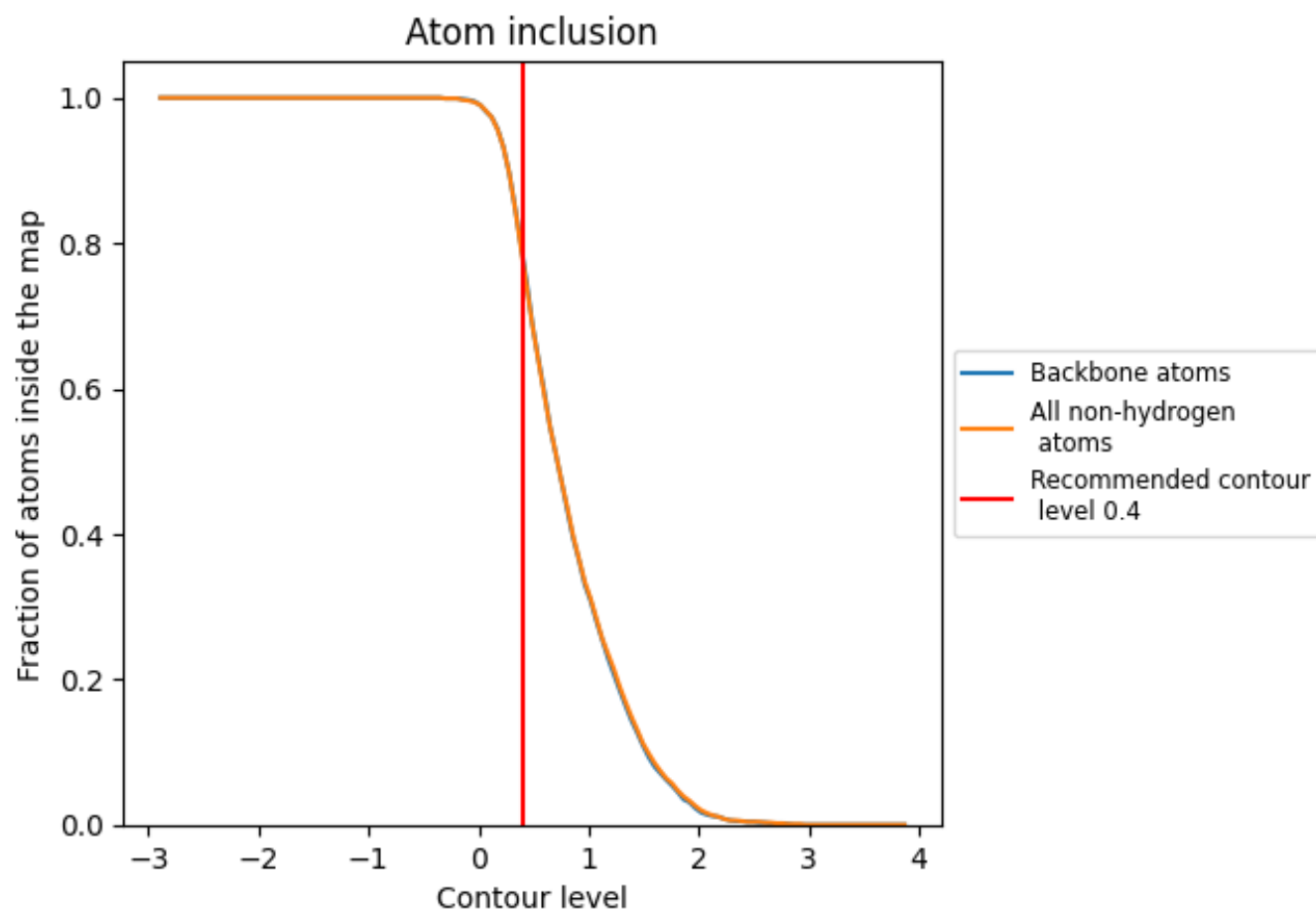
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7780	0.4520
A	0.6260	0.3740
B	0.8430	0.4750
C	0.8740	0.4990
D	0.8660	0.4930
E	0.6270	0.3760
F	0.8440	0.4760
G	0.8740	0.5000
H	0.8660	0.4920

