



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:38 PM UTC

PDB ID : 9QO5 / pdb_00009qo5
EMDB ID : EMD-53257
Title : Dissociation-state-4 of 9-subunit CSN and SCF (SKP1-SKP2-CKS1) complex
Authors : Ding, S.; Clapperton, J.A.; Maeots, M.E.; Enchev, R.I.
Deposited on : 2025-03-25
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

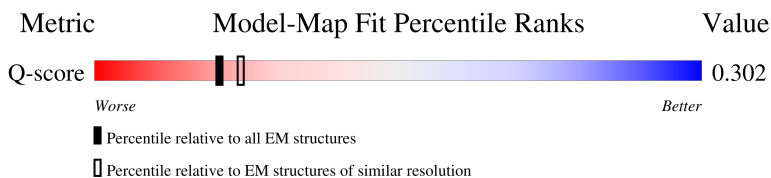
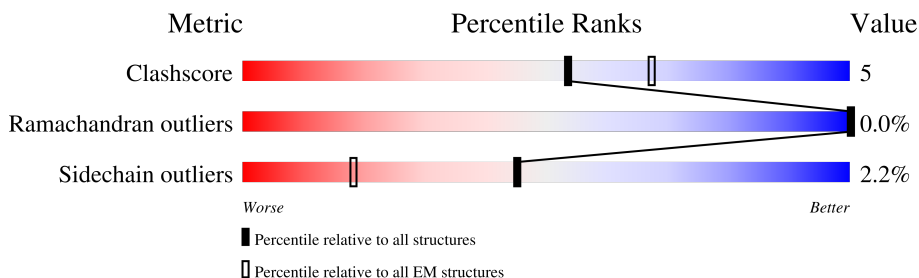
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



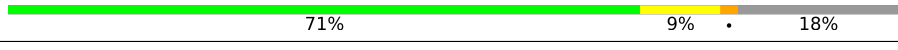
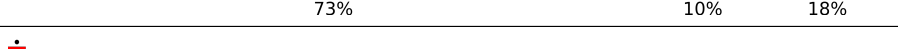
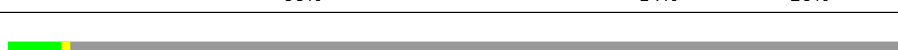
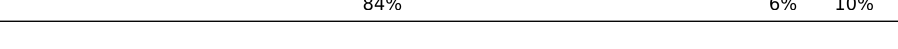
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	
2	B	443	
3	C	423	
4	D	406	

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Mol	Chain	Length	Quality of chain
5	F	327	
6	G	264	
7	H	209	
8	I	776	
9	J	108	
10	L	163	
11	M	424	
12	N	79	
13	E	334	
14	P	57	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 29818 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 COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3308	2090	576	620	22		

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	398	Total	C	N	O	S	0	0
			3267	2082	559	611	15		

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	400	Total	C	N	O	S	0	0
			3191	2032	536	596	27		

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	351	Total	C	N	O	S	0	0
			2833	1789	490	540	14		

- Molecule 5 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	282	Total	C	N	O	S	0	0
			2244	1434	373	422	15		

- Molecule 6 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	216	Total	C	N	O	S	0	0
			1705	1080	290	329	6		

- Molecule 7 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	172	Total	C	N	O	S	0	0
			1374	880	239	251	4		

- Molecule 8 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	618	Total	C	N	O	S	0	0
			5042	3199	859	959	25		

- Molecule 9 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	7	Total	C	N	O	0	0
			65	43	13	9		

- Molecule 10 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	127	Total	C	N	O	S	0	0
			1021	651	167	198	5		

- Molecule 11 is a protein called S-phase kinase-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	324	Total	C	N	O	S	0	0
			2565	1630	442	477	16		

- Molecule 12 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	71	Total	C	N	O	S	0	0
			614	398	105	108	3		

- Molecule 13 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	300	Total	C	N	O	S	0	0
			2381	1522	395	450	14		

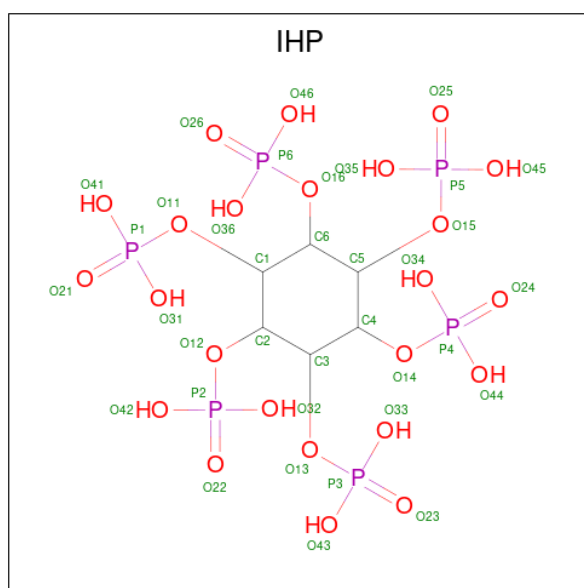
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	104	ALA	GLU	conflict	UNP Q92905

- Molecule 14 is a protein called COP9 signalosome complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	P	20	Total	C	N	O	0	0
			170	107	24	39		

- Molecule 15 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	E	1	Total	Zn	0
			1	1	

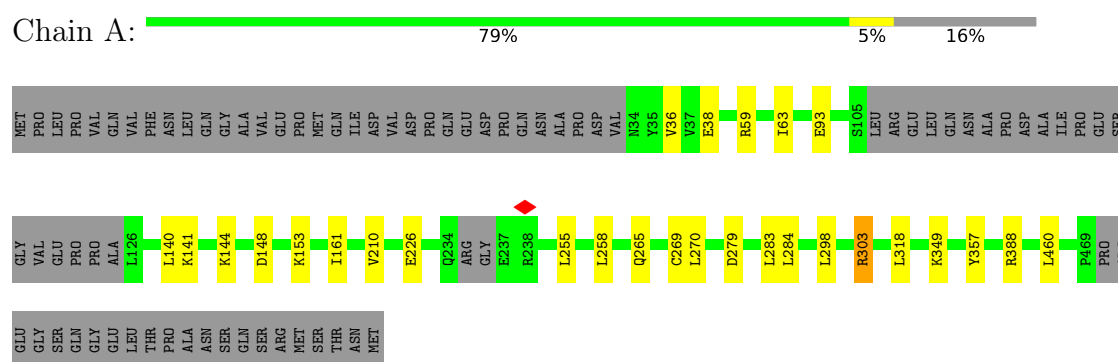
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	E	1	Total	O	0
			1	1	

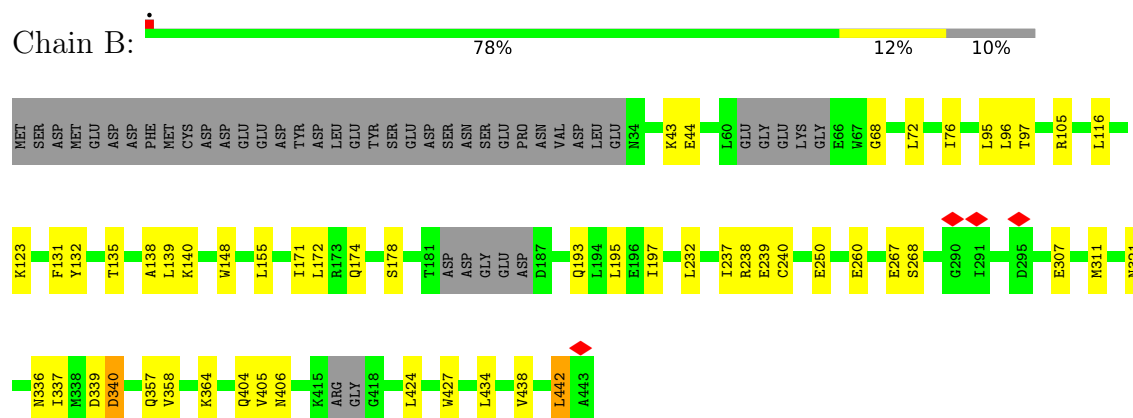
3 Residue-property plots

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

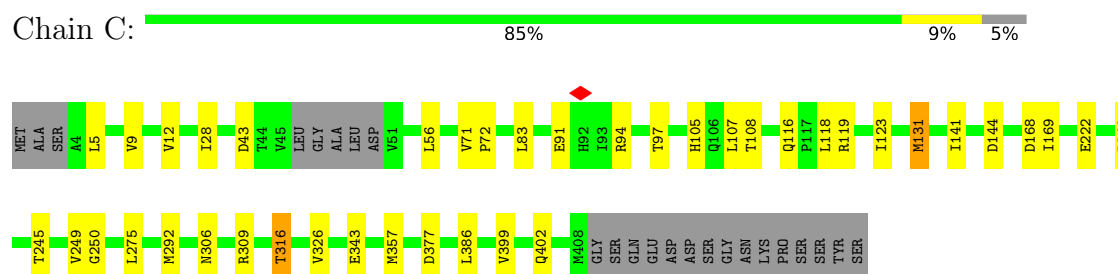
• Molecule 1: COP9 signalosome complex subunit 1



• Molecule 2: COP9 signalosome complex subunit 2



• Molecule 3: COP9 signalosome complex subunit 3



Chain D:

68% 17% 14%

Amino Acid
MET
ALA
ALA
ALA
VAL
ARG
GLN
ASP
LEU
ALA
GLN
LEU
MET
ASN
SER
SER
GLY
SER
HIS
LYS
ASP
LEU
GLY
GLY
LYS
TYR
ARG
GLN
ILE
LEU
GLU
LYS
ALA
ILE
GLN
SER
GLY
ALA
E40
Q41
L42
L45
V49
E50
A51
M52
V53
ASN
GLU
ASN
VAL
SER
LEU
VAL
ILE
S62
D68
F69
C70
T71
L76
P77
D78
S79
I84
T88
K91
I92
Q93
P94
R95
V96
F99
E100
E101
A104
Q108
H109
L110
A111
R121
A124
Q125
V126
L127
P131
LEU
GLU
THR
GLY
GLN
LYS
GLN
TYR
N140
V141
D142
Y143
K144
L145
Y148
L154
D158
Y167
A171
L174
Q175
M176
E177
L183
Q184
I185
H186
Y187
R193
Q206
R207
T208
N209
S212
T216
E219
L230
Q241
L264
D270
A283
M284
L285
M286
P287
H288
T293
A294
D295
G296
S297
L309
I338
M342
I343
T344
E345
V346
V347

[illegible]

Chain G:

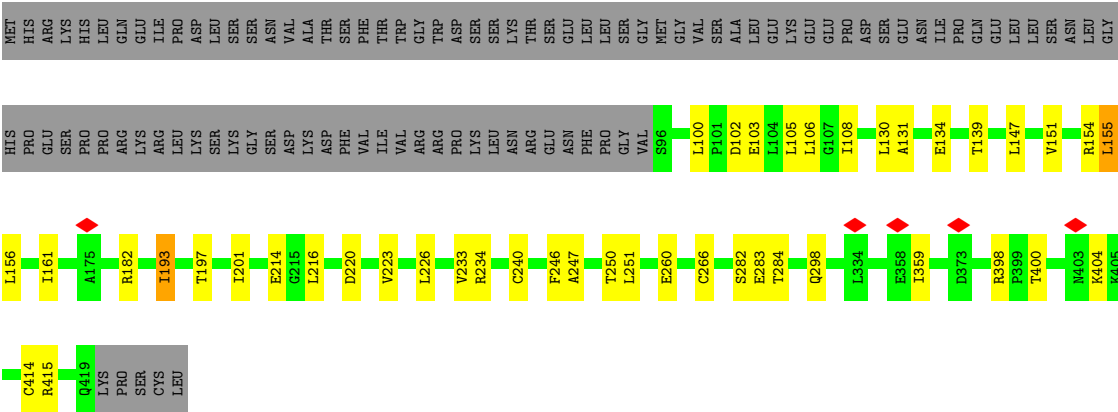
Chain H:

73% 10% 18%

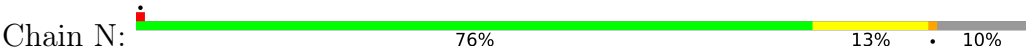
Amino Acid	Approx. Information Content (bits)
MET	0.05
PRO	0.05
VAL	0.05
ALA	0.05
VAL	0.05
MET	0.05
GLU	0.05
GLU	0.05
SER	0.05
ALA	0.05
F11	0.15
D18	0.15
N22	0.15
Q39	0.15
L40	0.15
L41	0.15
A42	0.15
L43	0.15
Y44	0.15
L45	0.15
L46	0.15
R84	0.15
I89	0.15
I93	0.15
N94	0.15
M106	0.15
R110	0.15
L120	0.15
V141	0.15
V145	0.15
T159	0.15
P167	0.25
VAL	0.05
ALA	0.05
GLY	0.05
ALA	0.05
LEU	0.05
ASP	0.05
VAL	0.05
SER	0.05
PHE	0.05
ASN	0.05
LYS	0.05
PHE	0.05
ILE	0.05
PRO	0.05
LEU	0.05

Amino Acid	Approx. Information Content (bits)
SER	0.05
GLU	0.05
PRO	0.05
ALA	0.05
PRO	0.05
VAL	0.05
PRO	0.05
PRO	0.05
ILE	0.05
PRO	0.05
ASN	0.05
GLU	0.05
Q195	0.15
Y203	0.15
V204	0.15
Y209	0.15

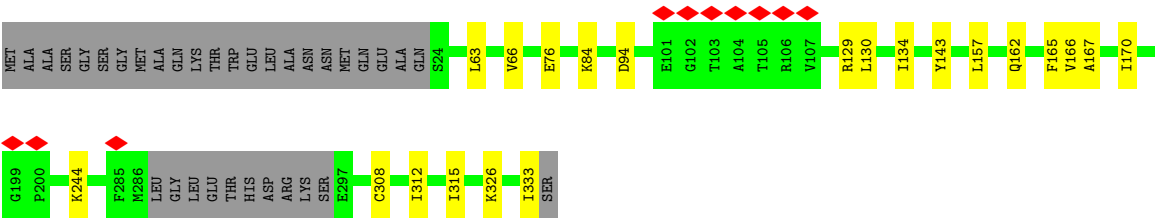
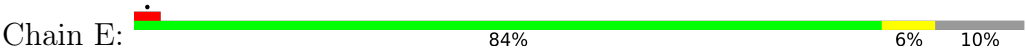




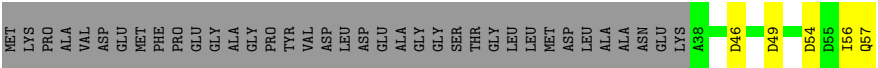
• Molecule 12: Cyclin-dependent kinases regulatory subunit 1



• Molecule 13: COP9 signalosome complex subunit 5



• Molecule 14: COP9 signalosome complex subunit 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131512	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	50	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.922	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.00984	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.19	0/3362	0.40	1/4531 (0.0%)
2	B	0.16	0/3322	0.41	2/4467 (0.0%)
3	C	0.15	0/3249	0.34	0/4385
4	D	0.16	0/2880	0.38	0/3889
5	F	0.18	0/2291	0.36	0/3104
6	G	0.26	0/1725	0.52	3/2334 (0.1%)
7	H	0.13	0/1407	0.32	0/1912
8	I	0.16	0/5126	0.38	0/6898
9	J	0.10	0/65	0.24	0/82
10	L	0.20	0/1036	0.52	1/1398 (0.1%)
11	M	0.16	0/2615	0.34	1/3548 (0.0%)
12	N	0.14	0/635	0.37	0/860
13	E	0.17	0/2433	0.34	0/3287
14	P	0.49	0/174	0.72	0/234
All	All	0.17	0/30320	0.39	8/40929 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	179	ASP	N-CA-C	-9.30	101.22	111.36
6	G	178	CYS	CB-CA-C	6.26	121.74	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	ASP	CB-CA-C	6.26	120.15	109.82
10	L	116	LEU	N-CA-C	-6.08	104.65	111.28
6	G	181	CYS	N-CA-C	-6.01	103.90	111.11
1	A	303	ARG	N-CA-C	-5.38	106.55	113.23
11	M	134	GLU	N-CA-C	-5.14	107.03	113.15
2	B	339	ASP	N-CA-C	-5.01	103.88	111.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3308	0	3335	16	0
2	B	3267	0	3323	34	0
3	C	3191	0	3212	29	0
4	D	2833	0	2819	53	0
5	F	2244	0	2234	21	0
6	G	1705	0	1745	11	0
7	H	1374	0	1360	18	0
8	I	5042	0	5020	72	0
9	J	65	0	75	1	0
10	L	1021	0	1023	21	0
11	M	2565	0	2596	24	0
12	N	614	0	594	7	0
13	E	2381	0	2357	19	0
14	P	170	0	131	4	0
15	B	36	0	6	1	0
16	E	1	0	0	0	0
17	E	1	0	0	0	0
All	All	29818	0	29830	308	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 (308) 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)
8:I:558:GLU:OE1	8:I:558:GLU:N	2.19	0.76
4:D:345:GLU:OE1	4:D:347:ARG:NH2	2.20	0.75
3:C:306:ASN:OD1	3:C:309:ARG:NH2	2.20	0.73
4:D:126:VAL:HG23	4:D:127:LEU:HD22	1.69	0.73
1:A:255:LEU:HD11	1:A:357:TYR:CD2	2.25	0.72
2:B:96:LEU:HD13	2:B:138:ALA:HB1	1.71	0.72
8:I:460:ASP:OD1	8:I:461:VAL:N	2.23	0.72
7:H:195:GLN:OE1	13:E:326:LYS:NZ	2.23	0.71
4:D:52:MET:N	4:D:52:MET:HE2	2.05	0.70
8:I:538:GLN:N	8:I:538:GLN:OE1	2.25	0.70
8:I:602:GLN:OE1	8:I:602:GLN:N	2.24	0.70
14:P:56:ILE:O	14:P:57:GLN:OXT	2.09	0.70
1:A:38:GLU:N	1:A:38:GLU:OE1	2.24	0.70
8:I:300:LEU:O	8:I:304:HIS:ND1	2.25	0.70
10:L:158:GLN:NE2	10:L:158:GLN:O	2.25	0.69
8:I:566:PHE:O	8:I:568:ALA:N	2.26	0.68
8:I:463:GLN:NE2	8:I:500:TYR:O	2.27	0.68
8:I:271:GLU:O	8:I:275:VAL:HG23	1.93	0.68
5:F:88:GLU:N	5:F:88:GLU:OE2	2.27	0.67
8:I:100:LEU:HD11	8:I:170:CYS:HB2	1.76	0.67
5:F:249:GLU:N	5:F:249:GLU:OE1	2.27	0.67
5:F:162:ASP:O	5:F:163:LEU:C	2.38	0.66
2:B:193:GLN:O	2:B:197:ILE:HG23	1.95	0.66
4:D:101:GLU:OE1	4:D:101:GLU:N	2.28	0.66
11:M:414:CYS:SG	11:M:415:ARG:N	2.70	0.65
3:C:107:LEU:HD21	3:C:123:ILE:HD11	1.79	0.65
2:B:44:GLU:N	2:B:44:GLU:OE1	2.31	0.64
4:D:342:MET:HE2	4:D:342:MET:HA	1.78	0.64
2:B:307:GLU:OE1	2:B:336:ASN:ND2	2.32	0.63
11:M:105:LEU:HD23	11:M:108:ILE:HD11	1.81	0.62
8:I:259:GLU:N	8:I:259:GLU:OE1	2.30	0.62
14:P:56:ILE:O	14:P:57:GLN:C	2.43	0.61
3:C:343:GLU:OE2	7:H:120:LEU:HD22	1.99	0.61
4:D:93:GLN:O	4:D:96:VAL:HG22	2.00	0.61
8:I:98:ASN:OD1	8:I:99:TYR:N	2.33	0.61
2:B:76:ILE:HD11	2:B:95:LEU:HD21	1.83	0.61
4:D:167:TYR:O	4:D:171:ALA:N	2.33	0.61
4:D:104:ALA:O	4:D:108:GLN:NE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:103:LEU:CD1	10:L:119:THR:HG21	2.30	0.61
2:B:405:VAL:HG23	2:B:406:ASN:OD1	2.00	0.61
4:D:283:ALA:HB3	4:D:284:MET:CE	2.31	0.61
4:D:230:LEU:CD1	4:D:264:LEU:HD13	2.31	0.60
4:D:230:LEU:HD11	4:D:264:LEU:HD13	1.83	0.60
2:B:311:MET:HE1	2:B:337:ILE:HD13	1.83	0.60
7:H:94:ASN:OD1	7:H:110:ARG:NH2	2.34	0.60
1:A:140:LEU:HD12	1:A:141:LYS:N	2.17	0.59
2:B:139:LEU:HD12	2:B:148:TRP:HB2	1.84	0.59
11:M:214:GLU:OE2	11:M:398:ARG:NH1	2.35	0.59
10:L:115:LEU:O	10:L:119:THR:HG23	2.03	0.59
3:C:316:THR:HG22	3:C:357:MET:HE3	1.83	0.59
13:E:162:GLN:N	13:E:162:GLN:OE1	2.36	0.59
1:A:59:ARG:O	1:A:63:ILE:HD12	2.03	0.58
10:L:27:ILE:HD12	10:L:28:LYS:N	2.16	0.58
1:A:269:CYS:SG	1:A:270:LEU:N	2.75	0.58
2:B:105:ARG:NH2	8:I:481:SER:OG	2.36	0.58
4:D:209:ASN:O	4:D:212:SER:OG	2.20	0.58
11:M:298:GLN:N	11:M:298:GLN:OE1	2.36	0.58
11:M:139:THR:HG1	11:M:415:ARG:H	1.53	0.57
10:L:51:ASN:OD1	10:L:53:ALA:N	2.37	0.57
3:C:28:ILE:HD12	3:C:56:LEU:HD21	1.86	0.57
2:B:434:LEU:O	2:B:438:VAL:HG23	2.04	0.57
4:D:283:ALA:HB3	4:D:284:MET:HE2	1.87	0.57
13:E:94:ASP:OD2	13:E:129:ARG:NH2	2.37	0.57
2:B:171:ILE:HG23	2:B:172:LEU:HD22	1.86	0.57
8:I:474:LEU:HD22	8:I:545:TRP:HH2	1.69	0.56
11:M:220:ASP:OD1	11:M:247:ALA:HB2	2.05	0.56
2:B:139:LEU:HD13	2:B:139:LEU:O	2.06	0.56
3:C:97:THR:HG22	3:C:97:THR:O	2.05	0.56
3:C:377:ASP:OD1	7:H:203:TYR:OH	2.23	0.56
4:D:148:TYR:CD2	4:D:174:LEU:HD11	2.41	0.56
8:I:158:GLU:O	8:I:162:LEU:N	2.34	0.56
4:D:111:ALA:HB2	4:D:127:LEU:HD21	1.89	0.55
13:E:66:VAL:HG22	13:E:170:ILE:HD11	1.89	0.55
4:D:193:ARG:O	4:D:193:ARG:NH1	2.39	0.55
5:F:49:LEU:HD22	13:E:63:LEU:HD12	1.88	0.55
11:M:246:PHE:O	11:M:250:THR:HG23	2.06	0.55
1:A:63:ILE:HD12	1:A:63:ILE:H	1.71	0.55
8:I:541:SER:OG	8:I:542:SER:N	2.38	0.55
4:D:219:GLU:OE1	4:D:219:GLU:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:103:LEU:HD11	10:L:119:THR:HG21	1.87	0.55
2:B:72:LEU:O	2:B:76:ILE:HD12	2.08	0.54
8:I:439:GLU:OE1	8:I:439:GLU:N	2.38	0.54
3:C:91:GLU:N	3:C:91:GLU:OE1	2.41	0.54
8:I:100:LEU:HD11	8:I:170:CYS:CB	2.38	0.54
1:A:388:ARG:NH1	2:B:404:GLN:OE1	2.41	0.54
7:H:204:VAL:HG23	13:E:315:ILE:HG21	1.89	0.54
10:L:67:ASP:OD1	10:L:67:ASP:N	2.40	0.53
5:F:126:THR:OG1	5:F:127:THR:N	2.41	0.53
6:G:202:HIS:O	6:G:205:THR:HG22	2.08	0.53
11:M:193:ILE:HG22	11:M:197:THR:HG23	1.91	0.53
3:C:94:ARG:O	3:C:97:THR:OG1	2.25	0.53
4:D:206:GLN:NE2	4:D:241:GLN:OE1	2.42	0.53
6:G:79:ILE:HD12	6:G:80:ALA:N	2.24	0.53
8:I:123:TRP:CD1	8:I:207:SER:HG	2.27	0.53
8:I:215:GLU:N	8:I:215:GLU:OE1	2.41	0.53
4:D:68:ASP:O	4:D:71:THR:OG1	2.27	0.52
1:A:144:LYS:NZ	1:A:148:ASP:OD2	2.41	0.52
6:G:14:GLN:N	6:G:14:GLN:OE1	2.42	0.52
4:D:95:ARG:O	4:D:99:PHE:N	2.42	0.52
4:D:359:VAL:O	4:D:359:VAL:HG13	2.09	0.52
8:I:134:ASN:OD1	8:I:160:TYR:N	2.42	0.52
5:F:186:LEU:HD23	5:F:187:THR:N	2.25	0.51
8:I:130:SER:O	8:I:134:ASN:ND2	2.44	0.51
8:I:411:MET:SD	8:I:411:MET:N	2.80	0.51
11:M:223:VAL:HB	11:M:247:ALA:HB1	1.92	0.51
11:M:283:GLU:OE1	11:M:283:GLU:N	2.41	0.51
3:C:402:GLN:OE1	3:C:402:GLN:N	2.44	0.51
12:N:71:ARG:NH1	12:N:73:LEU:HD12	2.25	0.51
8:I:499:GLU:OE1	8:I:499:GLU:N	2.43	0.51
2:B:364:LYS:HZ1	4:D:344:THR:CB	2.23	0.51
4:D:51:ALA:C	4:D:52:MET:HE2	2.36	0.51
8:I:555:LEU:HD23	8:I:556:PRO:O	2.11	0.51
11:M:156:LEU:HD12	11:M:201:ILE:HD11	1.92	0.51
6:G:11:LEU:HD13	6:G:11:LEU:O	2.10	0.50
3:C:169:ILE:N	3:C:169:ILE:HD12	2.26	0.50
4:D:377:LEU:O	4:D:381:VAL:HG23	2.11	0.50
3:C:131:MET:HE1	3:C:141:ILE:HD12	1.93	0.50
3:C:222:GLU:N	3:C:222:GLU:OE1	2.45	0.50
11:M:233:VAL:O	11:M:260:GLU:N	2.42	0.50
2:B:424:LEU:HD23	2:B:427:TRP:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:GLN:O	4:D:45:LEU:HD12	2.11	0.50
2:B:116:LEU:HD21	2:B:132:TYR:CZ	2.46	0.50
7:H:89:ILE:HG22	7:H:93:ILE:HD12	1.93	0.50
5:F:41:VAL:HG12	5:F:81:ILE:HB	1.94	0.50
8:I:363:PRO:O	8:I:367:VAL:HG12	2.11	0.49
13:E:84:LYS:HA	13:E:134:ILE:HD12	1.94	0.49
15:B:501:IHP:O36	15:B:501:IHP:O31	2.30	0.49
7:H:141:VAL:O	7:H:145:VAL:HG13	2.13	0.49
6:G:69:LEU:O	6:G:73:GLY:N	2.41	0.49
3:C:131:MET:CE	3:C:141:ILE:HD12	2.43	0.49
4:D:50:GLU:OE1	4:D:50:GLU:N	2.45	0.49
8:I:460:ASP:OD1	8:I:461:VAL:HG13	2.13	0.49
5:F:152:LEU:HD12	5:F:166:SER:O	2.13	0.49
5:F:199:GLY:O	5:F:203:VAL:HG13	2.12	0.49
8:I:28:ILE:HD11	8:I:133:LEU:CD2	2.42	0.49
7:H:106:MET:HE2	7:H:106:MET:HA	1.94	0.48
4:D:389:SER:O	4:D:389:SER:OG	2.28	0.48
8:I:438:GLU:N	8:I:438:GLU:OE1	2.46	0.48
4:D:110:LEU:HD22	4:D:126:VAL:HG11	1.95	0.48
11:M:233:VAL:HG23	11:M:234:ARG:HG3	1.94	0.48
4:D:286:MET:HE3	4:D:288:HIS:H	1.78	0.48
5:F:190:LEU:HG	13:E:244:LYS:HZ2	1.78	0.48
11:M:282:SER:OG	11:M:284:THR:HG22	2.14	0.48
4:D:45:LEU:O	4:D:49:VAL:HG22	2.14	0.48
10:L:115:LEU:HA	10:L:118:VAL:HG12	1.96	0.48
1:A:258:LEU:HD23	1:A:258:LEU:O	2.14	0.48
5:F:49:LEU:HD22	13:E:63:LEU:CD1	2.44	0.48
7:H:41:LEU:HD23	7:H:45:LEU:HD13	1.96	0.48
3:C:242:PRO:O	3:C:245:THR:OG1	2.28	0.47
4:D:142:ASP:OD1	4:D:143:TYR:N	2.45	0.47
8:I:304:HIS:O	8:I:308:GLN:NE2	2.47	0.47
2:B:239:GLU:OE1	2:B:240:CYS:N	2.47	0.47
5:F:72:LEU:N	5:F:123:GLY:O	2.45	0.47
5:F:217:VAL:HG12	7:H:204:VAL:HG11	1.97	0.47
2:B:68:GLY:O	2:B:72:LEU:HG	2.15	0.47
5:F:185:GLU:OE2	5:F:186:LEU:N	2.48	0.47
8:I:310:LEU:HD22	8:I:322:MET:HE1	1.96	0.47
10:L:33:ASP:OD1	10:L:33:ASP:N	2.47	0.47
10:L:126:MET:SD	10:L:126:MET:N	2.87	0.47
12:N:52:GLN:O	12:N:71:ARG:NH2	2.47	0.47
3:C:5:LEU:O	3:C:9:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:LEU:HD12	4:D:45:LEU:H	1.80	0.46
8:I:257:VAL:HG13	8:I:306:GLU:HG3	1.96	0.46
3:C:105:HIS:ND1	3:C:144:ASP:OD2	2.48	0.46
11:M:359:ILE:HD12	11:M:359:ILE:H	1.81	0.46
5:F:61:GLN:CD	13:E:130:LEU:HD11	2.40	0.46
6:G:162:ILE:HD12	6:G:162:ILE:O	2.16	0.46
8:I:241:GLU:OE1	8:I:294:VAL:HG11	2.16	0.46
10:L:21:ALA:HA	10:L:27:ILE:HD13	1.98	0.46
4:D:93:GLN:HA	4:D:96:VAL:HG13	1.98	0.46
2:B:232:LEU:HD13	2:B:268:SER:OG	2.16	0.46
4:D:121:ARG:NE	4:D:121:ARG:O	2.49	0.46
14:P:46:ASP:OD1	14:P:46:ASP:N	2.49	0.46
2:B:132:TYR:CD1	2:B:155:LEU:HD13	2.51	0.46
3:C:343:GLU:OE1	7:H:84:ARG:NH1	2.46	0.45
4:D:78:ASP:OD1	4:D:79:SER:N	2.49	0.45
8:I:608:MET:HE3	9:J:24:VAL:HG23	1.99	0.45
8:I:633:MET:HE3	8:I:633:MET:O	2.16	0.45
13:E:76:GLU:OE1	13:E:143:TYR:OH	2.34	0.45
2:B:174:GLN:O	2:B:178:SER:OG	2.28	0.45
6:G:122:MET:HE1	6:G:128:LEU:HA	1.99	0.45
11:M:151:VAL:O	11:M:155:LEU:HD13	2.15	0.45
3:C:116:GLN:OE1	3:C:119:ARG:NH1	2.49	0.45
11:M:102:ASP:OD1	11:M:103:GLU:N	2.49	0.45
2:B:238:ARG:NH2	2:B:260:GLU:OE2	2.48	0.45
2:B:250:GLU:N	2:B:250:GLU:OE2	2.49	0.45
4:D:342:MET:HE1	4:D:347:ARG:HH21	1.81	0.45
8:I:230:GLU:N	8:I:230:GLU:OE1	2.47	0.45
8:I:271:GLU:N	8:I:271:GLU:OE1	2.50	0.45
11:M:240:CYS:N	11:M:266:CYS:SG	2.89	0.45
7:H:46:LEU:HD12	7:H:46:LEU:O	2.16	0.45
8:I:46:TYR:N	8:I:136:ILE:HD11	2.31	0.45
10:L:27:ILE:HD12	10:L:28:LYS:H	1.79	0.45
8:I:28:ILE:HD11	8:I:133:LEU:HD23	1.98	0.45
8:I:377:TYR:HA	8:I:380:LEU:HD23	1.99	0.45
1:A:298:LEU:O	1:A:298:LEU:HD12	2.17	0.45
8:I:338:LYS:O	8:I:342:THR:HG23	2.17	0.45
8:I:367:VAL:HG11	8:I:425:TYR:CD2	2.52	0.45
13:E:66:VAL:HG22	13:E:170:ILE:CD1	2.46	0.45
4:D:145:LEU:HG	4:D:174:LEU:HD13	1.99	0.45
8:I:450:MET:HE1	8:I:492:LEU:HA	1.99	0.45
8:I:474:LEU:C	8:I:474:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:478:ASN:OD1	8:I:478:ASN:N	2.49	0.45
2:B:442:LEU:HD13	2:B:442:LEU:O	2.17	0.44
1:A:460:LEU:HD12	2:B:442:LEU:CD1	2.47	0.44
4:D:176:ASN:OD1	4:D:176:ASN:N	2.51	0.44
8:I:296:ILE:HD12	8:I:297:GLU:N	2.32	0.44
12:N:24:LEU:HD12	12:N:65:HIS:O	2.17	0.44
4:D:49:VAL:HG23	4:D:91:LYS:NZ	2.32	0.44
12:N:24:LEU:HD11	12:N:67:LEU:HG	1.99	0.44
6:G:89:SER:OG	6:G:90:THR:N	2.50	0.44
6:G:146:ASP:OD1	6:G:146:ASP:N	2.50	0.44
7:H:204:VAL:CG2	13:E:315:ILE:HG21	2.47	0.44
2:B:195:LEU:HD22	2:B:237:ILE:HD13	1.99	0.44
4:D:68:ASP:OD1	4:D:69:PHE:N	2.51	0.44
7:H:18:ASP:O	7:H:22:ASN:OD1	2.36	0.44
11:M:161:ILE:HD12	11:M:161:ILE:H	1.82	0.44
8:I:271:GLU:OE1	8:I:272:GLN:N	2.51	0.44
10:L:103:LEU:HD13	10:L:103:LEU:C	2.43	0.44
1:A:36:VAL:HG23	1:A:36:VAL:O	2.17	0.43
1:A:255:LEU:HD11	1:A:357:TYR:HD2	1.74	0.43
5:F:190:LEU:HD12	13:E:244:LYS:HG3	2.00	0.43
8:I:441:GLU:O	8:I:445:THR:HG23	2.18	0.43
3:C:326:VAL:HG12	3:C:326:VAL:O	2.16	0.43
3:C:292:MET:O	14:P:49:ASP:OD2	2.35	0.43
8:I:485:GLU:OE1	8:I:485:GLU:N	2.45	0.43
5:F:181:MET:C	5:F:182:LEU:HD12	2.42	0.43
1:A:460:LEU:HD12	2:B:442:LEU:HD11	2.00	0.43
2:B:140:LYS:HD2	2:B:140:LYS:O	2.19	0.43
8:I:430:LEU:HD22	8:I:484:ALA:HB1	2.01	0.43
10:L:107:ALA:O	10:L:111:ASP:N	2.51	0.43
8:I:600:THR:O	8:I:600:THR:OG1	2.34	0.42
8:I:311:LEU:HD23	8:I:343:HIS:ND1	2.34	0.42
2:B:131:PHE:O	2:B:135:THR:HG23	2.20	0.42
4:D:84:ILE:O	4:D:88:THR:HG23	2.19	0.42
8:I:18:ASP:OD1	8:I:18:ASP:N	2.52	0.42
8:I:422:LEU:HD21	8:I:453:PHE:HB2	2.02	0.42
10:L:156:GLU:OE2	11:M:154:ARG:NH2	2.52	0.42
11:M:226:LEU:HD23	11:M:251:LEU:HD21	2.01	0.42
10:L:19:GLU:OE2	10:L:20:ILE:N	2.52	0.42
11:M:404:LYS:O	11:M:406:ASN:ND2	2.51	0.42
3:C:71:VAL:N	3:C:72:PRO:CD	2.83	0.42
3:C:83:LEU:O	3:C:83:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:55:LEU:HA	10:L:58:VAL:HG22	2.01	0.42
11:M:156:LEU:CD1	11:M:201:ILE:HD11	2.50	0.42
3:C:107:LEU:HD21	3:C:123:ILE:CD1	2.47	0.42
8:I:388:ASP:OD1	8:I:390:GLY:N	2.53	0.42
10:L:126:MET:HA	10:L:126:MET:HE3	2.01	0.42
12:N:71:ARG:HH12	12:N:73:LEU:HD12	1.85	0.42
13:E:166:VAL:HG12	13:E:167:ALA:N	2.34	0.42
1:A:265:GLN:OE1	1:A:265:GLN:HA	2.20	0.42
8:I:201:ILE:HD13	8:I:278:TYR:CE1	2.55	0.42
8:I:236:PHE:HE2	8:I:279:LEU:HD11	1.85	0.42
8:I:474:LEU:HD22	8:I:545:TRP:CH2	2.51	0.42
8:I:501:THR:O	8:I:501:THR:HG22	2.20	0.42
3:C:28:ILE:HD12	3:C:56:LEU:CD2	2.48	0.41
3:C:43:ASP:OD1	3:C:43:ASP:N	2.53	0.41
5:F:138:VAL:O	5:F:142:VAL:HG23	2.19	0.41
10:L:63:THR:O	10:L:66:LYS:NZ	2.51	0.41
11:M:130:LEU:O	11:M:131:ALA:C	2.63	0.41
2:B:96:LEU:HD12	2:B:97:THR:N	2.36	0.41
2:B:321:ASN:ND2	2:B:357:GLN:OE1	2.53	0.41
4:D:396:THR:O	4:D:400:MET:HG3	2.20	0.41
8:I:17:LEU:HD13	8:I:88:LEU:HD11	2.02	0.41
8:I:232:PHE:CD1	8:I:232:PHE:C	2.98	0.41
10:L:61:TRP:CD2	10:L:115:LEU:HD13	2.56	0.41
4:D:293:THR:HG22	4:D:294:ALA:N	2.36	0.41
6:G:129:GLU:OE2	6:G:147:GLN:NE2	2.53	0.41
1:A:153:LYS:HA	1:A:161:ILE:HD11	2.01	0.41
5:F:135:ASP:OD1	5:F:135:ASP:N	2.52	0.41
8:I:111:MET:HE3	8:I:112:ASP:H	1.86	0.41
8:I:261:MET:SD	8:I:261:MET:N	2.93	0.41
7:H:39:GLN:O	7:H:43:LEU:HD23	2.19	0.41
4:D:51:ALA:HB3	4:D:52:MET:CE	2.50	0.41
7:H:41:LEU:CD2	7:H:45:LEU:HD13	2.51	0.41
8:I:331:ASP:OD1	8:I:331:ASP:N	2.54	0.41
12:N:9:SER:OG	12:N:21:HIS:O	2.32	0.41
3:C:399:VAL:O	3:C:399:VAL:HG12	2.20	0.41
7:H:195:GLN:CD	13:E:326:LYS:NZ	2.78	0.41
7:H:195:GLN:HE22	13:E:326:LYS:NZ	2.19	0.41
2:B:76:ILE:CD1	2:B:95:LEU:HD11	2.51	0.41
13:E:308:CYS:O	13:E:312:ILE:HG13	2.20	0.41
4:D:148:TYR:N	4:D:148:TYR:CD1	2.89	0.41
4:D:400:MET:O	4:D:404:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:111:MET:HE3	8:I:112:ASP:N	2.35	0.41
8:I:190:GLU:OE2	8:I:267:ARG:NH2	2.54	0.41
8:I:264:ALA:O	8:I:268:LEU:HD23	2.21	0.41
2:B:43:LYS:N	2:B:43:LYS:HD3	2.36	0.41
4:D:124:ALA:HB2	4:D:154:LEU:HD13	2.03	0.41
4:D:207:ARG:NE	4:D:207:ARG:HA	2.36	0.41
4:D:309:LEU:HD23	4:D:342:MET:HG3	2.03	0.41
8:I:475:VAL:HG21	8:I:547:PHE:HE2	1.85	0.41
3:C:168:ASP:C	3:C:169:ILE:HD12	2.46	0.40
8:I:286:GLU:OE1	8:I:286:GLU:N	2.54	0.40
10:L:7:GLN:HB3	10:L:13:ILE:HD13	2.03	0.40
4:D:49:VAL:HG23	4:D:91:LYS:HZ2	1.85	0.40
4:D:352:ILE:HG12	4:D:359:VAL:HG23	2.03	0.40
8:I:175:LEU:HD23	8:I:175:LEU:O	2.21	0.40
8:I:666:ASP:OD1	8:I:666:ASP:N	2.53	0.40
12:N:28:ILE:HG23	12:N:46:LEU:HD22	2.04	0.40
3:C:249:VAL:HG13	3:C:250:GLY:N	2.37	0.40
4:D:286:MET:HE3	4:D:288:HIS:HB3	2.04	0.40
5:F:41:VAL:HG22	5:F:186:LEU:HD22	2.03	0.40
6:G:207:GLN:HA	6:G:207:GLN:OE1	2.22	0.40
8:I:144:TRP:HZ3	8:I:156:ILE:HD12	1.85	0.40
4:D:175:GLN:OE1	4:D:177:GLU:N	2.55	0.40
5:F:190:LEU:HG	13:E:244:LYS:NZ	2.35	0.40
8:I:569:PHE:CD1	8:I:569:PHE:C	2.98	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	408/491 (83%)	386 (95%)	22 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	390/443 (88%)	375 (96%)	14 (4%)	1 (0%)	36	70
3	C	396/423 (94%)	378 (96%)	18 (4%)	0	100	100
4	D	345/406 (85%)	332 (96%)	13 (4%)	0	100	100
5	F	278/327 (85%)	272 (98%)	6 (2%)	0	100	100
6	G	214/264 (81%)	204 (95%)	10 (5%)	0	100	100
7	H	168/209 (80%)	166 (99%)	2 (1%)	0	100	100
8	I	604/776 (78%)	580 (96%)	24 (4%)	0	100	100
9	J	5/108 (5%)	5 (100%)	0	0	100	100
10	L	121/163 (74%)	112 (93%)	9 (7%)	0	100	100
11	M	322/424 (76%)	309 (96%)	13 (4%)	0	100	100
12	N	69/79 (87%)	67 (97%)	2 (3%)	0	100	100
13	E	296/334 (89%)	279 (94%)	17 (6%)	0	100	100
14	P	18/57 (32%)	17 (94%)	1 (6%)	0	100	100
All	All	3634/4504 (81%)	3482 (96%)	151 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	123	LYS

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	362/429 (84%)	354 (98%)	8 (2%)	45	65
2	B	364/405 (90%)	360 (99%)	4 (1%)	65	74
3	C	359/377 (95%)	352 (98%)	7 (2%)	50	67
4	D	303/347 (87%)	292 (96%)	11 (4%)	31	53
5	F	252/276 (91%)	247 (98%)	5 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	187/229 (82%)	175 (94%)	12 (6%)	16	40
7	H	143/173 (83%)	142 (99%)	1 (1%)	76	79
8	I	556/698 (80%)	548 (99%)	8 (1%)	59	71
9	J	7/90 (8%)	7 (100%)	0	100	100
10	L	115/150 (77%)	111 (96%)	4 (4%)	32	54
11	M	300/392 (76%)	292 (97%)	8 (3%)	39	60
12	N	68/76 (90%)	66 (97%)	2 (3%)	37	58
13	E	256/282 (91%)	253 (99%)	3 (1%)	63	73
14	P	18/45 (40%)	17 (94%)	1 (6%)	19	43
All	All	3290/3969 (83%)	3216 (98%)	74 (2%)	45	65

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLU
1	A	210	VAL
1	A	226	GLU
1	A	279	ASP
1	A	283	LEU
1	A	284	LEU
1	A	318	LEU
1	A	349	LYS
2	B	267	GLU
2	B	340	ASP
2	B	358	VAL
2	B	442	LEU
3	C	12	VAL
3	C	108	THR
3	C	118	LEU
3	C	131	MET
3	C	275	LEU
3	C	316	THR
3	C	386	LEU
4	D	42	LEU
4	D	71	THR
4	D	76	LEU
4	D	95	ARG
4	D	99	PHE
4	D	158	ASP

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Mol	Chain	Res	Type
4	D	185	ILE
4	D	270	ASP
4	D	338	ILE
4	D	365	GLU
4	D	385	LEU
5	F	56	ILE
5	F	126	THR
5	F	206	MET
5	F	216	THR
5	F	281	ASP
6	G	11	LEU
6	G	17	LEU
6	G	53	GLN
6	G	74	THR
6	G	122	MET
6	G	145	LEU
6	G	155	ASP
6	G	162	ILE
6	G	178	CYS
6	G	194	ARG
6	G	210	GLU
6	G	214	THR
7	H	159	THR
8	I	170	CYS
8	I	225	LEU
8	I	240	THR
8	I	319	LEU
8	I	325	LEU
8	I	344	ILE
8	I	371	LEU
8	I	618	ASP
10	L	16	VAL
10	L	29	THR
10	L	50	VAL
10	L	111	ASP
11	M	100	LEU
11	M	106	LEU
11	M	147	LEU
11	M	155	LEU
11	M	182	ARG
11	M	193	ILE
11	M	216	LEU

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Mol	Chain	Res	Type
11	M	400	THR
12	N	41	SER
12	N	73	LEU
13	E	157	LEU
13	E	165	PHE
13	E	333	ILE
14	P	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	217	HIS
1	A	406	GLN
2	B	84	ASN
2	B	176	HIS
2	B	353	ASN
3	C	7	GLN
3	C	180	HIS
3	C	271	ASN
3	C	353	GLN
4	D	72	HIS
4	D	163	GLN
4	D	406	GLN
5	F	303	ASN
6	G	53	GLN
6	G	68	ASN
8	I	48	HIS
8	I	436	ASN
10	L	65	HIS
10	L	157	ASN
11	M	273	HIS
11	M	311	ASN
12	N	65	HIS
13	E	248	ASN
13	E	275	GLN
13	E	321	GLN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	IHP	B	501	-	36,36,36	0.76	2 (5%)	60,60,60	0.85	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	IHP	B	501	-	-	8/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	501	IHP	P3-O13	3.05	1.64	1.59
15	B	501	IHP	P1-O11	2.29	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	501	IHP	P6-O16-C6	3.75	133.46	123.43
15	B	501	IHP	P2-O12-C2	2.74	130.75	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	501	IHP	P4-O14-C4	2.63	130.47	123.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

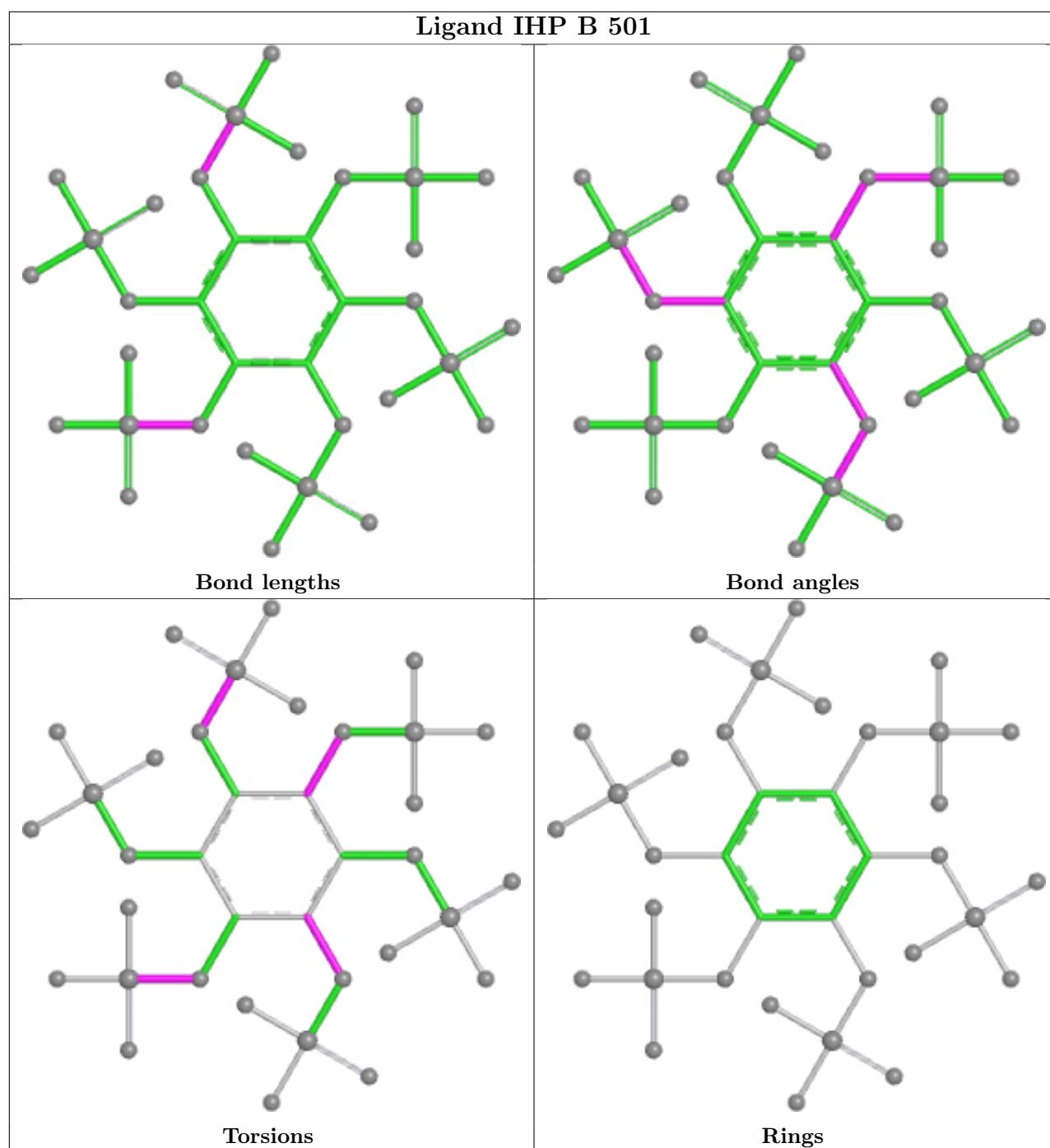
Mol	Chain	Res	Type	Atoms
15	B	501	IHP	C3-C4-O14-P4
15	B	501	IHP	C5-C4-O14-P4
15	B	501	IHP	C1-C6-O16-P6
15	B	501	IHP	C3-O13-P3-O23
15	B	501	IHP	C1-O11-P1-O41
15	B	501	IHP	C1-O11-P1-O21
15	B	501	IHP	C1-O11-P1-O31
15	B	501	IHP	C3-O13-P3-O33

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	501	IHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

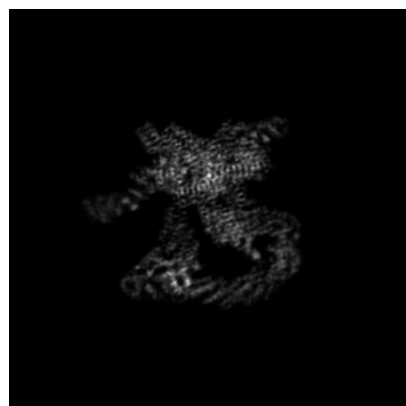
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53257. These allow visual inspection of the internal detail of the map and identification of artifacts.

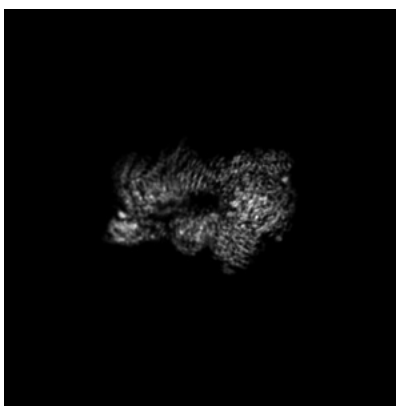
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

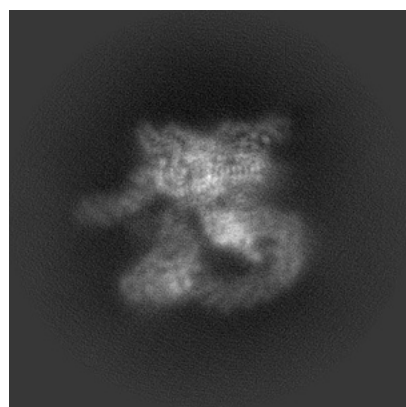


Y

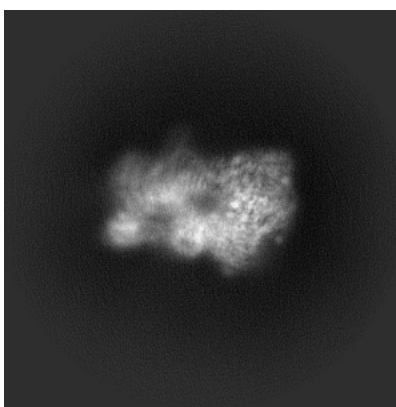


Z

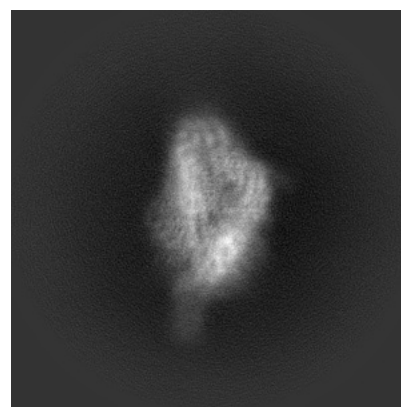
6.1.2 Raw map



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: 160

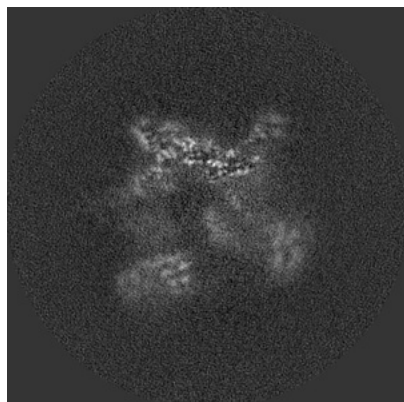


Y Index: 160

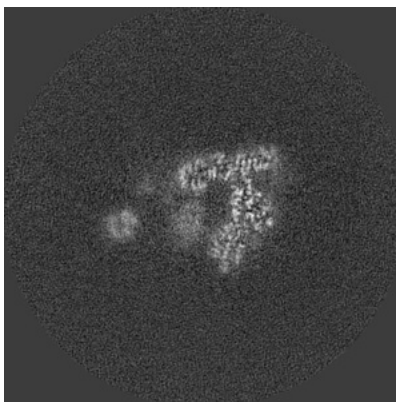


Z Index: 160

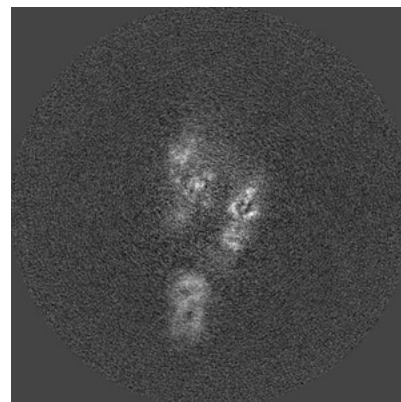
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

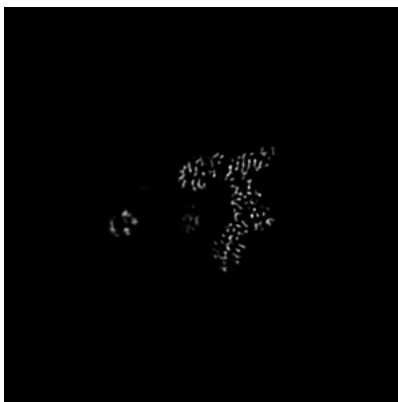
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 146

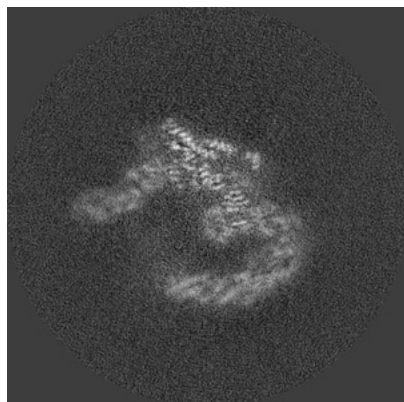


Y Index: 159

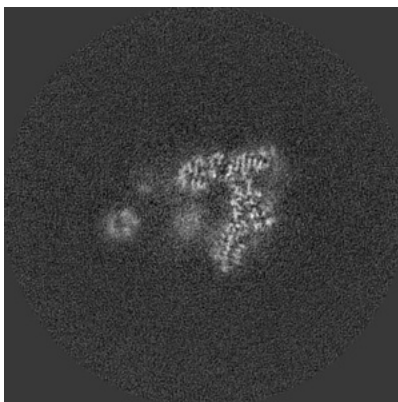


Z Index: 196

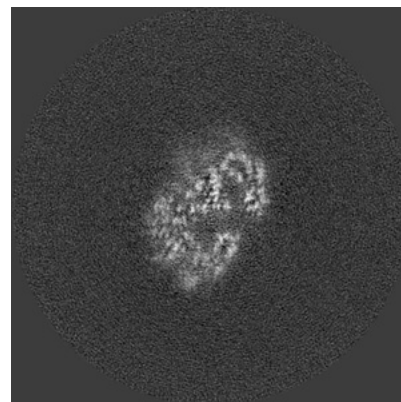
6.3.2 Raw map



X Index: 145



Y Index: 159

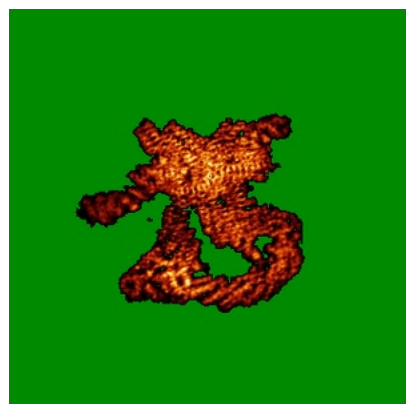


Z Index: 186

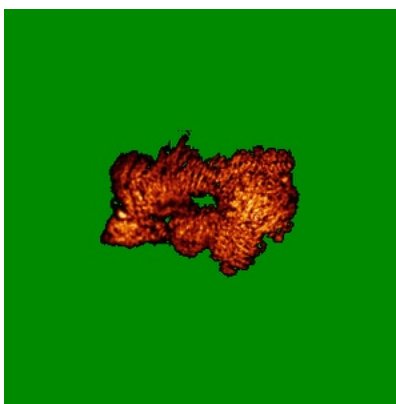
The images above show the largest variance slices of the map in three orthogonal directions.

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

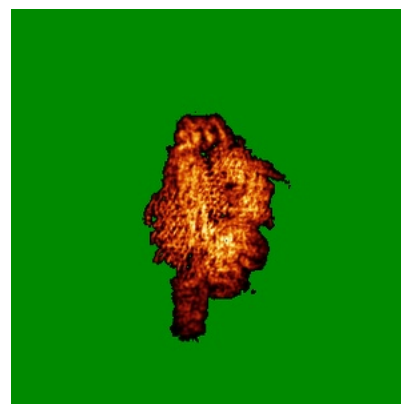
6.4.1 Primary map



X

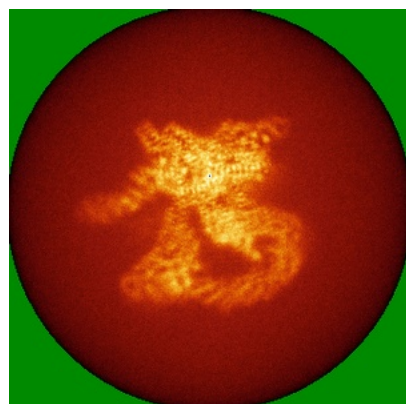


Y

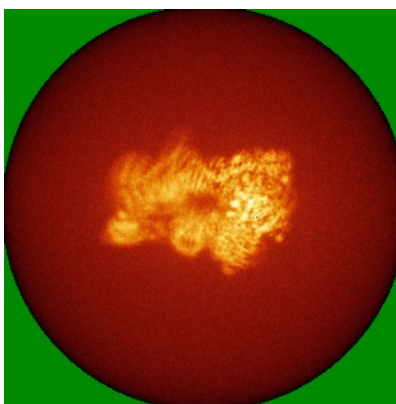


Z

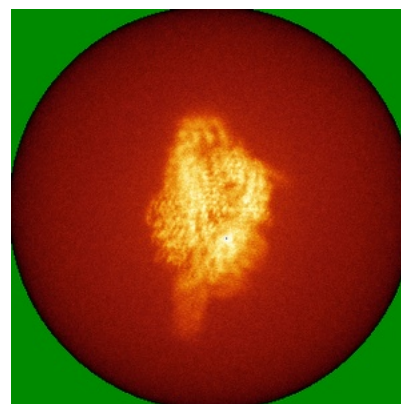
6.4.2 Raw map



X



Y

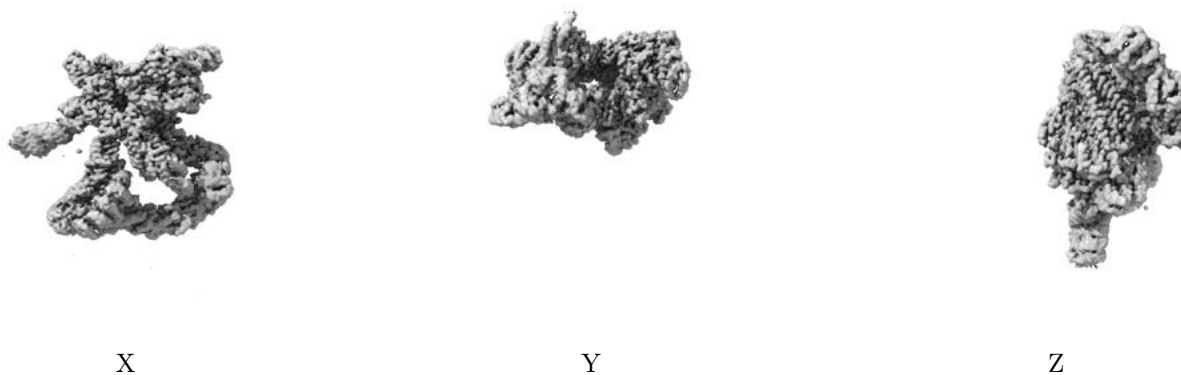


Z

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.

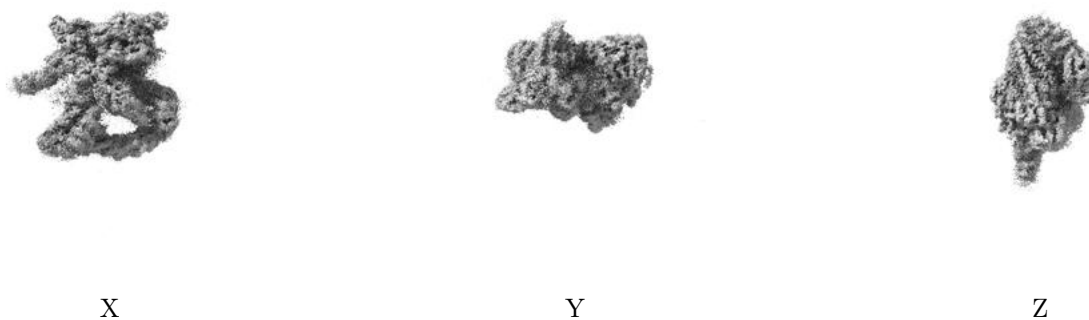
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00984. 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.

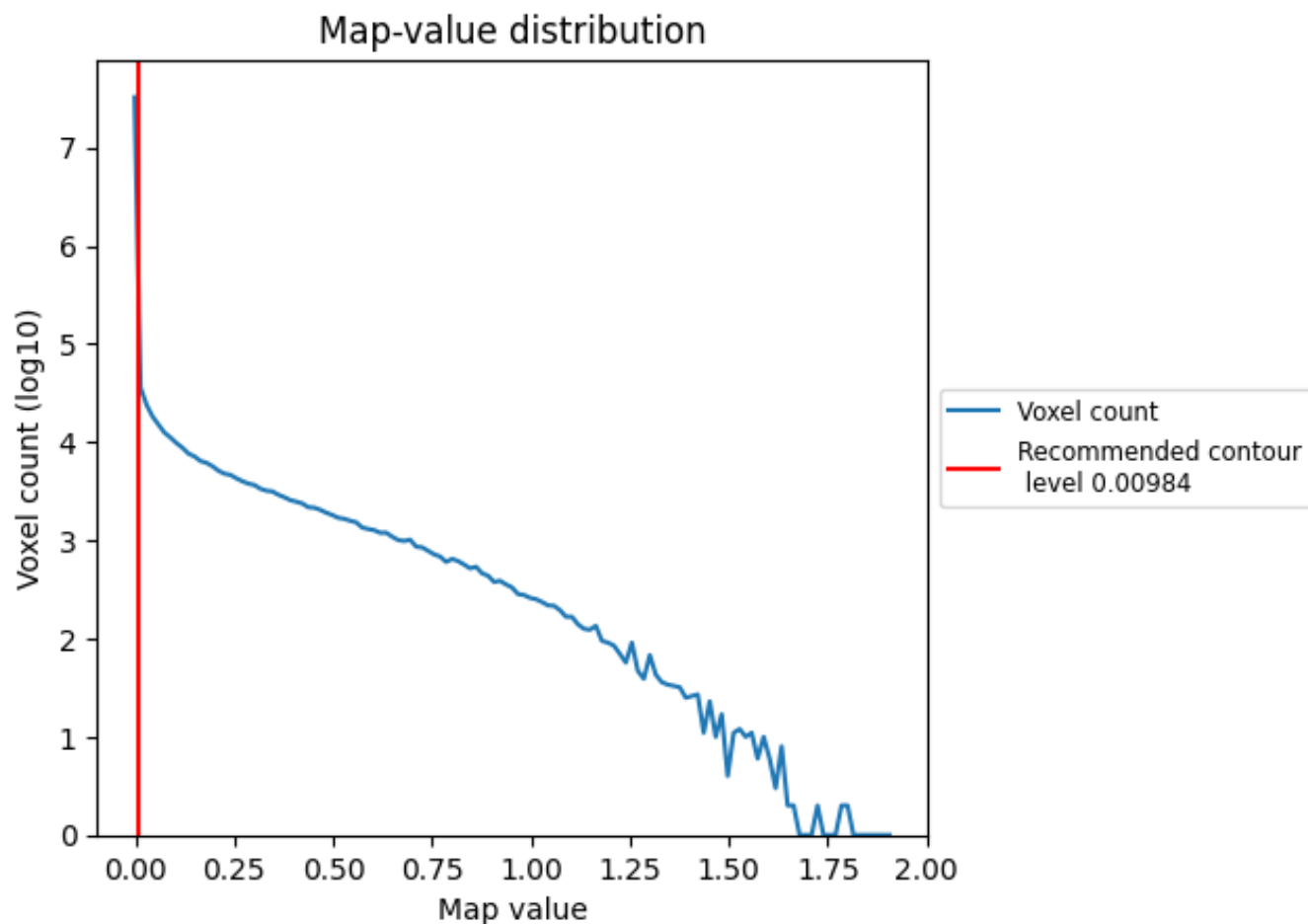
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

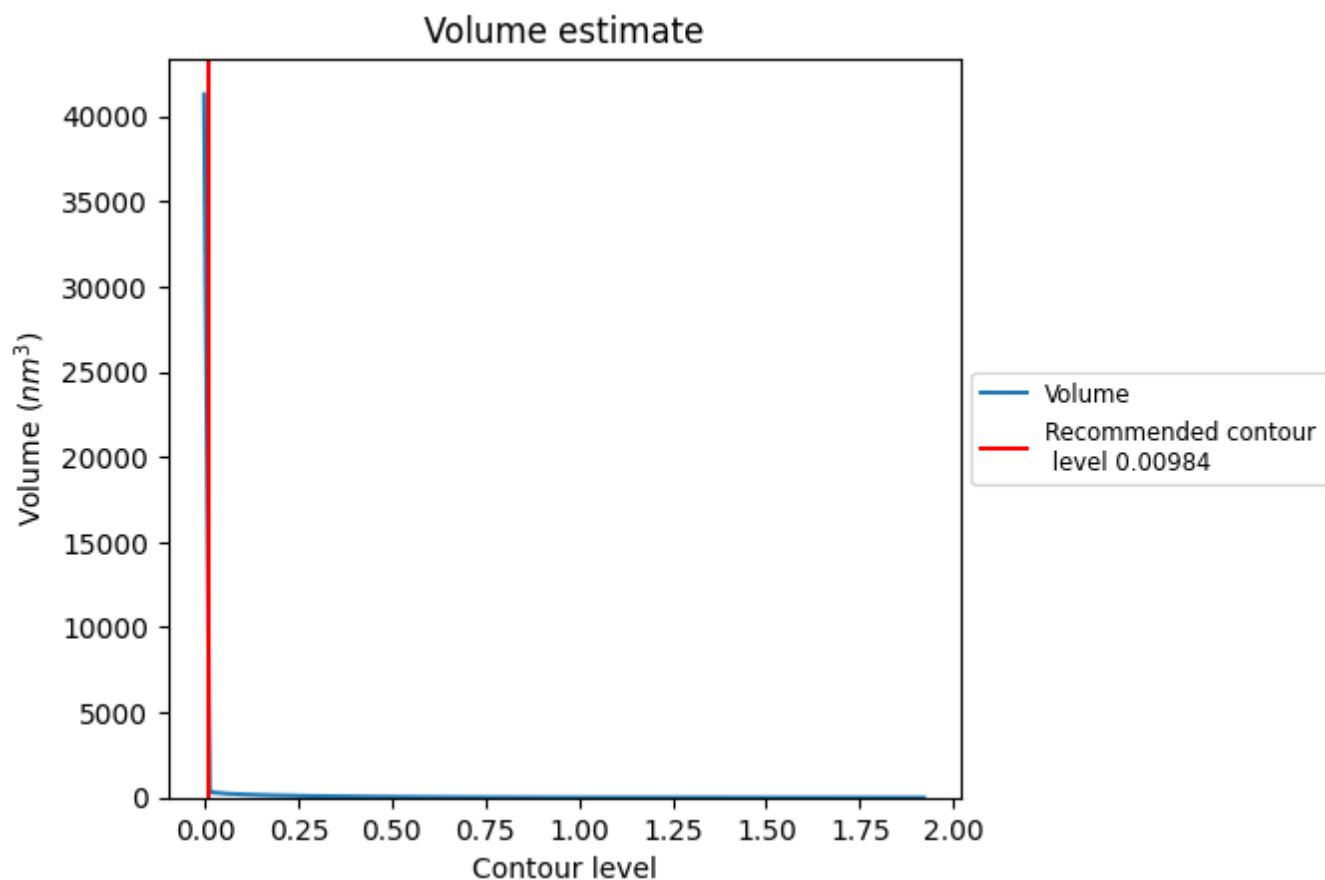
This section contains the results of statistical analysis of the map.

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.

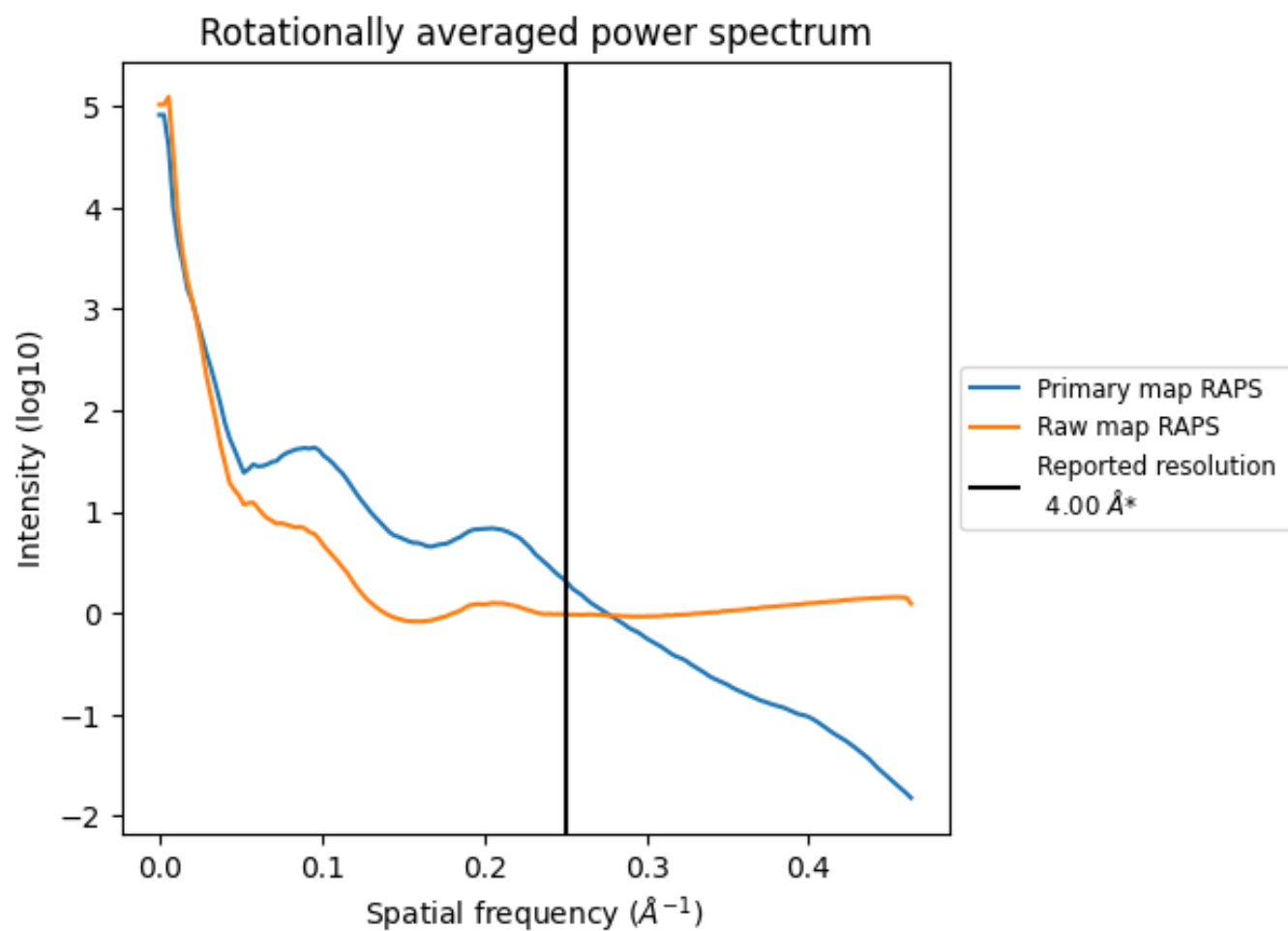
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9745 nm³; this corresponds to an approximate mass of 8803 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 ⓘ

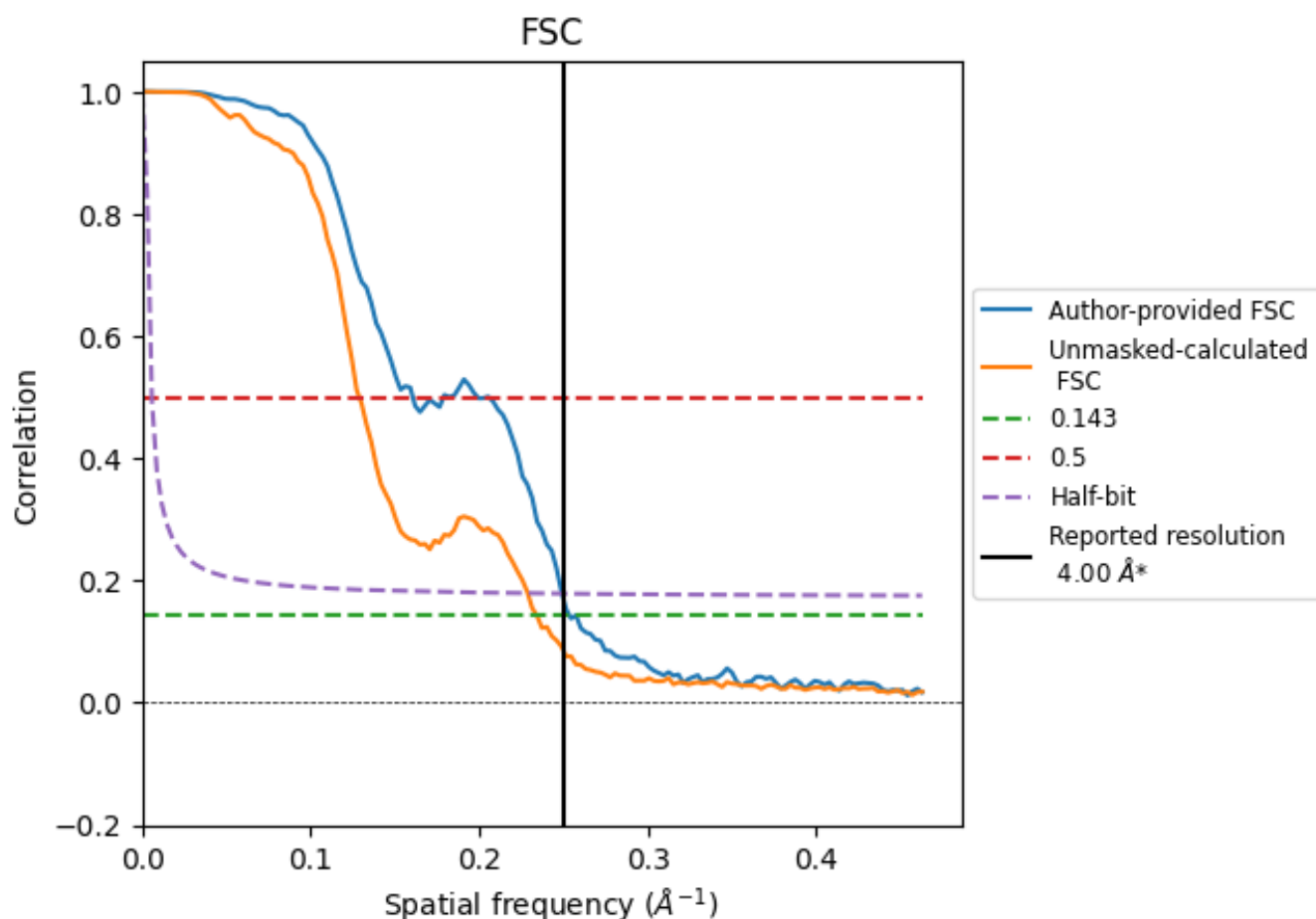


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

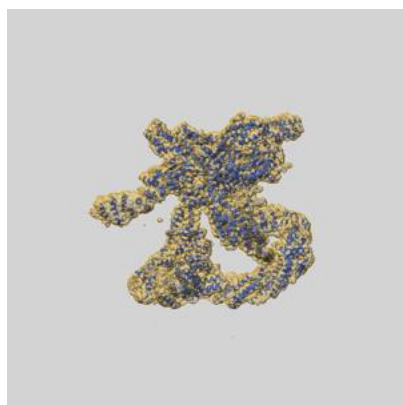
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.94	6.22	4.01
Unmasked-calculated*	4.27	7.76	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

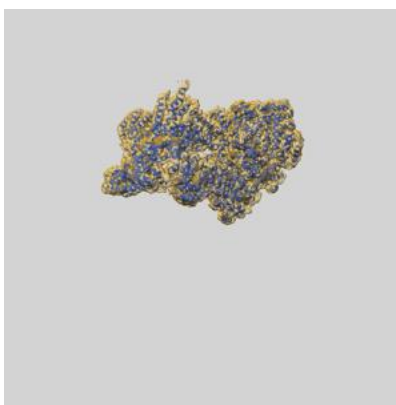
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53257 and PDB model 9QO5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

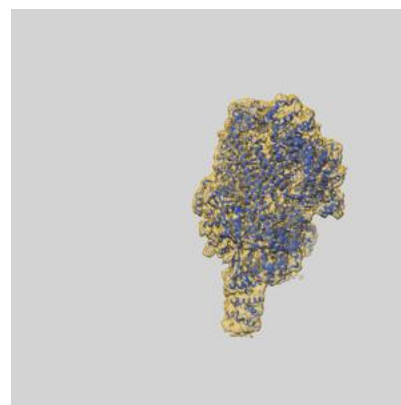
9.1 Map-model overlay [i](#)



X



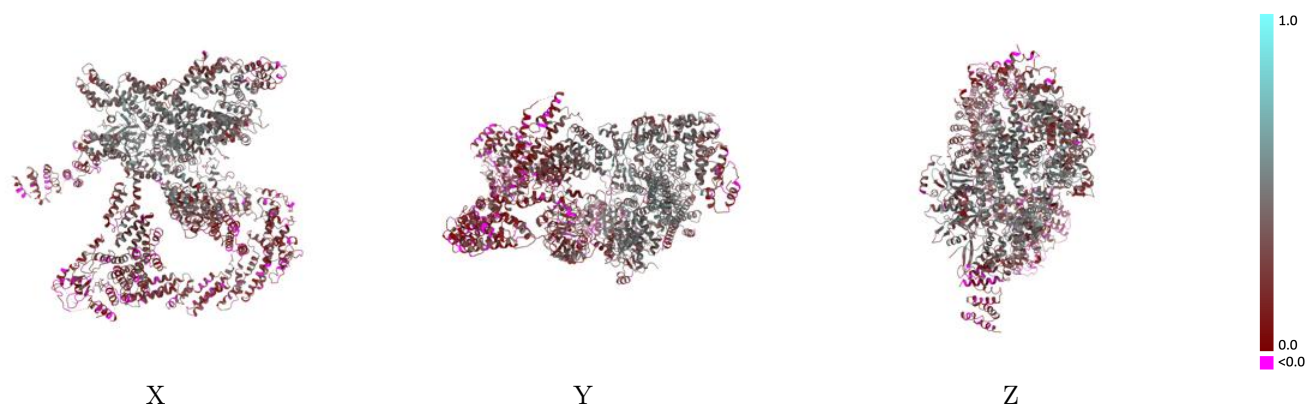
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00984 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

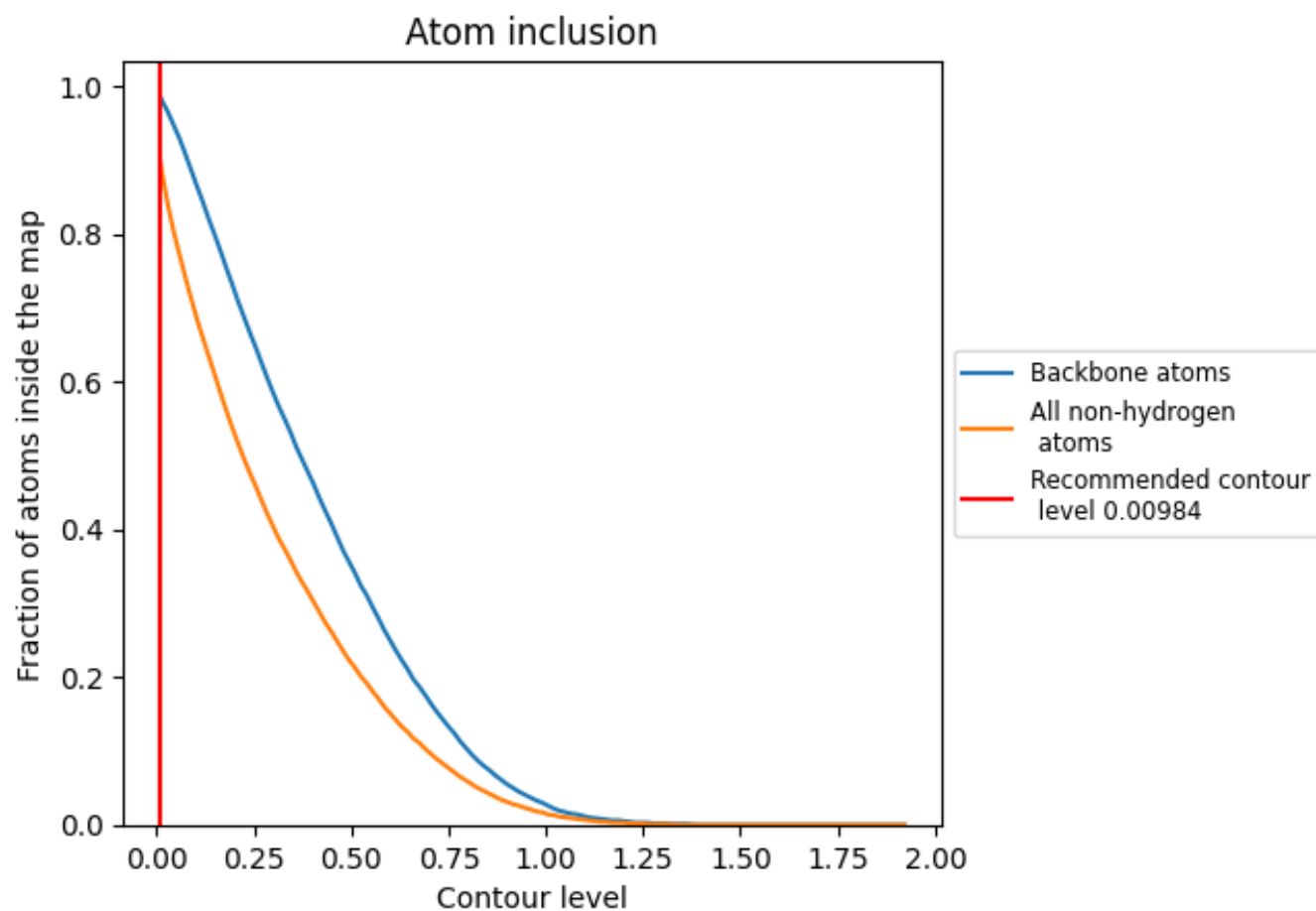


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 90% 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 (0.00984) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.3020
A	 0.9040	 0.3160
B	 0.8680	 0.2530
C	 0.9330	 0.3870
D	 0.9010	 0.2710
E	 0.9090	 0.3860
F	 0.9450	 0.4250
G	 0.9240	 0.3890
H	 0.9130	 0.3660
I	 0.8670	 0.1790
J	 0.7300	 0.0340
L	 0.8240	 0.1550
M	 0.8880	 0.2860
N	 0.8950	 0.3790
P	 0.8650	 0.3470

