



## Full wwPDB EM Validation Report ⓘ

Nov 18, 2025 – 10:31 AM JST

PDB ID : 9LXH / pdb\_00009lhx  
EMDB ID : EMD-63477  
Title : DOCK5/ELMO1 complex with RhoG and Rac1 on lipid membrane  
Authors : Shinoda, T.; Katsura, K.; Kukimoto-Niino, M.; Shirouzu, M.  
Deposited on : 2025-02-18  
Resolution : 7.52 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

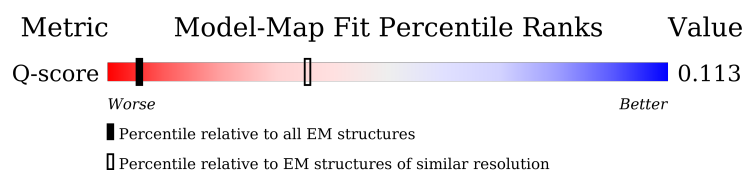
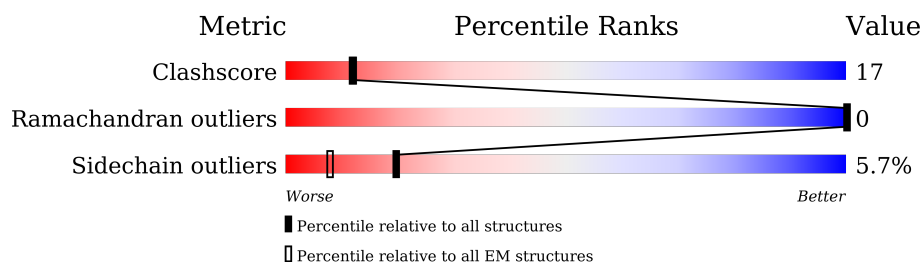
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.52 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	377 ( 7.02 - 8.01 )

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  $\geq 3$ , 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	733	<div> <div>75%</div> <div>72%</div> <div>26%</div> <div>..</div> </div>
2	B	1876	<div> <div>18%</div> <div>35%</div> <div>29%</div> <div>33%</div> </div>
3	C	214	<div> <div>69%</div> <div>63%</div> <div>21%</div> <div>15%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17437 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 Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	727	5814	3686	995	1093	40	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q92556
A	-4	GLY	-	expression tag	UNP Q92556
A	-3	SER	-	expression tag	UNP Q92556
A	-2	VAL	-	expression tag	UNP Q92556
A	-1	GLY	-	expression tag	UNP Q92556
A	0	SER	-	expression tag	UNP Q92556

- Molecule 2 is a protein called Deducator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1254	10207	6536	1733	1882	56	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9H7D0
B	-4	GLY	-	expression tag	UNP Q9H7D0
B	-3	SER	-	expression tag	UNP Q9H7D0
B	-2	GLY	-	expression tag	UNP Q9H7D0
B	-1	GLY	-	expression tag	UNP Q9H7D0
B	0	SER	-	expression tag	UNP Q9H7D0
B	1285	ARG	LYS	variant	UNP Q9H7D0

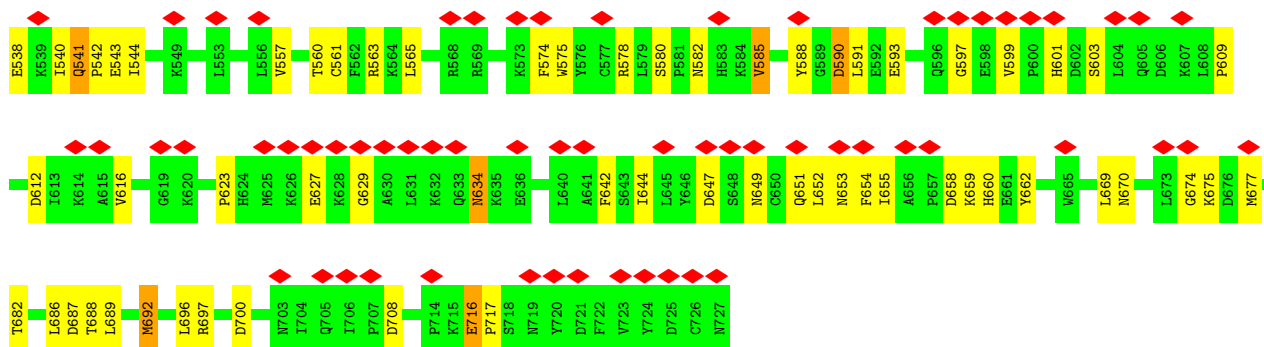
- Molecule 3 is a protein called Rho-related GTP-binding protein RhoG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	181	Total	C	N	O	S	0	0
			1416	897	248	263	8		

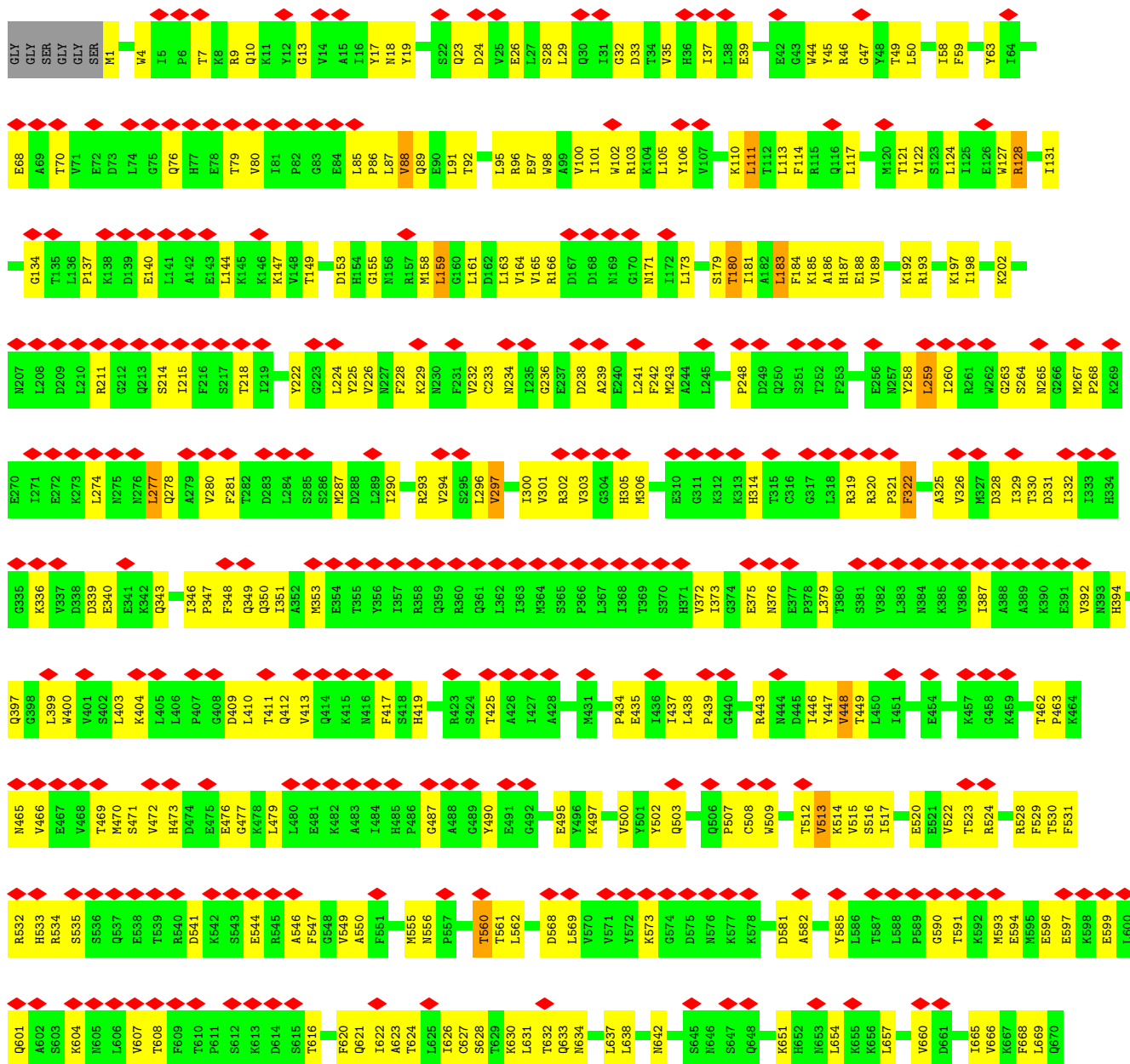
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP P84095
C	-5	SER	-	expression tag	UNP P84095
C	-4	SER	-	expression tag	UNP P84095
C	-3	GLY	-	expression tag	UNP P84095
C	-2	SER	-	expression tag	UNP P84095
C	-1	SER	-	expression tag	UNP P84095
C	0	GLY	-	expression tag	UNP P84095
C	61	LEU	GLN	engineered mutation	UNP P84095
C	192	SER	-	expression tag	UNP P84095
C	193	GLY	-	expression tag	UNP P84095
C	194	PRO	-	expression tag	UNP P84095
C	195	SER	-	expression tag	UNP P84095
C	196	SER	-	expression tag	UNP P84095
C	197	GLY	-	expression tag	UNP P84095
C	198	HIS	-	expression tag	UNP P84095
C	199	HIS	-	expression tag	UNP P84095
C	200	HIS	-	expression tag	UNP P84095
C	201	HIS	-	expression tag	UNP P84095
C	202	HIS	-	expression tag	UNP P84095
C	203	HIS	-	expression tag	UNP P84095
C	204	HIS	-	expression tag	UNP P84095
C	205	HIS	-	expression tag	UNP P84095
C	206	HIS	-	expression tag	UNP P84095
C	207	HIS	-	expression tag	UNP P84095



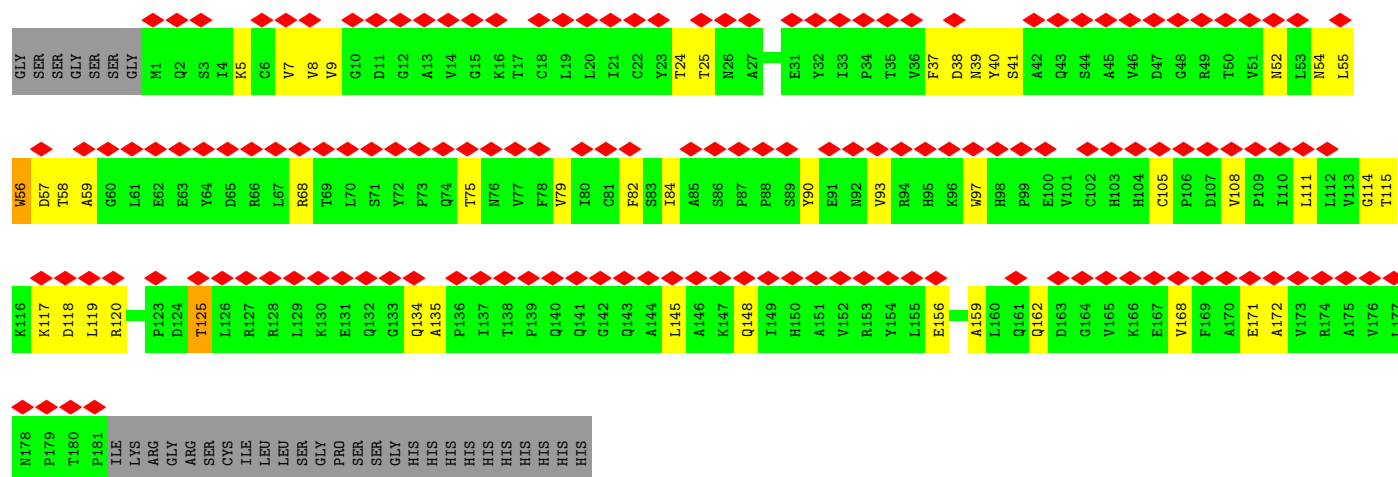


• Molecule 2: Dedicator of cytokinesis protein 5





- Molecule 3: Rho-related GTP-binding protein RhoG





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55365	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.181	Depositor
Minimum map value	-3.568	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	478.80002, 478.80002, 478.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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	0.11	0/5926	0.27	0/8005
2	B	0.14	0/10408	0.40	6/14037 (0.0%)
3	C	0.11	0/1449	0.27	0/1977
All	All	0.13	0/17783	0.35	6/24019 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1168	TYR	CA-C-N	-8.02	110.06	120.65
2	B	1168	TYR	C-N-CA	-8.02	110.06	120.65
2	B	673	LEU	CA-C-N	-7.45	110.82	120.65
2	B	673	LEU	C-N-CA	-7.45	110.82	120.65
2	B	1155	LEU	O-C-N	6.49	129.82	122.22
2	B	1169	LYS	N-CA-C	-5.34	105.15	110.97

There are no chirality outliers.

There are no planarity outliers.

### 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	5814	0	5799	135	0
2	B	10207	0	10318	448	0
3	C	1416	0	1414	36	0
All	All	17437	0	17531	598	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 17.

All (598) 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:871:GLN:HG3	2:B:918:VAL:HG13	1.62	0.81
2:B:868:LEU:HD13	2:B:878:LEU:HD23	1.64	0.80
2:B:1110:LEU:HD21	2:B:1158:GLU:HB2	1.65	0.77
2:B:1081:LYS:HA	2:B:1120:LEU:HD22	1.66	0.77
3:C:119:LEU:HB3	3:C:125:THR:HG21	1.67	0.77
2:B:757:LEU:HA	2:B:760:LEU:HG	1.68	0.75
2:B:1169:LYS:HD3	2:B:1201:LEU:HB3	1.68	0.75
2:B:1152:ILE:HD11	2:B:1197:VAL:HG22	1.67	0.75
3:C:8:VAL:HG22	3:C:79:VAL:HB	1.68	0.75
2:B:1238:ASP:OD1	2:B:1238:ASP:N	2.20	0.75
1:A:306:GLU:HA	1:A:309:MET:HG2	1.68	0.74
2:B:128:ARG:O	2:B:128:ARG:NH1	2.21	0.74
1:A:580:SER:HB2	1:A:585:VAL:HG12	1.70	0.72
2:B:4:TRP:HB3	2:B:39:GLU:HB3	1.73	0.71
1:A:52:GLN:HA	1:A:60:TYR:HA	1.72	0.71
2:B:166:ARG:HG2	2:B:173:LEU:HB2	1.73	0.71
1:A:340:ASN:ND2	1:A:351:MET:SD	2.64	0.71
2:B:1193:PHE:HA	2:B:1196:LEU:HD12	1.72	0.70
2:B:1057:GLU:O	2:B:1080:ARG:NH1	2.24	0.70
2:B:1183:HIS:HE1	2:B:1186:LEU:HB2	1.55	0.70
2:B:343:GLN:HB3	2:B:400:TRP:HB3	1.73	0.69
2:B:860:MET:HE3	2:B:864:VAL:HG12	1.72	0.69
2:B:940:VAL:O	2:B:944:ASN:ND2	2.26	0.69
1:A:717:PRO:O	2:B:1:MET:N	2.26	0.69
2:B:1176:LEU:HD22	2:B:1194:ALA:HB1	1.75	0.68
2:B:91:LEU:HD11	2:B:124:LEU:HD11	1.74	0.68
2:B:889:GLN:HE22	2:B:898:ASP:HB3	1.58	0.68
2:B:471:SER:HG	2:B:473:HIS:HE2	1.39	0.68
2:B:258:TYR:HE1	2:B:490:TYR:HB2	1.58	0.68
3:C:39:ASN:ND2	3:C:55:LEU:O	2.27	0.67
2:B:471:SER:HB2	2:B:479:LEU:HD13	1.76	0.67
2:B:569:LEU:HB2	2:B:620:PHE:HB3	1.77	0.67
2:B:734:SER:O	2:B:738:ASN:ND2	2.25	0.67
2:B:671:ASP:N	2:B:671:ASP:OD1	2.26	0.67
2:B:681:MET:HE1	2:B:728:LEU:H	1.58	0.67
2:B:1169:LYS:HZ2	2:B:1201:LEU:HG	1.60	0.66
1:A:537:LYS:O	1:A:541:GLN:NE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:LEU:HA	2:B:909:ILE:HG12	1.77	0.66
2:B:376:ASN:ND2	2:B:502:TYR:O	2.29	0.66
2:B:1028:LEU:HA	2:B:1032:PHE:HD2	1.61	0.66
2:B:590:GLY:N	2:B:594:GLU:OE2	2.27	0.66
2:B:1059:LEU:HD12	2:B:1116:PRO:HB2	1.77	0.66
2:B:233:CYS:SG	2:B:234:ASN:N	2.68	0.65
2:B:879:LEU:HA	2:B:882:LEU:HD12	1.78	0.65
1:A:563:ARG:HB2	1:A:655:ILE:HB	1.79	0.65
2:B:158:MET:HG3	2:B:159:LEU:HD22	1.79	0.65
1:A:202:LEU:HD12	1:A:246:VAL:HG21	1.78	0.65
2:B:448:VAL:HG23	2:B:513:VAL:HG23	1.78	0.65
2:B:560:THR:HG23	2:B:638:LEU:HD23	1.79	0.64
2:B:300:ILE:HB	2:B:302:ARG:HH22	1.62	0.64
2:B:439:PRO:HD3	2:B:711:HIS:HB3	1.78	0.64
2:B:1183:HIS:CG	2:B:1184:LYS:H	2.15	0.64
2:B:1030:ARG:O	2:B:1030:ARG:NH1	2.30	0.64
2:B:1133:GLN:O	2:B:1137:ASN:ND2	2.31	0.64
3:C:93:VAL:HA	3:C:97:TRP:HD1	1.62	0.64
2:B:1081:LYS:HE3	2:B:1117:GLU:HG2	1.80	0.63
2:B:886:LEU:HD13	2:B:935:ARG:HE	1.64	0.63
2:B:469:THR:O	2:B:528:ARG:NH1	2.32	0.63
1:A:294:LEU:HD22	1:A:441:PHE:HB2	1.81	0.63
2:B:265:ASN:HB2	2:B:267:MET:HE1	1.80	0.63
2:B:449:THR:HB	2:B:623:ALA:HB3	1.81	0.63
1:A:532:PRO:HD2	1:A:533:ILE:HD12	1.81	0.63
1:A:533:ILE:HA	1:A:536:LEU:HD22	1.81	0.63
2:B:471:SER:OG	2:B:473:HIS:NE2	2.32	0.62
1:A:543:GLU:OE1	2:B:103:ARG:NH2	2.30	0.62
2:B:1148:GLU:OE1	2:B:1148:GLU:N	2.25	0.62
2:B:929:MET:HE2	2:B:968:HIS:HB3	1.80	0.62
2:B:1224:THR:HB	2:B:1247:LEU:HD21	1.81	0.62
2:B:340:GLU:HA	2:B:404:LYS:HE3	1.82	0.62
2:B:379:LEU:H	2:B:508:CYS:HB2	1.64	0.62
2:B:294:VAL:H	2:B:330:THR:HG22	1.64	0.62
2:B:350:GLN:HE22	2:B:353:MET:HG3	1.63	0.62
1:A:575:TRP:HZ3	1:A:588:TYR:HB2	1.65	0.62
2:B:463:PRO:HD2	2:B:503:GLN:HB3	1.82	0.62
2:B:761:LYS:NZ	2:B:822:SER:O	2.31	0.61
1:A:18:TYR:HE2	3:C:7:VAL:HG23	1.65	0.61
1:A:280:ILE:HD11	1:A:446:PHE:HB2	1.81	0.61
2:B:651:LYS:NZ	2:B:688:THR:OG1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:ASN:HB3	2:B:534:ARG:H	1.66	0.61
1:A:450:ARG:HG2	1:A:453:GLU:HB2	1.82	0.61
2:B:373:ILE:HG23	2:B:376:ASN:HB2	1.83	0.61
2:B:1226:ASN:O	2:B:1229:ASN:ND2	2.31	0.61
2:B:654:LEU:HA	2:B:657:LEU:HD12	1.82	0.60
2:B:887:SER:HB3	2:B:931:ARG:HH12	1.66	0.60
3:C:59:ALA:H	3:C:68:ARG:HD2	1.66	0.60
2:B:573:LYS:HD2	2:B:616:THR:HG21	1.84	0.60
2:B:1065:SER:OG	2:B:1068:LYS:NZ	2.33	0.60
3:C:82:PHE:O	3:C:115:THR:N	2.26	0.60
2:B:306:MET:HG2	2:B:314:HIS:HB3	1.83	0.60
2:B:102:TRP:HA	2:B:105:LEU:HB2	1.83	0.60
2:B:935:ARG:HG2	2:B:936:ILE:N	2.15	0.60
2:B:1110:LEU:HD22	2:B:1154:LYS:HG3	1.83	0.60
1:A:536:LEU:HD11	2:B:17:TYR:HB2	1.84	0.60
1:A:13:GLU:N	1:A:75:LEU:O	2.23	0.59
2:B:225:TYR:HE1	2:B:278:GLN:HA	1.67	0.59
2:B:329:ILE:HG22	2:B:332:ILE:HD12	1.83	0.59
2:B:905:LEU:O	2:B:909:ILE:HG23	2.02	0.59
2:B:302:ARG:HH11	2:B:322:PHE:HB2	1.67	0.59
1:A:565:LEU:HD11	1:A:653:ASN:HB2	1.85	0.59
2:B:533:HIS:HB3	2:B:544:GLU:HG2	1.85	0.59
2:B:607:VAL:HG12	2:B:608:THR:HG23	1.85	0.59
3:C:52:ASN:ND2	3:C:54:ASN:OD1	2.35	0.59
1:A:461:GLN:OE1	1:A:503:LYS:NZ	2.33	0.59
1:A:670:ASN:CG	1:A:675:LYS:HB2	2.27	0.59
2:B:677:PHE:HA	2:B:680:MET:HE2	1.85	0.59
2:B:732:LYS:HD3	2:B:733:LEU:HD12	1.85	0.59
2:B:263:GLY:N	2:B:267:MET:O	2.26	0.58
2:B:9:ARG:HB3	2:B:68:GLU:HG3	1.86	0.58
2:B:760:LEU:HD23	2:B:763:LEU:HD21	1.85	0.58
2:B:1183:HIS:CE1	2:B:1186:LEU:HB2	2.37	0.58
2:B:1223:CYS:O	2:B:1227:VAL:HG13	2.04	0.58
1:A:336:SER:HB3	1:A:340:ASN:HD21	1.68	0.58
2:B:909:ILE:HG13	2:B:910:LEU:N	2.16	0.58
3:C:38:ASP:H	3:C:57:ASP:HB3	1.69	0.58
1:A:80:SER:OG	1:A:83:GLN:OE1	2.22	0.58
1:A:682:THR:O	1:A:686:LEU:N	2.35	0.58
2:B:529:PHE:HB2	2:B:550:ALA:HB3	1.85	0.58
2:B:1169:LYS:HA	2:B:1172:LEU:HD12	1.85	0.57
2:B:79:THR:HG22	2:B:85:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:666:VAL:HA	2:B:669:LEU:HD23	1.86	0.57
2:B:730:TYR:HB3	2:B:770:SER:HB3	1.87	0.57
2:B:886:LEU:HD22	2:B:935:ARG:HH21	1.70	0.57
2:B:795:PHE:O	2:B:799:ASN:ND2	2.34	0.57
2:B:1121:ARG:HH21	2:B:1125:ILE:HD13	1.69	0.57
2:B:950:ILE:HA	2:B:953:PHE:CD2	2.40	0.57
2:B:1071:LYS:O	2:B:1075:LYS:HG2	2.05	0.57
1:A:644:ILE:HB	1:A:652:LEU:HB2	1.87	0.57
2:B:211:ARG:NH2	2:B:336:LYS:O	2.37	0.57
3:C:84:ILE:HD12	3:C:117:LYS:HB2	1.86	0.57
2:B:528:ARG:NH1	2:B:530:THR:OG1	2.38	0.56
2:B:23:GLN:HB2	2:B:26:GLU:HB2	1.87	0.56
2:B:473:HIS:HB3	2:B:477:GLY:HA2	1.87	0.56
2:B:890:LEU:HD21	2:B:935:ARG:HG3	1.86	0.56
1:A:289:GLU:OE2	1:A:293:GLN:NE2	2.39	0.56
2:B:532:ARG:HA	2:B:546:ALA:HA	1.87	0.56
2:B:680:MET:SD	2:B:732:LYS:NZ	2.76	0.56
1:A:274:ILE:HA	1:A:277:THR:HG22	1.88	0.56
2:B:18:ASN:ND2	2:B:29:LEU:O	2.38	0.56
2:B:826:ASP:HA	2:B:829:LEU:HD13	1.87	0.56
1:A:537:LYS:NZ	1:A:538:GLU:OE1	2.36	0.56
2:B:621:GLN:NE2	2:B:622:ILE:O	2.39	0.56
2:B:1169:LYS:NZ	2:B:1201:LEU:HG	2.21	0.55
2:B:828:LYS:HE2	2:B:833:PRO:HG3	1.86	0.55
2:B:960:LEU:HG	2:B:964:MET:HE2	1.87	0.55
2:B:745:ASP:OD1	2:B:745:ASP:N	2.39	0.55
3:C:117:LYS:HG3	3:C:120:ARG:HH21	1.71	0.55
1:A:306:GLU:O	1:A:310:MET:N	2.36	0.55
2:B:871:GLN:NE2	2:B:918:VAL:O	2.39	0.55
2:B:1117:GLU:OE2	2:B:1121:ARG:N	2.38	0.55
1:A:26:GLN:OE1	1:A:66:ARG:NH2	2.28	0.55
2:B:720:ILE:HG23	2:B:769:GLN:HG3	1.87	0.55
2:B:466:VAL:HG22	2:B:547:PHE:HZ	1.72	0.55
2:B:654:LEU:HB3	2:B:692:LEU:HB3	1.89	0.55
3:C:159:ALA:O	3:C:162:GLN:NE2	2.40	0.55
2:B:1085:PHE:O	2:B:1088:ARG:HG3	2.07	0.54
2:B:1169:LYS:O	2:B:1172:LEU:N	2.40	0.54
1:A:363:ASN:ND2	1:A:366:ASN:O	2.41	0.54
2:B:517:ILE:HD12	2:B:522:VAL:HG23	1.89	0.54
2:B:929:MET:HE1	2:B:972:TYR:HB3	1.88	0.54
2:B:1078:ASP:OD2	2:B:1080:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ILE:HG23	1:A:515:LEU:HD22	1.89	0.54
2:B:630:LYS:HA	2:B:668:PHE:HZ	1.72	0.54
2:B:1091:TRP:HA	2:B:1094:LEU:HD12	1.89	0.54
2:B:674:ASP:O	2:B:677:PHE:N	2.40	0.54
2:B:910:LEU:HD23	2:B:913:LEU:HD12	1.89	0.54
2:B:1044:ASN:OD1	2:B:1044:ASN:N	2.39	0.54
1:A:351:MET:HA	1:A:354:ARG:HG2	1.90	0.54
1:A:627:GLU:HG3	1:A:629:GLY:H	1.72	0.54
2:B:1114:LEU:O	2:B:1163:ARG:NH2	2.40	0.54
2:B:535:SER:H	2:B:541:ASP:HA	1.72	0.54
2:B:198:ILE:HG13	2:B:202:LYS:HE3	1.89	0.53
1:A:14:TRP:HB2	1:A:17:ALA:HB3	1.91	0.53
1:A:411:CYS:SG	1:A:416:SER:OG	2.63	0.53
2:B:239:ALA:HB1	2:B:302:ARG:HH21	1.73	0.53
2:B:449:THR:HA	2:B:512:THR:HA	1.90	0.53
2:B:1147:PHE:CZ	2:B:1151:LEU:HD22	2.43	0.53
1:A:491:ALA:HB1	1:A:502:PHE:HE1	1.73	0.53
2:B:24:ASP:OD1	2:B:24:ASP:N	2.35	0.53
3:C:5:LYS:HA	3:C:54:ASN:HD22	1.73	0.53
2:B:319:ARG:HH21	2:B:497:LYS:HB2	1.74	0.53
1:A:529:GLN:HA	1:A:534:LEU:HD13	1.90	0.53
2:B:660:VAL:HB	2:B:665:ILE:HD11	1.90	0.53
2:B:1028:LEU:HA	2:B:1032:PHE:CD2	2.43	0.53
2:B:1119:GLU:HA	2:B:1122:LYS:HD3	1.89	0.53
1:A:320:GLN:OE1	1:A:321:ARG:NH1	2.42	0.53
1:A:289:GLU:O	1:A:293:GLN:HG2	2.09	0.53
1:A:527:ASP:HA	1:A:537:LYS:HE2	1.91	0.53
2:B:466:VAL:HG13	2:B:531:PHE:HB3	1.91	0.53
2:B:958:ILE:HB	2:B:1016:VAL:HG21	1.91	0.53
2:B:1098:LYS:HA	2:B:1101:PHE:CD2	2.44	0.53
2:B:1128:PHE:HA	2:B:1131:MET:HG3	1.91	0.53
2:B:349:GLN:HB2	2:B:392:VAL:HG11	1.91	0.52
1:A:407:ASP:O	1:A:409:HIS:ND1	2.42	0.52
2:B:928:ILE:HG23	2:B:932:LEU:HD13	1.92	0.52
2:B:959:ALA:HA	2:B:962:GLN:HE21	1.75	0.52
2:B:446:ILE:O	2:B:515:VAL:N	2.38	0.52
1:A:670:ASN:O	1:A:674:GLY:N	2.42	0.52
2:B:215:ILE:O	2:B:218:THR:OG1	2.24	0.52
1:A:687:ASP:OD1	1:A:688:THR:N	2.42	0.52
2:B:320:ARG:HD3	2:B:500:VAL:HB	1.91	0.52
2:B:934:ARG:HD2	2:B:938:ARG:HH12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1062:GLU:HG3	2:B:1069:ARG:HG3	1.92	0.52
2:B:166:ARG:O	2:B:171:ASN:HA	2.10	0.52
2:B:268:PRO:HG2	2:B:274:LEU:HB2	1.91	0.52
2:B:1184:LYS:O	2:B:1187:SER:OG	2.22	0.52
1:A:623:PRO:HG2	1:A:651:GLN:HG2	1.91	0.51
2:B:882:LEU:HD23	2:B:885:GLN:NE2	2.24	0.51
2:B:925:ILE:HA	2:B:928:ILE:HD12	1.92	0.51
2:B:471:SER:OG	2:B:528:ARG:NE	2.38	0.51
2:B:568:ASP:HA	2:B:621:GLN:HA	1.91	0.51
2:B:155:GLY:HA2	2:B:158:MET:HG2	1.92	0.51
2:B:1175:LEU:O	2:B:1179:HIS:ND1	2.44	0.51
1:A:560:THR:OG1	1:A:561:CYS:N	2.43	0.51
2:B:59:PHE:CE2	2:B:63:TYR:HB3	2.45	0.51
2:B:926:GLN:HG3	2:B:929:MET:HE3	1.92	0.51
1:A:279:VAL:HG21	1:A:290:MET:HE3	1.91	0.51
2:B:1156:ASP:OD2	2:B:1157:GLN:NE2	2.44	0.51
2:B:745:ASP:OD1	2:B:804:ARG:NH1	2.36	0.51
2:B:853:VAL:O	2:B:856:LYS:HG3	2.10	0.51
2:B:410:LEU:HA	2:B:413:VAL:HG22	1.92	0.51
2:B:242:PHE:HE2	2:B:301:VAL:HB	1.74	0.51
2:B:909:ILE:O	2:B:912:VAL:HG22	2.11	0.51
2:B:917:ASP:OD1	2:B:917:ASP:N	2.37	0.51
2:B:297:VAL:HA	2:B:326:VAL:HG22	1.92	0.51
3:C:40:TYR:O	3:C:55:LEU:N	2.43	0.51
1:A:540:ILE:HD11	2:B:28:SER:HB2	1.93	0.51
2:B:556:ASN:N	2:B:560:THR:O	2.44	0.51
3:C:134:GLN:NE2	3:C:135:ALA:O	2.44	0.51
2:B:322:PHE:O	2:B:350:GLN:HB2	2.12	0.50
2:B:844:ILE:HA	2:B:847:ILE:HG12	1.92	0.50
2:B:37:ILE:HA	2:B:47:GLY:HA3	1.92	0.50
2:B:111:LEU:H	2:B:111:LEU:HD23	1.76	0.50
2:B:411:THR:OG1	2:B:412:GLN:OE1	2.25	0.50
2:B:581:ASP:OD1	2:B:581:ASP:N	2.44	0.50
3:C:24:THR:HG23	3:C:25:THR:HG23	1.91	0.50
1:A:216:TYR:HE2	1:A:258:ARG:HH22	1.59	0.50
2:B:520:GLU:O	2:B:524:ARG:NH1	2.44	0.50
2:B:601:GLN:HA	2:B:604:LYS:HG2	1.93	0.50
2:B:638:LEU:O	2:B:642:ASN:N	2.38	0.50
2:B:730:TYR:HB2	2:B:767:ILE:HG23	1.93	0.50
2:B:908:ASN:ND2	2:B:911:GLU:OE2	2.41	0.50
2:B:37:ILE:HD13	2:B:45:TYR:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:O	1:A:118:GLN:HG2	2.12	0.50
1:A:374:THR:HG22	1:A:377:GLY:HA3	1.92	0.50
1:A:582:ASN:OD1	2:B:1213:GLN:NE2	2.44	0.50
2:B:180:THR:HA	2:B:183:LEU:HB2	1.93	0.50
2:B:822:SER:O	2:B:825:ASN:ND2	2.45	0.50
2:B:412:GLN:OE1	2:B:412:GLN:N	2.44	0.50
2:B:305:HIS:HB3	2:B:314:HIS:HB2	1.94	0.49
2:B:228:PHE:HB3	2:B:277:LEU:HD13	1.92	0.49
2:B:446:ILE:HB	2:B:515:VAL:HB	1.93	0.49
2:B:45:TYR:O	2:B:59:PHE:N	2.38	0.49
2:B:46:ARG:HB3	2:B:58:ILE:HG13	1.95	0.49
2:B:89:GLN:O	2:B:92:THR:OG1	2.25	0.49
2:B:110:LYS:O	2:B:114:PHE:N	2.31	0.49
2:B:707:ILE:C	2:B:710:GLN:HE22	2.21	0.49
3:C:111:LEU:HD13	3:C:172:ALA:HB2	1.94	0.49
2:B:961:LEU:O	2:B:969:TYR:OH	2.25	0.49
2:B:534:ARG:NE	2:B:541:ASP:OD1	2.39	0.49
2:B:934:ARG:NH1	2:B:938:ARG:HH22	2.10	0.49
1:A:378:MET:SD	1:A:378:MET:N	2.85	0.49
2:B:1169:LYS:O	2:B:1170:VAL:C	2.56	0.49
2:B:1199:SER:O	2:B:1202:GLU:HG2	2.12	0.49
1:A:184:ILE:HG13	1:A:204:ILE:HG21	1.95	0.49
1:A:536:LEU:HD21	2:B:17:TYR:HB2	1.95	0.49
2:B:140:GLU:N	2:B:140:GLU:OE1	2.45	0.49
1:A:203:ALA:O	1:A:206:GLU:HG3	2.13	0.49
1:A:248:ASN:HD21	1:A:297:LEU:HG	1.77	0.49
2:B:7:THR:HG22	2:B:9:ARG:H	1.78	0.49
2:B:957:MET:HE2	2:B:957:MET:HB3	1.78	0.49
2:B:1047:PHE:HZ	2:B:1090:MET:HG2	1.77	0.49
1:A:541:GLN:N	1:A:542:PRO:HD3	2.28	0.48
2:B:287:MET:HE2	2:B:435:GLU:HB2	1.95	0.48
2:B:514:LYS:NZ	2:B:516:SER:OG	2.34	0.48
2:B:706:ASP:HB2	2:B:709:PHE:CD2	2.48	0.48
1:A:266:LEU:HD22	1:A:271:LEU:HD22	1.95	0.48
1:A:291:ALA:HA	1:A:441:PHE:HB3	1.93	0.48
2:B:1183:HIS:CG	2:B:1184:LYS:N	2.81	0.48
2:B:582:ALA:HA	2:B:585:TYR:CZ	2.48	0.48
2:B:961:LEU:HD13	2:B:964:MET:HE3	1.94	0.48
2:B:1087:ILE:O	2:B:1091:TRP:HD1	1.97	0.48
2:B:1188:SER:O	2:B:1191:GLU:HG3	2.12	0.48
2:B:1169:LYS:O	2:B:1172:LEU:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PHE:O	1:A:259:ARG:NH2	2.47	0.48
1:A:272:ARG:NH1	1:A:273:SER:OG	2.46	0.48
1:A:582:ASN:ND2	2:B:1214:ASP:HB2	2.29	0.48
2:B:720:ILE:HA	2:B:724:PHE:HB2	1.95	0.48
2:B:872:SER:OG	2:B:873:GLU:OE1	2.28	0.48
2:B:979:ARG:HA	2:B:982:ILE:HG22	1.94	0.48
3:C:38:ASP:N	3:C:57:ASP:HB3	2.28	0.48
2:B:908:ASN:O	2:B:912:VAL:HG13	2.14	0.48
2:B:300:ILE:HB	2:B:302:ARG:NH2	2.29	0.48
2:B:438:LEU:HD23	2:B:438:LEU:H	1.78	0.48
2:B:896:LYS:O	2:B:899:HIS:ND1	2.47	0.48
2:B:996:LEU:HD12	2:B:1017:PHE:CZ	2.49	0.48
2:B:1057:GLU:HA	2:B:1061:LEU:HD22	1.96	0.48
2:B:1236:ARG:NH2	2:B:1237:GLU:OE2	2.47	0.48
3:C:168:VAL:O	3:C:171:GLU:HG3	2.14	0.48
2:B:928:ILE:HG23	2:B:932:LEU:HD22	1.94	0.48
2:B:1200:LEU:HD13	2:B:1230:PHE:CD2	2.49	0.48
1:A:281:ARG:O	1:A:283:GLN:NE2	2.46	0.48
2:B:763:LEU:HA	2:B:766:PHE:CD2	2.49	0.48
2:B:95:LEU:HD13	2:B:98:TRP:CD1	2.49	0.47
2:B:325:ALA:HB2	2:B:348:PHE:HD1	1.78	0.47
2:B:394:HIS:O	2:B:397:GLN:NE2	2.47	0.47
2:B:876:GLU:OE1	2:B:924:HIS:NE2	2.39	0.47
2:B:935:ARG:O	2:B:939:THR:HG23	2.14	0.47
1:A:18:TYR:CG	3:C:5:LYS:HB2	2.49	0.47
2:B:821:PRO:HG2	2:B:863:ILE:HG12	1.97	0.47
2:B:860:MET:HA	2:B:863:ILE:HB	1.96	0.47
2:B:932:LEU:HG	2:B:935:ARG:CZ	2.45	0.47
2:B:986:LEU:HD12	2:B:990:PHE:CZ	2.49	0.47
2:B:1247:LEU:O	2:B:1251:HIS:CG	2.67	0.47
2:B:4:TRP:CH2	2:B:46:ARG:HG2	2.50	0.47
2:B:569:LEU:N	2:B:620:PHE:O	2.32	0.47
2:B:945:ARG:HH11	2:B:946:GLN:H	1.62	0.47
3:C:37:PHE:HB2	3:C:56:TRP:HZ3	1.80	0.47
2:B:187:HIS:HB3	2:B:1006:TRP:CE2	2.49	0.47
2:B:193:ARG:O	2:B:197:LYS:HG2	2.15	0.47
2:B:1040:LEU:HA	2:B:1043:TRP:CE3	2.50	0.47
2:B:1099:ILE:HD12	2:B:1099:ILE:H	1.80	0.47
1:A:588:TYR:N	1:A:603:SER:OG	2.48	0.47
2:B:719:TYR:HA	2:B:722:LYS:HG2	1.97	0.47
2:B:899:HIS:HB2	2:B:953:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1079:MET:O	2:B:1082:GLU:HG2	2.15	0.47
2:B:1099:ILE:HG12	2:B:1138:PHE:HB2	1.95	0.47
3:C:114:GLY:H	3:C:156:GLU:HG2	1.79	0.47
2:B:1153:THR:O	2:B:1157:GLN:HG2	2.15	0.47
1:A:670:ASN:ND2	1:A:675:LYS:HB2	2.29	0.47
2:B:10:GLN:NE2	2:B:37:ILE:O	2.42	0.47
1:A:244:ILE:HG21	1:A:293:GLN:HB3	1.96	0.46
1:A:18:TYR:CD2	3:C:5:LYS:HB2	2.50	0.46
1:A:18:TYR:CE2	3:C:7:VAL:HG23	2.48	0.46
2:B:35:VAL:HG12	2:B:49:THR:HG22	1.97	0.46
2:B:95:LEU:HA	2:B:98:TRP:CD1	2.50	0.46
2:B:1125:ILE:N	2:B:1126:PRO:HD2	2.30	0.46
2:B:1233:GLU:HB3	2:B:1234:LYS:HE2	1.97	0.46
2:B:1215:GLU:HB2	2:B:1220:ARG:HH12	1.81	0.46
1:A:321:ARG:HD3	1:A:324:ILE:HD11	1.96	0.46
2:B:144:LEU:HA	2:B:147:LYS:HG2	1.98	0.46
1:A:113:ASP:OD1	1:A:114:VAL:N	2.49	0.46
2:B:149:THR:HG23	2:B:164:VAL:HG21	1.98	0.46
2:B:1090:MET:HE3	2:B:1094:LEU:HG	1.97	0.46
2:B:713:ASN:O	2:B:717:GLU:HG2	2.16	0.46
2:B:859:CYS:O	2:B:863:ILE:HG13	2.16	0.46
1:A:689:LEU:HD21	2:B:106:TYR:CE2	2.50	0.45
2:B:1117:GLU:OE1	2:B:1120:LEU:N	2.47	0.45
1:A:172:SER:HB3	1:A:175:THR:HG23	1.98	0.45
2:B:1227:VAL:HA	2:B:1230:PHE:HD2	1.81	0.45
1:A:575:TRP:HA	1:A:591:LEU:HB2	1.98	0.45
2:B:446:ILE:HG13	2:B:626:ILE:HG23	1.98	0.45
2:B:889:GLN:NE2	2:B:898:ASP:HB3	2.26	0.45
2:B:1054:LEU:HB2	2:B:1083:ILE:HG21	1.98	0.45
2:B:1224:THR:HG21	2:B:1247:LEU:HD11	1.98	0.45
1:A:356:TYR:HB3	1:A:361:PHE:HB2	1.99	0.45
1:A:574:PHE:HB2	1:A:593:GLU:HA	1.97	0.45
2:B:520:GLU:O	2:B:523:THR:OG1	2.33	0.45
2:B:1216:SER:OG	2:B:1219:ASN:OD1	2.35	0.45
2:B:248:PRO:HG3	2:B:387:ILE:HD13	1.99	0.45
2:B:596:GLU:O	2:B:599:GLU:HG3	2.16	0.45
2:B:694:PHE:HE1	2:B:733:LEU:HG	1.81	0.45
2:B:1086:ARG:HA	2:B:1089:ASP:OD2	2.17	0.45
1:A:236:ASP:HB3	1:A:239:ILE:HG22	1.99	0.45
1:A:325:PHE:HB2	1:A:348:ARG:HH21	1.82	0.45
2:B:328:ASP:N	2:B:328:ASP:OD1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:842:LYS:O	2:B:845:GLN:HG2	2.17	0.45
3:C:40:TYR:HB2	3:C:55:LEU:HD12	1.98	0.45
2:B:1098:LYS:HD3	2:B:1101:PHE:CE2	2.52	0.45
1:A:609:PRO:HB2	1:A:612:ASP:HB2	1.99	0.45
2:B:447:TYR:HE2	2:B:627:CYS:HB2	1.81	0.45
2:B:707:ILE:O	2:B:710:GLN:NE2	2.49	0.45
2:B:1193:PHE:O	2:B:1197:VAL:HG23	2.17	0.45
1:A:647:ASP:O	1:A:649:ASN:ND2	2.50	0.45
2:B:181:ILE:O	2:B:185:LYS:HG2	2.17	0.45
2:B:229:LYS:HB2	2:B:400:TRP:HB2	1.99	0.45
2:B:1238:ASP:O	2:B:1242:ARG:HG2	2.17	0.45
1:A:642:PHE:HB3	1:A:662:TYR:HE1	1.80	0.45
2:B:97:GLU:O	2:B:101:ILE:HG12	2.17	0.45
2:B:593:MET:O	2:B:596:GLU:HG3	2.17	0.45
1:A:216:TYR:CE1	1:A:250:LEU:HA	2.52	0.44
1:A:329:ARG:NH2	1:A:351:MET:SD	2.90	0.44
2:B:1169:LYS:HB2	2:B:1169:LYS:HE2	1.71	0.44
2:B:1224:THR:O	2:B:1227:VAL:HG22	2.17	0.44
1:A:459:CYS:O	1:A:463:LEU:HG	2.18	0.44
2:B:88:VAL:O	2:B:92:THR:HG23	2.18	0.44
2:B:909:ILE:O	2:B:913:LEU:HG	2.18	0.44
2:B:1154:LYS:HA	2:B:1154:LYS:HD3	1.83	0.44
2:B:1215:GLU:HA	2:B:1220:ARG:HH22	1.83	0.44
2:B:1237:GLU:HA	2:B:1240:TYR:HB3	1.98	0.44
1:A:578:ARG:HH22	1:A:601:HIS:H	1.66	0.44
2:B:731:VAL:HA	2:B:787:PHE:HE1	1.82	0.44
2:B:1073:VAL:HA	2:B:1077:GLY:HA2	1.99	0.44
2:B:1:MET:C	2:B:4:TRP:HE1	2.26	0.44
2:B:165:VAL:O	2:B:171:ASN:ND2	2.36	0.44
2:B:1133:GLN:NE2	2:B:1134:CYS:SG	2.90	0.44
2:B:1135:GLU:OE2	2:B:1147:PHE:HB3	2.18	0.44
1:A:18:TYR:CE1	3:C:5:LYS:HD3	2.53	0.44
1:A:206:GLU:HB3	1:A:246:VAL:HG22	1.99	0.44
2:B:351:ILE:HD13	2:B:375:GLU:HA	1.98	0.44
2:B:674:ASP:O	2:B:675:ALA:C	2.61	0.44
2:B:906:LEU:HA	2:B:906:LEU:HD22	1.77	0.44
2:B:1150:GLU:OE1	2:B:1150:GLU:N	2.44	0.44
2:B:1204:LEU:HD13	2:B:1204:LEU:HA	1.84	0.44
2:B:110:LYS:HB3	2:B:113:LEU:HB2	1.99	0.44
2:B:749:LYS:HG2	2:B:753:LEU:HG	1.99	0.44
2:B:1091:TRP:O	2:B:1098:LYS:NZ	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1206:ASP:HA	2:B:1209:THR:HG22	2.00	0.44
3:C:7:VAL:HB	3:C:75:THR:HG21	2.00	0.44
2:B:1208:ARG:HG3	2:B:1209:THR:N	2.33	0.44
1:A:237:GLN:CD	1:A:237:GLN:H	2.26	0.44
1:A:700:ASP:HB2	2:B:32:GLY:HA2	1.99	0.44
2:B:634:ASN:HB3	2:B:637:LEU:HB2	1.99	0.44
2:B:876:GLU:CD	2:B:876:GLU:H	2.25	0.43
2:B:1106:VAL:HG11	2:B:1150:GLU:OE2	2.18	0.43
1:A:115:THR:O	1:A:119:GLU:HG2	2.18	0.43
1:A:168:HIS:HB3	1:A:170:ILE:HG13	2.00	0.43
1:A:230:PRO:HA	1:A:233:GLN:HG2	2.01	0.43
2:B:768:ILE:HD11	2:B:827:VAL:HG22	2.00	0.43
2:B:825:ASN:OD1	2:B:826:ASP:N	2.49	0.43
2:B:1213:GLN:HG3	2:B:1214:ASP:H	1.83	0.43
1:A:148:LYS:NZ	1:A:192:ALA:O	2.34	0.43
1:A:216:TYR:OH	1:A:250:LEU:O	2.28	0.43
2:B:906:LEU:O	2:B:910:LEU:HG	2.18	0.43
2:B:913:LEU:HB3	2:B:925:ILE:HD11	2.00	0.43
2:B:1168:TYR:O	2:B:1169:LYS:C	2.58	0.43
1:A:465:LYS:HE3	1:A:465:LYS:HB3	1.84	0.43
2:B:746:ASP:HB3	2:B:749:LYS:HB2	2.01	0.43
2:B:1180:CYS:HB2	2:B:1187:SER:HB3	2.00	0.43
1:A:402:ASN:OD1	1:A:403:SER:N	2.51	0.43
2:B:241:LEU:HD23	2:B:260:ILE:HD12	2.00	0.43
2:B:1023:GLN:O	2:B:1026:GLU:HG2	2.19	0.43
2:B:1202:GLU:HA	2:B:1205:LEU:HB2	2.01	0.43
2:B:1241:ILE:HA	2:B:1244:LEU:HG	1.99	0.43
3:C:40:TYR:HB2	3:C:55:LEU:HB2	1.98	0.43
2:B:306:MET:SD	2:B:320:ARG:NH1	2.91	0.43
2:B:1023:GLN:HA	2:B:1026:GLU:HG2	2.01	0.43
2:B:1121:ARG:O	2:B:1125:ILE:HG12	2.18	0.43
1:A:172:SER:O	1:A:175:THR:OG1	2.37	0.43
1:A:688:THR:O	1:A:692:MET:N	2.36	0.43
1:A:689:LEU:HD23	1:A:689:LEU:HA	1.77	0.43
2:B:1120:LEU:O	2:B:1124:THR:OG1	2.27	0.43
3:C:145:LEU:HA	3:C:148:GLN:HG2	2.00	0.43
1:A:697:ARG:HB3	2:B:32:GLY:H	1.84	0.43
2:B:86:PRO:HA	2:B:89:GLN:HG2	2.00	0.43
2:B:654:LEU:HD23	2:B:657:LEU:HD12	2.01	0.43
2:B:801:LEU:O	2:B:804:ARG:HG2	2.18	0.43
1:A:634:ASN:OD1	1:A:634:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:GLY:C	2:B:264:SER:HB2	2.44	0.43
2:B:986:LEU:O	2:B:989:THR:OG1	2.32	0.43
2:B:45:TYR:N	2:B:59:PHE:O	2.46	0.43
2:B:1222:SER:O	2:B:1225:VAL:HG12	2.18	0.43
2:B:92:THR:O	2:B:96:ARG:HG3	2.19	0.42
2:B:301:VAL:HA	2:B:321:PRO:HA	2.00	0.42
2:B:339:ASP:OD1	2:B:339:ASP:N	2.50	0.42
2:B:1121:ARG:HH21	2:B:1125:ILE:HA	1.84	0.42
2:B:1200:LEU:O	2:B:1203:ASN:HB3	2.19	0.42
1:A:616:VAL:HG21	1:A:669:LEU:HD13	2.01	0.42
1:A:658:ASP:OD2	1:A:660:HIS:ND1	2.52	0.42
1:A:697:ARG:HH21	2:B:32:GLY:C	2.27	0.42
2:B:224:LEU:HB3	2:B:403:LEU:HD11	2.02	0.42
2:B:594:GLU:O	2:B:597:GLU:HG3	2.19	0.42
2:B:994:LYS:HB3	2:B:1049:LEU:HD13	2.01	0.42
2:B:1018:LEU:HD22	2:B:1079:MET:HG3	2.00	0.42
1:A:202:LEU:HD13	1:A:205:LEU:HD12	2.00	0.42
1:A:312:LYS:NZ	1:A:374:THR:OG1	2.39	0.42
2:B:810:VAL:HG23	2:B:811:LYS:H	1.84	0.42
2:B:1210:ILE:HD12	2:B:1213:GLN:HB3	2.01	0.42
3:C:41:SER:HB2	3:C:52:ASN:HD21	1.84	0.42
1:A:297:LEU:HD23	1:A:300:LEU:HD12	2.00	0.42
2:B:153:ASP:HB3	2:B:163:LEU:HD23	2.00	0.42
2:B:955:ALA:HA	2:B:958:ILE:HG12	2.01	0.42
2:B:1099:ILE:HB	2:B:1100:LYS:HZ1	1.85	0.42
3:C:105:CYS:O	3:C:108:VAL:HG12	2.19	0.42
2:B:180:THR:OG1	2:B:959:ALA:HB2	2.19	0.42
2:B:530:THR:HG22	2:B:549:VAL:HG22	2.01	0.42
2:B:555:MET:HA	2:B:561:THR:HA	2.02	0.42
2:B:1220:ARG:O	2:B:1224:THR:HG23	2.19	0.42
1:A:557:VAL:O	1:A:578:ARG:HG3	2.19	0.42
1:A:659:LYS:HB3	1:A:659:LYS:HE3	1.78	0.42
2:B:186:ALA:HA	2:B:189:VAL:HG22	2.02	0.42
2:B:1002:TYR:HD2	2:B:1010:ASN:HD21	1.67	0.42
2:B:127:TRP:O	2:B:131:ILE:HG12	2.20	0.42
2:B:187:HIS:HB3	2:B:1006:TRP:CD2	2.55	0.42
2:B:224:LEU:HD22	2:B:403:LEU:HD11	2.02	0.42
2:B:349:GLN:NE2	2:B:350:GLN:O	2.52	0.42
2:B:732:LYS:O	2:B:736:VAL:HG23	2.20	0.42
2:B:1191:GLU:O	2:B:1195:LEU:HG	2.20	0.42
2:B:1199:SER:HB2	2:B:1230:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:VAL:HA	3:C:97:TRP:CD1	2.49	0.42
1:A:245:ALA:HB2	1:A:293:GLN:HE22	1.84	0.42
2:B:628:SER:HB2	2:B:631:LEU:HD22	2.02	0.42
2:B:761:LYS:O	2:B:765:ARG:HG3	2.20	0.42
2:B:877:VAL:C	2:B:880:PRO:HD2	2.45	0.42
2:B:1097:HIS:C	2:B:1100:LYS:HZ2	2.27	0.42
2:B:1114:LEU:HD22	2:B:1158:GLU:HG2	2.02	0.42
1:A:183:LYS:HG3	1:A:187:PHE:CZ	2.55	0.42
1:A:677:MET:HG3	1:A:682:THR:HG21	2.02	0.42
2:B:241:LEU:O	2:B:259:LEU:HA	2.19	0.42
2:B:287:MET:O	2:B:290:ILE:HG22	2.20	0.42
2:B:331:ASP:O	2:B:336:LYS:NZ	2.52	0.42
2:B:413:VAL:HG12	2:B:417:PHE:HD2	1.84	0.42
2:B:417:PHE:HD1	2:B:419:HIS:HE1	1.68	0.42
2:B:434:PRO:HD3	2:B:443:ARG:CZ	2.50	0.42
2:B:711:HIS:O	2:B:714:PRO:HD2	2.20	0.42
2:B:886:LEU:O	2:B:890:LEU:HG	2.19	0.42
1:A:258:ARG:O	1:A:262:MET:HG2	2.20	0.42
2:B:13:GLY:HA3	2:B:35:VAL:HG23	2.01	0.42
2:B:44:TRP:CE3	2:B:58:ILE:HG22	2.55	0.42
2:B:128:ARG:HD3	2:B:128:ARG:C	2.45	0.42
2:B:761:LYS:HD2	2:B:823:ILE:HB	2.00	0.42
2:B:1008:VAL:O	2:B:1011:MET:HG2	2.19	0.42
2:B:1217:LYS:HA	2:B:1220:ARG:HD2	2.02	0.42
1:A:462:LEU:HD22	1:A:506:LEU:HD13	2.02	0.41
1:A:716:GLU:HG3	2:B:44:TRP:NE1	2.35	0.41
2:B:95:LEU:HD21	2:B:124:LEU:HD21	2.02	0.41
2:B:409:ASP:N	2:B:409:ASP:OD1	2.52	0.41
2:B:717:GLU:OE2	2:B:765:ARG:NH1	2.52	0.41
2:B:824:ILE:HG21	2:B:840:PHE:CZ	2.55	0.41
2:B:1166:GLU:CD	2:B:1166:GLU:H	2.28	0.41
1:A:652:LEU:HB3	1:A:654:PHE:CZ	2.55	0.41
2:B:85:LEU:O	2:B:88:VAL:HG22	2.20	0.41
2:B:95:LEU:HA	2:B:98:TRP:HD1	1.84	0.41
2:B:631:LEU:HD12	2:B:633:GLN:HG3	2.02	0.41
3:C:90:TYR:HE1	3:C:145:LEU:HD13	1.85	0.41
1:A:536:LEU:HD11	2:B:18:ASN:H	1.86	0.41
2:B:841:CYS:SG	2:B:842:LYS:N	2.94	0.41
1:A:526:GLU:HA	1:A:530:SER:HB3	2.02	0.41
1:A:590:ASP:OD1	1:A:590:ASP:N	2.54	0.41
2:B:469:THR:O	2:B:530:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:PRO:HG2	2:B:509:TRP:CH2	2.55	0.41
2:B:651:LYS:HE2	2:B:692:LEU:HD12	2.03	0.41
2:B:19:TYR:HD2	2:B:26:GLU:HB3	1.85	0.41
2:B:179:SER:O	2:B:183:LEU:HD23	2.20	0.41
2:B:472:VAL:O	2:B:479:LEU:HA	2.20	0.41
2:B:731:VAL:HG23	2:B:735:LYS:HZ3	1.84	0.41
2:B:907:SER:O	2:B:911:GLU:HG3	2.20	0.41
2:B:1181:ARG:HA	2:B:1181:ARG:NE	2.35	0.41
1:A:204:ILE:HD13	1:A:204:ILE:HA	1.92	0.41
1:A:214:ASP:OD1	1:A:214:ASP:N	2.52	0.41
1:A:708:ASP:OD1	1:A:708:ASP:N	2.48	0.41
2:B:214:SER:O	2:B:218:THR:HG23	2.21	0.41
2:B:514:LYS:HE3	2:B:514:LYS:HB3	1.85	0.41
2:B:1079:MET:HE3	2:B:1083:ILE:HD11	2.02	0.41
2:B:1251:HIS:O	2:B:1252:ARG:C	2.63	0.41
1:A:199:GLN:HG2	1:A:239:ILE:HD13	2.03	0.41
2:B:85:LEU:HA	2:B:88:VAL:HG13	2.01	0.41
2:B:224:LEU:HB2	2:B:281:PHE:HD2	1.86	0.41
2:B:243:MET:HB2	2:B:296:LEU:HD21	2.01	0.41
2:B:961:LEU:HA	2:B:964:MET:HE3	2.02	0.41
2:B:1042:LEU:HD12	2:B:1042:LEU:HA	1.88	0.41
2:B:1082:GLU:OE1	2:B:1082:GLU:N	2.53	0.41
2:B:1169:LYS:HG3	2:B:1201:LEU:HD23	2.02	0.41
2:B:1184:LYS:O	2:B:1187:SER:N	2.35	0.41
3:C:79:VAL:HG22	3:C:111:LEU:HD23	2.02	0.41
2:B:4:TRP:HZ3	2:B:45:TYR:HA	1.85	0.41
2:B:753:LEU:O	2:B:757:LEU:HG	2.21	0.41
2:B:860:MET:HG2	2:B:885:GLN:HE22	1.86	0.41
2:B:950:ILE:HA	2:B:953:PHE:HD2	1.85	0.41
1:A:14:TRP:HE1	1:A:77:LEU:HD23	1.86	0.41
1:A:19:PRO:HD2	3:C:39:ASN:ND2	2.36	0.41
1:A:129:LEU:O	1:A:132:MET:HG3	2.21	0.41
2:B:184:PHE:O	2:B:188:GLU:HG3	2.21	0.41
2:B:280:VAL:HG23	2:B:425:THR:HG21	2.03	0.41
2:B:293:ARG:NH2	2:B:328:ASP:HB3	2.36	0.41
2:B:783:ASP:O	2:B:786:GLU:HG3	2.21	0.41
2:B:947:SER:N	2:B:948:PRO:HD2	2.36	0.41
2:B:238:ASP:HB2	2:B:303:VAL:HB	2.02	0.41
2:B:258:TYR:HA	2:B:487:GLY:HA2	2.03	0.41
2:B:1024:PHE:HB3	2:B:1046:TYR:HE2	1.85	0.41
2:B:1134:CYS:HA	2:B:1137:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:GLU:OE1	1:A:535:GLU:N	2.54	0.40
2:B:10:GLN:N	2:B:10:GLN:OE1	2.54	0.40
2:B:80:VAL:HG21	2:B:134:GLY:H	1.86	0.40
2:B:346:ILE:HD12	2:B:347:PRO:HD2	2.03	0.40
3:C:9:VAL:HG12	3:C:58:THR:HG21	2.03	0.40
1:A:54:ALA:HB3	1:A:75:LEU:HA	2.03	0.40
1:A:470:MET:HG2	2:B:137:PRO:HB3	2.02	0.40
1:A:536:LEU:HA	2:B:18:ASN:OD1	2.21	0.40
2:B:857:LEU:O	2:B:861:THR:OG1	2.32	0.40
1:A:476:ASP:HB2	1:A:479:LYS:HB2	2.03	0.40
1:A:491:ALA:O	1:A:494:THR:OG1	2.37	0.40
2:B:98:TRP:HZ3	2:B:117:LEU:HG	1.85	0.40
2:B:353:MET:HE3	2:B:353:MET:HB3	1.87	0.40
2:B:562:LEU:HD21	2:B:624:THR:HG21	2.03	0.40
2:B:1111:GLU:OE1	2:B:1111:GLU:N	2.46	0.40
2:B:9:ARG:NH1	2:B:76:GLN:OE1	2.55	0.40
2:B:137:PRO:HG2	2:B:140:GLU:OE1	2.22	0.40
2:B:1229:ASN:O	2:B:1232:LYS:HG3	2.22	0.40
2:B:1251:HIS:O	2:B:1254:CYS:N	2.44	0.40
1:A:265:ILE:O	1:A:268:GLN:HG2	2.21	0.40
1:A:561:CYS:SG	1:A:597:GLY:HA2	2.62	0.40
2:B:189:VAL:O	2:B:192:LYS:HG3	2.21	0.40
2:B:465:ASN:O	2:B:533:HIS:HA	2.20	0.40
2:B:470:MET:O	2:B:495:GLU:HG2	2.21	0.40
2:B:555:MET:HE2	2:B:555:MET:HB2	1.96	0.40
2:B:932:LEU:HA	2:B:935:ARG:HD3	2.04	0.40
2:B:1079:MET:O	2:B:1083:ILE:HG13	2.22	0.40
2:B:1235:LYS:O	2:B:1236:ARG:HD2	2.22	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	725/733 (99%)	697 (96%)	28 (4%)	0	100	100
2	B	1252/1876 (67%)	1172 (94%)	80 (6%)	0	100	100
3	C	179/214 (84%)	173 (97%)	6 (3%)	0	100	100
All	All	2156/2823 (76%)	2042 (95%)	114 (5%)	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	645/665 (97%)	621 (96%)	24 (4%)	29	49
2	B	1140/1703 (67%)	1057 (93%)	83 (7%)	11	31
3	C	157/184 (85%)	154 (98%)	3 (2%)	52	69
All	All	1942/2552 (76%)	1832 (94%)	110 (6%)	20	38

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	52	GLN
1	A	79	THR
1	A	114	VAL
1	A	168	HIS
1	A	178	VAL
1	A	195	ILE
1	A	260	GLN
1	A	270	GLN
1	A	290	MET
1	A	379	LEU
1	A	406	GLU
1	A	490	ARG
1	A	509	LEU
1	A	536	LEU

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Mol	Chain	Res	Type
1	A	541	GLN
1	A	544	ILE
1	A	585	VAL
1	A	590	ASP
1	A	599	VAL
1	A	634	ASN
1	A	692	MET
1	A	696	LEU
1	A	716	GLU
2	B	33	ASP
2	B	50	LEU
2	B	70	THR
2	B	87	LEU
2	B	88	VAL
2	B	100	VAL
2	B	111	LEU
2	B	121	THR
2	B	122	TYR
2	B	128	ARG
2	B	159	LEU
2	B	161	LEU
2	B	180	THR
2	B	183	LEU
2	B	222	TYR
2	B	226	VAL
2	B	232	VAL
2	B	259	LEU
2	B	277	LEU
2	B	297	VAL
2	B	322	PHE
2	B	372	VAL
2	B	399	LEU
2	B	437	ILE
2	B	448	VAL
2	B	462	THR
2	B	476	GLU
2	B	513	VAL
2	B	560	THR
2	B	591	THR
2	B	632	THR
2	B	671	ASP
2	B	710	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	745	ASP
2	B	754	PHE
2	B	810	VAL
2	B	841	CYS
2	B	843	PHE
2	B	861	THR
2	B	864	VAL
2	B	881	LEU
2	B	896	LYS
2	B	905	LEU
2	B	906	LEU
2	B	909	ILE
2	B	912	VAL
2	B	917	ASP
2	B	932	LEU
2	B	933	LEU
2	B	934	ARG
2	B	935	ARG
2	B	936	ILE
2	B	943	MET
2	B	964	MET
2	B	970	SER
2	B	977	LYS
2	B	986	LEU
2	B	1000	ASN
2	B	1001	VAL
2	B	1013	GLN
2	B	1018	LEU
2	B	1019	ARG
2	B	1033	MET
2	B	1044	ASN
2	B	1045	ASN
2	B	1062	GLU
2	B	1094	LEU
2	B	1100	LYS
2	B	1110	LEU
2	B	1118	VAL
2	B	1132	MET
2	B	1145	HIS
2	B	1147	PHE
2	B	1154	LYS
2	B	1156	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1158	GLU
2	B	1169	LYS
2	B	1199	SER
2	B	1223	CYS
2	B	1227	VAL
2	B	1229	ASN
2	B	1238	ASP
2	B	1247	LEU
3	C	56	TRP
3	C	118	ASP
3	C	125	THR

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	71	ASN
1	A	199	GLN
1	A	283	GLN
1	A	340	ASN
1	A	383	ASN
1	A	541	GLN
1	A	582	ASN
1	A	649	ASN
2	B	23	GLN
2	B	130	GLN
2	B	278	GLN
2	B	350	GLN
2	B	556	ASN
2	B	576	ASN
2	B	710	GLN
2	B	885	GLN
2	B	889	GLN
2	B	1023	GLN
2	B	1066	GLN
2	B	1133	GLN
2	B	1137	ASN
2	B	1213	GLN
2	B	1226	ASN
2	B	1229	ASN
3	C	104	HIS
3	C	132	GLN

### 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.

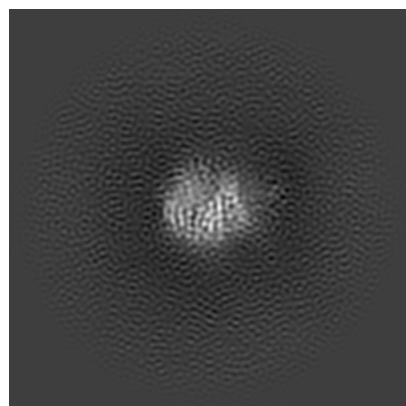
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63477. These allow visual inspection of the internal detail of the map and identification of artifacts.

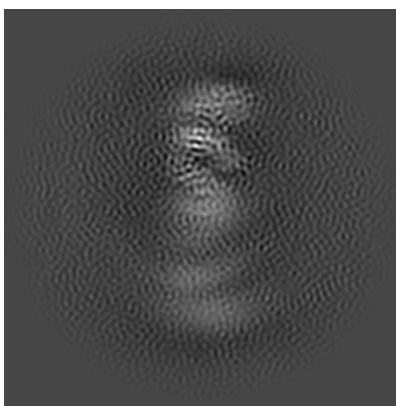
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

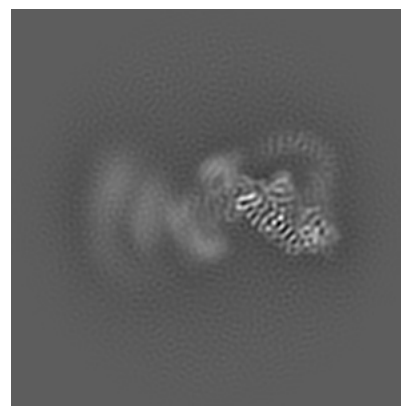
#### 6.1.1 Primary map



X

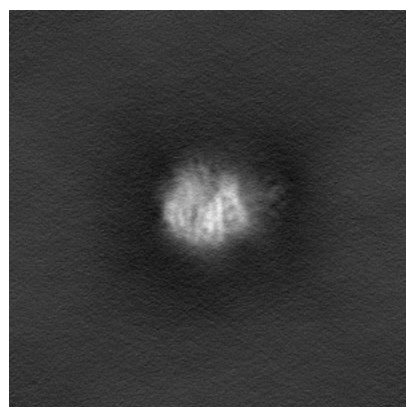


Y

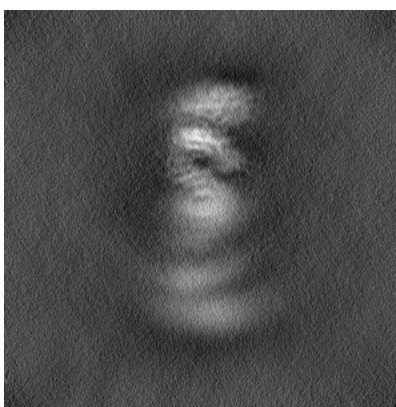


Z

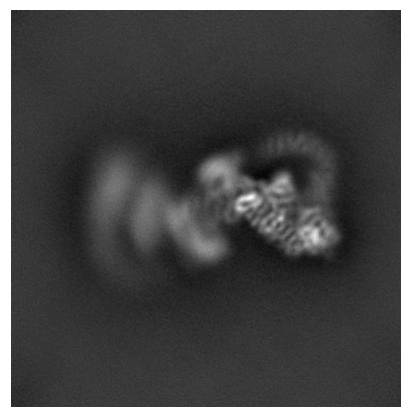
#### 6.1.2 Raw map



X



Y

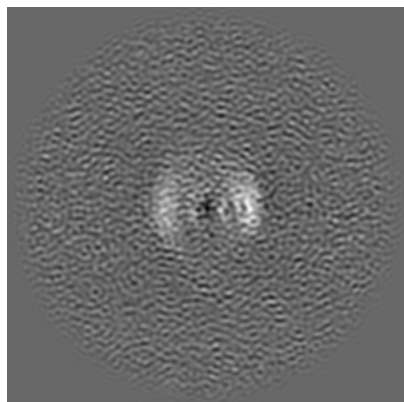


Z

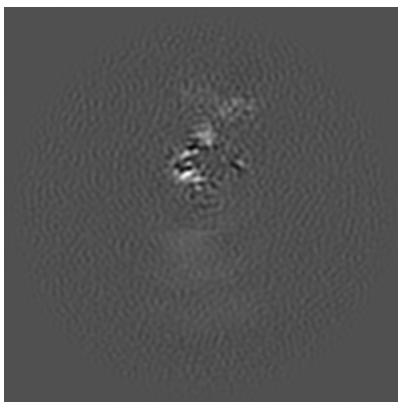
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

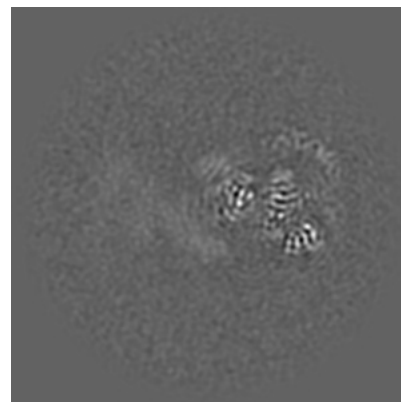
### 6.2.1 Primary map



X Index: 180

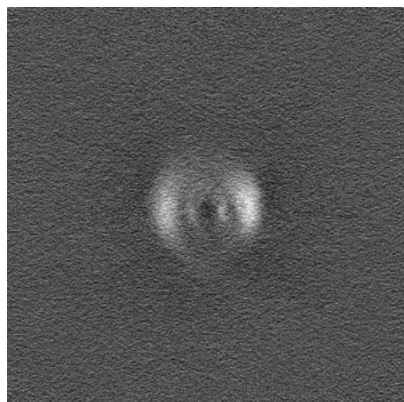


Y Index: 180

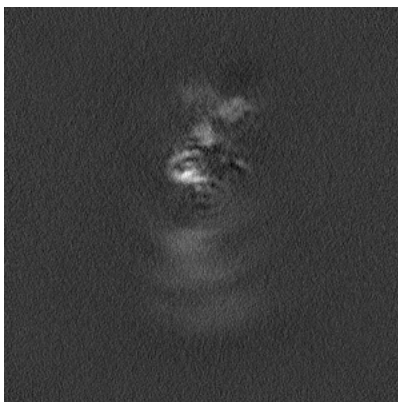


Z Index: 180

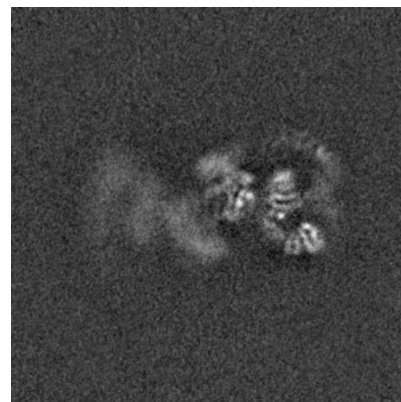
### 6.2.2 Raw map



X Index: 180



Y Index: 180



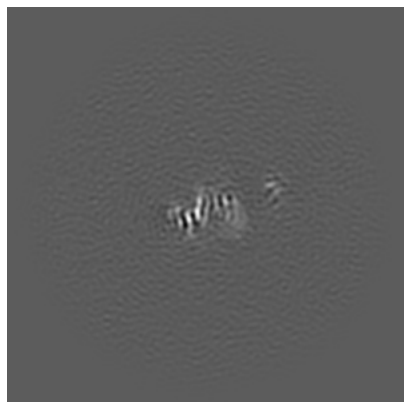
Z Index: 180

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

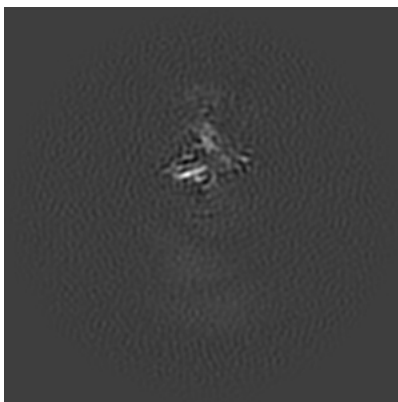


## 6.3 Largest variance slices [i](#)

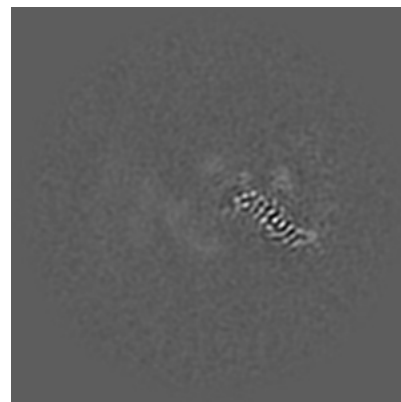
### 6.3.1 Primary map



X Index: 243



Y Index: 189

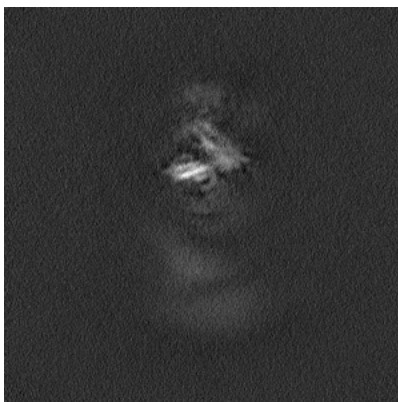


Z Index: 168

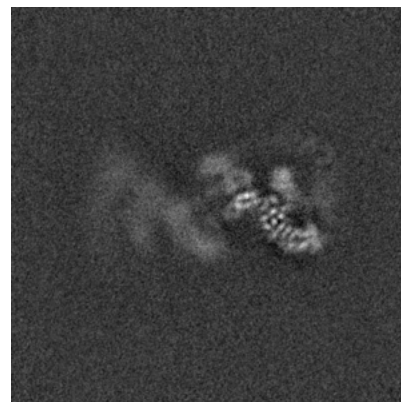
### 6.3.2 Raw map



X Index: 243



Y Index: 190

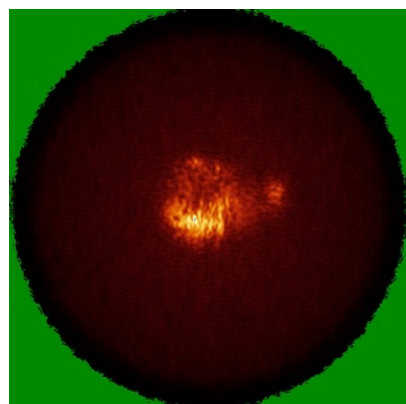


Z Index: 172

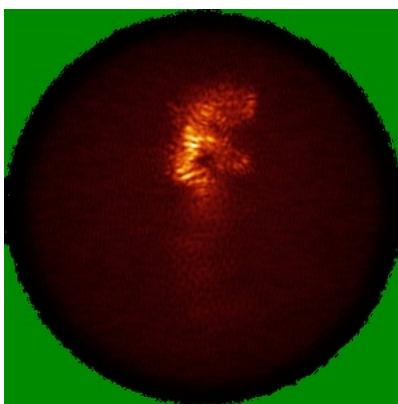
The images above show the largest variance slices of the map in three orthogonal directions.

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

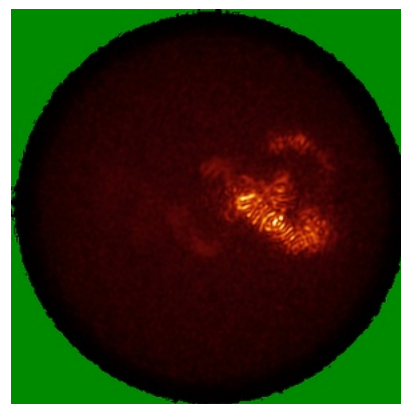
### 6.4.1 Primary map



X

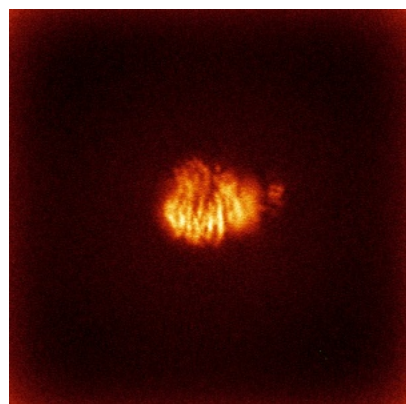


Y

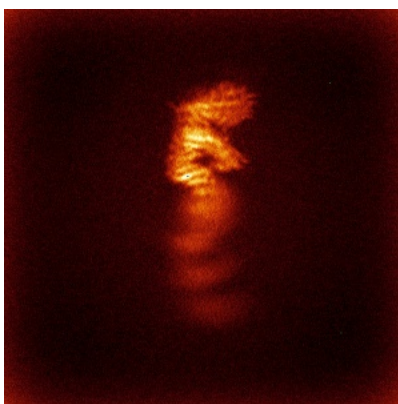


Z

### 6.4.2 Raw map



X



Y

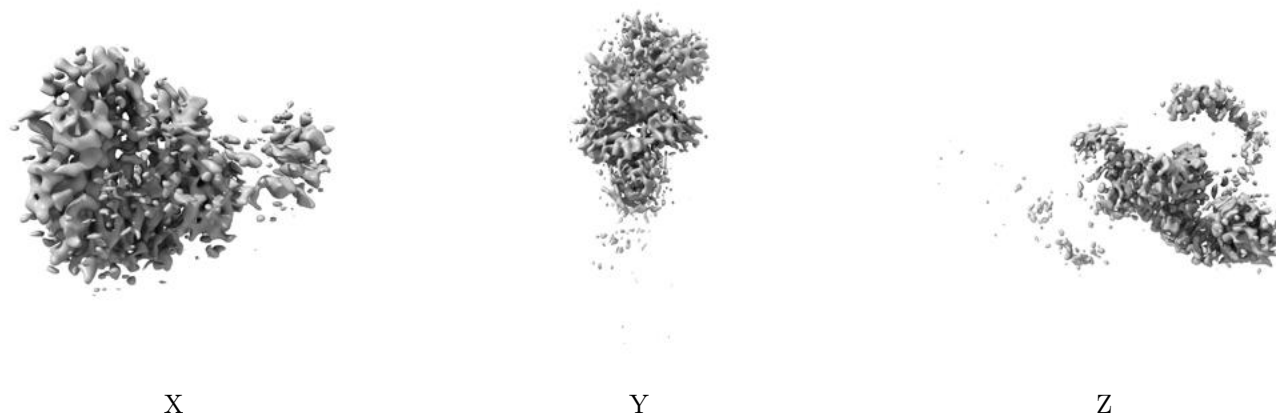


Z

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.

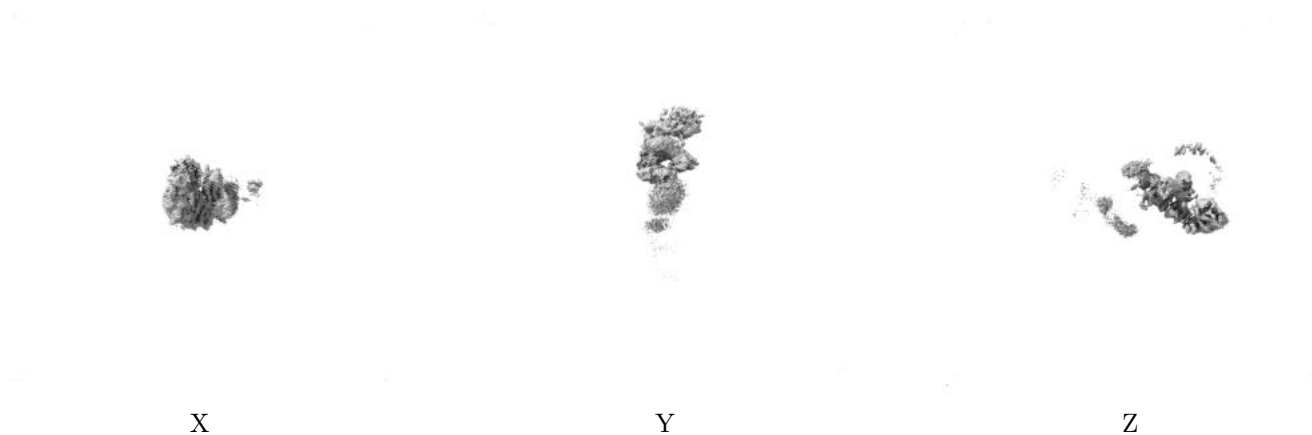
## 6.5 Orthogonal surface views [i](#)

### 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.

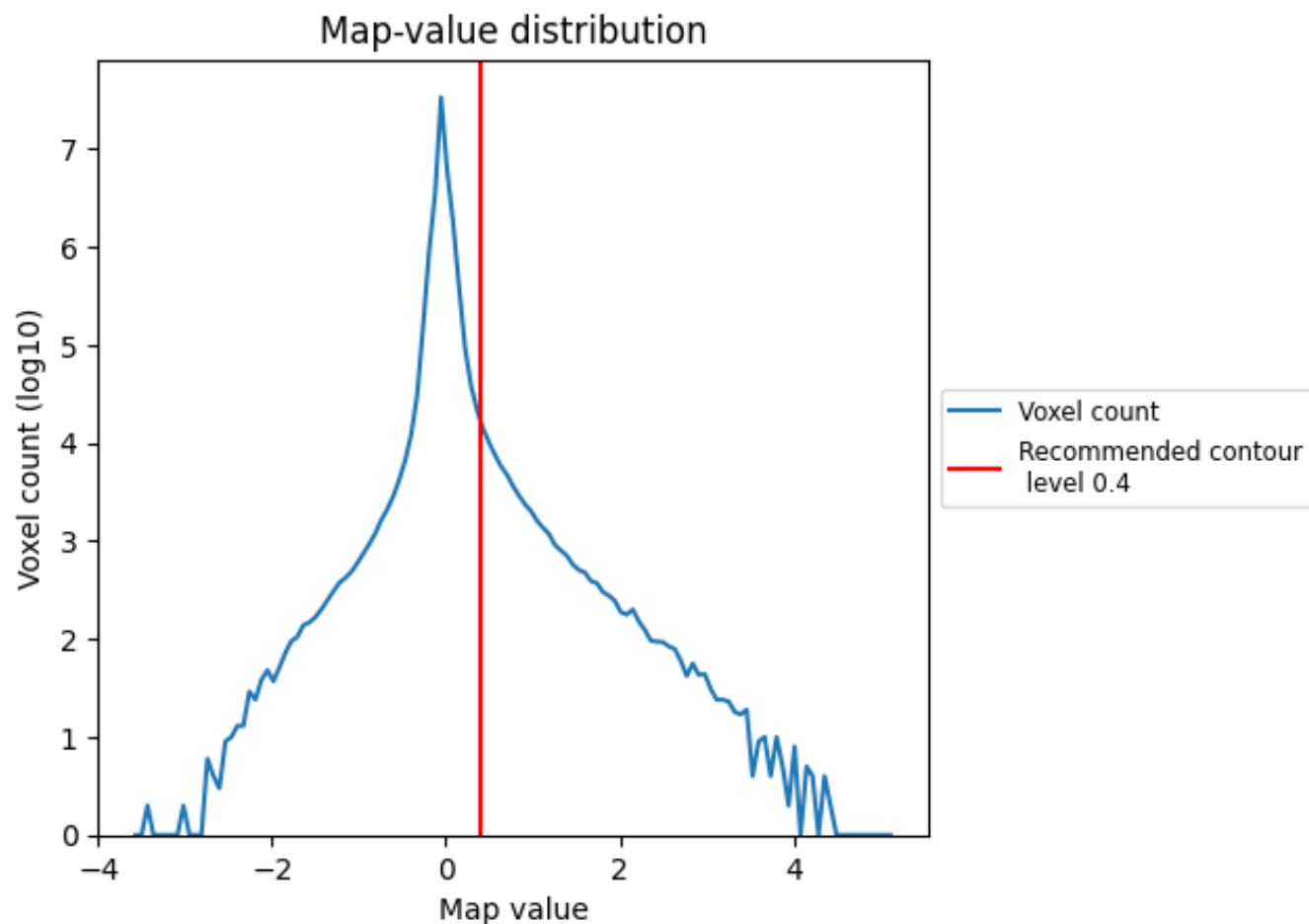
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

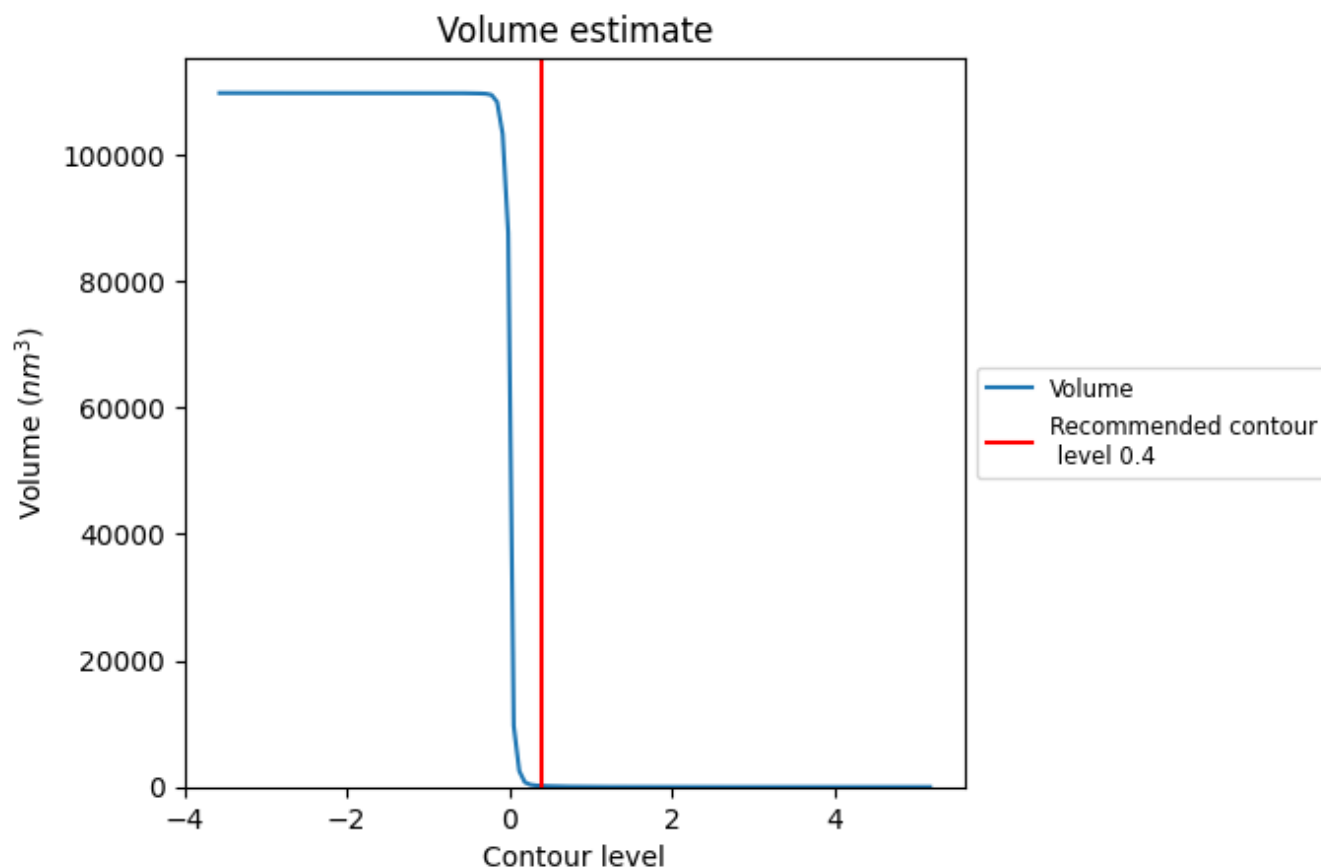
This section contains the results of statistical analysis of the map.

### 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.

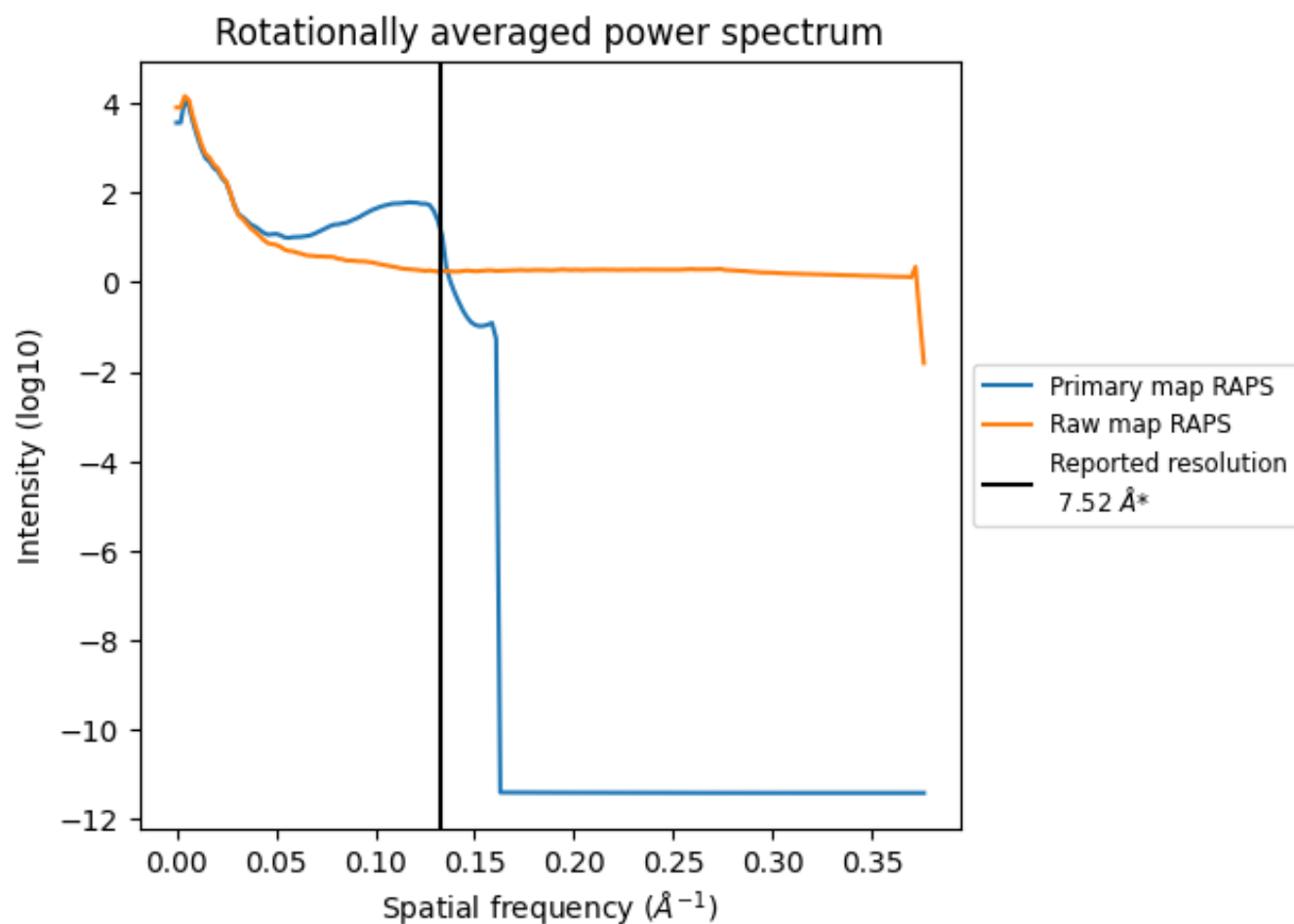
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170  $\text{nm}^3$ ; this corresponds to an approximate mass of 153 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](#)

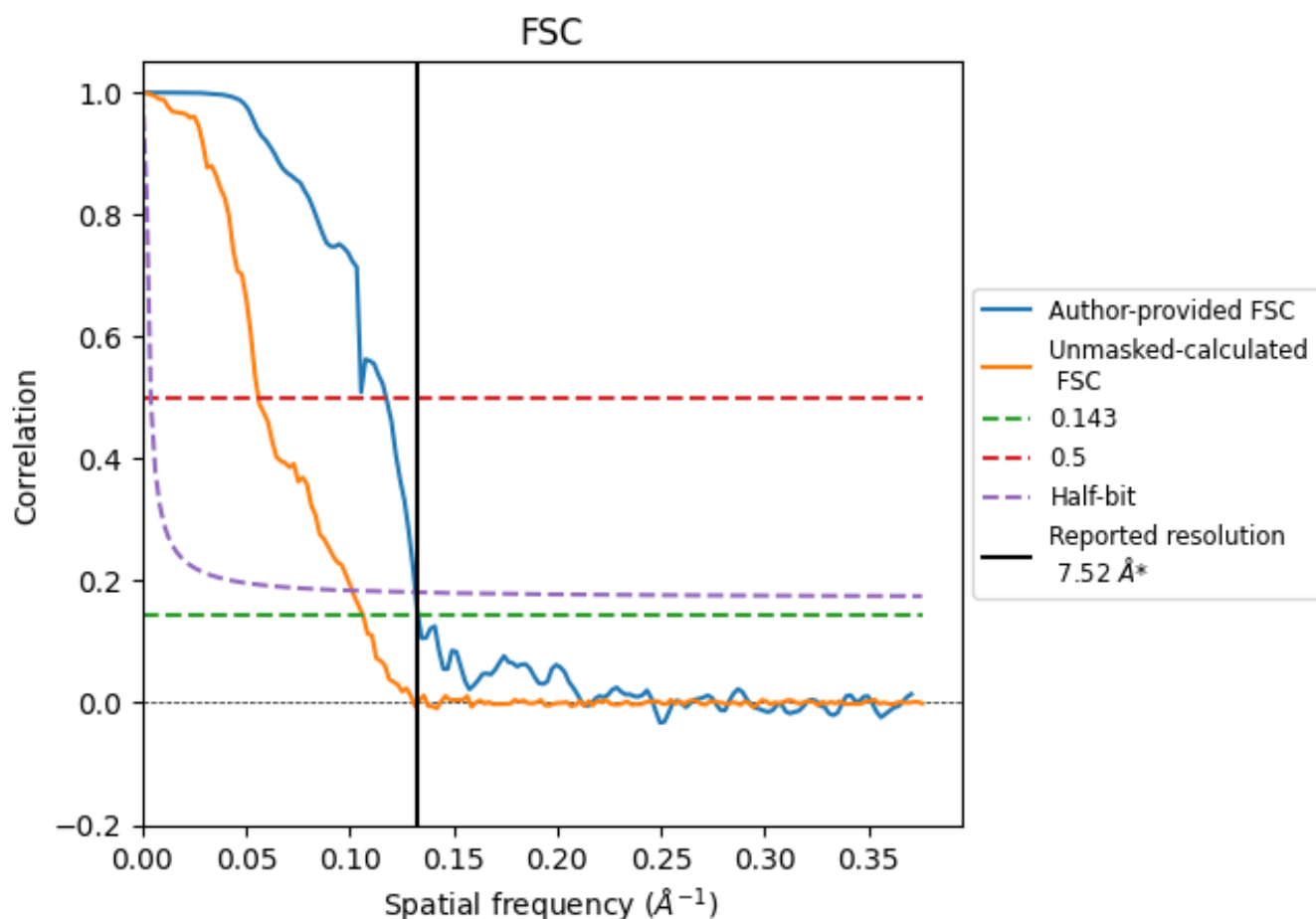


\*Reported resolution corresponds to spatial frequency of 0.133 Å<sup>-1</sup>

## 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 0.133  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.52	-	-
Author-provided FSC curve	7.52	8.50	7.59
Unmasked-calculated*	9.39	17.86	9.88

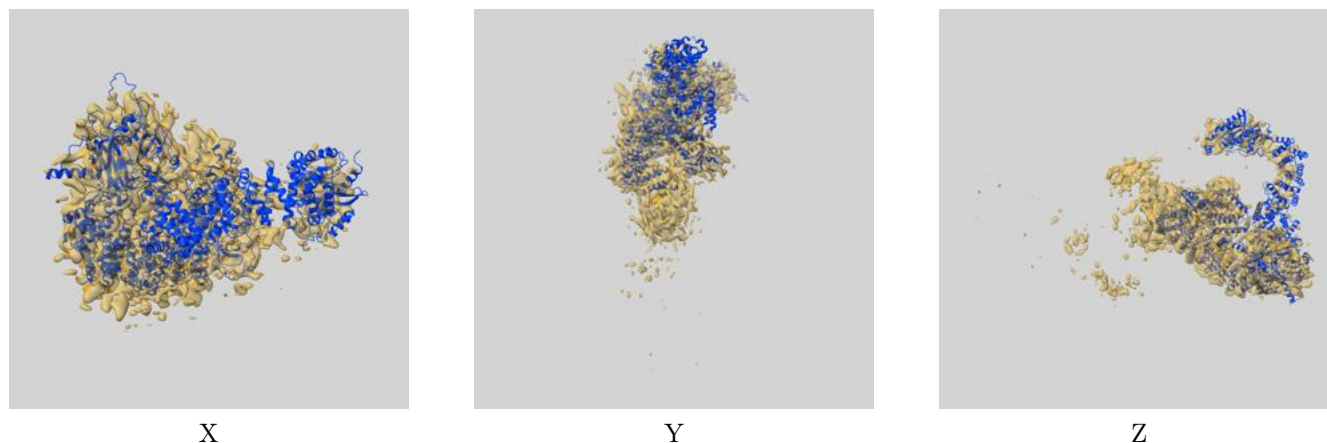
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.39 differs from the reported value 7.52 by more than 10 %



## 9 Map-model fit [i](#)

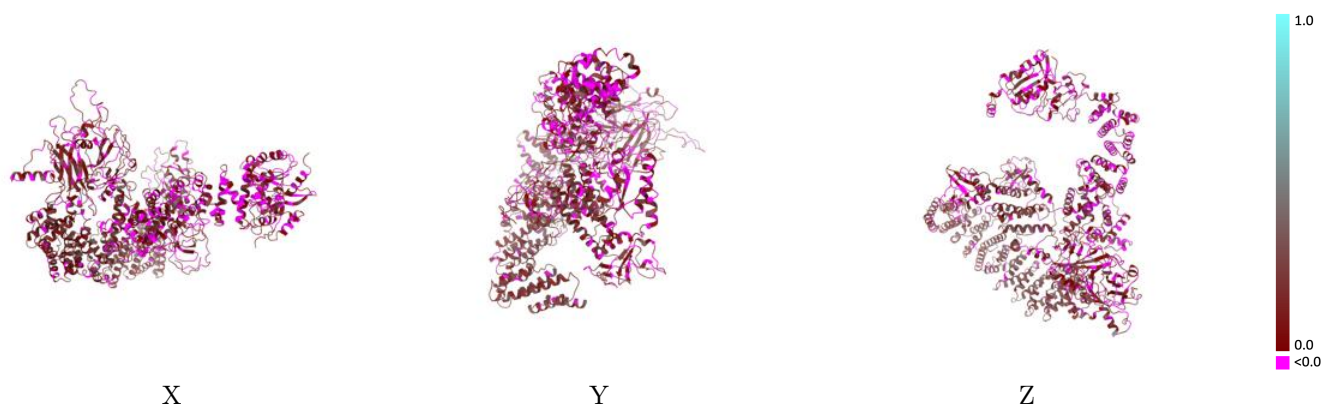
This section contains information regarding the fit between EMDB map EMD-63477 and PDB model 9LXH. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



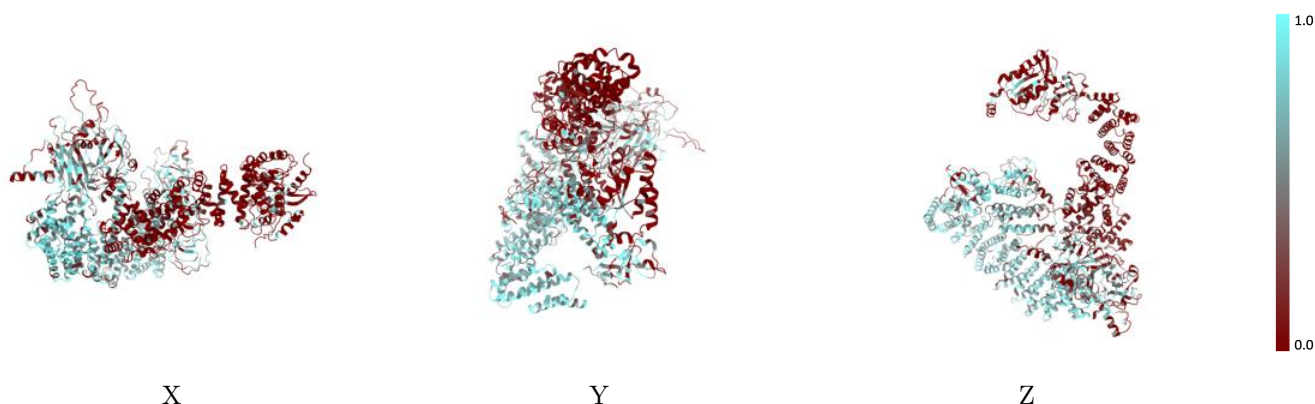
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



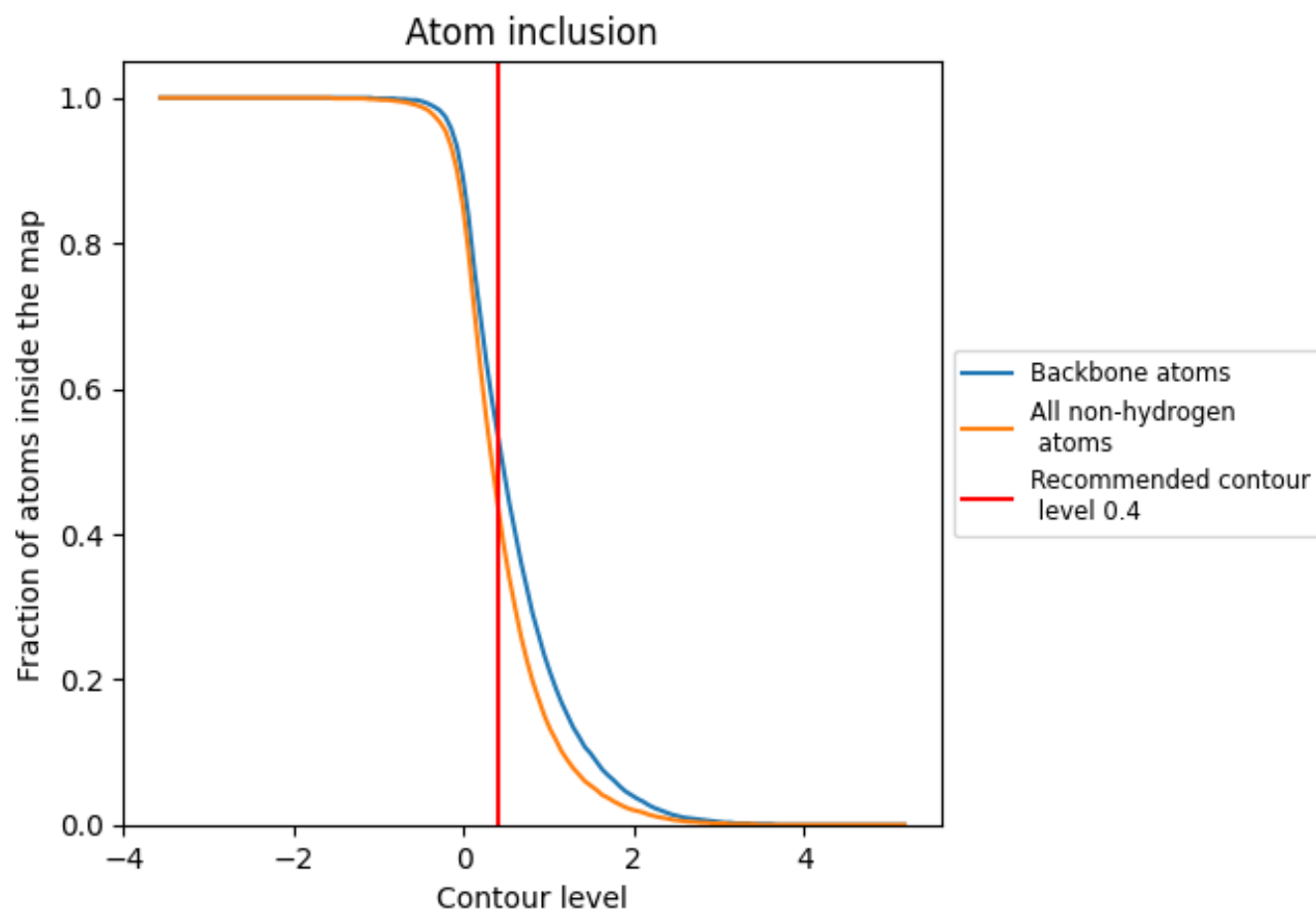
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 54% of all backbone atoms, 44% 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	<div></div> 0.4390	<div></div> 0.1130
A	<div></div> 0.2180	<div></div> 0.0730
B	<div></div> 0.6000	<div></div> 0.1450
C	<div></div> 0.1840	<div></div> 0.0560

