



Full wwPDB EM Validation Report ⓘ

Apr 14, 2025 – 01:52 PM JST

PDB ID : 8Z5P / pdb_00008z5p
EMDB ID : EMD-39777
Title : human phosphorylase kinase - inactive state
Authors : Ma, R.; Yan, K.
Deposited on : 2024-04-18
Resolution : 3.41 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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

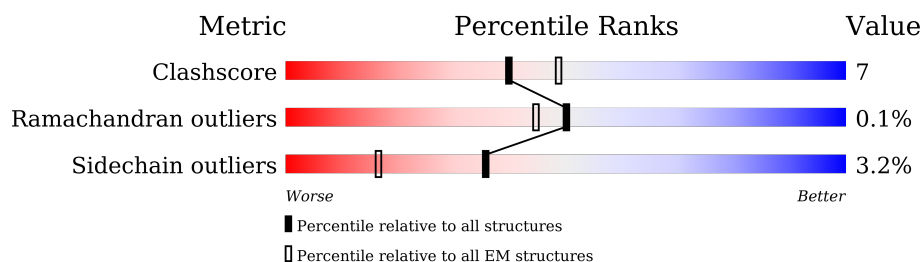
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1223	
1	E	1223	
2	B	1093	
2	F	1093	
3	C	387	
3	G	387	
4	D	168	
4	H	168	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40126 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 Phosphorylase b kinase regulatory subunit alpha, skeletal muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	995	Total	C	N	O	S	0	0
			7852	5004	1327	1475	46		
1	E	995	Total	C	N	O	S	0	0
			7852	5004	1327	1475	46		

- Molecule 2 is a protein called Phosphorylase b kinase regulatory subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1001	Total	C	N	O	S	0	0
			8049	5159	1378	1476	36		
2	F	1001	Total	C	N	O	S	0	0
			8049	5159	1378	1476	36		

- Molecule 3 is a protein called Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	376	Total	C	N	O	S	0	0
			3065	1965	527	558	15		
3	G	376	Total	C	N	O	S	0	0
			3065	1965	527	558	15		

- Molecule 4 is a protein called Calmodulin-3.

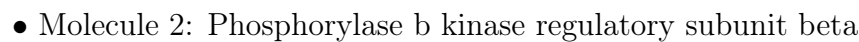
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1097	674	178	236	9		
4	H	144	Total	C	N	O	S	0	0
			1097	674	178	236	9		

There are 38 discrepancies between the modelled and reference sequences:

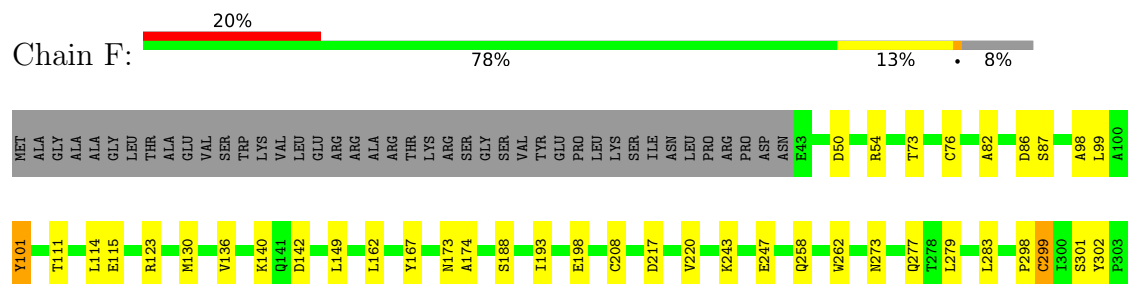
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	ASP	-	expression tag	UNP P0DP25
D	-17	TYR	-	expression tag	UNP P0DP25
D	-16	LYS	-	expression tag	UNP P0DP25
D	-15	ASP	-	expression tag	UNP P0DP25
D	-14	ASP	-	expression tag	UNP P0DP25
D	-13	ASP	-	expression tag	UNP P0DP25
D	-12	ASP	-	expression tag	UNP P0DP25
D	-11	LYS	-	expression tag	UNP P0DP25
D	-10	SER	-	expression tag	UNP P0DP25
D	-9	GLY	-	expression tag	UNP P0DP25
D	-8	PRO	-	expression tag	UNP P0DP25
D	-7	ASP	-	expression tag	UNP P0DP25
D	-6	GLU	-	expression tag	UNP P0DP25
D	-5	VAL	-	expression tag	UNP P0DP25
D	-4	ASP	-	expression tag	UNP P0DP25
D	-3	ALA	-	expression tag	UNP P0DP25
D	-2	SER	-	expression tag	UNP P0DP25
D	-1	GLY	-	expression tag	UNP P0DP25
D	0	ARG	-	expression tag	UNP P0DP25
H	-18	ASP	-	expression tag	UNP P0DP25
H	-17	TYR	-	expression tag	UNP P0DP25
H	-16	LYS	-	expression tag	UNP P0DP25
H	-15	ASP	-	expression tag	UNP P0DP25
H	-14	ASP	-	expression tag	UNP P0DP25
H	-13	ASP	-	expression tag	UNP P0DP25
H	-12	ASP	-	expression tag	UNP P0DP25
H	-11	LYS	-	expression tag	UNP P0DP25
H	-10	SER	-	expression tag	UNP P0DP25
H	-9	GLY	-	expression tag	UNP P0DP25
H	-8	PRO	-	expression tag	UNP P0DP25
H	-7	ASP	-	expression tag	UNP P0DP25
H	-6	GLU	-	expression tag	UNP P0DP25
H	-5	VAL	-	expression tag	UNP P0DP25
H	-4	ASP	-	expression tag	UNP P0DP25
H	-3	ALA	-	expression tag	UNP P0DP25
H	-2	SER	-	expression tag	UNP P0DP25
H	-1	GLY	-	expression tag	UNP P0DP25
H	0	ARG	-	expression tag	UNP P0DP25

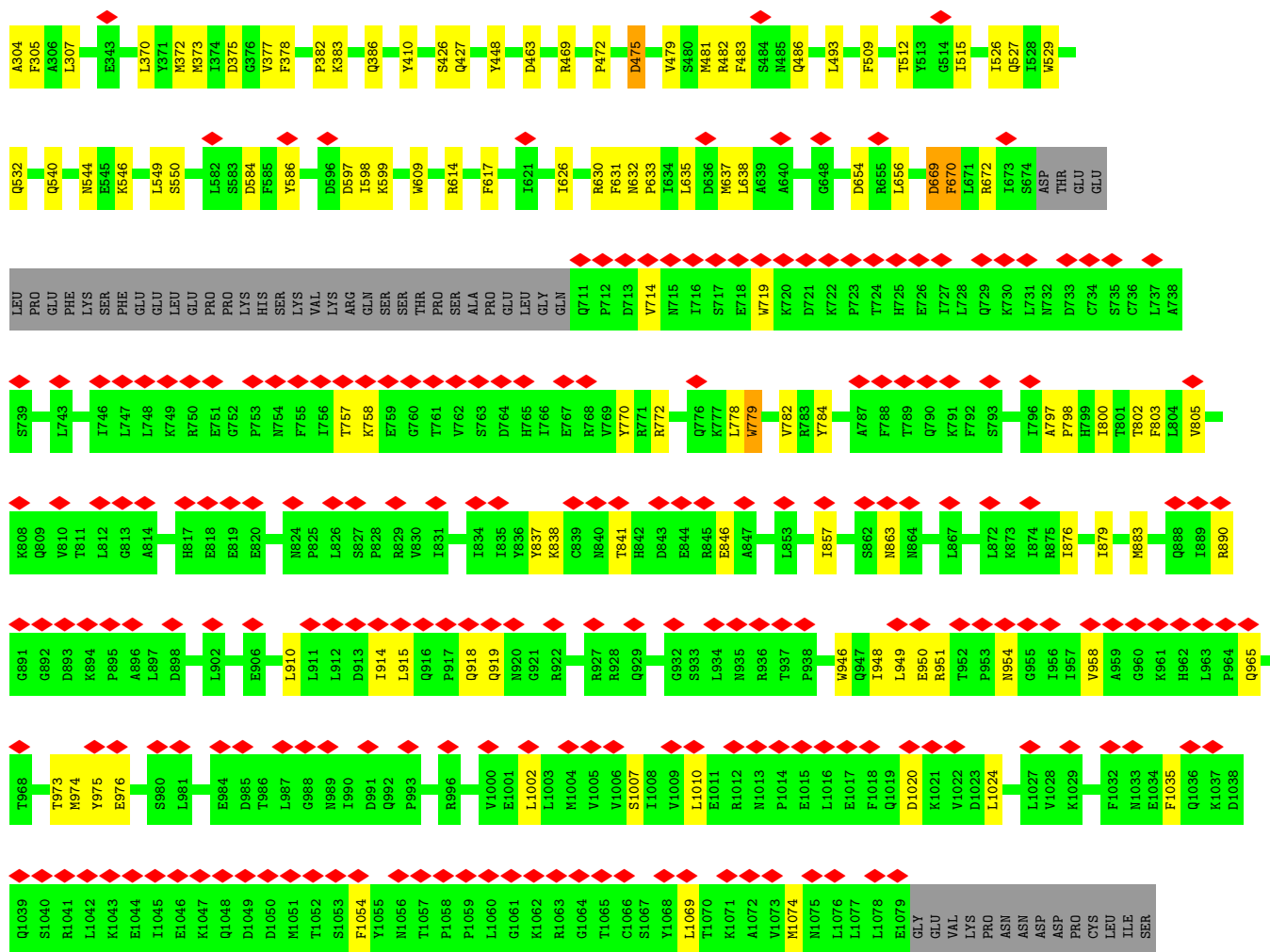


Chain B:



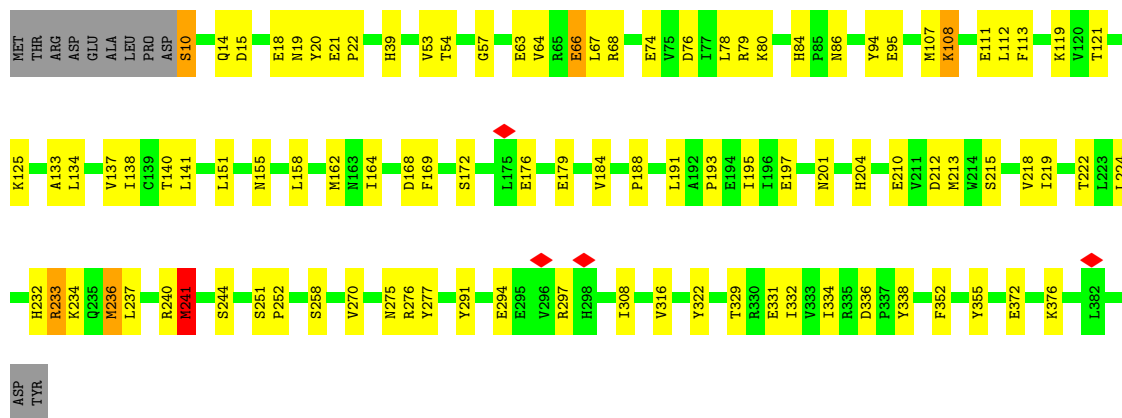
Chain F:





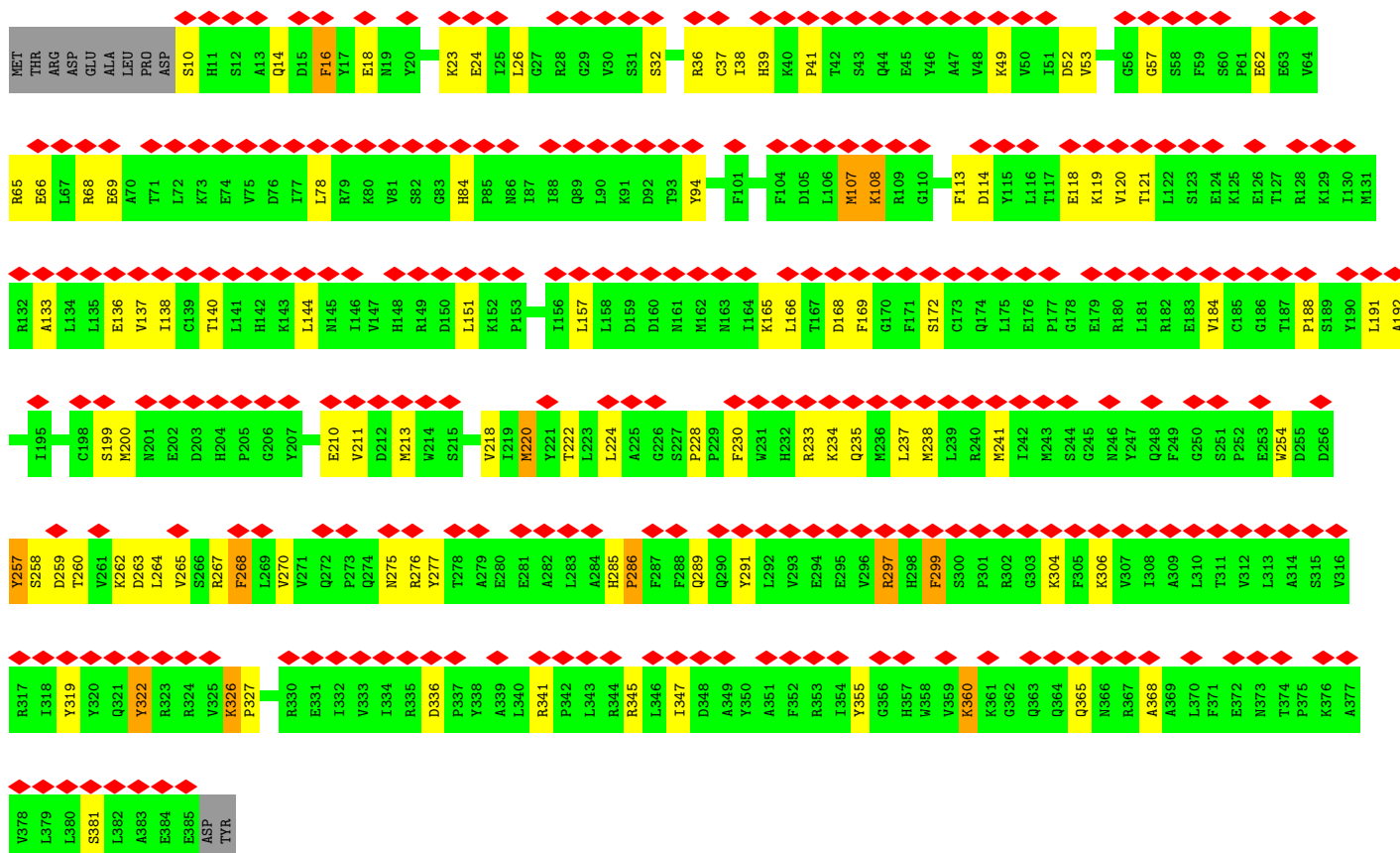
- Molecule 3: Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform

Chain C: 72% 24%

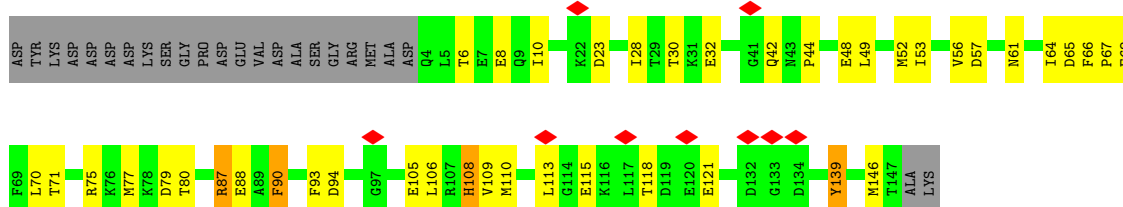


- Molecule 3: Phosphorylase b kinase gamma catalytic chain, skeletal muscle/heart isoform

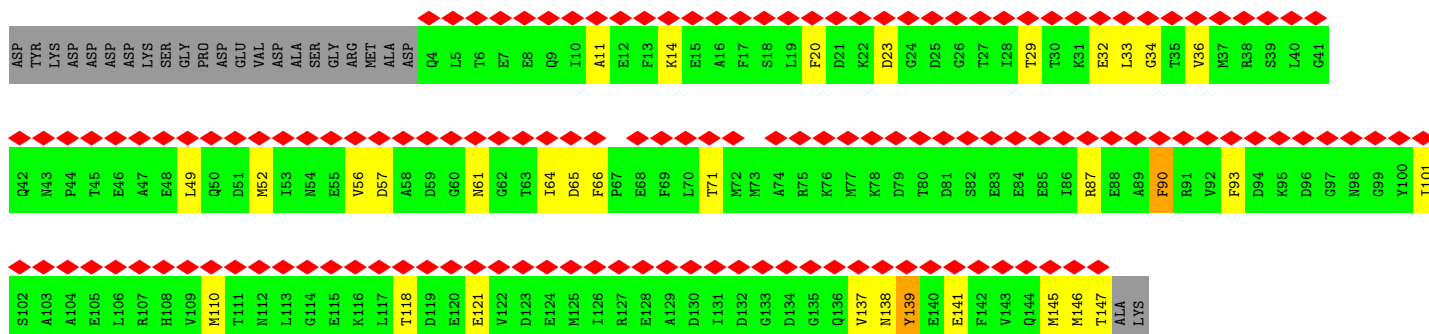
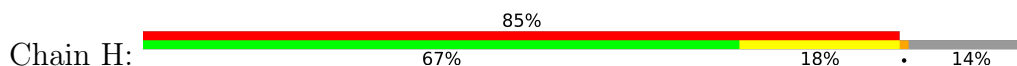
Chain G: 73% 71% 24%



• Molecule 4: Calmodulin-3



• Molecule 4: Calmodulin-3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.610	Depositor
Minimum map value	-1.814	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.25	0/8012	0.51	2/10854 (0.0%)
1	E	0.25	0/8012	0.50	3/10854 (0.0%)
2	B	0.25	0/8230	0.49	1/11158 (0.0%)
2	F	0.25	0/8230	0.49	0/11158
3	C	0.26	0/3136	0.53	1/4243 (0.0%)
3	G	0.27	0/3136	0.55	2/4243 (0.0%)
4	D	0.26	0/1109	0.54	0/1493
4	H	0.25	0/1109	0.48	0/1493
All	All	0.25	0/40974	0.50	9/55496 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	862	PRO	CA-N-CD	-12.44	94.08	111.50
1	A	224	PRO	CA-N-CD	-6.97	101.74	111.50
3	G	286	PRO	CA-N-CD	-6.58	102.29	111.50
1	E	946	LEU	CA-CB-CG	6.15	129.45	115.30
3	C	241	MET	CA-CB-CG	6.14	123.74	113.30
2	B	284	PRO	CA-N-CD	-5.87	103.28	111.50
3	G	286	PRO	N-CD-CG	-5.78	94.54	103.20
1	E	425	PRO	CA-N-CD	-5.76	103.43	111.50
1	E	901	LEU	CA-CB-CG	5.72	128.45	115.30

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	7852	0	7885	77	0
1	E	7852	0	7885	93	0
2	B	8049	0	8041	126	0
2	F	8049	0	8041	86	0
3	C	3065	0	3063	70	0
3	G	3065	0	3063	73	0
4	D	1097	0	1002	29	0
4	H	1097	0	1002	23	0
All	All	40126	0	39982	549	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 7.

All (549) 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)
4:D:42:GLN:HG3	4:D:44:PRO:HD3	1.50	0.93
1:A:861:GLU:HG2	1:A:864:GLU:HB2	1.57	0.84
3:G:286:PRO:HA	3:G:289:GLN:HG2	1.61	0.83
2:F:283:LEU:HD11	2:F:307:LEU:HD11	1.67	0.77
1:E:253:LYS:HD2	1:E:256:ASP:HB2	1.66	0.76
2:B:811:THR:HG22	2:B:821:VAL:HA	1.69	0.74
1:A:1142:ILE:O	1:A:1143:HIS:ND1	2.20	0.74
3:C:138:ILE:HD11	3:C:212:ASP:HB3	1.71	0.72
2:B:254:LEU:HD22	2:B:265:ILE:HD11	1.72	0.70
1:A:1187:LEU:HD12	3:C:376:LYS:HE3	1.73	0.70
2:B:586:TYR:HB2	2:B:779:TRP:HZ3	1.57	0.69
2:B:166:GLU:OE1	2:B:166:GLU:N	2.27	0.68
1:E:18:VAL:HG13	1:E:22:ILE:HD12	1.75	0.68
1:A:884:SER:HB2	1:A:890:ILE:HG23	1.75	0.68
2:B:586:TYR:HB2	2:B:779:TRP:CZ3	2.29	0.67
1:E:144:PHE:O	1:E:148:MET:HG2	1.94	0.67
3:C:111:GLU:N	3:C:111:GLU:OE1	2.26	0.66
3:C:270:VAL:O	3:C:276:ARG:NH1	2.29	0.66
2:B:579:ILE:HG13	2:B:580:PHE:HD1	1.61	0.66
3:C:15:ASP:O	3:C:19:ASN:HB2	1.96	0.65
3:C:232:HIS:CE1	3:C:234:LYS:HB2	2.32	0.65
3:C:232:HIS:HE1	3:C:237:LEU:HD12	1.61	0.65
3:C:79:ARG:NH1	3:C:79:ARG:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:LYS:NZ	2:F:550:SER:OG	2.30	0.65
2:B:105:ASP:OD1	2:F:486:GLN:NE2	2.30	0.65
3:G:210:GLU:HB3	3:G:276:ARG:HH21	1.62	0.65
2:B:846:GLU:OE1	2:B:846:GLU:N	2.28	0.64
3:G:107:MET:HG2	3:G:108:LYS:H	1.62	0.64
3:G:270:VAL:O	3:G:276:ARG:NH1	2.31	0.64
3:C:210:GLU:HB3	3:C:276:ARG:HH21	1.63	0.64
1:A:290:ARG:NH2	1:A:391:ASP:OD1	2.30	0.63
1:E:290:ARG:NH2	1:E:391:ASP:OD1	2.30	0.63
3:C:53:VAL:HG12	3:C:67:LEU:HD22	1.81	0.63
1:E:395:MET:SD	1:E:396:GLY:N	2.71	0.63
3:C:64:VAL:O	3:C:68:ARG:HG3	1.99	0.63
4:D:53:ILE:HD12	4:D:64:ILE:HD11	1.81	0.63
2:B:810:VAL:HG12	2:B:874:ILE:HD12	1.80	0.62
1:E:814:TYR:OH	1:E:830:SER:OG	2.17	0.62
2:B:515:ILE:HD13	2:B:638:LEU:HD23	1.81	0.62
2:F:283:LEU:HD21	2:F:307:LEU:HD21	1.81	0.62
1:E:527:GLN:OE1	1:E:527:GLN:N	2.25	0.62
4:H:87:ARG:NH1	4:H:139:TYR:OH	2.33	0.62
2:B:362:GLU:O	2:B:429:ARG:NH2	2.33	0.62
1:A:1107:PHE:O	1:A:1111:VAL:HG23	2.00	0.61
3:C:169:PHE:O	3:C:172:SER:OG	2.15	0.61
1:E:378:ASP:OD1	1:E:379:ARG:N	2.32	0.61
2:B:332:ARG:HH21	2:B:333:PHE:HE1	1.48	0.61
1:A:1192:ALA:HB3	3:C:372:GLU:HG2	1.82	0.61
2:B:944:ARG:HA	2:B:947:GLN:HG2	1.82	0.61
3:C:107:MET:O	3:C:108:LYS:HB2	2.00	0.61
1:A:86:ARG:NH1	1:A:155:ILE:O	2.34	0.61
2:F:879:ILE:HG22	2:F:883:MET:HE1	1.83	0.61
1:A:1076:TRP:NE1	1:A:1097:THR:OG1	2.34	0.61
3:C:219:ILE:HA	3:C:222:THR:HG22	1.82	0.61
2:F:846:GLU:OE1	2:F:846:GLU:N	2.26	0.60
1:A:1151:VAL:HA	1:A:1154:ILE:HG12	1.82	0.60
4:D:106:LEU:O	4:D:110:MET:HG2	2.01	0.60
2:F:162:LEU:HD11	2:F:167:TYR:HB2	1.82	0.60
2:B:140:LYS:NZ	2:B:550:SER:OG	2.34	0.60
3:C:232:HIS:CE1	3:C:237:LEU:HD12	2.36	0.60
1:E:51:ILE:HD11	1:E:84:LEU:HD13	1.84	0.60
2:F:73:THR:HG23	2:F:82:ALA:HA	1.84	0.60
2:F:1002:LEU:HD13	2:F:1069:LEU:HD22	1.84	0.60
2:B:973:THR:HG22	2:B:974:MET:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:SER:HB3	4:D:71:THR:HG23	1.83	0.59
1:E:268:PHE:O	1:E:428:ARG:NH2	2.35	0.59
1:E:216:ASP:HB3	1:E:227:VAL:HG12	1.83	0.59
2:B:50:ASP:O	2:B:54:ARG:HG3	2.01	0.59
1:E:323:ASN:HD21	1:E:387:PRO:HB3	1.68	0.59
1:E:585:ALA:O	1:E:589:MET:HG2	2.02	0.59
3:G:258:SER:HB3	4:H:71:THR:HG23	1.83	0.59
3:G:286:PRO:HA	3:G:289:GLN:CG	2.33	0.59
1:E:45:ARG:NH1	1:E:134:GLN:OE1	2.35	0.58
2:F:954:ASN:ND2	2:F:1020:ASP:OD1	2.36	0.58
3:G:264:LEU:HG	3:G:268:PHE:CZ	2.39	0.58
3:G:297:ARG:HH22	4:H:14:LYS:HD3	1.68	0.58
3:C:331:GLU:HA	3:C:334:ILE:HD12	1.85	0.58
2:B:541:LEU:HB2	2:B:670:PHE:CE1	2.39	0.58
2:B:829:ARG:O	2:B:833:ASN:ND2	2.37	0.58
1:E:397:LYS:HG3	1:E:399:PRO:HD2	1.84	0.58
2:F:98:ALA:HB2	2:F:114:LEU:HB2	1.85	0.57
2:B:544:ASN:H	2:B:549:LEU:HB2	1.68	0.57
1:A:51:ILE:HD13	1:A:84:LEU:HD13	1.87	0.57
1:A:451:ILE:O	1:A:455:LEU:HG	2.03	0.57
2:B:101:TYR:HB3	2:B:111:THR:HG22	1.87	0.57
2:B:780:LEU:HD23	2:B:781:ALA:H	1.69	0.57
2:F:111:THR:O	2:F:115:GLU:HG2	2.04	0.57
2:F:798:PRO:O	2:F:802:THR:HG22	2.04	0.57
2:F:633:PRO:O	2:F:637:MET:HG2	2.04	0.57
3:G:65:ARG:O	3:G:69:GLU:HG2	2.04	0.57
1:A:124:VAL:HG23	1:A:125:VAL:HG13	1.87	0.57
2:B:108:LYS:HE2	1:E:224:PRO:HD2	1.87	0.57
2:B:820:GLU:OE2	2:B:820:GLU:N	2.37	0.57
3:G:263:ASP:HB3	3:G:267:ARG:HH21	1.69	0.57
3:C:236:MET:CE	3:C:236:MET:H	2.18	0.57
3:G:26:LEU:HD21	3:G:36:ARG:HD2	1.85	0.57
2:F:50:ASP:O	2:F:54:ARG:HG3	2.04	0.57
3:G:264:LEU:HD13	3:G:285:HIS:CG	2.40	0.57
3:G:137:VAL:HG11	3:G:166:LEU:HD13	1.87	0.56
1:E:1076:TRP:NE1	1:E:1097:THR:OG1	2.38	0.56
2:B:846:GLU:HA	2:B:849:ILE:HD12	1.88	0.56
1:A:1086:SER:HB2	1:A:1091:VAL:HG12	1.86	0.56
2:B:495:VAL:HG23	2:B:615:PRO:HG2	1.88	0.56
4:D:75:ARG:HH11	4:D:77:MET:HE1	1.70	0.56
2:B:88:LEU:HD23	2:B:177:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:829:ARG:HG2	2:B:833:ASN:HD21	1.70	0.56
1:E:582:ILE:HD12	1:E:582:ILE:H	1.71	0.56
1:A:1191:SER:OG	3:C:376:LYS:NZ	2.38	0.56
1:E:511:TYR:HD2	1:E:520:PHE:HE2	1.53	0.56
2:B:954:ASN:ND2	2:B:1020:ASP:OD1	2.36	0.55
1:A:920:ILE:O	1:A:924:ILE:HG13	2.07	0.55
3:G:23:LYS:HD2	3:G:36:ARG:NH1	2.21	0.55
1:A:1092:LEU:HD12	1:A:1114:VAL:HG21	1.88	0.55
2:B:626:ILE:HB	2:B:631:PHE:HB2	1.87	0.55
3:C:162:MET:SD	3:C:162:MET:N	2.80	0.55
4:D:30:THR:HB	4:D:49:LEU:HD21	1.89	0.55
4:D:48:GLU:O	4:D:52:MET:HG3	2.07	0.55
3:G:24:GLU:CD	3:G:36:ARG:HD3	2.26	0.55
1:A:43:TRP:O	1:A:47:ASN:ND2	2.37	0.55
1:A:359:LEU:HD21	1:A:367:PRO:HB3	1.88	0.55
1:A:1106:LYS:HZ3	1:A:1110:HIS:HB2	1.72	0.55
1:E:336:ILE:HG23	1:E:348:VAL:HG13	1.88	0.55
1:E:897:ILE:O	1:E:901:LEU:HD12	2.06	0.55
1:E:1200:MET:HE1	3:G:347:ILE:HG23	1.89	0.55
3:G:23:LYS:NZ	3:G:38:ILE:HG12	2.22	0.55
1:A:319:LYS:O	1:A:384:TYR:OH	2.20	0.54
2:B:250:ASN:ND2	2:B:481:MET:SD	2.77	0.54
2:B:440:LEU:HD22	2:B:445:GLN:NE2	2.21	0.54
1:E:572:ASP:OD1	1:E:575:GLY:N	2.39	0.54
2:B:568:ILE:HD11	2:B:668:LEU:HD13	1.90	0.54
2:B:1002:LEU:HD13	2:B:1069:LEU:HD22	1.89	0.54
4:D:8:GLU:OE1	4:D:8:GLU:N	2.37	0.54
2:F:101:TYR:HB3	2:F:111:THR:HG22	1.90	0.54
4:D:79:ASP:OD1	4:D:80:THR:N	2.40	0.54
3:G:53:VAL:HG21	3:G:68:ARG:HH21	1.72	0.54
3:G:84:HIS:HD2	3:G:140:THR:HG21	1.72	0.54
3:C:84:HIS:HD2	3:C:140:THR:HG21	1.73	0.54
2:F:540:GLN:HB3	2:F:670:PHE:HZ	1.73	0.54
1:E:506:GLY:HA2	1:E:509:LYS:HE3	1.90	0.53
1:A:309:ASN:OD1	1:A:309:ASN:N	2.40	0.53
3:C:112:LEU:HD23	3:C:158:LEU:HD11	1.91	0.53
4:H:90:PHE:CE1	4:H:101:ILE:HD11	2.43	0.53
2:B:1023:ASP:HB2	2:B:1026:ARG:HB2	1.91	0.53
1:A:51:ILE:HG12	1:A:81:VAL:HG23	1.90	0.53
2:F:586:TYR:HB3	2:F:782:VAL:HG11	1.90	0.53
1:E:47:ASN:HD21	1:E:84:LEU:HD11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:GLN:N	2:F:258:GLN:OE1	2.41	0.53
2:F:626:ILE:HB	2:F:631:PHE:HB2	1.89	0.53
2:B:944:ARG:HG2	2:B:947:GLN:HE21	1.73	0.53
1:A:370:PRO:HA	1:A:398:LEU:HB2	1.91	0.53
3:C:329:THR:HB	3:C:332:ILE:HG12	1.90	0.53
1:A:808:GLU:O	1:A:812:GLU:HG2	2.09	0.52
1:A:1100:MET:SD	1:A:1106:LYS:HG3	2.49	0.52
2:F:669:ASP:HB2	2:F:672:ARG:HH22	1.74	0.52
2:F:526:ILE:HG21	2:F:656:LEU:HD21	1.90	0.52
3:G:228:PRO:HD2	3:G:368:ALA:HB2	1.91	0.52
4:D:23:ASP:OD1	4:D:23:ASP:N	2.42	0.52
1:A:514:ARG:NH1	1:A:619:MET:O	2.43	0.52
3:C:193:PRO:O	3:C:197:GLU:HG2	2.10	0.52
2:F:779:TRP:HE3	2:F:779:TRP:H	1.57	0.52
2:B:148:CYS:HB2	2:B:170:LEU:HD13	1.91	0.52
3:C:86:ASN:ND2	3:C:164:ILE:O	2.43	0.52
3:C:201:ASN:HB3	3:C:204:HIS:CE1	2.45	0.52
2:F:597:ASP:OD1	2:F:598:ILE:N	2.43	0.52
2:B:546:LYS:HE2	1:E:28:PRO:HD2	1.91	0.52
3:C:270:VAL:HG11	3:C:275:ASN:HB2	1.91	0.52
1:A:263:VAL:HG12	1:A:263:VAL:O	2.10	0.52
1:A:526:ASP:OD1	1:A:528:GLN:HG2	2.10	0.52
1:A:173:GLU:OE2	1:A:500:ARG:NH1	2.44	0.51
1:A:268:PHE:O	1:A:428:ARG:NH2	2.39	0.51
1:A:336:ILE:HG13	1:A:348:VAL:HG13	1.91	0.51
2:B:778:LEU:O	2:B:782:VAL:HG23	2.10	0.51
3:G:270:VAL:HG11	3:G:275:ASN:HB2	1.91	0.51
3:C:215:SER:O	3:C:219:ILE:HG23	2.11	0.51
1:E:44:VAL:O	1:E:48:VAL:HG23	2.10	0.51
2:F:584:ASP:HB2	2:F:770:TYR:HE2	1.74	0.51
2:B:467:VAL:O	2:B:468:GLN:NE2	2.44	0.51
3:G:297:ARG:NH2	4:H:14:LYS:HD3	2.25	0.51
2:B:877:GLY:O	2:B:880:ILE:HG22	2.10	0.51
3:C:188:PRO:HA	3:C:191:LEU:HD23	1.91	0.51
4:H:56:VAL:HG21	4:H:64:ILE:HD11	1.91	0.51
2:F:273:ASN:O	2:F:277:GLN:HG2	2.11	0.51
2:B:847:ALA:O	2:B:851:GLN:HG3	2.11	0.51
1:E:1059:ARG:NH2	1:E:1122:GLU:OE2	2.44	0.51
2:F:879:ILE:O	2:F:883:MET:HE2	2.11	0.51
2:B:223:ARG:HD2	2:B:338:TYR:CE2	2.47	0.50
3:C:10:SER:OG	3:C:95:GLU:OE1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1051:MET:O	2:B:1051:MET:HG2	2.11	0.50
3:C:119:LYS:O	3:C:121:THR:N	2.45	0.50
2:F:883:MET:HB3	2:F:910:LEU:HG	1.93	0.50
3:G:234:LYS:HB2	3:G:237:LEU:HG	1.94	0.50
1:E:586:LEU:HA	1:E:589:MET:HG2	1.92	0.50
1:A:68:ASP:OD1	1:A:68:ASP:N	2.37	0.50
2:F:838:LYS:O	2:F:841:THR:OG1	2.23	0.50
3:C:237:LEU:HD22	3:C:240:ARG:HH11	1.77	0.50
1:E:583:LEU:HG	1:E:587:ARG:HE	1.77	0.50
3:G:39:HIS:CD2	3:G:41:PRO:HD2	2.47	0.50
2:B:418:GLU:OE1	2:B:418:GLU:N	2.39	0.50
2:B:441:PHE:H	2:B:445:GLN:HE22	1.59	0.50
2:B:1052:THR:HA	2:B:1055:TYR:CD2	2.47	0.50
1:E:584:ALA:O	1:E:588:LYS:HG3	2.11	0.50
2:B:98:ALA:HB2	2:B:114:LEU:HB2	1.94	0.50
3:C:308:ILE:HD11	4:D:113:LEU:HD13	1.93	0.50
2:F:299:CYS:HA	2:F:304:ALA:CB	2.42	0.50
2:F:958:VAL:HG23	2:F:1024:LEU:HD11	1.92	0.50
3:G:235:GLN:HA	3:G:238:MET:SD	2.52	0.50
3:C:74:GLU:O	3:C:78:LEU:HG	2.12	0.49
2:F:632:ASN:HA	2:F:635:LEU:HD12	1.94	0.49
3:G:23:LYS:HB2	3:G:36:ARG:HG3	1.93	0.49
3:C:232:HIS:CD2	3:C:233:ARG:N	2.80	0.49
1:A:572:ASP:OD1	1:A:575:GLY:N	2.46	0.49
3:C:316:VAL:HG21	4:D:88:GLU:HB3	1.94	0.49
4:H:65:ASP:OD1	4:H:66:PHE:N	2.40	0.49
3:G:16:PHE:HB2	3:G:94:TYR:HD2	1.77	0.49
1:E:1086:SER:HB2	1:E:1091:VAL:HG12	1.93	0.49
1:A:453:THR:HG23	1:A:456:LYS:HE2	1.94	0.49
1:A:847:LEU:HD23	1:A:854:LEU:HD11	1.94	0.49
3:C:237:LEU:O	3:C:241:MET:SD	2.71	0.49
3:C:336:ASP:OD1	3:C:336:ASP:N	2.45	0.49
1:E:1200:MET:HE1	3:G:347:ILE:HG12	1.95	0.49
2:F:515:ILE:HG12	2:F:638:LEU:HD22	1.94	0.49
1:E:502:MET:SD	1:E:502:MET:N	2.85	0.49
1:E:584:ALA:HB2	3:G:57:GLY:HA3	1.95	0.49
2:F:946:TRP:NE1	2:F:950:GLU:OE2	2.45	0.49
2:B:838:LYS:O	2:B:841:THR:OG1	2.22	0.49
2:F:193:ILE:HD12	2:F:198:GLU:HB3	1.95	0.49
1:A:859:PRO:O	1:A:863:ARG:NH2	2.46	0.48
2:B:173:ASN:HD22	2:B:220:VAL:HG22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:373:MET:O	2:F:377:VAL:HG12	2.13	0.48
2:B:134:ASP:OD1	2:B:135:LYS:N	2.45	0.48
1:E:51:ILE:HG13	1:E:84:LEU:HD22	1.94	0.48
1:E:359:LEU:HD21	1:E:367:PRO:HB3	1.95	0.48
1:E:22:ILE:HG23	1:E:401:MET:SD	2.53	0.48
2:F:382:PRO:O	2:F:386:GLN:HG3	2.13	0.48
3:G:213:MET:SD	3:G:213:MET:N	2.85	0.48
2:F:426:SER:OG	2:F:427:GLN:OE1	2.23	0.48
3:G:107:MET:HG2	3:G:108:LYS:N	2.27	0.48
4:D:110:MET:HB3	4:D:115:GLU:HB2	1.94	0.48
2:F:279:LEU:O	2:F:283:LEU:HB2	2.14	0.48
2:F:472:PRO:HG2	2:F:475:ASP:OD1	2.14	0.48
3:G:169:PHE:O	3:G:172:SER:OG	2.32	0.48
2:F:914:ILE:HG13	2:F:915:LEU:N	2.28	0.48
3:G:319:TYR:HA	4:H:52:MET:HE1	1.95	0.48
1:A:894:THR:HG23	1:A:920:ILE:HG21	1.96	0.48
3:G:336:ASP:N	3:G:336:ASP:OD1	2.47	0.48
2:B:890:ARG:O	2:B:890:ARG:NE	2.46	0.48
2:F:951:ARG:HD2	2:F:1010:LEU:HD21	1.96	0.48
2:B:499:LEU:H	2:B:499:LEU:HD23	1.79	0.48
2:F:949:LEU:O	2:F:965:GLN:NE2	2.46	0.48
3:G:299:PHE:HE1	3:G:304:LYS:HG2	1.77	0.48
2:B:173:ASN:OD1	2:B:174:ALA:N	2.47	0.47
2:B:331:LYS:HD2	2:B:332:ARG:H	1.78	0.47
3:C:74:GLU:HA	3:C:74:GLU:OE1	2.14	0.47
4:D:66:PHE:HB3	4:D:67:PRO:HD3	1.94	0.47
3:G:192:ALA:HB3	3:G:211:VAL:HG12	1.96	0.47
2:B:497:VAL:HG23	2:B:617:PHE:HB3	1.95	0.47
4:H:90:PHE:HE1	4:H:101:ILE:HD11	1.79	0.47
2:B:52:TYR:HD1	2:B:55:ILE:HD11	1.79	0.47
1:E:847:LEU:HB3	1:E:854:LEU:HD11	1.96	0.47
2:F:50:ASP:OD2	2:F:54:ARG:NH2	2.40	0.47
3:G:114:ASP:O	3:G:118:GLU:HG2	2.14	0.47
2:B:440:LEU:HD22	2:B:445:GLN:HE21	1.79	0.47
2:B:859:TRP:CZ3	2:B:863:ASN:HB3	2.48	0.47
3:C:234:LYS:HB3	3:C:236:MET:SD	2.54	0.47
2:F:544:ASN:H	2:F:549:LEU:HB2	1.79	0.47
3:C:15:ASP:HB2	3:C:94:TYR:HE2	1.79	0.47
1:E:583:LEU:O	1:E:586:LEU:HG	2.15	0.47
1:E:847:LEU:HD13	1:E:854:LEU:HD11	1.95	0.47
2:F:778:LEU:O	2:F:782:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:119:LYS:O	3:G:121:THR:N	2.46	0.47
3:G:319:TYR:HA	4:H:52:MET:CE	2.44	0.47
1:A:464:THR:OG1	1:A:465:ILE:N	2.46	0.47
2:B:154:ASN:HB2	2:B:161:LEU:HD23	1.96	0.47
2:B:283:LEU:HD21	2:B:307:LEU:HD11	1.97	0.47
1:E:1131:ILE:O	1:E:1135:THR:HG23	2.15	0.47
1:A:837:VAL:HG12	1:A:895:GLN:HE21	1.80	0.47
2:F:890:ARG:O	2:F:890:ARG:NE	2.45	0.47
4:H:57:ASP:OD2	4:H:61:ASN:ND2	2.47	0.47
1:A:220:VAL:HG13	1:A:221:LYS:HG3	1.97	0.47
1:A:1106:LYS:HD2	1:A:1106:LYS:O	2.15	0.47
2:B:298:PRO:O	2:B:303:PRO:HG2	2.15	0.47
2:B:779:TRP:CE3	2:B:779:TRP:HA	2.50	0.47
2:B:946:TRP:NE1	2:B:950:GLU:OE2	2.48	0.47
3:C:215:SER:HA	3:C:218:VAL:HG12	1.97	0.47
1:E:1130:ALA:O	1:E:1133:VAL:HG12	2.15	0.47
2:F:243:LYS:O	2:F:247:GLU:HG3	2.15	0.47
3:C:251:SER:HB3	3:C:252:PRO:HD3	1.97	0.47
1:E:129:GLN:HA	1:E:129:GLN:OE1	2.14	0.47
2:F:299:CYS:HA	2:F:304:ALA:HB3	1.97	0.47
3:G:84:HIS:CD2	3:G:140:THR:HG21	2.50	0.47
1:E:349:GLN:O	1:E:353:GLU:HG2	2.15	0.47
1:E:90:HIS:O	1:E:94:ARG:HG2	2.15	0.46
2:F:797:ALA:HA	2:F:800:ILE:HG12	1.97	0.46
3:G:254:TRP:HA	3:G:257:TYR:HE1	1.79	0.46
1:E:36:SER:HB3	1:E:399:PRO:HG2	1.96	0.46
1:E:887:ASP:O	1:E:889:SER:N	2.48	0.46
2:B:383:LYS:H	2:B:383:LYS:HD2	1.80	0.46
2:B:1052:THR:HA	2:B:1055:TYR:HD2	1.80	0.46
1:E:827:ARG:NH1	1:E:947:MET:O	2.48	0.46
2:B:576:TYR:HD2	2:B:618:LEU:HD23	1.80	0.46
1:E:191:ASN:HB2	1:E:313:TYR:HB2	1.95	0.46
1:E:1100:MET:HE2	1:E:1107:PHE:H	1.80	0.46
2:F:304:ALA:O	2:F:469:ARG:NH2	2.44	0.46
3:G:297:ARG:HE	4:H:11:ALA:HB1	1.80	0.46
1:A:538:MET:O	1:A:542:MET:HG3	2.16	0.46
1:A:1132:LEU:HA	1:A:1132:LEU:HD23	1.78	0.46
1:E:61:TYR:HE2	1:E:70:ASP:HA	1.79	0.46
1:E:294:CYS:SG	1:E:295:ARG:N	2.88	0.46
1:E:1133:VAL:HA	1:E:1136:MET:HE3	1.97	0.46
2:F:974:MET:HG3	2:F:975:TYR:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:ARG:NH1	1:E:415:GLU:OE2	2.49	0.46
2:F:630:ARG:NH1	2:F:633:PRO:HG2	2.31	0.46
3:G:254:TRP:HA	3:G:257:TYR:CE1	2.51	0.46
2:B:501:ALA:HB2	2:B:517:THR:HB	1.98	0.46
2:B:656:LEU:O	2:B:660:ILE:HG12	2.15	0.46
3:C:54:THR:HG22	3:C:57:GLY:H	1.81	0.46
1:E:191:ASN:O	1:E:192:GLN:HG2	2.16	0.46
2:F:86:ASP:OD1	2:F:87:SER:N	2.48	0.46
2:F:918:GLN:O	2:F:919:GLN:NE2	2.48	0.46
2:F:948:ILE:HD11	2:F:1007:SER:HB2	1.98	0.46
2:B:498:ALA:N	2:B:617:PHE:O	2.35	0.46
2:B:589:GLN:O	2:B:630:ARG:NH1	2.48	0.46
2:F:302:TYR:HA	2:F:305:PHE:CE2	2.50	0.46
2:F:631:PHE:CE2	2:F:635:LEU:HD11	2.50	0.46
1:A:554:TRP:NE1	1:A:558:GLY:O	2.43	0.46
1:A:924:ILE:HA	1:A:927:MET:HG3	1.98	0.46
1:A:1129:GLU:OE2	3:C:355:TYR:OH	2.28	0.46
3:C:184:VAL:HG22	3:C:195:ILE:HG22	1.98	0.46
4:D:105:GLU:HA	4:D:108:HIS:ND1	2.31	0.46
2:F:283:LEU:CD2	2:F:307:LEU:HD21	2.46	0.46
2:F:527:GLN:CB	2:F:529:TRP:HE1	2.29	0.46
2:B:811:THR:OG1	2:B:875:ARG:HD2	2.16	0.45
2:F:757:THR:OG1	2:F:758:LYS:N	2.50	0.45
3:G:326:LYS:HE3	3:G:326:LYS:HB2	1.60	0.45
1:A:453:THR:HA	1:A:456:LYS:HD3	1.97	0.45
1:E:817:VAL:HG11	1:E:826:ILE:HB	1.97	0.45
2:F:509:PHE:O	2:F:512:THR:OG1	2.33	0.45
4:H:32:GLU:O	4:H:36:VAL:HG23	2.17	0.45
2:B:803:PHE:HZ	2:B:857:ILE:HG22	1.81	0.45
2:B:780:LEU:HD23	2:B:781:ALA:N	2.30	0.45
2:B:974:MET:SD	2:B:975:TYR:N	2.89	0.45
3:C:14:GLN:O	3:C:18:GLU:HG3	2.16	0.45
1:E:19:GLN:HA	1:E:23:LEU:HB2	1.99	0.45
1:E:263:VAL:HG12	1:E:263:VAL:O	2.15	0.45
1:E:480:SER:HB2	1:E:502:MET:SD	2.57	0.45
3:G:14:GLN:O	3:G:18:GLU:HG3	2.17	0.45
1:A:29:VAL:HG21	2:F:130:MET:HG2	1.98	0.45
1:A:345:ALA:O	1:A:349:GLN:HG2	2.16	0.45
1:A:1106:LYS:HA	1:A:1109:VAL:HG12	1.98	0.45
3:C:241:MET:HA	3:C:244:SER:OG	2.16	0.45
1:E:1133:VAL:HA	1:E:1136:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:ASN:HD22	2:F:220:VAL:HG22	1.81	0.45
2:B:554:ASP:OD1	2:B:554:ASP:N	2.48	0.45
3:G:218:VAL:O	3:G:222:THR:OG1	2.22	0.45
2:B:387:GLU:O	2:B:391:LEU:HG	2.16	0.45
3:C:20:TYR:HE1	3:C:39:HIS:HD1	1.65	0.45
1:E:1159:ASN:ND2	1:E:1184:ILE:HA	2.31	0.45
1:A:584:ALA:HB2	3:C:57:GLY:HA3	1.98	0.45
1:A:604:LEU:H	1:A:604:LEU:HD12	1.80	0.45
1:E:1052:GLY:O	1:E:1056:ARG:NH1	2.50	0.45
1:A:397:LYS:HG3	1:A:399:PRO:HD2	1.99	0.45
2:B:278:THR:HG23	2:B:805:VAL:HG21	1.99	0.45
2:B:538:TYR:HB3	2:B:552:ARG:HD3	1.98	0.45
2:B:757:THR:OG1	2:B:758:LYS:N	2.50	0.45
4:D:93:PHE:CE1	4:D:109:VAL:HG11	2.52	0.45
1:E:535:ASP:HB3	1:E:538:MET:HB2	1.99	0.45
1:E:1129:GLU:OE2	3:G:355:TYR:OH	2.29	0.45
1:A:1172:ASP:OD1	1:A:1174:THR:OG1	2.29	0.44
2:B:382:PRO:O	2:B:385:VAL:HG22	2.18	0.44
2:B:672:ARG:HA	2:B:672:ARG:HD2	1.77	0.44
1:E:60:ALA:HB2	1:E:418:LEU:HG	1.98	0.44
1:E:119:LYS:O	1:E:120:THR:OG1	2.26	0.44
1:E:336:ILE:HD12	1:E:336:ILE:H	1.82	0.44
1:E:905:MET:HG3	1:E:912:PHE:CE1	2.53	0.44
1:A:763:PHE:HA	1:A:766:LEU:HD12	1.99	0.44
2:B:165:GLU:N	2:B:165:GLU:OE1	2.50	0.44
2:B:194:TYR:CD1	1:E:79:GLN:HG3	2.52	0.44
2:B:410:TYR:HB3	2:B:429:ARG:HD3	1.98	0.44
1:E:184:TRP:CZ2	1:E:295:ARG:HG2	2.52	0.44
3:G:16:PHE:HB2	3:G:94:TYR:CD2	2.52	0.44
4:H:118:THR:HG23	4:H:121:GLU:H	1.82	0.44
2:F:383:LYS:H	2:F:383:LYS:HG2	1.61	0.44
2:B:73:THR:OG1	2:B:83:LYS:NZ	2.38	0.44
2:B:335:ARG:NH1	2:B:359:ASP:OD2	2.51	0.44
4:D:87:ARG:HG3	4:D:139:TYR:OH	2.18	0.44
3:G:265:VAL:HA	3:G:268:PHE:CE2	2.52	0.44
3:C:372:GLU:O	3:C:372:GLU:HG3	2.18	0.44
4:D:57:ASP:OD2	4:D:61:ASN:ND2	2.50	0.44
2:B:225:SER:HA	2:B:233:GLU:OE2	2.18	0.44
1:E:96:VAL:HG21	1:E:492:MET:SD	2.57	0.44
2:F:493:LEU:HD11	2:F:609:TRP:HD1	1.83	0.44
2:B:253:ASN:HD21	2:B:259:GLY:HA3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:ALA:O	3:C:137:VAL:HG23	2.18	0.44
1:E:438:VAL:HG11	1:E:554:TRP:HD1	1.83	0.44
3:G:133:ALA:O	3:G:136:GLU:HG2	2.17	0.44
3:G:341:ARG:O	3:G:345:ARG:HG3	2.18	0.44
4:H:33:LEU:HD11	4:H:49:LEU:HG	2.00	0.44
1:A:139:SER:HB2	1:A:204:MET:HG3	1.99	0.43
1:A:825:LEU:O	1:A:829:ILE:HG23	2.18	0.43
2:B:86:ASP:OD1	2:B:87:SER:N	2.51	0.43
2:B:999:VAL:HG13	2:B:1024:LEU:HD21	2.00	0.43
3:C:294:GLU:O	3:C:297:ARG:NH2	2.38	0.43
2:B:918:GLN:O	2:B:919:GLN:NE2	2.49	0.43
2:F:479:VAL:HG11	2:F:482:ARG:HB2	2.00	0.43
3:G:37:CYS:O	3:G:38:ILE:HD13	2.18	0.43
2:B:193:ILE:HD12	2:B:254:LEU:HG	2.00	0.43
2:B:880:ILE:HD12	2:B:883:MET:SD	2.59	0.43
3:C:155:ASN:ND2	3:C:168:ASP:OD2	2.51	0.43
1:E:216:ASP:N	1:E:216:ASP:OD1	2.51	0.43
3:G:220:MET:O	3:G:224:LEU:HG	2.17	0.43
3:G:108:LYS:HA	3:G:108:LYS:HD3	1.73	0.43
2:B:300:ILE:O	2:B:300:ILE:HG22	2.17	0.43
2:B:312:LEU:O	2:B:315:GLN:HG2	2.18	0.43
2:F:99:LEU:HD21	2:F:463:ASP:HB3	1.99	0.43
2:B:802:THR:HA	2:B:805:VAL:HG12	2.01	0.43
3:C:232:HIS:CE1	3:C:237:LEU:HB2	2.53	0.43
4:D:52:MET:O	4:D:56:VAL:HG12	2.19	0.43
4:D:118:THR:HG23	4:D:121:GLU:H	1.83	0.43
2:F:529:TRP:N	2:F:529:TRP:CD1	2.85	0.43
2:B:493:LEU:HD12	2:B:494:VAL:N	2.33	0.43
4:D:49:LEU:O	4:D:53:ILE:HG12	2.19	0.43
1:E:162:VAL:HG22	1:E:217:LEU:HD12	2.00	0.43
3:G:238:MET:HA	3:G:241:MET:SD	2.59	0.43
1:A:378:ASP:OD1	1:A:379:ARG:N	2.52	0.43
4:D:65:ASP:CG	4:D:66:PHE:H	2.23	0.43
2:F:527:GLN:HB2	2:F:529:TRP:HE1	1.84	0.43
2:B:293:ASP:OD1	2:B:293:ASP:N	2.51	0.42
2:B:367:ILE:H	2:B:367:ILE:HG13	1.60	0.42
2:B:772:ARG:HA	2:B:772:ARG:HD2	1.86	0.42
3:G:62:GLU:O	3:G:65:ARG:HG2	2.18	0.42
3:C:224:LEU:HD23	3:C:224:LEU:HA	1.84	0.42
4:D:68:GLU:OE1	4:D:68:GLU:N	2.42	0.42
1:E:336:ILE:HG13	1:E:351:TYR:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:SER:OG	3:G:49:LYS:NZ	2.52	0.42
1:A:450:GLU:O	1:A:454:ILE:HG12	2.19	0.42
1:A:582:ILE:O	1:A:586:LEU:HD23	2.18	0.42
2:B:549:LEU:HD23	2:B:549:LEU:HA	1.74	0.42
3:C:213:MET:SD	3:C:213:MET:N	2.92	0.42
4:D:6:THR:O	4:D:10:ILE:HG12	2.19	0.42
4:D:28:ILE:O	4:D:32:GLU:HB2	2.19	0.42
4:D:66:PHE:O	4:D:70:LEU:HD13	2.19	0.42
2:F:370:LEU:HD22	2:F:448:TYR:HA	2.01	0.42
3:G:184:VAL:HG21	3:G:199:SER:HB3	2.01	0.42
3:C:63:GLU:O	3:C:66:GLU:HG3	2.19	0.42
3:C:141:LEU:HD23	3:C:141:LEU:HA	1.91	0.42
1:E:894:THR:HG23	1:E:920:ILE:HG21	2.01	0.42
2:F:802:THR:HA	2:F:805:VAL:HG12	2.02	0.42
2:F:803:PHE:HZ	2:F:857:ILE:HG22	1.84	0.42
3:G:157:LEU:HD21	3:G:165:LYS:HG3	2.01	0.42
2:B:307:LEU:HD23	2:B:307:LEU:HA	1.75	0.42
3:C:236:MET:SD	3:C:236:MET:N	2.91	0.42
1:E:302:LYS:HD3	1:E:395:MET:HG3	2.02	0.42
2:F:173:ASN:OD1	2:F:174:ALA:N	2.53	0.42
2:F:546:LYS:HD3	2:F:546:LYS:HA	1.88	0.42
3:G:291:TYR:HB3	4:H:14:LYS:HE2	2.00	0.42
1:A:916:PHE:HZ	1:A:1105:ILE:HG23	1.84	0.42
2:B:104:ILE:HG22	2:B:106:ASP:H	1.84	0.42
2:B:264:VAL:C	2:B:265:ILE:HD13	2.40	0.42
2:B:442:LEU:HA	2:B:445:GLN:OE1	2.19	0.42
2:B:876:ILE:HA	2:B:879:ILE:HD12	2.00	0.42
2:B:951:ARG:HD2	2:B:1010:LEU:HD21	2.02	0.42
1:E:217:LEU:HD11	1:E:228:ILE:HD11	2.00	0.42
1:A:437:ASP:N	1:A:437:ASP:OD1	2.53	0.42
3:C:176:GLU:HB3	3:C:179:GLU:HG2	2.01	0.42
4:D:75:ARG:HD3	4:D:77:MET:HE3	2.01	0.42
1:E:28:PRO:O	1:E:29:VAL:HB	2.20	0.42
3:G:306:LYS:CE	4:H:147:THR:HB	2.48	0.42
1:A:306:GLU:HB2	1:A:321:PHE:CE1	2.55	0.42
3:C:169:PHE:HB3	3:C:172:SER:OG	2.19	0.42
3:G:52:ASP:OD1	3:G:52:ASP:N	2.45	0.42
1:A:1163:LEU:HD13	1:A:1176:LEU:HD12	2.01	0.42
2:B:123:ARG:HE	2:B:194:TYR:HE2	1.67	0.42
2:B:328:TYR:CE2	2:B:429:ARG:HD2	2.55	0.42
3:C:151:LEU:HD13	3:C:151:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:ARG:NH2	1:E:71:LYS:HG2	2.35	0.42
3:G:265:VAL:HA	3:G:268:PHE:CD2	2.55	0.42
3:G:322:TYR:HB2	4:H:52:MET:SD	2.60	0.42
1:A:216:ASP:OD1	1:A:216:ASP:N	2.52	0.41
2:B:328:TYR:CD2	2:B:429:ARG:HD2	2.55	0.41
2:B:590:ASP:HB3	2:B:593:LEU:HB2	2.02	0.41
2:B:714:VAL:HG13	2:B:719:TRP:CD2	2.55	0.41
1:E:363:LYS:HD2	1:E:364:ASN:N	2.35	0.41
1:E:554:TRP:NE1	1:E:558:GLY:O	2.45	0.41
2:B:837:TYR:O	2:B:841:THR:HG23	2.20	0.41
2:B:880:ILE:O	2:B:884:GLU:HG3	2.20	0.41
4:D:106:LEU:HD23	4:D:106:LEU:HA	1.90	0.41
1:E:425:PRO:HD2	1:E:426:LEU:N	2.35	0.41
2:F:837:TYR:O	2:F:841:THR:HG23	2.19	0.41
3:G:254:TRP:HB3	3:G:262:LYS:HE2	2.02	0.41
2:B:309:ASP:HB3	2:B:312:LEU:CD2	2.50	0.41
2:B:798:PRO:HA	2:B:801:THR:HG22	2.02	0.41
3:C:237:LEU:O	3:C:240:ARG:N	2.52	0.41
1:E:130:TRP:HB3	1:E:132:HIS:CE1	2.55	0.41
2:F:772:ARG:HA	2:F:772:ARG:HD2	1.85	0.41
2:B:441:PHE:H	2:B:445:GLN:NE2	2.17	0.41
3:C:134:LEU:HD12	3:C:134:LEU:HA	1.93	0.41
2:F:142:ASP:N	2:F:142:ASP:OD1	2.54	0.41
2:F:714:VAL:HG13	2:F:719:TRP:CD2	2.55	0.41
2:B:1002:LEU:HD13	2:B:1069:LEU:HB3	2.03	0.41
1:E:774:SER:OG	1:E:775:SER:N	2.53	0.41
1:A:386:ASN:O	1:A:389:THR:OG1	2.31	0.41
3:G:78:LEU:HD12	3:G:78:LEU:HA	1.86	0.41
3:G:138:ILE:HD13	3:G:151:LEU:HD11	2.01	0.41
2:B:876:ILE:H	2:B:876:ILE:HD12	1.85	0.41
1:E:326:CYS:HB3	1:E:373:TYR:O	2.21	0.41
3:C:210:GLU:HB3	3:C:276:ARG:HE	1.85	0.41
4:D:90:PHE:O	4:D:94:ASP:N	2.54	0.41
1:E:776:LEU:HD21	1:E:817:VAL:HG22	2.03	0.41
2:F:973:THR:HG22	2:F:976:GLU:HG3	2.03	0.41
3:G:133:ALA:HA	3:G:136:GLU:OE2	2.20	0.41
1:A:19:GLN:HA	1:A:23:LEU:HB2	2.03	0.41
1:A:398:LEU:N	1:A:399:PRO:HD3	2.35	0.41
1:A:1106:LYS:NZ	1:A:1110:HIS:HB2	2.34	0.41
2:B:327:LYS:HG3	2:B:328:TYR:CD1	2.55	0.41
1:E:592:GLY:HA2	1:E:599:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:VAL:HG22	2:F:149:LEU:HD21	2.02	0.41
2:F:876:ILE:HD12	2:F:876:ILE:H	1.85	0.41
3:G:188:PRO:HA	3:G:191:LEU:HG	2.02	0.41
3:G:326:LYS:H	3:G:326:LYS:HG3	1.74	0.41
4:H:33:LEU:HD12	4:H:34:GLY:N	2.36	0.41
4:H:101:ILE:HD13	4:H:137:VAL:HB	2.02	0.41
4:H:137:VAL:HG22	4:H:141:GLU:OE1	2.21	0.41
2:B:579:ILE:HG13	2:B:580:PHE:CD1	2.50	0.41
1:E:306:GLU:HB3	1:E:321:PHE:HE1	1.85	0.41
1:A:321:PHE:HA	1:A:324:ILE:HD11	2.02	0.40
1:A:1186:THR:HA	1:A:1189:TYR:HD2	1.85	0.40
3:G:259:ASP:OD1	3:G:260:THR:N	2.54	0.40
1:A:326:CYS:HB3	1:A:373:TYR:O	2.21	0.40
1:A:438:VAL:HG21	1:A:554:TRP:HD1	1.86	0.40
1:A:1127:LEU:HD12	1:A:1127:LEU:HA	1.85	0.40
2:B:1059:PRO:HA	2:B:1065:THR:HG23	2.02	0.40
3:C:21:GLU:HA	3:C:22:PRO:HD3	1.94	0.40
1:E:6:ASN:O	1:E:10:ARG:HG3	2.21	0.40
1:E:305:LYS:HG3	1:E:306:GLU:H	1.85	0.40
2:F:298:PRO:HA	2:F:301:SER:HG	1.86	0.40
2:F:598:ILE:HG13	2:F:599:LYS:N	2.35	0.40
4:H:23:ASP:OD1	4:H:23:ASP:N	2.42	0.40
3:G:306:LYS:HE2	4:H:147:THR:HB	2.04	0.40
2:B:146:THR:HG22	2:B:164:TYR:OH	2.22	0.40
2:B:443:TRP:NE1	2:B:447:LEU:HD11	2.36	0.40
3:C:79:ARG:HG3	3:C:80:LYS:HD2	2.03	0.40
3:C:236:MET:H	3:C:236:MET:HE3	1.84	0.40
2:F:123:ARG:HD2	2:F:123:ARG:HA	1.89	0.40
2:F:307:LEU:HD23	2:F:307:LEU:HA	1.61	0.40
3:G:360:LYS:H	3:G:365:GLN:HG3	1.87	0.40
1:A:774:SER:OG	1:A:775:SER:N	2.54	0.40
1:A:855:THR:HB	1:A:919:ARG:HA	2.04	0.40
2:B:258:GLN:OE1	1:E:71:LYS:HB3	2.21	0.40
2:B:974:MET:SD	2:B:975:TYR:HB2	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	989/1223 (81%)	917 (93%)	71 (7%)	1 (0%)	48	78
1	E	989/1223 (81%)	913 (92%)	75 (8%)	1 (0%)	48	78
2	B	997/1093 (91%)	971 (97%)	26 (3%)	0	100	100
2	F	997/1093 (91%)	965 (97%)	32 (3%)	0	100	100
3	C	374/387 (97%)	356 (95%)	17 (4%)	1 (0%)	37	67
3	G	374/387 (97%)	355 (95%)	16 (4%)	3 (1%)	16	45
4	D	142/168 (84%)	137 (96%)	5 (4%)	0	100	100
4	H	142/168 (84%)	138 (97%)	3 (2%)	1 (1%)	19	48
All	All	5004/5742 (87%)	4752 (95%)	245 (5%)	7 (0%)	50	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	108	LYS
3	G	108	LYS
3	G	327	PRO
1	A	775	SER
1	E	775	SER
4	H	29	THR
3	G	120	VAL

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	864/1068 (81%)	843 (98%)	21 (2%)	44	66
1	E	864/1068 (81%)	844 (98%)	20 (2%)	45	67
2	B	885/975 (91%)	859 (97%)	26 (3%)	37	61
2	F	885/975 (91%)	859 (97%)	26 (3%)	37	61
3	C	336/349 (96%)	323 (96%)	13 (4%)	27	53
3	G	336/349 (96%)	316 (94%)	20 (6%)	16	41
4	D	114/143 (80%)	109 (96%)	5 (4%)	24	50
4	H	114/143 (80%)	106 (93%)	8 (7%)	12	37
All	All	4398/5070 (87%)	4259 (97%)	139 (3%)	36	59

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	26	GLN
1	A	98	LYS
1	A	105	SER
1	A	272	ASP
1	A	310	ARG
1	A	341	PHE
1	A	483	TYR
1	A	488	CYS
1	A	490	ASN
1	A	502	MET
1	A	530	PHE
1	A	537	LYS
1	A	604	LEU
1	A	612	CYS
1	A	849	SER
1	A	898	MET
1	A	904	TYR
1	A	927	MET
1	A	1110	HIS
1	A	1123	TYR
2	B	76	CYS
2	B	101	TYR
2	B	153	PHE
2	B	167	TYR
2	B	188	SER
2	B	262	TRP

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Mol	Chain	Res	Type
2	B	305	PHE
2	B	313	PHE
2	B	338	TYR
2	B	371	TYR
2	B	378	PHE
2	B	410	TYR
2	B	411	TYR
2	B	480	SER
2	B	576	TYR
2	B	587	MET
2	B	604	PHE
2	B	614	ARG
2	B	617	PHE
2	B	654	ASP
2	B	780	LEU
2	B	784	TYR
2	B	974	MET
2	B	996	ARG
2	B	1035	PHE
2	B	1054	PHE
3	C	10	SER
3	C	66	GLU
3	C	76	ASP
3	C	113	PHE
3	C	125	LYS
3	C	233	ARG
3	C	236	MET
3	C	241	MET
3	C	277	TYR
3	C	291	TYR
3	C	322	TYR
3	C	338	TYR
3	C	352	PHE
4	D	87	ARG
4	D	90	PHE
4	D	108	HIS
4	D	139	TYR
4	D	146	MET
1	E	46	ASP
1	E	66	ASP
1	E	105	SER
1	E	204	MET

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Mol	Chain	Res	Type
1	E	240	SER
1	E	253	LYS
1	E	272	ASP
1	E	341	PHE
1	E	344	ASN
1	E	435	LYS
1	E	437	ASP
1	E	443	SER
1	E	483	TYR
1	E	488	CYS
1	E	492	MET
1	E	530	PHE
1	E	578	LEU
1	E	814	TYR
1	E	946	LEU
1	E	1123	TYR
2	F	76	CYS
2	F	101	TYR
2	F	188	SER
2	F	208	CYS
2	F	217	ASP
2	F	262	TRP
2	F	299	CYS
2	F	372	MET
2	F	375	ASP
2	F	378	PHE
2	F	410	TYR
2	F	475	ASP
2	F	481	MET
2	F	483	PHE
2	F	532	GLN
2	F	614	ARG
2	F	617	PHE
2	F	654	ASP
2	F	669	ASP
2	F	670	PHE
2	F	779	TRP
2	F	784	TYR
2	F	863	ASN
2	F	1035	PHE
2	F	1054	PHE
2	F	1074	MET

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Mol	Chain	Res	Type
3	G	10	SER
3	G	16	PHE
3	G	66	GLU
3	G	107	MET
3	G	113	PHE
3	G	144	LEU
3	G	168	ASP
3	G	200	MET
3	G	220	MET
3	G	230	PHE
3	G	233	ARG
3	G	257	TYR
3	G	268	PHE
3	G	277	TYR
3	G	297	ARG
3	G	299	PHE
3	G	322	TYR
3	G	326	LYS
3	G	360	LYS
3	G	381	SER
4	H	20	PHE
4	H	90	PHE
4	H	93	PHE
4	H	110	MET
4	H	138	ASN
4	H	139	TYR
4	H	145	MET
4	H	146	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
2	B	171	GLN
2	B	833	ASN
2	B	947	GLN
3	C	232	HIS
1	E	47	ASN
1	E	323	ASN
3	G	19	ASN
3	G	39	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

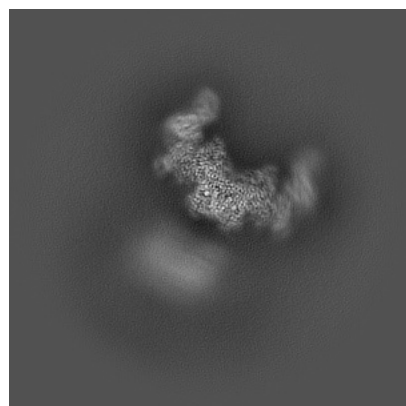
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39777. These allow visual inspection of the internal detail of the map and identification of artifacts.

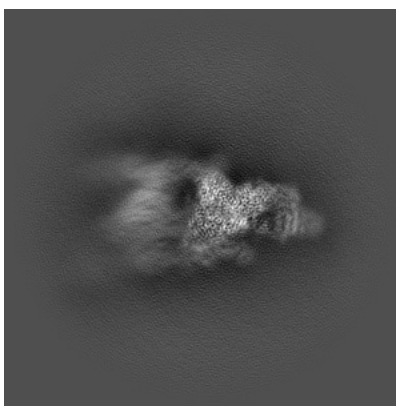
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

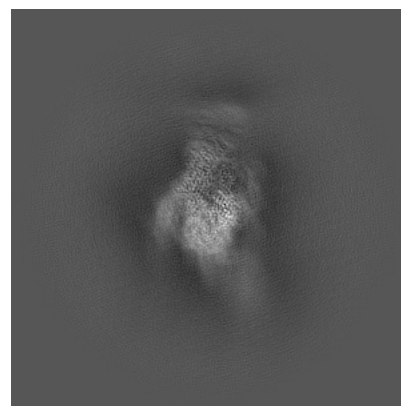
6.1.1 Primary map



X

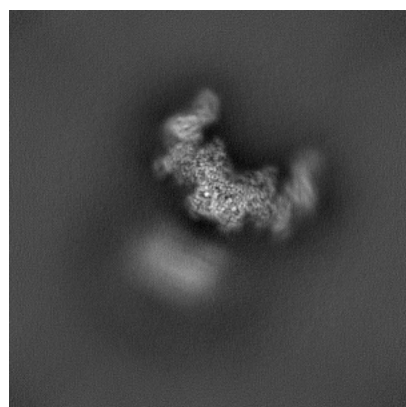


Y

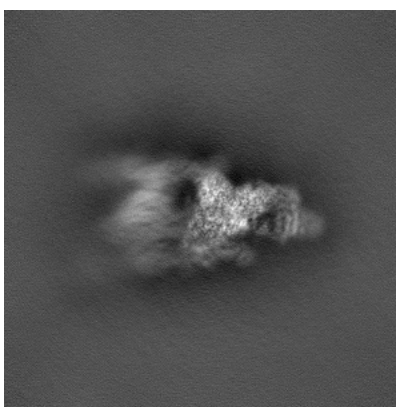


Z

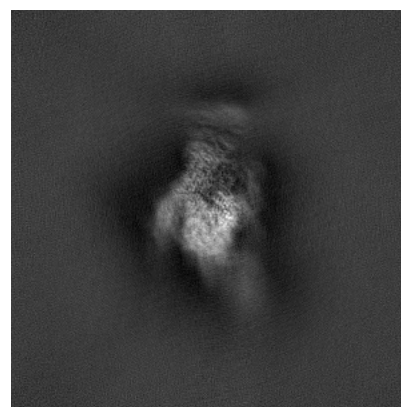
6.1.2 Raw map



X



Y

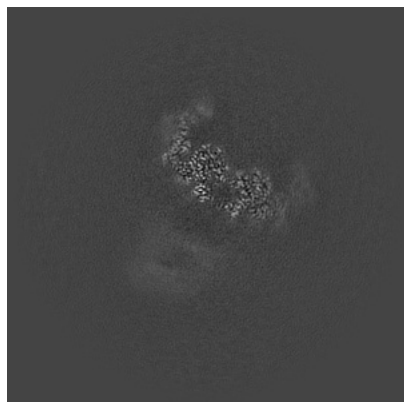


Z

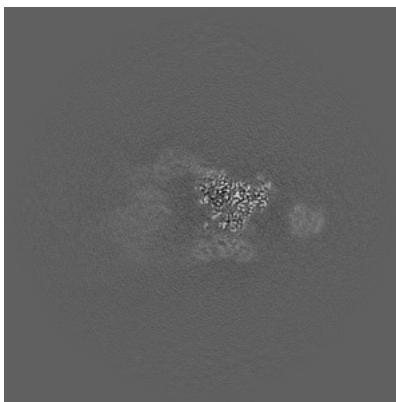
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

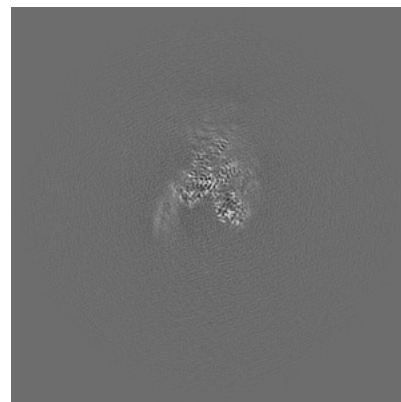
6.2.1 Primary map



X Index: 240



Y Index: 240

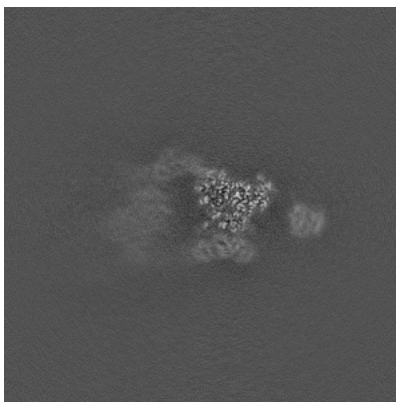


Z Index: 240

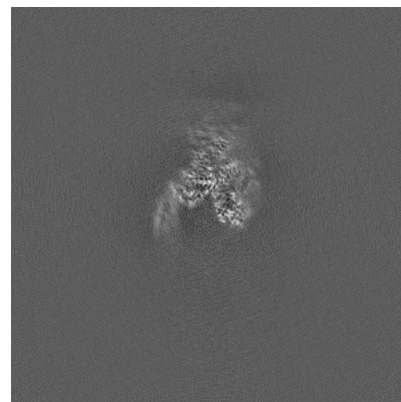
6.2.2 Raw map



X Index: 240



Y Index: 240

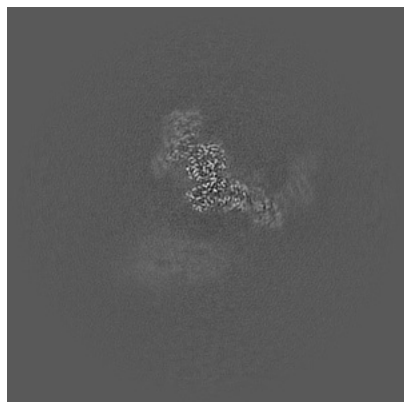


Z Index: 240

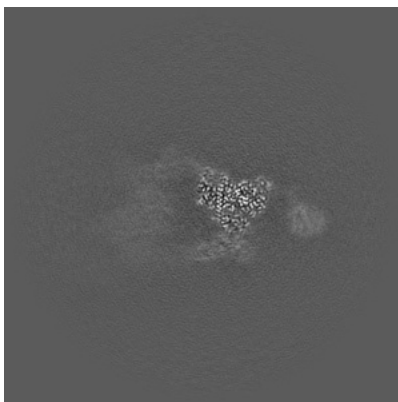
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

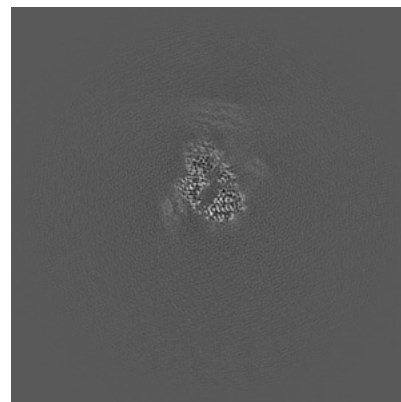
6.3.1 Primary map



X Index: 251



Y Index: 236

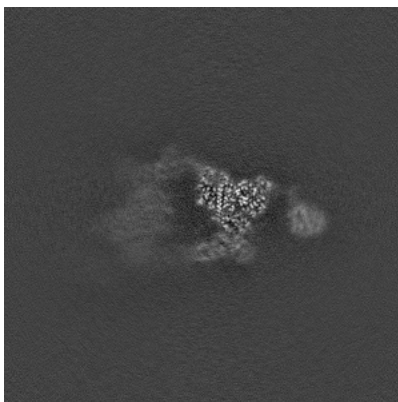


Z Index: 260

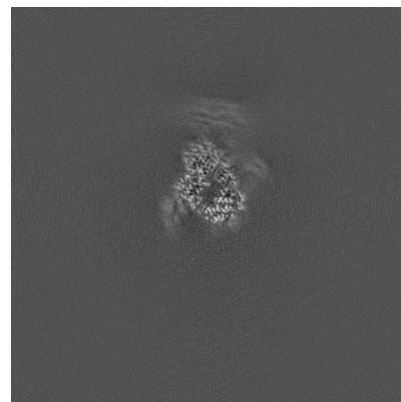
6.3.2 Raw map



X Index: 251



Y Index: 236

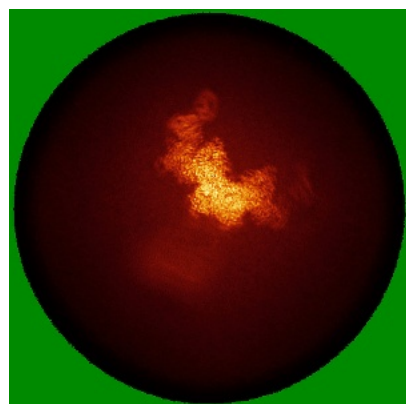


Z Index: 259

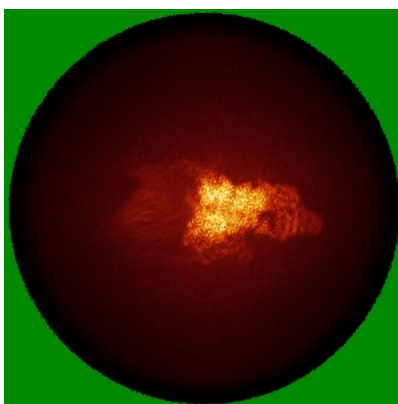
The images above show the largest variance slices of the map in three orthogonal directions.

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

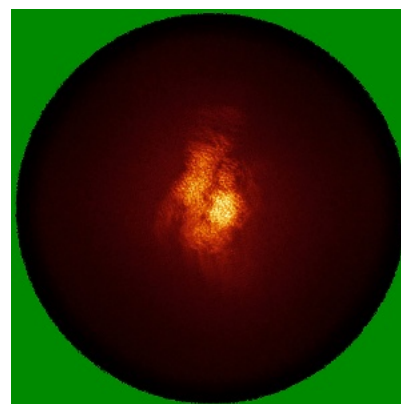
6.4.1 Primary map



X

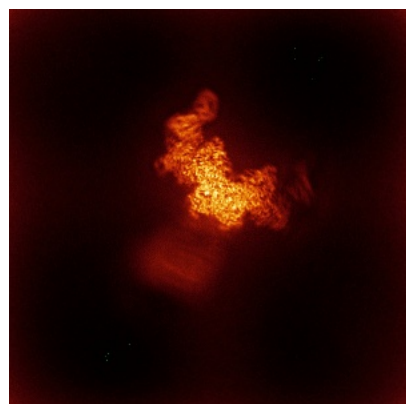


Y

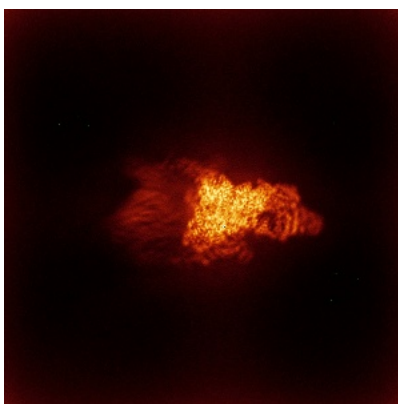


Z

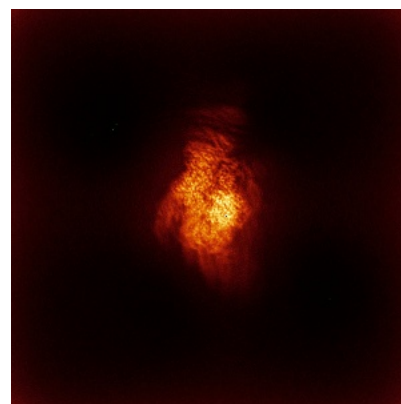
6.4.2 Raw map



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.

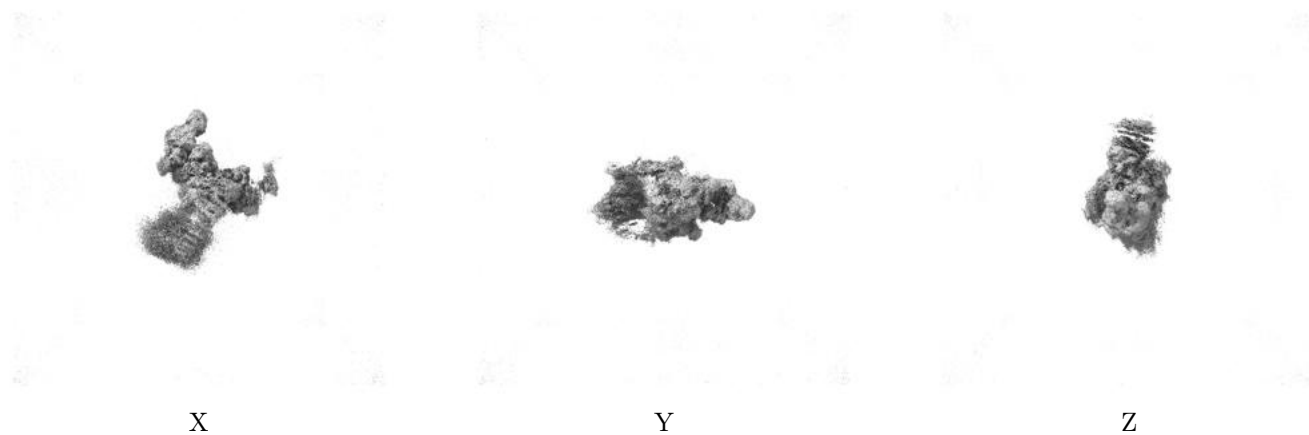
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

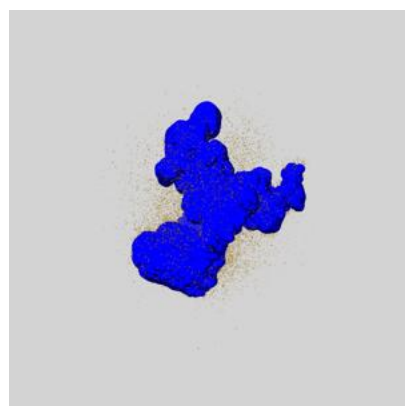
6.6 Mask visualisation [i](#)

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

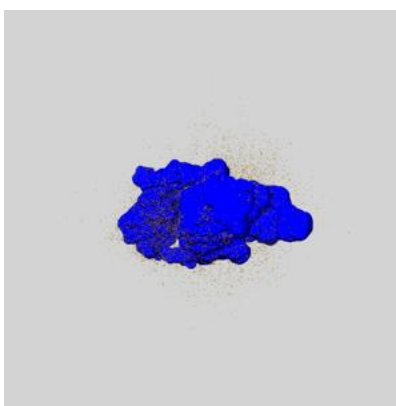
A mask typically either:

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

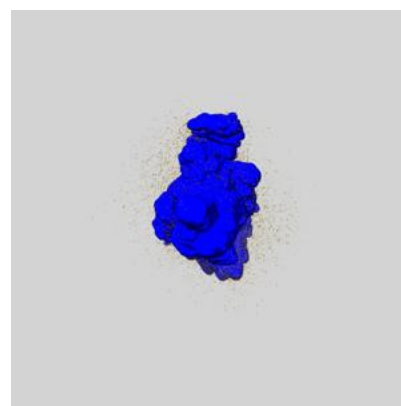
6.6.1 emd_39777_msk_1.map [i](#)



X



Y

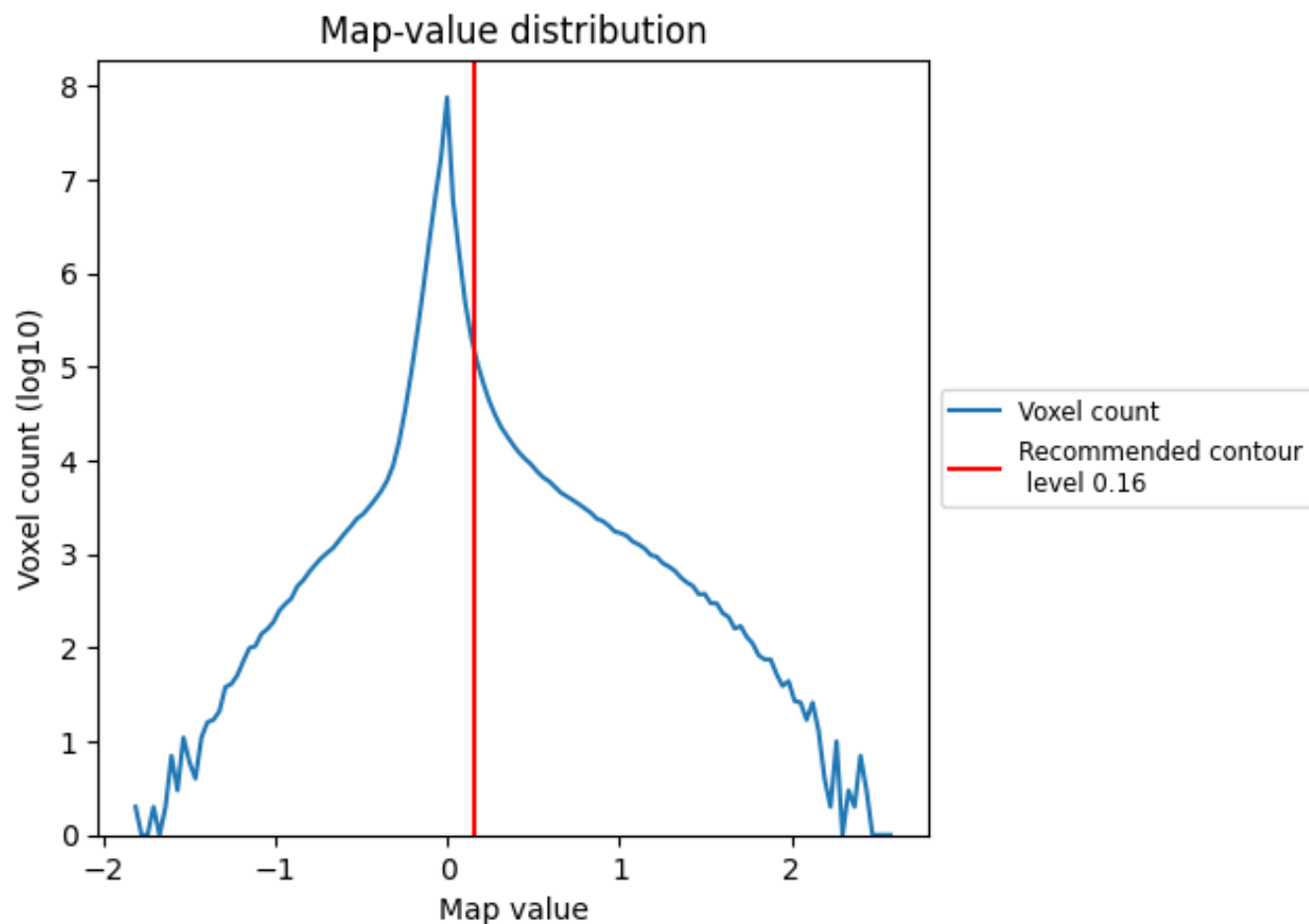


Z

7 Map analysis [i](#)

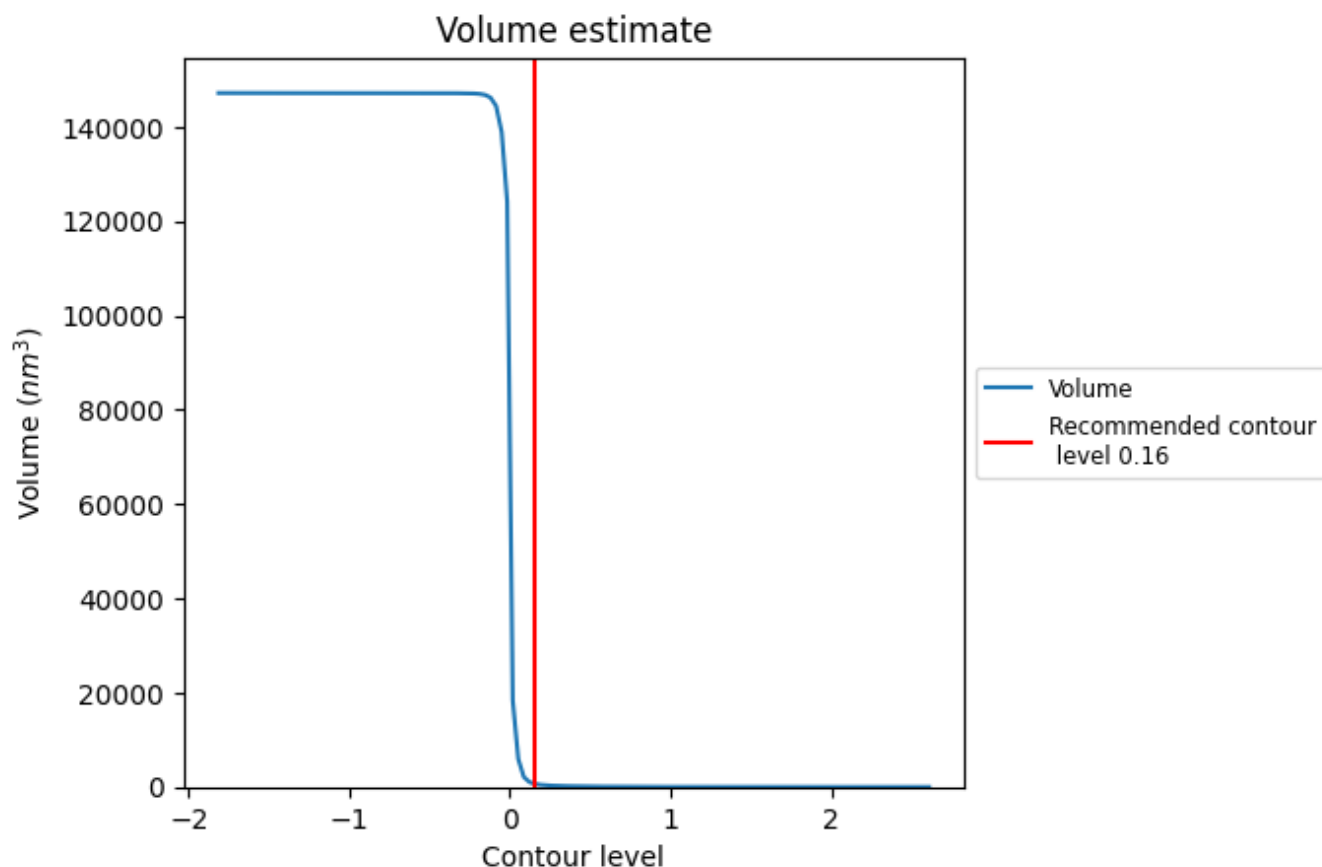
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

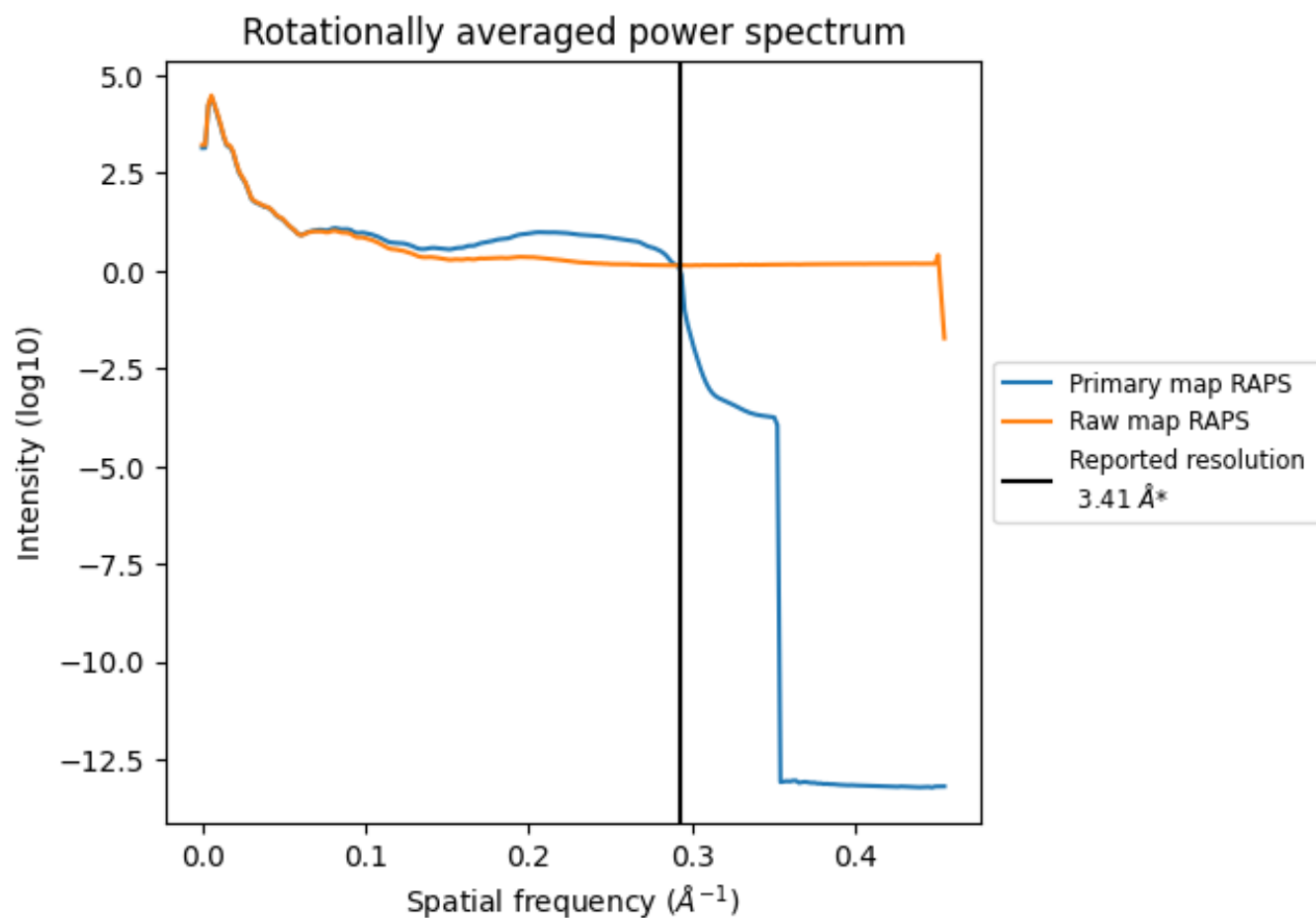
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 631 nm^3 ; this corresponds to an approximate mass of 570 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 ⓘ

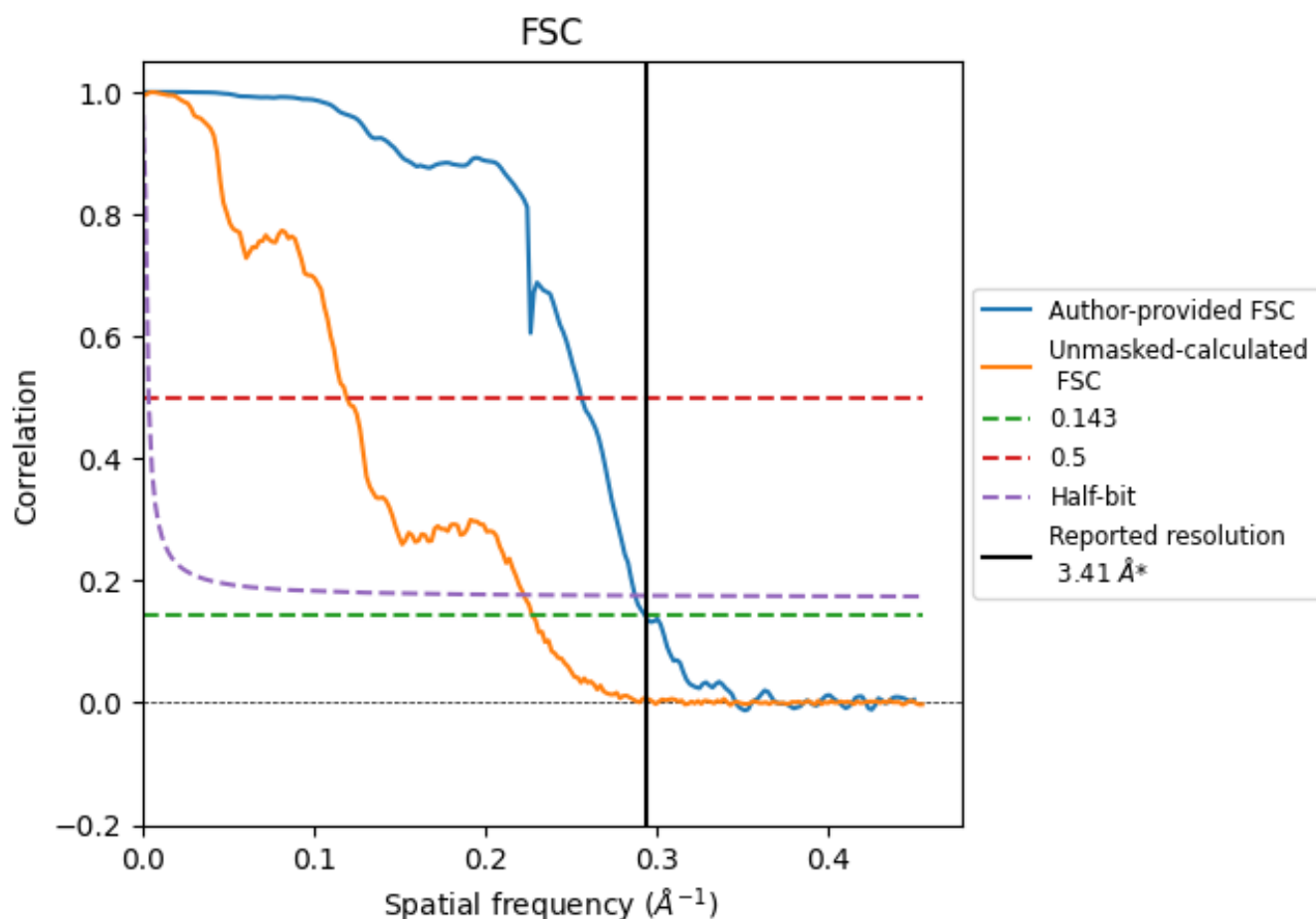


*Reported resolution corresponds to spatial frequency of 0.293 Å⁻¹

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 0.293 \AA^{-1}

8.2 Resolution estimates [i](#)

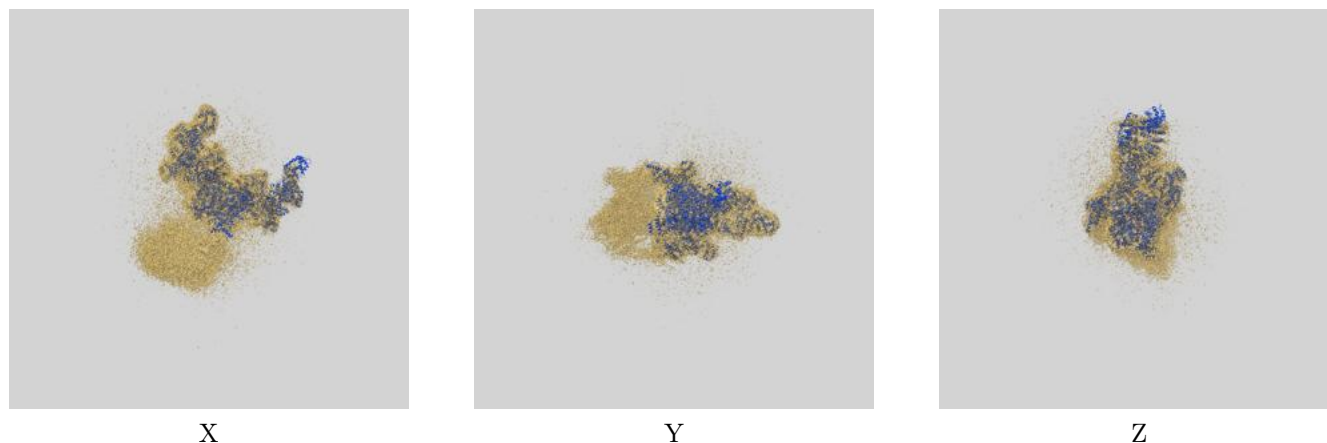
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.41	3.90	3.48
Unmasked-calculated*	4.40	8.39	4.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.40 differs from the reported value 3.41 by more than 10 %

9 Map-model fit [i](#)

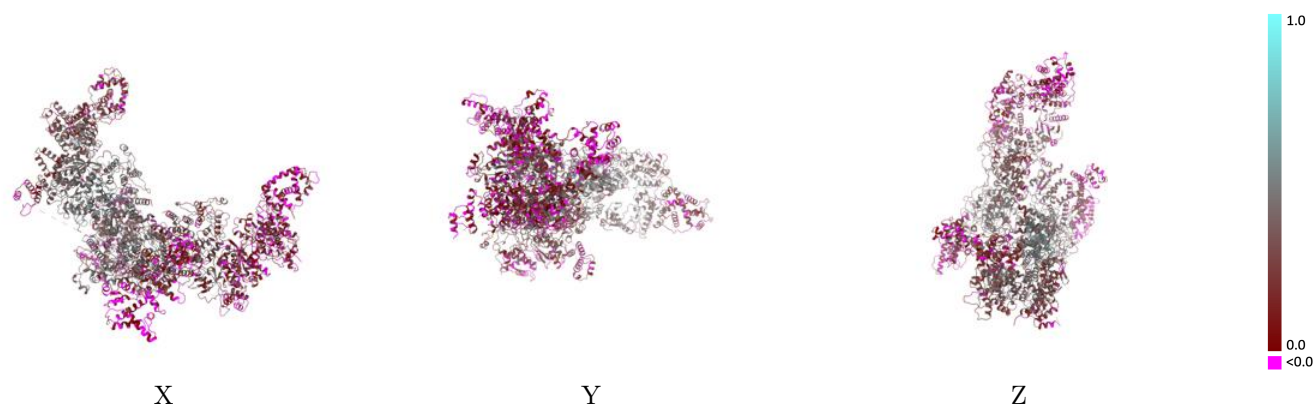
This section contains information regarding the fit between EMDB map EMD-39777 and PDB model 8Z5P. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



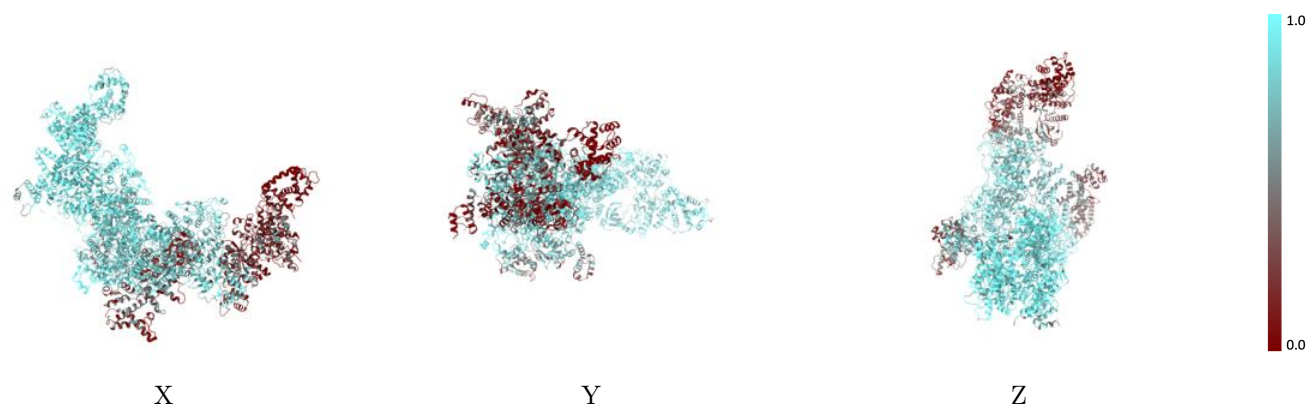
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



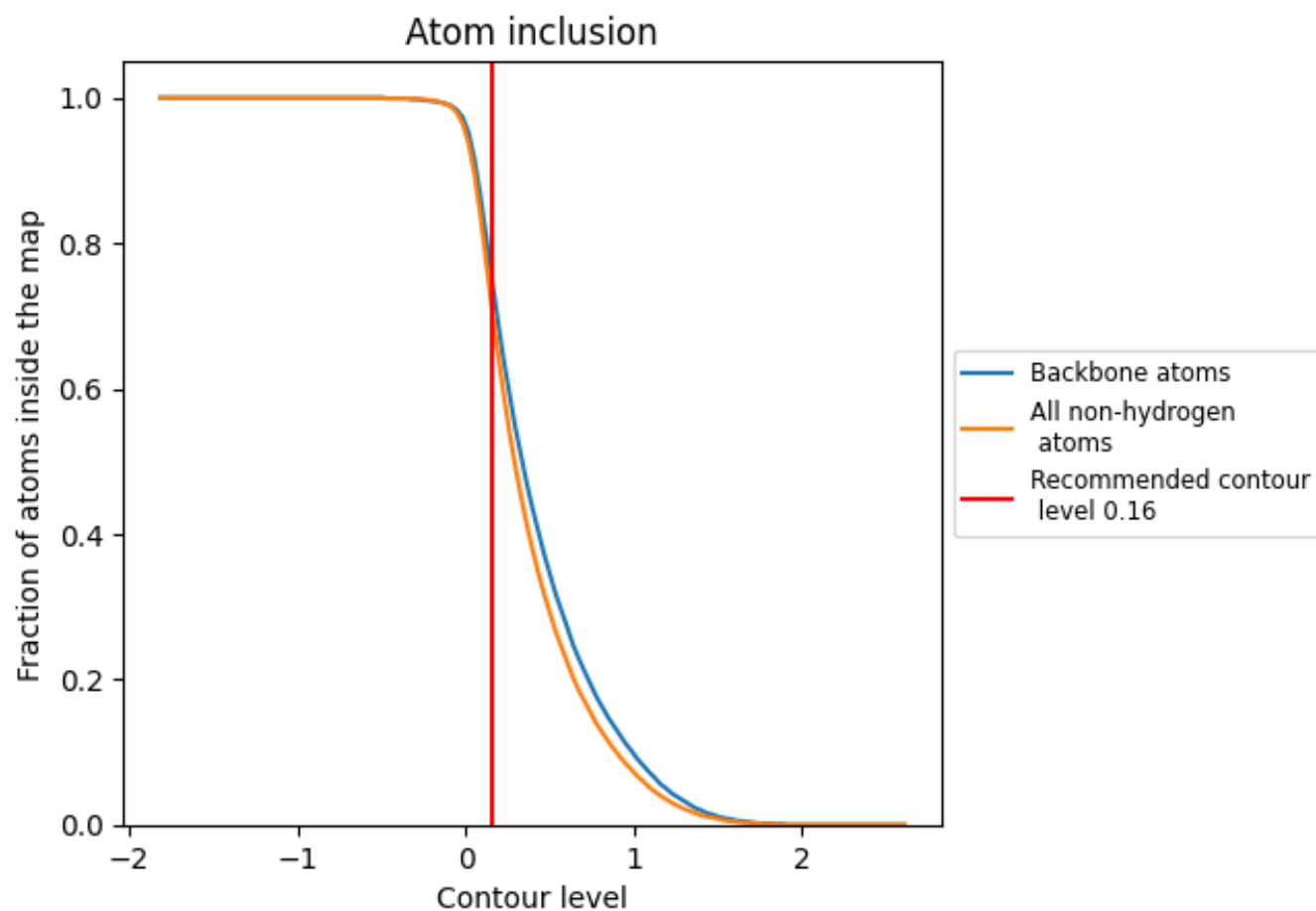
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 70% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7030	<div></div> 0.2640
A	<div></div> 0.9220	<div></div> 0.3890
B	<div></div> 0.7720	<div></div> 0.2600
C	<div></div> 0.9060	<div></div> 0.3110
D	<div></div> 0.8410	<div></div> 0.1860
E	<div></div> 0.5870	<div></div> 0.2120
F	<div></div> 0.7020	<div></div> 0.2650
G	<div></div> 0.2500	<div></div> 0.1380
H	<div></div> 0.0420	<div></div> 0.0670

1.0

0.0

<0.0