



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:06 AM UTC

PDB ID : 7BST / pdb_00007bst
EMDB ID : EMD-30166
Title : EcoR124I-Ocr in the Intermediate State
Authors : Gao, Y.; Gao, P.
Deposited on : 2020-03-31
Resolution : 4.37 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

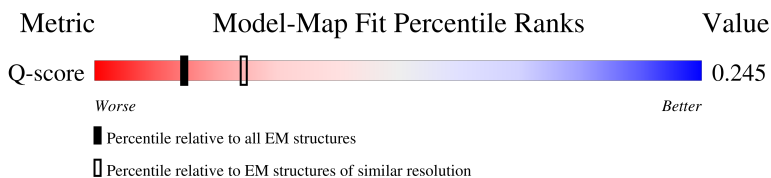
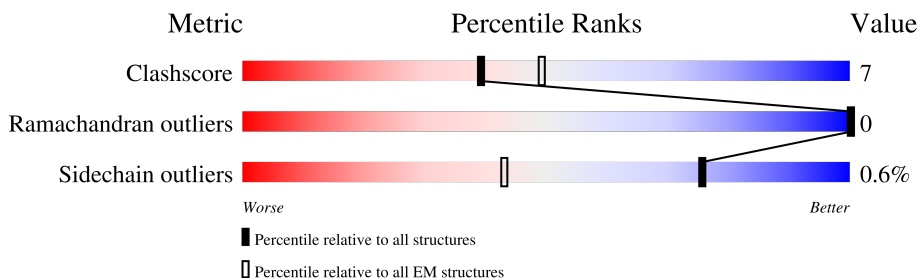
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.37 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3738 (3.87 - 4.87)

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	B	1038	
1	C	1038	
2	D	520	
2	E	520	

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Mol	Chain	Length	Quality of chain
3	F	117	76% 15% 9%
3	G	117	74% 16% 9%
4	A	404	48% 73% 21% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28266 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 Type I restriction enzyme R Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	975	Total	C	N	O	S	0	0
			7906	5022	1343	1524	17		
1	C	992	Total	C	N	O	S	0	0
			8042	5108	1363	1554	17		

- Molecule 2 is a protein called Type I restriction enzyme EcoR124II M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	472	Total	C	N	O	S	0	0
			3732	2390	623	713	6		
2	E	473	Total	C	N	O	S	0	0
			3735	2391	623	715	6		

- Molecule 3 is a protein called Overcome classical restriction gp0.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	106	Total	C	N	O	S	0	0
			876	550	136	185	5		
3	G	106	Total	C	N	O	S	0	0
			876	550	136	185	5		

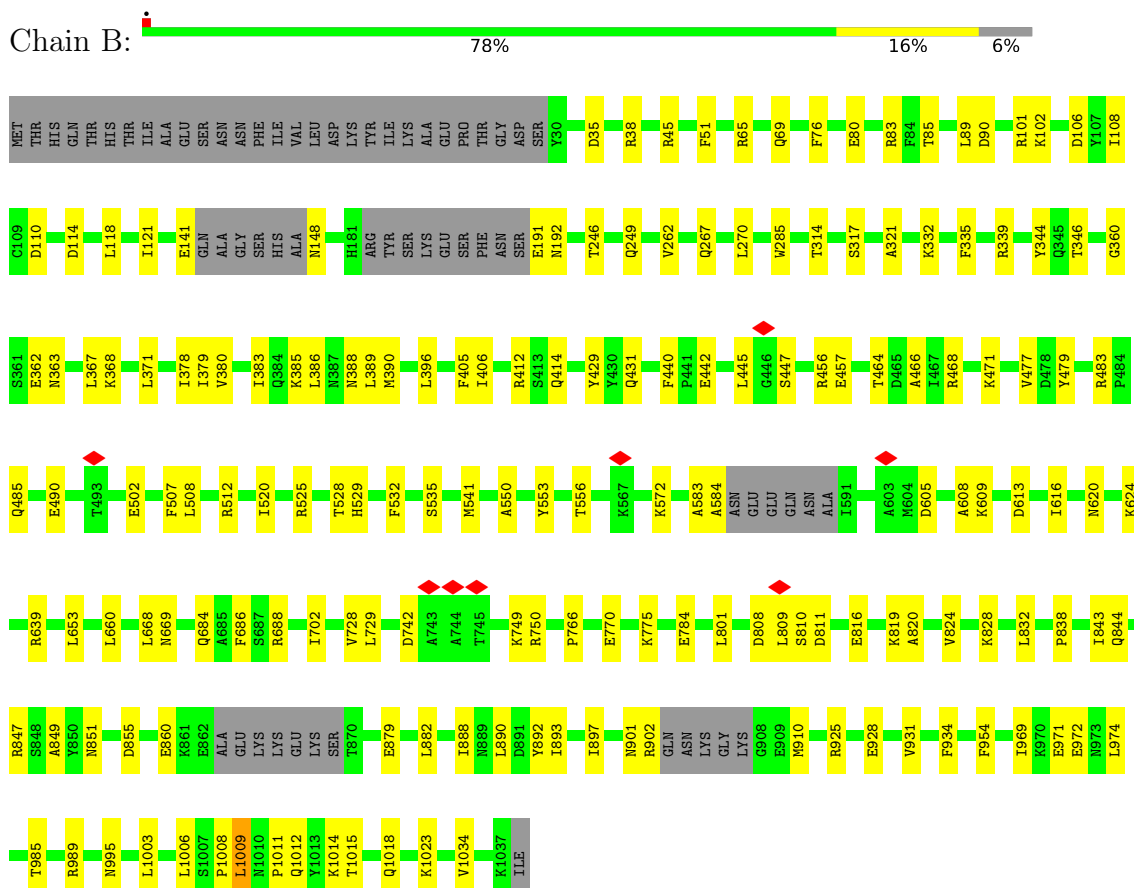
- Molecule 4 is a protein called Type-1 restriction enzyme EcoR124II specificity protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	384	Total	C	N	O	S	0	0
			3099	2001	505	585	8		

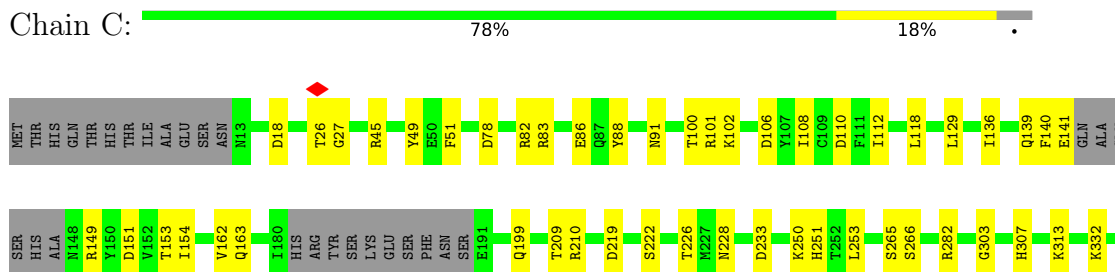
3 Residue-property plots

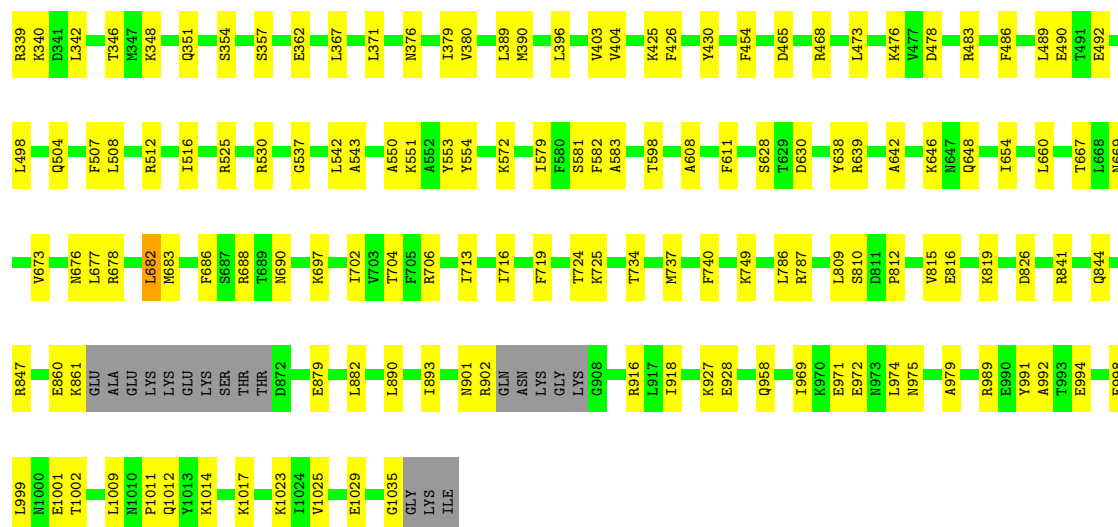
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Type I restriction enzyme R Protein

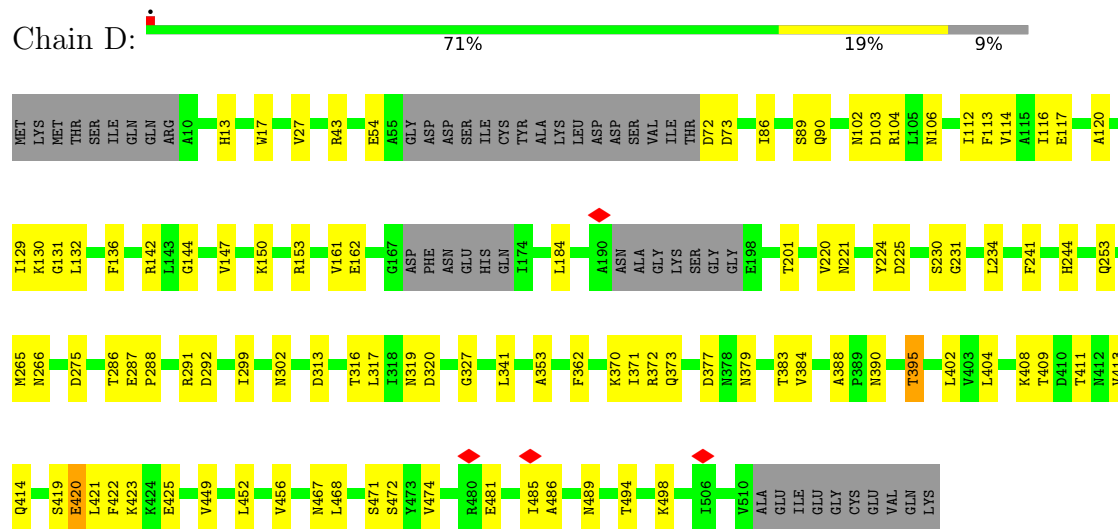


• Molecule 1: Type I restriction enzyme R Protein

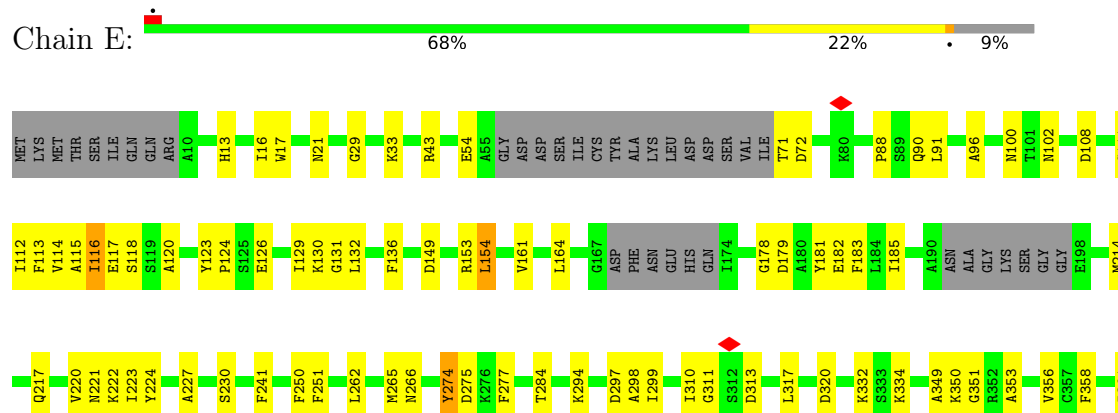


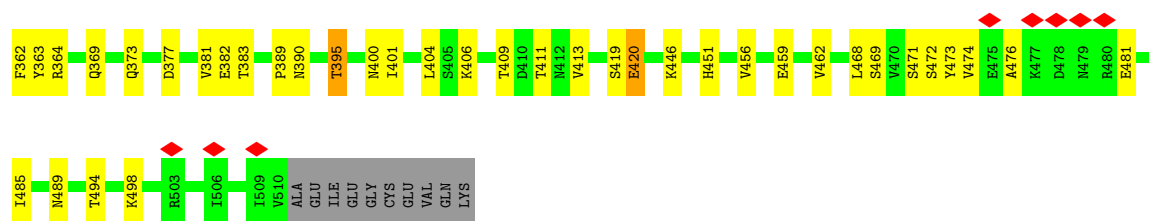


- Molecule 2: Type I restriction enzyme EcoR124II M protein



- Molecule 2: Type I restriction enzyme EcoR124II M protein





- Molecule 3: Overcome classical restriction gp0.3

Chain F:



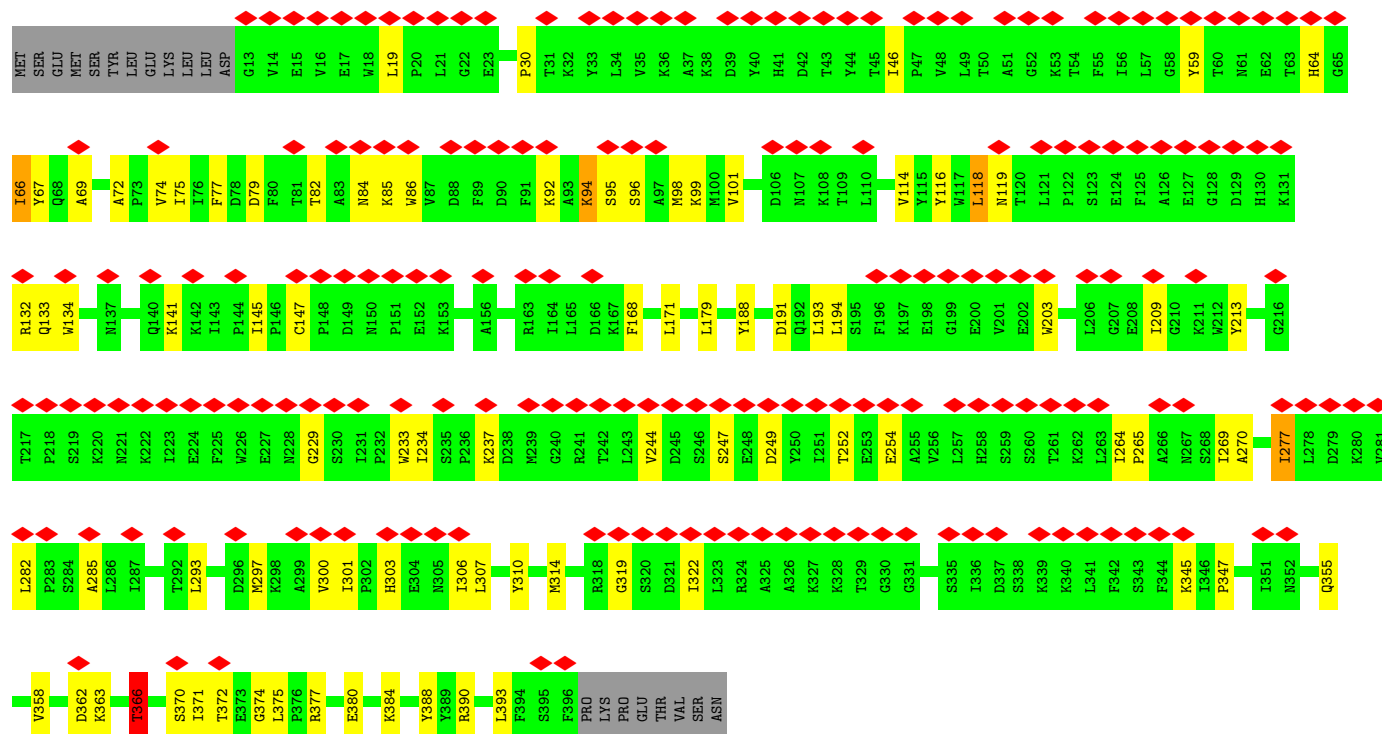
- Molecule 3: Overcome classical restriction gp0.3

Chain G:



- Molecule 4: Type-1 restriction enzyme EcoR124II specificity protein

Chain A:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64585	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 ($e^-/\text{\AA}^2$)	60, 60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	367.2, 367.2, 367.2	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	B	0.20	0/8050	0.55	6/10852 (0.1%)
1	C	0.20	0/8189	0.54	4/11043 (0.0%)
2	D	0.28	0/3809	0.74	8/5158 (0.2%)
2	E	0.25	0/3812	0.69	6/5164 (0.1%)
3	F	0.19	0/893	0.44	0/1213
3	G	0.18	0/893	0.45	0/1213
4	A	0.26	0/3173	0.73	4/4301 (0.1%)
All	All	0.23	0/28819	0.61	28/38944 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	3
2	E	0	3
4	A	0	5
All	All	0	12

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1008	PRO	CA-C-N	7.21	134.68	121.70
1	B	1008	PRO	C-N-CA	7.21	134.68	121.70
4	A	374	GLY	CA-C-N	6.80	128.16	120.06
4	A	374	GLY	C-N-CA	6.80	128.16	120.06
1	B	860	GLU	CA-C-N	6.51	133.42	121.70
1	B	860	GLU	C-N-CA	6.51	133.42	121.70
2	E	420	GLU	CA-C-N	5.84	132.22	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	420	GLU	C-N-CA	5.84	132.22	121.70
1	B	1003	LEU	C-N-CD	-5.79	107.87	120.60
2	D	409	THR	CA-C-N	5.78	132.10	121.70
2	D	409	THR	C-N-CA	5.78	132.10	121.70
2	E	409	THR	CA-C-N	5.72	132.00	121.70
2	E	409	THR	C-N-CA	5.72	132.00	121.70
2	D	395	THR	CA-C-N	5.64	131.85	121.70
2	D	395	THR	C-N-CA	5.64	131.85	121.70
1	C	27	GLY	CA-C-N	5.57	131.73	121.70
1	C	27	GLY	C-N-CA	5.57	131.73	121.70
2	D	420	GLU	CA-C-N	5.53	131.66	121.70
2	D	420	GLU	C-N-CA	5.53	131.66	121.70
2	E	395	THR	CA-C-N	5.53	131.65	121.70
2	E	395	THR	C-N-CA	5.53	131.65	121.70
1	C	26	THR	CA-C-N	5.35	131.34	121.70
1	C	26	THR	C-N-CA	5.35	131.34	121.70
2	D	27	VAL	CA-C-N	5.23	129.73	121.56
2	D	27	VAL	C-N-CA	5.23	129.73	121.56
4	A	141	LYS	CA-C-N	5.14	130.95	121.70
4	A	141	LYS	C-N-CA	5.14	130.95	121.70
1	B	1009	LEU	CA-CB-CG	5.11	134.19	116.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	191	ASP	Peptide
4	A	303	HIS	Peptide
4	A	366	THR	Peptide
4	A	72	ALA	Peptide
4	A	94	LYS	Peptide
1	C	678	ARG	Peptide
2	D	131	GLY	Peptide
2	D	313	ASP	Peptide
2	D	474	VAL	Peptide
2	E	274	TYR	Peptide
2	E	294	LYS	Peptide
2	E	474	VAL	Peptide

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	B	7906	0	7718	99	0
1	C	8042	0	7846	113	0
2	D	3732	0	3652	62	0
2	E	3735	0	3648	76	0
3	F	876	0	800	10	0
3	G	876	0	800	11	0
4	A	3099	0	3118	48	0
All	All	28266	0	27582	404	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 (404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:LEU:CD1	1:C:686:PHE:CE2	2.34	1.09
1:C:682:LEU:HD12	1:C:686:PHE:CE2	1.99	0.98
1:C:682:LEU:CD1	1:C:686:PHE:CZ	2.57	0.88
2:E:13:HIS:O	2:E:17:TRP:HB2	1.77	0.84
2:D:13:HIS:O	2:D:17:TRP:HB2	1.87	0.75
2:D:373:GLN:O	2:D:377:ASP:HB2	1.87	0.74
1:C:971:GLU:HG3	1:C:972:GLU:HG2	1.72	0.71
2:E:29:GLY:O	2:E:33:LYS:HB2	1.91	0.70
1:C:682:LEU:HD13	1:C:686:PHE:CZ	2.27	0.69
1:C:504:GLN:HA	1:C:508:LEU:HB2	1.75	0.69
4:A:69:ALA:HB3	4:A:92:LYS:H	1.58	0.69
2:E:334:LYS:HB3	2:E:364:ARG:HH21	1.58	0.68
2:D:224:TYR:HB3	2:D:299:ILE:HG22	1.77	0.67
1:B:108:ILE:HA	1:B:121:ILE:O	1.96	0.66
1:C:682:LEU:HD11	1:C:686:PHE:CZ	2.30	0.64
2:E:227:ALA:H	2:E:284:THR:HG21	1.62	0.64
1:B:405:PHE:HB2	1:B:431:GLN:HA	1.79	0.64
1:B:985:THR:O	1:B:989:ARG:HB2	1.98	0.63
2:E:178:GLY:O	2:E:181:TYR:HB3	1.99	0.63
2:D:136:PHE:HZ	2:D:265:MET:HB3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:372:THR:HA	4:A:377:ARG:HD3	1.81	0.62
2:D:129:ILE:HG23	2:D:130:LYS:HG3	1.80	0.62
1:B:766:PRO:HB3	1:B:849:ALA:HB2	1.82	0.62
1:C:1012:GLN:HG3	1:C:1014:LYS:H	1.64	0.62
2:E:185:ILE:HD11	2:E:262:LEU:HD13	1.81	0.62
1:C:129:LEU:HD11	1:C:251:HIS:HA	1.82	0.61
1:C:110:ASP:HB3	1:C:118:LEU:HD11	1.83	0.60
1:C:45:ARG:HH11	1:C:51:PHE:HB3	1.65	0.60
4:A:82:THR:HG21	4:A:134:TRP:HB2	1.83	0.60
1:B:335:PHE:HB2	1:B:378:ILE:HD11	1.82	0.60
1:B:246:THR:O	1:B:249:GLN:NE2	2.35	0.60
2:E:481:GLU:HG2	4:A:384:LYS:HB3	1.82	0.60
1:B:1012:GLN:HE22	1:B:1015:THR:H	1.50	0.60
1:B:995:ASN:ND2	2:D:90:GLN:O	2.35	0.59
4:A:168:PHE:HA	4:A:171:LEU:HG	1.84	0.59
4:A:145:ILE:HG22	4:A:147:CYS:H	1.67	0.59
2:E:481:GLU:HB2	4:A:388:TYR:HB2	1.85	0.59
1:B:477:VAL:HG22	1:B:702:ILE:HB	1.85	0.58
1:C:786:LEU:HB3	1:C:882:LEU:HD11	1.85	0.58
1:B:855:ASP:OD2	1:B:925:ARG:NH1	2.37	0.58
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.36	0.58
1:C:473:LEU:H	1:C:690:ASN:HB2	1.69	0.58
4:A:77:PHE:HB2	4:A:84:ASN:HB3	1.85	0.58
4:A:119:ASN:HB3	4:A:390:ARG:HH22	1.68	0.58
1:C:209:THR:O	1:C:228:ASN:ND2	2.36	0.58
1:B:971:GLU:HG3	1:B:972:GLU:HG2	1.86	0.57
1:C:233:ASP:O	1:C:468:ARG:NH2	2.37	0.57
1:C:819:LYS:NZ	1:C:826:ASP:OD1	2.35	0.57
3:G:68:SER:H	4:A:237:LYS:HD3	1.69	0.57
1:B:851:ASN:HB3	1:B:925:ARG:HH22	1.70	0.57
1:C:815:VAL:HG12	1:C:819:LYS:HE2	1.86	0.57
2:E:217:GLN:O	2:E:222:LYS:NZ	2.37	0.57
2:E:136:PHE:HZ	2:E:265:MET:HB3	1.69	0.57
4:A:85:LYS:HD2	4:A:118:LEU:HD12	1.85	0.57
1:B:101:ARG:HB2	1:B:267:GLN:HE22	1.70	0.56
2:E:224:TYR:HB3	2:E:299:ILE:HG22	1.86	0.56
2:E:356:VAL:HG12	2:E:401:ILE:HG12	1.88	0.56
1:B:35:ASP:OD1	1:B:38:ARG:NH1	2.37	0.56
1:C:639:ARG:NH2	2:E:320:ASP:O	2.37	0.56
2:E:88:PRO:HA	2:E:91:LEU:HB3	1.86	0.56
4:A:370:SER:HB2	4:A:371:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:ASN:OD1	1:C:706:ARG:NH1	2.39	0.56
2:E:349:ALA:HA	2:E:406:LYS:HB2	1.88	0.56
1:C:787:ARG:NH2	1:C:879:GLU:OE2	2.39	0.55
1:C:542:LEU:HD23	1:C:654:ILE:HG12	1.87	0.55
1:C:673:VAL:HB	1:C:704:THR:HG22	1.88	0.55
1:C:465:ASP:OD1	1:C:468:ARG:NH2	2.40	0.55
2:E:43:ARG:NH1	2:E:161:VAL:O	2.40	0.55
1:B:879:GLU:HB3	1:B:882:LEU:HB2	1.89	0.55
1:B:888:ILE:HG23	1:B:892:TYR:HB3	1.89	0.55
1:B:750:ARG:NH2	1:B:784:GLU:OE1	2.40	0.55
2:E:13:HIS:O	2:E:17:TRP:CB	2.52	0.55
4:A:75:ILE:HD11	4:A:86:TRP:HB2	1.89	0.55
2:E:131:GLY:O	2:E:274:TYR:OH	2.23	0.55
1:C:682:LEU:HD11	1:C:686:PHE:CE2	2.34	0.54
1:C:83:ARG:NH2	1:C:112:ILE:O	2.41	0.54
2:E:179:ASP:O	2:E:182:GLU:HB3	2.08	0.54
4:A:234:ILE:HB	4:A:293:LEU:HB3	1.90	0.54
1:B:897:ILE:HA	1:B:910:MET:HE1	1.88	0.54
1:C:108:ILE:HB	2:D:147:VAL:HG11	1.89	0.54
1:C:530:ARG:HE	1:C:537:GLY:HA3	1.71	0.54
2:E:382:GLU:HG2	2:E:383:THR:HG23	1.90	0.54
3:F:18:LEU:HD22	3:F:93:LEU:HD22	1.90	0.53
1:B:925:ARG:O	1:B:928:GLU:HB3	2.09	0.53
1:B:931:VAL:O	1:B:934:PHE:HB3	2.08	0.53
1:C:1014:LYS:HB3	1:C:1017:LYS:HE2	1.89	0.53
1:C:543:ALA:HB3	1:C:673:VAL:HA	1.91	0.53
4:A:67:TYR:H	4:A:94:LYS:HD3	1.73	0.53
1:B:528:THR:HA	1:B:669:ASN:HD21	1.74	0.53
1:B:770:GLU:O	1:B:775:LYS:NZ	2.41	0.53
1:C:716:ILE:HD13	1:C:725:LYS:HB3	1.89	0.53
1:B:363:ASN:O	1:B:385:LYS:NZ	2.39	0.53
2:E:381:VAL:HA	2:E:404:LEU:HG	1.90	0.53
4:A:79:ASP:OD1	4:A:133:GLN:NE2	2.42	0.53
1:B:80:GLU:HG2	1:B:83:ARG:HH21	1.74	0.52
3:G:18:LEU:HD22	3:G:93:LEU:HD22	1.90	0.52
1:B:89:LEU:O	1:B:102:LYS:NZ	2.42	0.52
2:D:383:THR:HG22	2:D:413:VAL:HG23	1.92	0.52
1:B:742:ASP:H	1:B:749:LYS:HG3	1.73	0.52
2:E:117:GLU:HA	2:E:120:ALA:HB3	1.92	0.52
4:A:358:VAL:O	4:A:362:ASP:HB2	2.10	0.52
1:C:101:ARG:NH1	1:C:106:ASP:OD2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:992:ALA:HB3	1:C:1025:VAL:HG12	1.91	0.52
1:C:581:SER:OG	1:C:598:THR:O	2.28	0.51
2:E:411:THR:OG1	2:E:456:VAL:O	2.28	0.51
1:B:620:ASN:HA	1:B:624:LYS:H	1.75	0.51
2:D:54:GLU:OE2	2:D:72:ASP:N	2.44	0.51
2:D:372:ARG:HH12	2:D:468:LEU:HB2	1.74	0.51
2:E:43:ARG:HH12	2:E:164:LEU:HB2	1.74	0.51
1:C:139:GLN:NE2	1:C:149:ARG:O	2.43	0.51
1:C:153:THR:OG1	1:C:163:GLN:NE2	2.43	0.51
1:C:219:ASP:HA	1:C:222:SER:HB3	1.93	0.51
1:C:713:ILE:HA	1:C:716:ILE:HD12	1.93	0.51
1:B:483:ARG:HD3	1:B:485:GLN:HB3	1.92	0.51
1:B:335:PHE:HB3	1:B:380:VAL:HA	1.93	0.51
2:D:43:ARG:NH1	2:D:161:VAL:O	2.43	0.51
1:B:525:ARG:HH22	1:B:572:LYS:H	1.58	0.51
1:B:45:ARG:HH11	1:B:51:PHE:HB3	1.76	0.51
1:C:210:ARG:NH1	1:C:226:THR:O	2.43	0.50
1:C:812:PRO:O	1:C:816:GLU:HB2	2.11	0.50
1:C:682:LEU:HD13	1:C:686:PHE:CE2	2.34	0.50
1:B:69:GLN:HE21	1:B:76:PHE:HD2	1.57	0.50
4:A:265:PRO:HD2	4:A:301:ILE:HG21	1.94	0.50
1:B:339:ARG:HD3	1:B:360:GLY:HA3	1.92	0.50
2:E:485:ILE:O	2:E:489:ASN:ND2	2.45	0.50
1:B:550:ALA:HA	1:B:553:TYR:HD2	1.77	0.50
2:D:411:THR:HG23	2:D:413:VAL:HG13	1.93	0.50
4:A:269:ILE:HG13	4:A:300:VAL:HB	1.94	0.50
1:B:529:HIS:ND1	1:B:820:ALA:O	2.35	0.50
1:B:819:LYS:HA	1:B:824:VAL:HB	1.94	0.49
1:C:507:PHE:O	1:C:512:ARG:NH1	2.44	0.49
1:C:404:VAL:HG22	1:C:430:TYR:HB2	1.92	0.49
4:A:30:PRO:HD3	4:A:99:LYS:HA	1.94	0.49
1:B:660:LEU:O	1:B:688:ARG:NH1	2.46	0.49
1:C:139:GLN:HB3	1:C:151:ASP:HB2	1.94	0.49
2:E:390:ASN:OD1	2:E:395:THR:OG1	2.30	0.49
1:C:958:GLN:HE21	1:C:1035:GLY:HA2	1.77	0.49
1:C:136:ILE:HG22	1:C:154:ILE:HG12	1.93	0.49
1:C:88:TYR:O	1:C:102:LYS:NZ	2.37	0.49
1:C:648:GLN:HE21	1:C:667:THR:HB	1.78	0.49
1:C:972:GLU:OE2	1:C:1023:LYS:NZ	2.46	0.49
2:E:54:GLU:OE1	2:E:72:ASP:N	2.45	0.49
2:E:353:ALA:HB3	2:E:404:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:MET:O	1:C:425:LYS:NZ	2.34	0.49
2:D:241:PHE:HB3	2:D:244:HIS:HB2	1.94	0.49
4:A:229:GLY:HA3	4:A:252:THR:HA	1.95	0.49
1:B:456:ARG:HH12	2:D:319:ASN:HB2	1.78	0.48
1:C:486:PHE:HD1	1:C:489:LEU:HD12	1.78	0.48
2:D:225:ASP:HB2	2:D:234:LEU:HD21	1.94	0.48
2:E:112:ILE:HA	2:E:113:PHE:HA	1.61	0.48
4:A:116:TYR:O	4:A:390:ARG:NH2	2.36	0.48
1:C:969:ILE:HG23	1:C:974:LEU:HB2	1.95	0.48
2:D:320:ASP:OD1	2:D:320:ASP:N	2.47	0.48
2:E:361:ILE:O	4:A:132:ARG:NH1	2.46	0.48
1:B:583:ALA:HA	1:B:584:ALA:HA	1.64	0.48
1:B:684:GLN:O	1:B:688:ARG:NH1	2.47	0.48
2:D:106:ASN:ND2	2:D:162:GLU:OE1	2.47	0.48
2:E:224:TYR:HA	2:E:251:PHE:HB2	1.94	0.48
1:B:141:GLU:OE2	1:B:148:ASN:N	2.47	0.48
1:B:728:VAL:HG12	1:B:729:LEU:HB2	1.96	0.48
1:B:808:ASP:HB3	1:B:811:ASP:HB2	1.96	0.48
2:D:253:GLN:NE2	2:D:287:GLU:O	2.39	0.48
2:E:220:VAL:HG23	2:E:221:ASN:HB3	1.95	0.48
4:A:252:THR:HG22	4:A:254:GLU:H	1.79	0.48
1:B:389:LEU:HD11	1:B:396:LEU:HD11	1.95	0.48
1:C:354:SER:O	1:C:376:ASN:ND2	2.40	0.48
1:C:927:LYS:NZ	1:C:1029:GLU:O	2.41	0.48
1:C:994:GLU:HA	1:C:999:LEU:HD23	1.96	0.48
2:D:231:GLY:H	2:D:266:ASN:HD22	1.60	0.48
2:D:384:VAL:HG12	2:D:402:LEU:HG	1.96	0.48
4:A:179:LEU:HD13	4:A:375:LEU:HD22	1.96	0.48
4:A:319:GLY:HA2	4:A:322:ILE:HG12	1.96	0.48
1:C:476:LYS:NZ	1:C:478:ASP:OD1	2.33	0.47
1:C:683:MET:HE2	1:C:719:PHE:HE2	1.79	0.47
2:E:115:ALA:O	2:E:118:SER:HB3	2.14	0.47
2:D:275:ASP:OD1	2:D:275:ASP:N	2.46	0.47
2:D:286:THR:HG22	2:D:317:LEU:HD11	1.95	0.47
1:B:383:ILE:HG12	1:B:414:GLN:HB3	1.96	0.47
1:B:844:GLN:OE1	1:B:847:ARG:NH1	2.47	0.47
3:F:71:MET:HG3	3:F:80:ILE:HG12	1.97	0.47
1:B:972:GLU:OE2	1:B:1023:LYS:NZ	2.48	0.47
1:C:844:GLN:OE1	1:C:847:ARG:NH1	2.47	0.47
2:E:43:ARG:HB2	2:E:102:ASN:HD22	1.79	0.47
4:A:277:ILE:HG23	4:A:282:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:LEU:HD23	1:B:893:ILE:HD12	1.97	0.47
1:B:901:ASN:HA	1:B:902:ARG:HA	1.63	0.47
1:C:554:TYR:HB3	1:C:611:PHE:HZ	1.78	0.47
2:D:390:ASN:OD1	2:D:395:THR:OG1	2.29	0.47
2:E:451:HIS:HE1	2:E:476:ALA:HB2	1.80	0.47
3:F:100:LEU:HA	3:F:103:GLU:HB3	1.97	0.47
1:B:344:TYR:HA	1:B:639:ARG:HH21	1.79	0.47
1:B:362:GLU:O	1:B:388:ASN:ND2	2.48	0.47
2:D:370:LYS:HA	2:D:373:GLN:HB3	1.97	0.47
2:E:29:GLY:O	2:E:33:LYS:CB	2.61	0.47
3:G:71:MET:HG3	3:G:80:ILE:HG12	1.97	0.47
1:B:367:LEU:HD21	1:B:389:LEU:HD22	1.96	0.47
1:B:1014:LYS:O	1:B:1018:GLN:N	2.47	0.47
1:C:86:GLU:O	1:C:91:ASN:ND2	2.48	0.47
1:C:357:SER:HA	1:C:379:ILE:HA	1.95	0.47
2:E:230:SER:OG	2:E:266:ASN:ND2	2.48	0.47
2:E:16:ILE:HG23	2:E:164:LEU:HD22	1.97	0.46
1:B:412:ARG:HH12	1:B:445:LEU:HB2	1.80	0.46
1:C:483:ARG:HH12	1:C:516:ILE:HG13	1.81	0.46
1:C:669:ASN:HB3	1:C:697:LYS:HE3	1.97	0.46
1:B:456:ARG:NH2	2:D:316:THR:OG1	2.47	0.46
2:D:384:VAL:HG23	2:D:414:GLN:HG3	1.96	0.46
2:E:311:GLY:HA2	2:E:313:ASP:HA	1.97	0.46
3:G:100:LEU:HA	3:G:103:GLU:HB3	1.97	0.46
1:B:285:TRP:HZ3	2:D:327:GLY:H	1.64	0.46
3:G:7:TYR:OH	3:G:92:ASP:OD2	2.29	0.46
1:C:110:ASP:HB2	2:D:142:ARG:HH21	1.81	0.46
1:B:85:THR:O	1:B:90:ASP:N	2.41	0.46
1:C:367:LEU:HD23	1:C:389:LEU:HD13	1.97	0.46
1:C:734:THR:HA	1:C:737:MET:HB2	1.98	0.46
2:E:451:HIS:CE1	2:E:476:ALA:HB2	2.50	0.46
4:A:19:LEU:HD13	4:A:145:ILE:HB	1.97	0.46
1:B:969:ILE:HD12	1:B:974:LEU:HD22	1.98	0.46
1:C:102:LYS:HA	1:C:106:ASP:HB2	1.97	0.46
3:G:28:ARG:HG2	3:G:105:LEU:HD22	1.98	0.46
3:F:91:ILE:HA	3:F:94:TRP:HD1	1.81	0.46
2:D:419:SER:HA	2:D:420:GLU:HA	1.64	0.46
1:B:405:PHE:HE2	1:B:429:TYR:HB2	1.82	0.45
1:C:140:PHE:HA	1:C:141:GLU:HA	1.74	0.45
1:C:307:HIS:HB2	1:C:313:LYS:HD3	1.98	0.45
1:C:483:ARG:NH2	1:C:490:GLU:OE2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:975:ASN:O	1:C:979:ALA:N	2.44	0.45
4:A:233:TRP:HB3	4:A:249:ASP:HB3	1.97	0.45
3:F:28:ARG:HG2	3:F:105:LEU:HD22	1.98	0.45
1:B:386:LEU:HG	1:B:390:MET:HE2	1.98	0.45
1:B:529:HIS:O	1:B:535:SER:OG	2.31	0.45
1:C:303:GLY:N	1:C:454:PHE:O	2.49	0.45
2:E:310:ILE:HA	2:E:332:LYS:HG3	1.97	0.45
1:B:541:MET:HG3	1:B:668:LEU:HD11	1.98	0.45
3:G:91:ILE:HA	3:G:94:TRP:HD1	1.81	0.45
4:A:114:VAL:O	4:A:118:LEU:HB2	2.17	0.45
1:C:357:SER:HB3	1:C:380:VAL:H	1.81	0.45
2:E:129:ILE:HG23	2:E:130:LYS:HG3	1.98	0.45
1:B:532:PHE:HD1	1:B:816:GLU:HG3	1.80	0.45
1:B:824:VAL:HG13	1:B:828:LYS:HB2	1.98	0.45
1:C:18:ASP:OD1	1:C:282:ARG:NH2	2.49	0.45
2:E:116:ILE:O	2:E:120:ALA:N	2.47	0.45
2:E:123:TYR:HA	2:E:126:GLU:HG3	1.99	0.45
1:B:110:ASP:HB2	1:B:118:LEU:HD11	1.98	0.45
1:B:969:ILE:HG23	1:B:974:LEU:HB2	1.98	0.45
2:E:468:LEU:HA	2:E:469:SER:HA	1.64	0.45
3:F:37:ILE:HD11	3:F:97:ALA:HB2	1.99	0.45
4:A:193:LEU:HD23	4:A:194:LEU:HB2	1.99	0.45
2:D:102:ASN:OD1	2:D:106:ASN:ND2	2.50	0.45
2:E:297:ASP:HA	2:E:351:GLY:HA3	1.98	0.45
1:B:368:LYS:HA	1:B:371:LEU:HB2	1.98	0.45
1:B:466:ALA:HB1	1:B:471:LYS:HB2	2.00	0.45
2:D:288:PRO:HG2	2:D:291:ARG:HD2	1.97	0.45
2:E:100:ASN:ND2	2:E:123:TYR:OH	2.50	0.45
4:A:363:LYS:HA	4:A:366:THR:HG22	1.99	0.45
1:C:348:LYS:HA	1:C:351:GLN:HG2	1.97	0.44
1:C:901:ASN:HA	1:C:902:ARG:HA	1.72	0.44
1:C:998:GLU:HA	1:C:1001:GLU:HB2	1.99	0.44
2:D:388:ALA:HB1	2:D:423:LYS:HG2	1.98	0.44
2:D:388:ALA:HB2	2:D:421:LEU:HB3	1.99	0.44
3:G:37:ILE:HD11	3:G:97:ALA:HB2	1.99	0.44
4:A:307:LEU:HD23	4:A:358:VAL:HG11	1.99	0.44
2:D:341:LEU:HD11	2:D:371:ILE:HD12	1.98	0.44
4:A:314:MET:HE2	4:A:347:PRO:HD2	1.99	0.44
1:C:579:ILE:HD13	1:C:638:TYR:HD1	1.81	0.44
2:D:379:ASN:HD22	2:D:408:LYS:HA	1.83	0.44
2:E:262:LEU:HA	2:E:265:MET:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:244:VAL:H	4:A:285:ALA:HB1	1.83	0.44
1:B:314:THR:HG23	1:B:346:THR:HG22	1.98	0.44
1:C:642:ALA:O	1:C:646:LYS:HB2	2.18	0.44
2:D:485:ILE:O	2:D:489:ASN:ND2	2.51	0.44
2:E:54:GLU:O	2:E:71:THR:N	2.49	0.44
2:E:361:ILE:HG13	2:E:364:ARG:HG2	1.99	0.44
1:B:1011:PRO:HA	1:B:1012:GLN:HA	1.75	0.44
2:D:86:ILE:HA	2:D:89:SER:HB3	2.00	0.44
2:D:112:ILE:HA	2:D:113:PHE:HA	1.66	0.44
1:B:332:LYS:HD2	1:B:379:ILE:HD11	1.99	0.44
1:B:686:PHE:HE1	1:B:702:ILE:HG21	1.82	0.44
1:C:809:LEU:HA	1:C:810:SER:HA	1.77	0.44
1:B:925:ARG:O	1:B:928:GLU:CB	2.65	0.44
1:C:339:ARG:HA	1:C:340:LYS:HA	1.73	0.44
1:C:389:LEU:HD11	1:C:396:LEU:HD11	1.99	0.44
4:A:64:HIS:HB2	4:A:66:ILE:HG23	1.98	0.44
1:B:507:PHE:HA	1:B:512:ARG:HH22	1.83	0.44
1:B:954:PHE:HD1	1:B:1034:VAL:HG23	1.82	0.43
2:D:86:ILE:O	2:D:90:GLN:N	2.47	0.43
2:E:317:LEU:HA	2:E:320:ASP:HB3	2.00	0.43
2:E:413:VAL:HG21	2:E:446:LYS:HZ2	1.82	0.43
2:E:419:SER:HA	2:E:420:GLU:HA	1.69	0.43
2:D:481:GLU:HB2	4:A:188:TYR:HB2	1.99	0.43
3:F:74:THR:HG23	3:F:76:ASP:H	1.83	0.43
1:C:478:ASP:N	1:C:702:ILE:O	2.45	0.43
2:D:220:VAL:HA	2:D:221:ASN:HA	1.52	0.43
1:B:321:ALA:HB1	1:B:378:ILE:HD13	2.00	0.43
2:E:362:PHE:HD2	2:E:363:TYR:HD1	1.66	0.43
1:B:65:ARG:NH2	1:B:76:PHE:O	2.50	0.43
4:A:95:SER:N	4:A:98:MET:SD	2.88	0.43
4:A:194:LEU:HD21	4:A:310:TYR:HE1	1.84	0.43
2:D:486:ALA:HA	2:D:489:ASN:HD22	1.83	0.43
2:E:33:LYS:HE2	2:E:33:LYS:HB3	1.92	0.43
1:C:100:THR:HG23	1:C:199:GLN:HE22	1.84	0.43
1:C:1009:LEU:O	1:C:1014:LYS:NZ	2.46	0.43
4:A:213:TYR:HD2	4:A:264:ILE:HG22	1.84	0.43
1:B:440:PHE:HB3	1:B:442:GLU:H	1.83	0.43
1:B:477:VAL:H	1:B:729:LEU:HD11	1.83	0.43
1:C:78:ASP:O	1:C:82:ARG:HB2	2.18	0.43
1:C:1009:LEU:HD12	1:C:1011:PRO:HG2	1.99	0.43
2:D:372:ARG:NH2	2:D:467:ASN:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:71:MET:HE1	3:G:75:LYS:HA	2.01	0.43
1:C:812:PRO:O	1:C:816:GLU:CB	2.67	0.43
2:D:117:GLU:HA	2:D:120:ALA:HB3	2.01	0.43
1:B:479:TYR:OH	1:B:490:GLU:O	2.37	0.42
1:C:362:GLU:N	3:F:107:GLU:OE2	2.41	0.42
2:D:129:ILE:HA	2:D:130:LYS:HA	1.79	0.42
2:E:275:ASP:N	2:E:275:ASP:OD1	2.51	0.42
2:D:13:HIS:O	2:D:17:TRP:CB	2.62	0.42
2:D:471:SER:HA	2:D:472:SER:HA	1.79	0.42
1:B:262:VAL:HB	1:B:270:LEU:HB2	2.01	0.42
2:D:54:GLU:OE2	2:D:73:ASP:N	2.44	0.42
2:E:459:GLU:HA	2:E:462:VAL:HG13	2.00	0.42
3:G:74:THR:HG23	3:G:76:ASP:H	1.83	0.42
2:D:102:ASN:O	2:D:106:ASN:ND2	2.52	0.42
2:D:103:ASP:HB3	2:D:104:ARG:HH21	1.85	0.42
2:D:449:VAL:HB	2:D:452:LEU:HD22	2.00	0.42
1:B:457:GLU:O	2:D:319:ASN:ND2	2.52	0.42
1:B:1006:LEU:HD12	1:B:1009:LEU:HD11	2.01	0.42
2:D:201:THR:OG1	2:D:302:ASN:ND2	2.50	0.42
2:E:21:ASN:HD21	2:E:183:PHE:HE2	1.68	0.42
4:A:233:TRP:O	4:A:247:SER:OG	2.30	0.42
1:B:191:GLU:HA	1:B:192:ASN:HA	1.84	0.42
1:C:162:VAL:HG21	1:C:253:LEU:HD21	2.01	0.42
1:C:332:LYS:O	1:C:403:VAL:HA	2.20	0.42
2:E:214:MET:HE2	2:E:241:PHE:HD2	1.84	0.42
2:E:222:LYS:HG3	2:E:298:ALA:HB3	2.01	0.42
4:A:94:LYS:O	4:A:96:SER:N	2.46	0.42
4:A:355:GLN:HA	4:A:358:VAL:HG12	2.02	0.42
1:B:541:MET:HG2	1:B:653:LEU:HB3	2.01	0.42
1:C:154:ILE:HB	1:C:162:VAL:HB	2.01	0.42
1:B:412:ARG:HH21	1:B:447:SER:HB2	1.85	0.42
2:D:144:GLY:HA3	2:D:150:LYS:HE2	2.01	0.42
2:E:250:PHE:H	2:E:277:PHE:HD1	1.67	0.42
1:C:740:PHE:H	1:C:749:LYS:HB2	1.85	0.42
1:C:890:LEU:HD23	1:C:893:ILE:HD12	2.02	0.42
1:C:265:SER:HA	1:C:266:SER:HA	1.59	0.41
2:D:411:THR:OG1	2:D:456:VAL:O	2.38	0.41
2:E:363:TYR:HB2	2:E:369:GLN:HB2	2.02	0.41
1:B:317:SER:HB2	1:B:406:ILE:HG21	2.01	0.41
1:C:525:ARG:NH2	1:C:572:LYS:O	2.50	0.41
1:C:841:ARG:HE	1:C:916:ARG:HH21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PHE:HD1	1:B:80:GLU:HB3	1.85	0.41
1:B:502:GLU:HG3	1:B:508:LEU:HD11	2.01	0.41
1:B:809:LEU:HA	1:B:810:SER:HA	1.71	0.41
1:C:342:LEU:O	1:C:346:THR:OG1	2.31	0.41
1:C:1009:LEU:HD21	1:C:1012:GLN:HE21	1.84	0.41
2:D:144:GLY:HA2	2:D:153:ARG:HH12	1.84	0.41
2:E:389:PRO:HA	2:E:390:ASN:HA	1.69	0.41
4:A:203:TRP:HB3	4:A:345:LYS:HB3	2.02	0.41
1:B:605:ASP:O	1:B:609:LYS:N	2.41	0.41
1:C:628:SER:OG	1:C:630:ASP:OD1	2.36	0.41
2:D:230:SER:OG	2:D:231:GLY:N	2.54	0.41
2:D:362:PHE:O	2:D:467:ASN:ND2	2.54	0.41
2:E:90:GLN:OE1	2:E:130:LYS:N	2.53	0.41
1:B:838:PRO:HG2	1:B:843:ILE:HD11	2.01	0.41
1:C:550:ALA:HA	1:C:553:TYR:HD2	1.85	0.41
2:E:217:GLN:NE2	2:E:350:LYS:O	2.53	0.41
1:C:677:LEU:HB2	1:C:682:LEU:HD22	2.03	0.41
2:E:469:SER:HB2	2:E:473:TYR:CZ	2.56	0.41
1:B:605:ASP:H	1:B:608:ALA:HB3	1.86	0.41
1:B:801:LEU:HD13	1:B:832:LEU:HD12	2.01	0.41
2:E:358:PHE:O	2:E:400:ASN:ND2	2.53	0.41
1:C:551:LYS:HD3	1:C:608:ALA:HA	2.02	0.41
1:C:918:ILE:HD13	1:C:928:GLU:HA	2.02	0.41
1:C:989:ARG:NE	1:C:991:TYR:O	2.50	0.41
2:E:108:ASP:HB3	2:E:111:SER:HB3	2.03	0.41
1:B:613:ASP:HA	1:B:616:ILE:HD12	2.03	0.41
1:C:332:LYS:HE2	1:C:371:LEU:HD23	2.02	0.41
1:C:390:MET:HE1	1:C:426:PHE:HE2	1.86	0.41
1:C:660:LEU:O	1:C:688:ARG:NH1	2.44	0.41
2:D:353:ALA:HB3	2:D:404:LEU:HB2	2.02	0.41
2:D:494:THR:O	2:D:498:LYS:HD2	2.21	0.41
2:E:113:PHE:HE2	2:E:115:ALA:HB3	1.86	0.41
2:E:114:VAL:HG23	2:E:154:LEU:HD13	2.03	0.41
2:E:149:ASP:OD2	2:E:153:ARG:NH2	2.52	0.41
2:E:222:LYS:HA	2:E:223:ILE:HA	1.89	0.41
2:E:494:THR:O	2:E:498:LYS:HD2	2.21	0.41
3:F:56:MET:HE2	3:F:81:LEU:HD22	2.03	0.41
4:A:270:ALA:HB1	4:A:297:MET:HE2	2.02	0.41
1:C:49:TYR:HE1	1:C:250:LYS:HB2	1.86	0.41
1:C:492:GLU:HB3	1:C:498:LEU:HD21	2.03	0.41
1:C:716:ILE:HG23	1:C:724:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:46:ILE:HG22	4:A:59:TYR:H	1.86	0.41
1:B:69:GLN:NE2	1:B:76:PHE:H	2.19	0.40
1:C:860:GLU:HA	1:C:861:LYS:HE2	2.02	0.40
2:E:471:SER:HA	2:E:472:SER:HA	1.73	0.40
3:G:33:LEU:HD23	3:G:33:LEU:HA	1.89	0.40
4:A:74:VAL:HG23	4:A:101:VAL:HB	2.02	0.40
1:B:80:GLU:OE2	1:B:114:ASP:N	2.51	0.40
1:C:998:GLU:O	1:C:1002:THR:N	2.54	0.40
2:D:292:ASP:OD1	2:D:292:ASP:N	2.54	0.40
2:E:373:GLN:O	2:E:377:ASP:HB2	2.22	0.40
4:A:209:ILE:H	4:A:209:ILE:HG13	1.77	0.40
1:B:464:THR:O	1:B:468:ARG:HB2	2.21	0.40
1:C:582:PHE:CD1	1:C:583:ALA:HB2	2.56	0.40
2:D:422:PHE:HE2	2:D:425:GLU:HG2	1.86	0.40
2:E:96:ALA:HB2	2:E:124:PRO:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	963/1038 (93%)	897 (93%)	66 (7%)	0	100	100
1	C	982/1038 (95%)	898 (91%)	84 (9%)	0	100	100
2	D	464/520 (89%)	385 (83%)	79 (17%)	0	100	100
2	E	465/520 (89%)	389 (84%)	76 (16%)	0	100	100
3	F	104/117 (89%)	102 (98%)	2 (2%)	0	100	100
3	G	104/117 (89%)	102 (98%)	2 (2%)	0	100	100
4	A	382/404 (95%)	333 (87%)	49 (13%)	0	100	100
All	All	3464/3754 (92%)	3106 (90%)	358 (10%)	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	B	847/927 (91%)	845 (100%)	2 (0%)	87	85
1	C	862/927 (93%)	861 (100%)	1 (0%)	88	88
2	D	399/439 (91%)	395 (99%)	4 (1%)	68	76
2	E	399/439 (91%)	396 (99%)	3 (1%)	73	77
3	F	95/105 (90%)	95 (100%)	0	100	100
3	G	95/105 (90%)	95 (100%)	0	100	100
4	A	344/364 (94%)	337 (98%)	7 (2%)	48	66
All	All	3041/3306 (92%)	3024 (99%)	17 (1%)	76	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	520	ILE
1	B	556	THR
1	C	682	LEU
2	D	114	VAL
2	D	116	ILE
2	D	132	LEU
2	D	184	LEU
2	E	116	ILE
2	E	132	LEU
2	E	154	LEU
4	A	66	ILE
4	A	118	LEU
4	A	277	ILE
4	A	306	ILE
4	A	366	THR
4	A	380	GLU
4	A	393	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	69	GLN
1	B	163	GLN
1	B	267	GLN
1	B	376	ASN
1	B	387	ASN
1	B	459	HIS
1	B	514	GLN
1	B	622	HIS
1	B	648	GLN
1	B	924	ASN
1	B	975	ASN
1	B	1000	ASN
1	C	42	GLN
1	C	47	GLN
1	C	57	GLN
1	C	69	GLN
1	C	91	ASN
1	C	163	GLN
1	C	345	GLN
1	C	522	ASN
1	C	622	HIS
1	C	680	HIS
1	C	726	ASN
1	C	806	GLN
1	C	958	GLN
1	C	975	ASN
1	C	995	ASN
1	C	1012	GLN
2	D	21	ASN
2	D	106	ASN
2	D	217	GLN
2	D	240	GLN
2	D	266	ASN
2	D	302	ASN
2	D	319	ASN
2	D	342	HIS
2	D	400	ASN
2	D	441	GLN
2	D	489	ASN
2	E	21	ASN

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Mol	Chain	Res	Type
2	E	100	ASN
2	E	102	ASN
2	E	141	ASN
2	E	217	GLN
2	E	379	ASN
2	E	438	GLN
2	E	451	HIS
3	F	43	ASN
3	G	82	GLN
4	A	130	HIS
4	A	258	HIS
4	A	313	HIS
4	A	354	GLN
4	A	383	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.

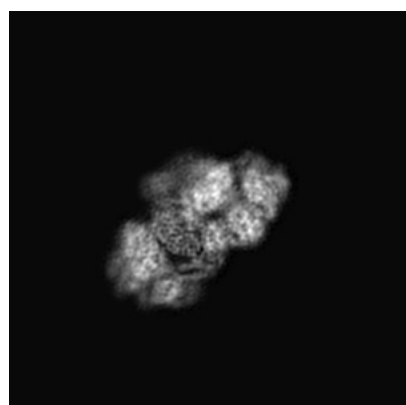
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30166. These allow visual inspection of the internal detail of the map and identification of artifacts.

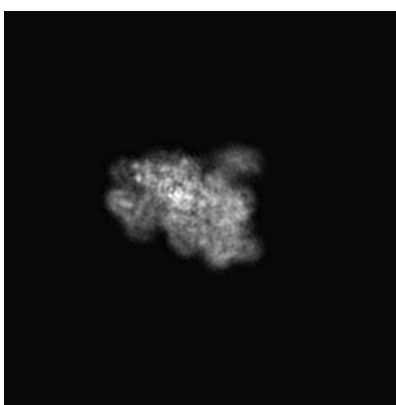
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

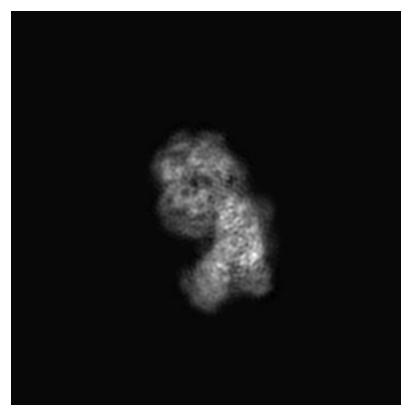
6.1.1 Primary map



X



Y

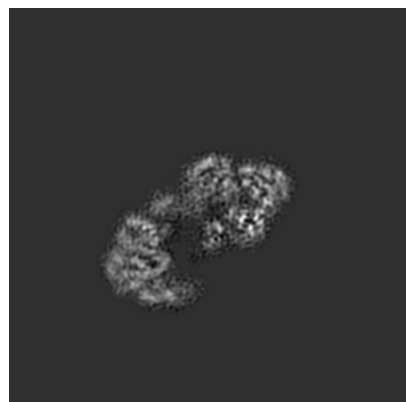


Z

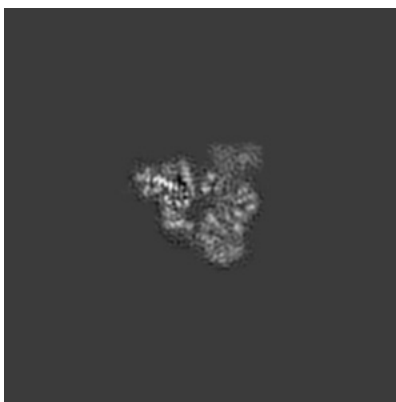
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

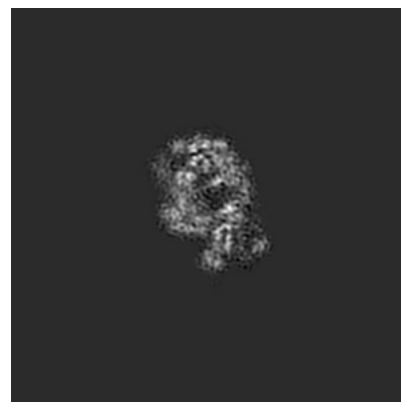
6.2.1 Primary map



X Index: 136



Y Index: 136

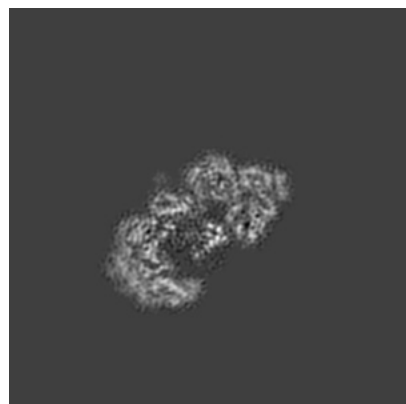


Z Index: 136

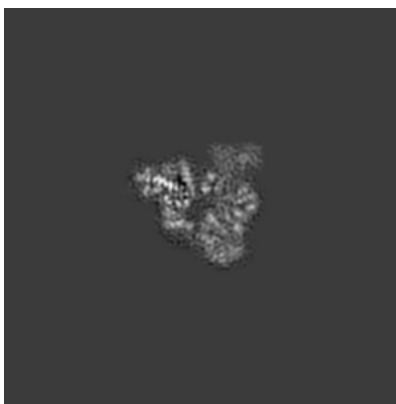
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

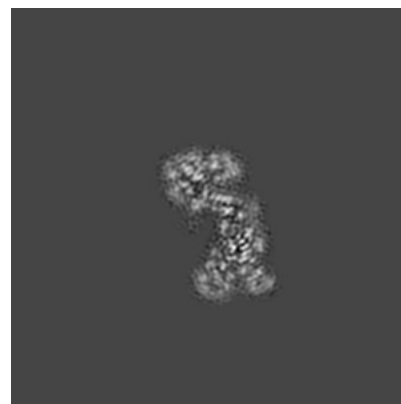
6.3.1 Primary map



X Index: 140



Y Index: 136

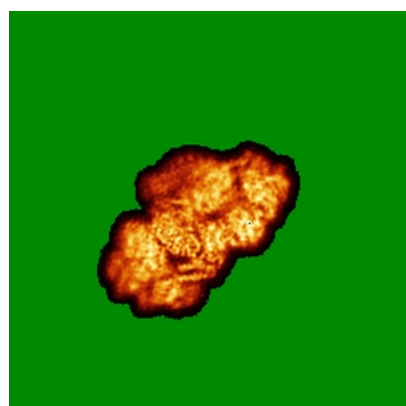


Z Index: 120

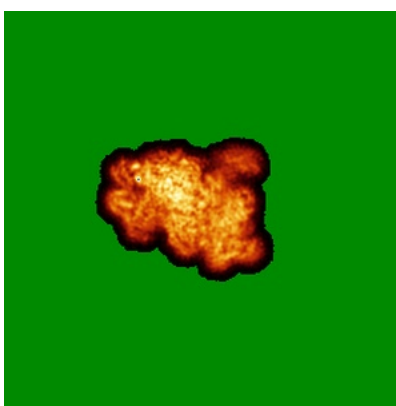
The images above show the largest variance slices of the map in three orthogonal directions.

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

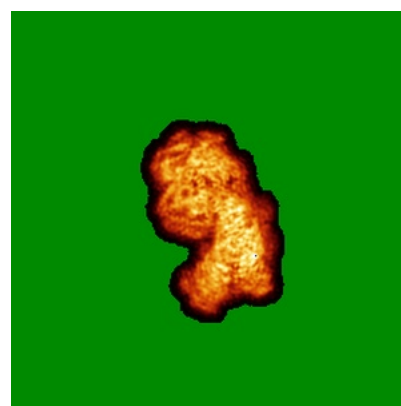
6.4.1 Primary map



X



Y

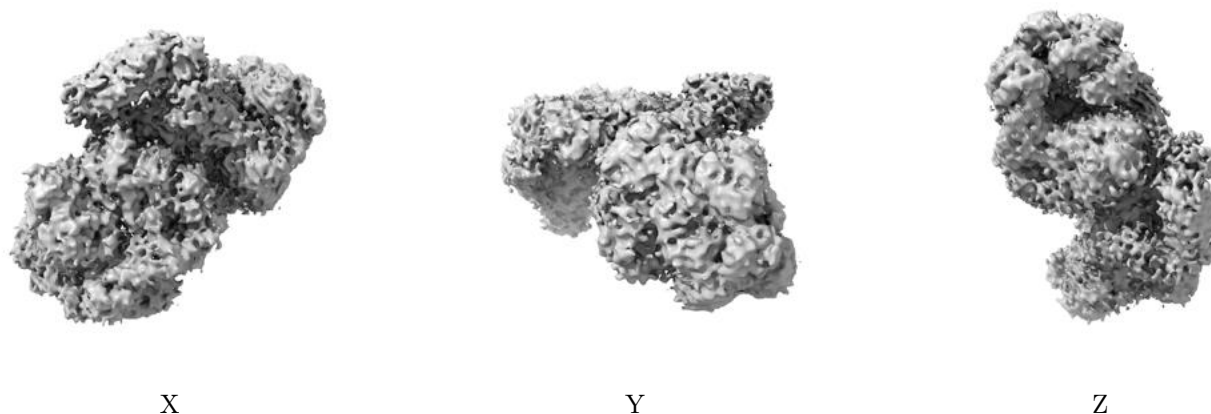


Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

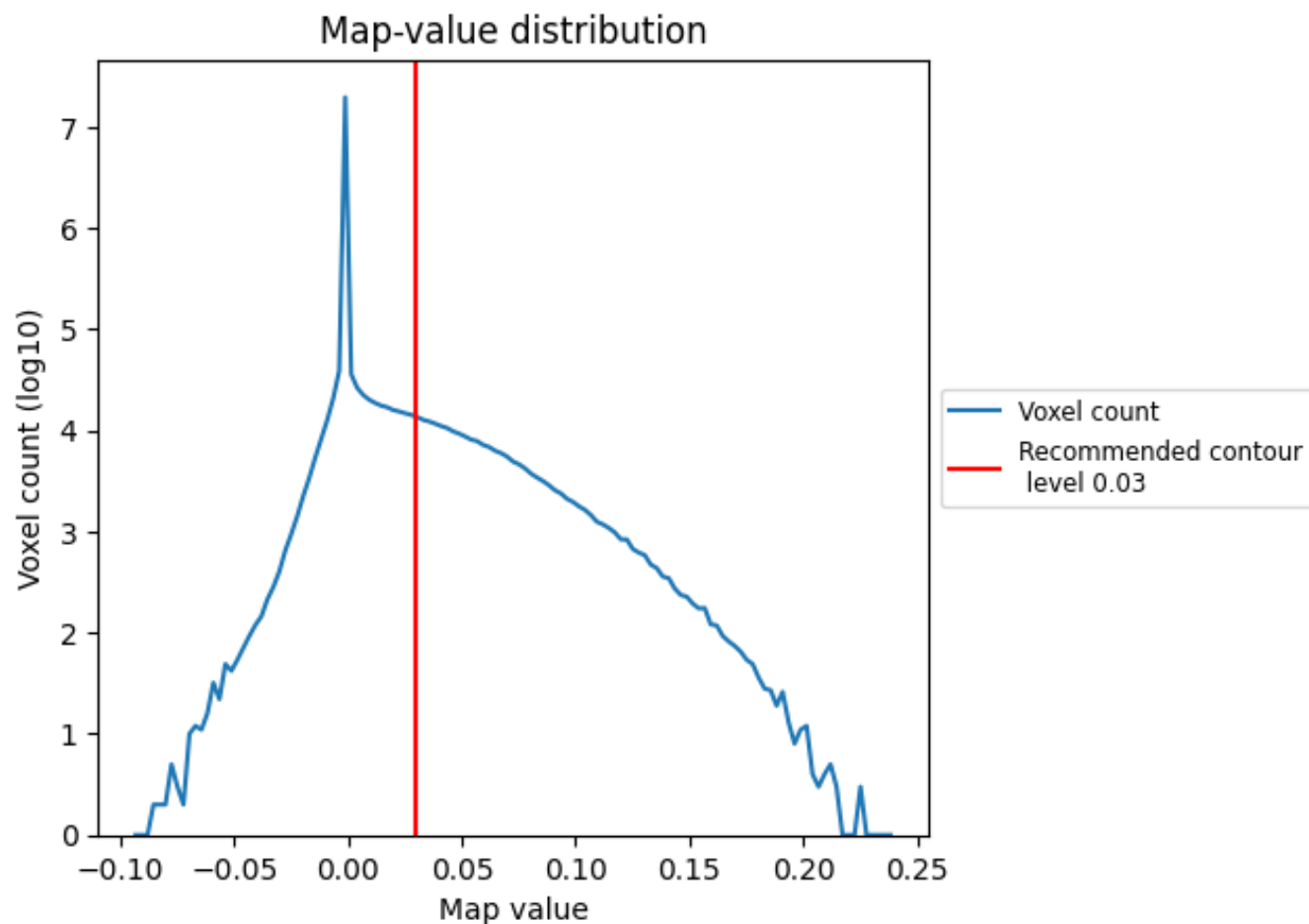
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

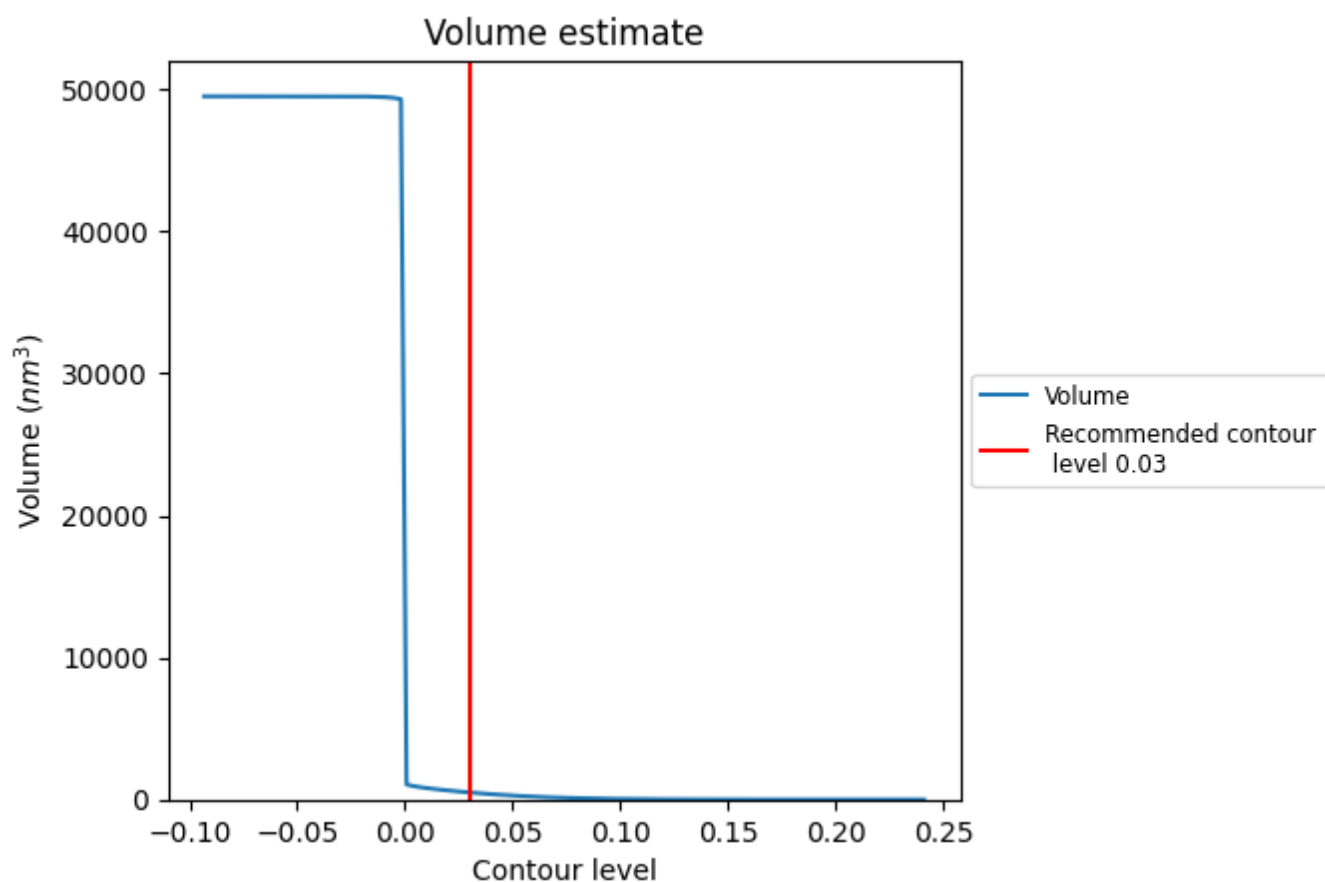
This section contains the results of statistical analysis of the map.

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.

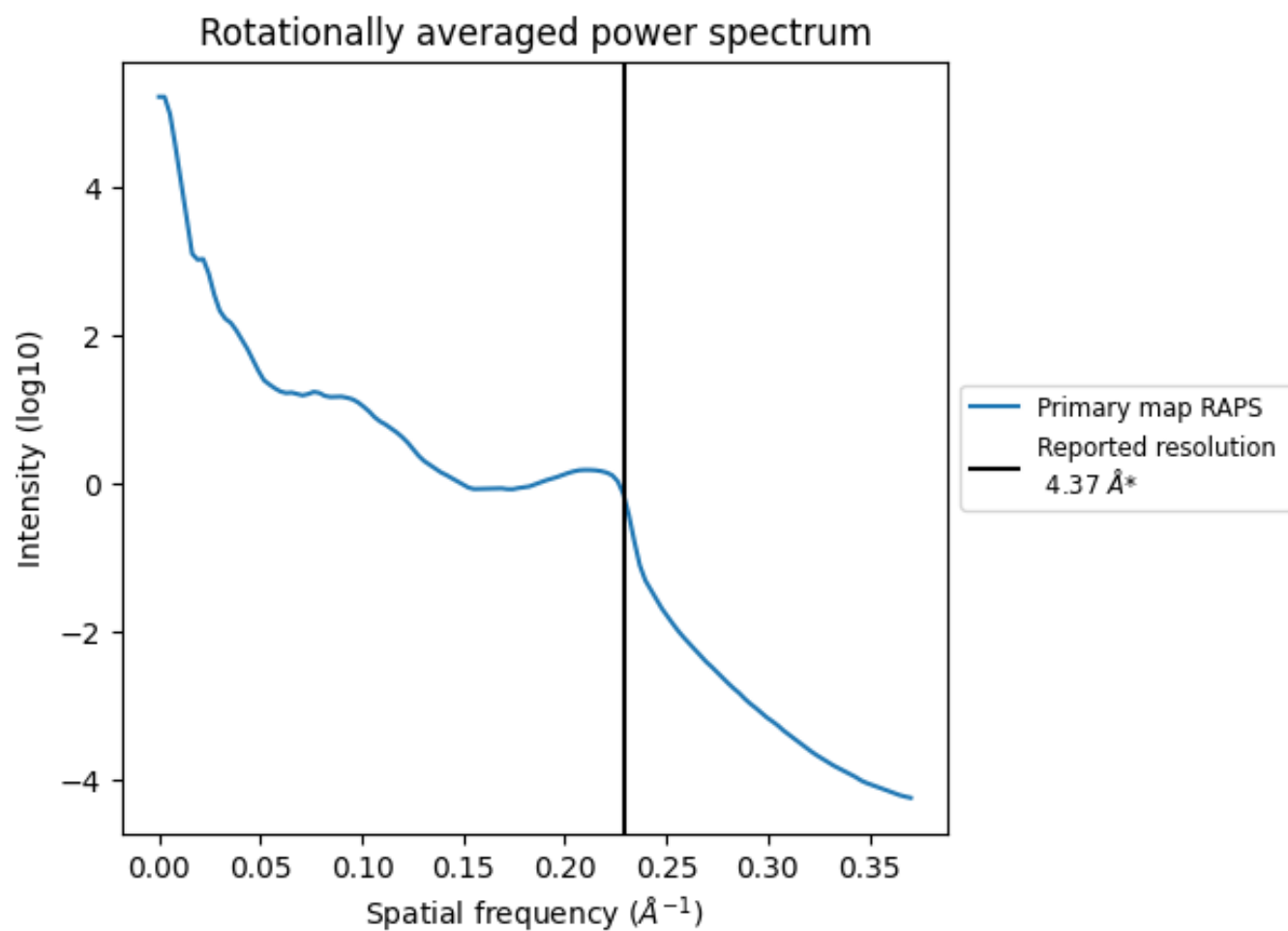
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 497 nm³; this corresponds to an approximate mass of 449 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 0.229 Å⁻¹

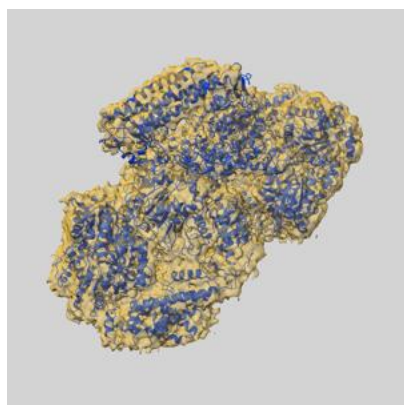
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

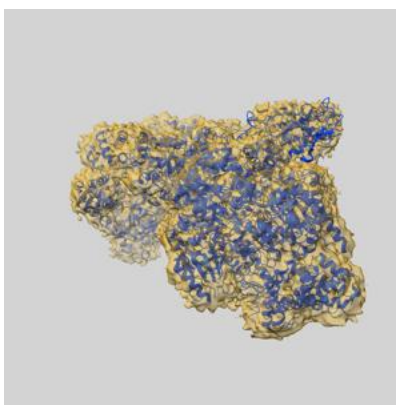
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30166 and PDB model 7BST. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

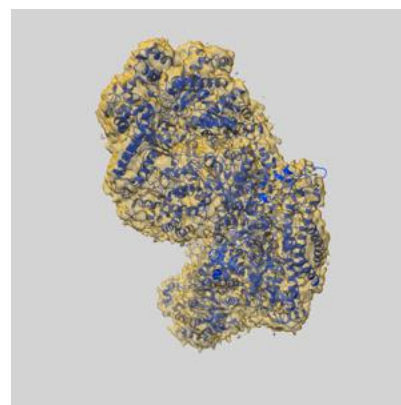
9.1 Map-model overlay [i](#)



X



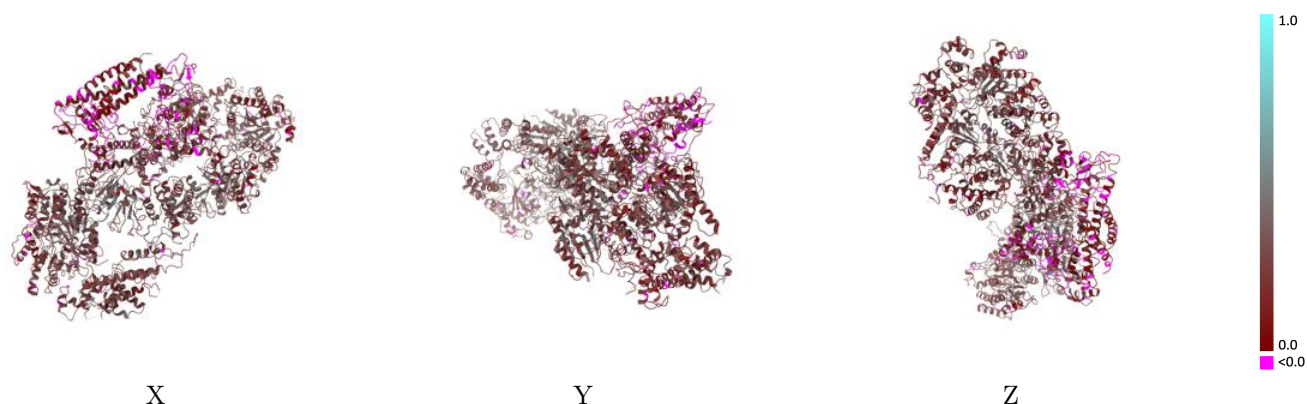
Y



Z

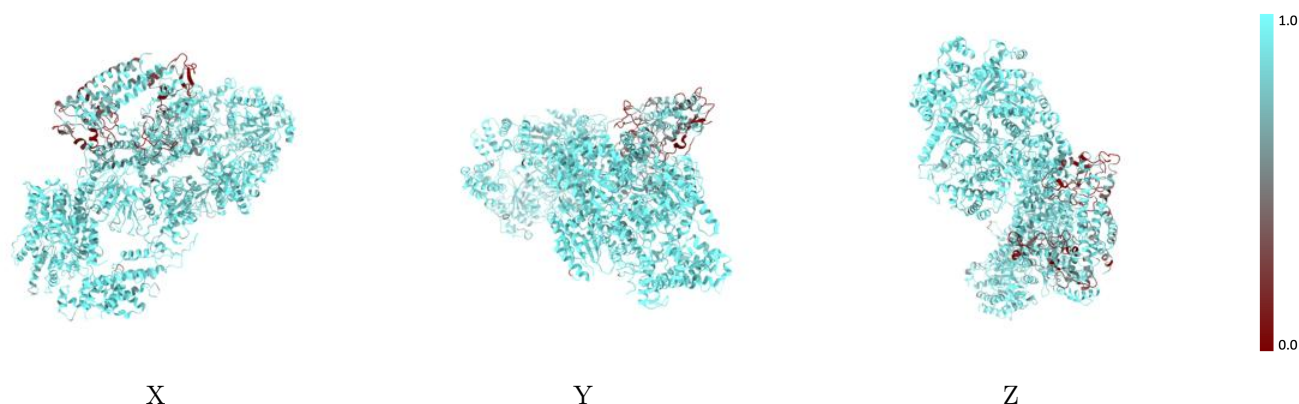
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



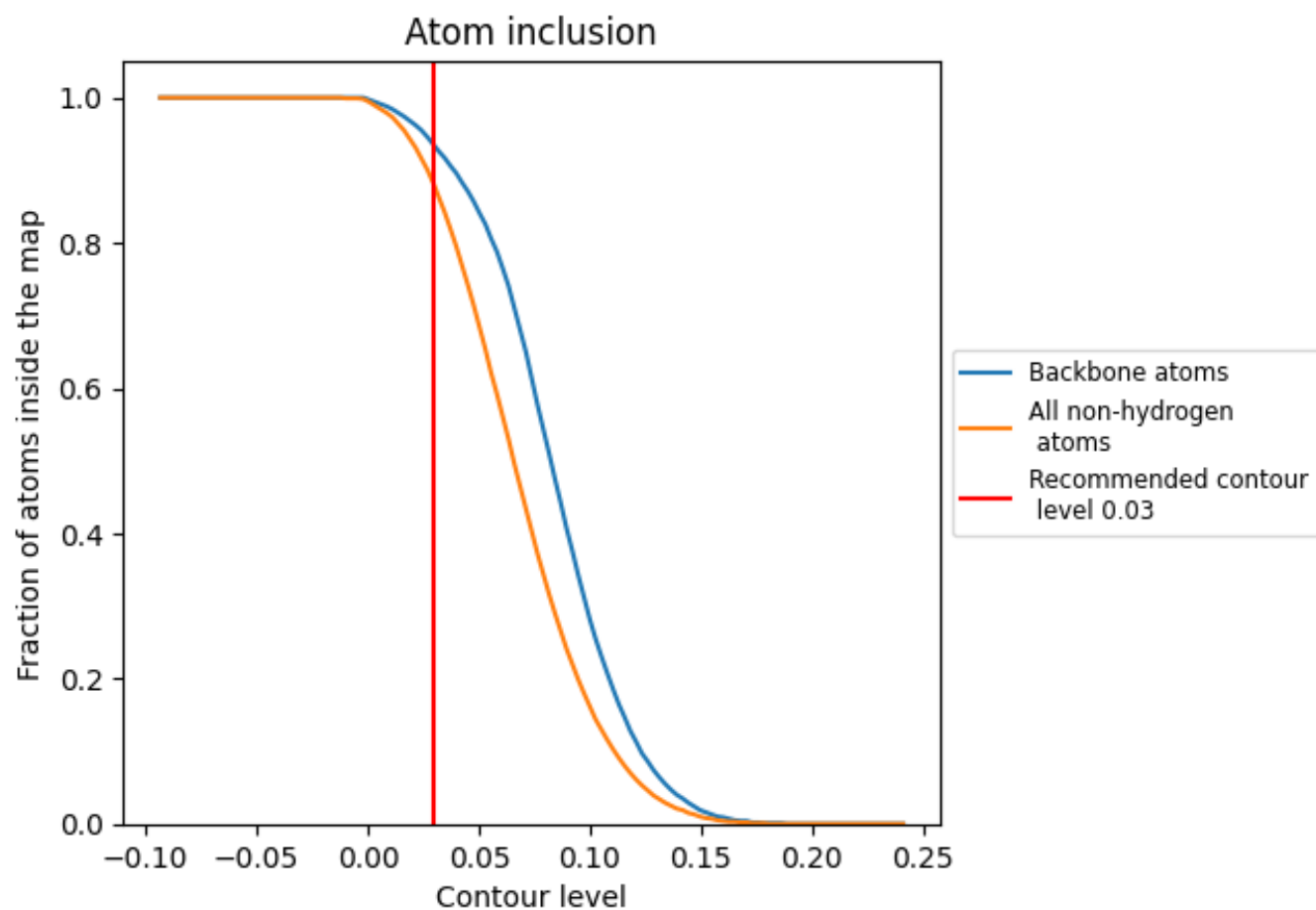
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.2450
A	0.4510	0.0720
B	0.9420	0.2710
C	0.9490	0.2750
D	0.9100	0.3010
E	0.9160	0.2220
F	0.8960	0.2210
G	0.8620	0.2260

1.0

0.0

<0.0