



Full wwPDB EM Validation Report ⓘ

Jun 1, 2026 – 11:03 AM EDT

PDB ID : 9PUV / pdb_00009puv
EMDB ID : EMD-71877
Title : Insulin receptor bound to S961
Authors : Vogel, A.; Blakely, A.; Hill, C.P.
Deposited on : 2025-07-31
Resolution : 3.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

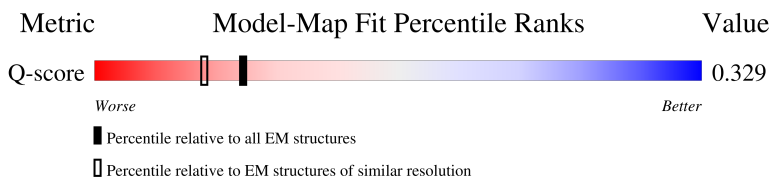
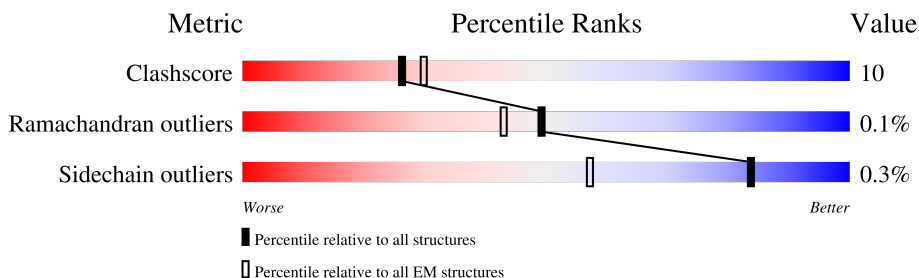
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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	11376 (3.18 - 4.18)

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	1371	
1	C	1371	
2	B	43	
2	D	43	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26242 atoms, of which 12914 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 Isoform Long of Insulin receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	788	Total	C	H	N	O	S	0	0
			12551	4032	6196	1101	1174	48		
1	C	788	Total	C	H	N	O	S	0	0
			12549	4032	6194	1101	1174	48		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	549	SER	ASN	conflict	UNP P06213
A	1346	ASP	-	expression tag	UNP P06213
A	1347	TYR	-	expression tag	UNP P06213
A	1348	LYS	-	expression tag	UNP P06213
A	1349	ASP	-	expression tag	UNP P06213
A	1350	ASP	-	expression tag	UNP P06213
A	1351	ASP	-	expression tag	UNP P06213
A	1352	ASP	-	expression tag	UNP P06213
A	1353	LYS	-	expression tag	UNP P06213
A	1354	ASP	-	expression tag	UNP P06213
A	1355	TYR	-	expression tag	UNP P06213
A	1356	LYS	-	expression tag	UNP P06213
A	1357	ASP	-	expression tag	UNP P06213
A	1358	ASP	-	expression tag	UNP P06213
A	1359	ASP	-	expression tag	UNP P06213
A	1360	ASP	-	expression tag	UNP P06213
A	1361	LYS	-	expression tag	UNP P06213
C	549	SER	ASN	conflict	UNP P06213
C	1346	ASP	-	expression tag	UNP P06213
C	1347	TYR	-	expression tag	UNP P06213
C	1348	LYS	-	expression tag	UNP P06213
C	1349	ASP	-	expression tag	UNP P06213
C	1350	ASP	-	expression tag	UNP P06213
C	1351	ASP	-	expression tag	UNP P06213
C	1352	ASP	-	expression tag	UNP P06213
C	1353	LYS	-	expression tag	UNP P06213

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1354	ASP	-	expression tag	UNP P06213
C	1355	TYR	-	expression tag	UNP P06213
C	1356	LYS	-	expression tag	UNP P06213
C	1357	ASP	-	expression tag	UNP P06213
C	1358	ASP	-	expression tag	UNP P06213
C	1359	ASP	-	expression tag	UNP P06213
C	1360	ASP	-	expression tag	UNP P06213
C	1361	LYS	-	expression tag	UNP P06213

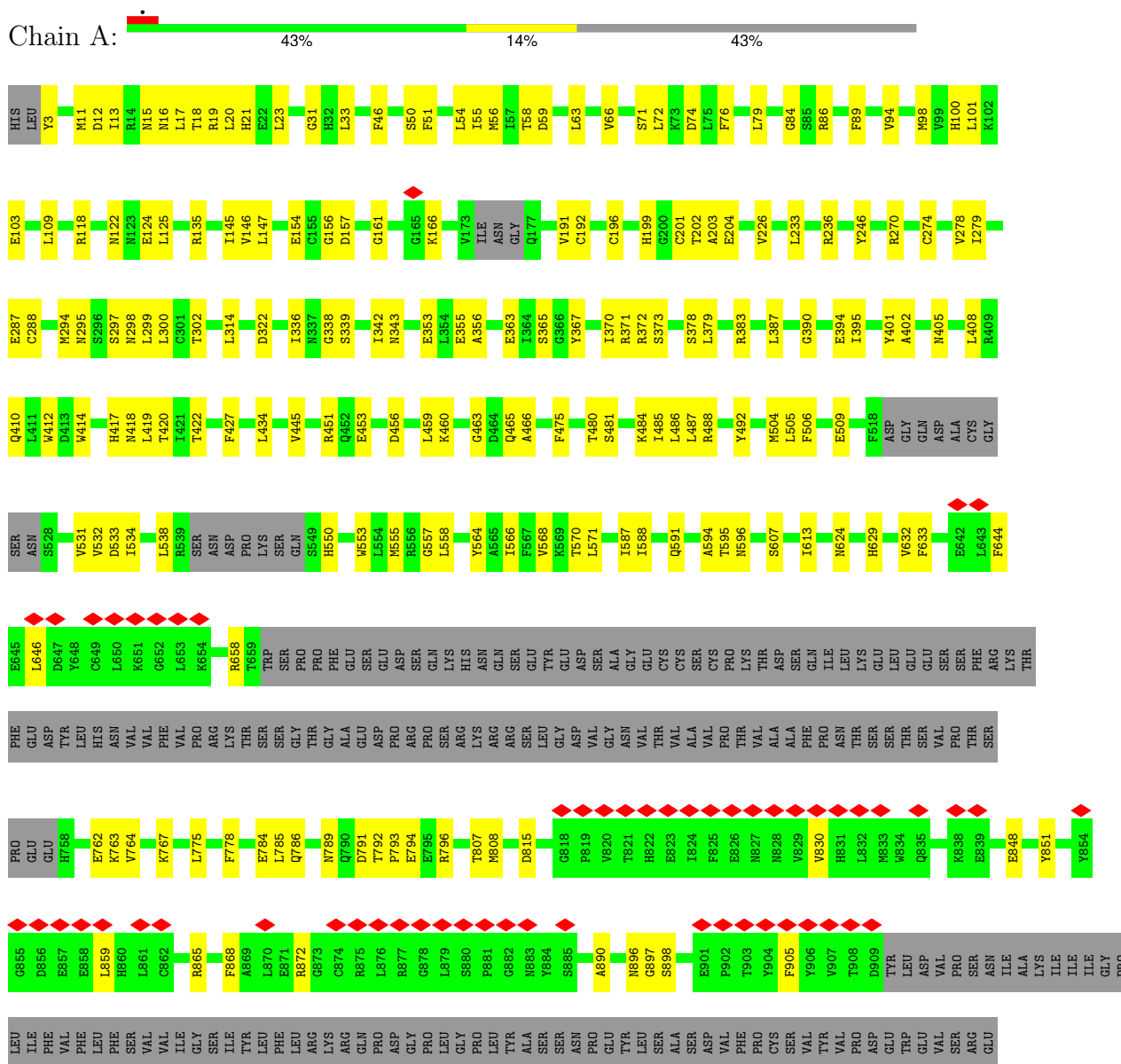
- Molecule 2 is a protein called S961 Insulin receptor antagonist.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	38	Total	C	H	N	O	S	0	0
			556	188	254	50	62	2		
2	D	40	Total	C	H	N	O	S	0	0
			586	197	270	52	65	2		

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.

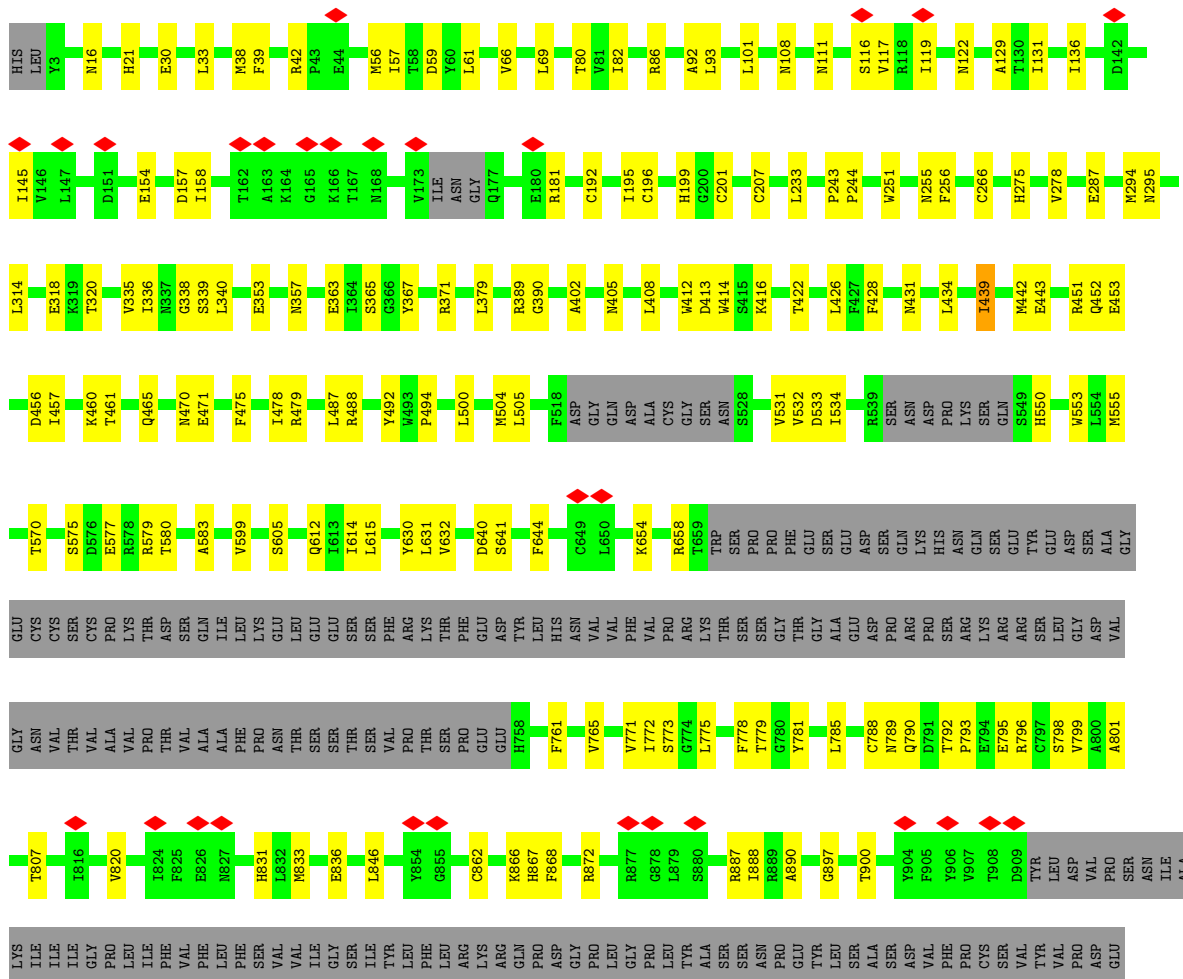
• Molecule 1: Isoform Long of Insulin receptor



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

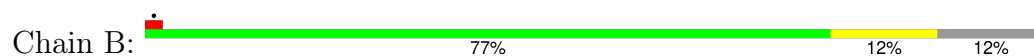
- Molecule 1: Isoform Long of Insulin receptor

Chain C: 45% 12% 43%

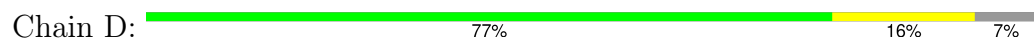


LEU	GLU	ASP	GLY	MET	TRP
PRO	LEU	GLN	LEU	ILE	GLU
ARG	GLU	PRO	LEU	GLN	VAL
SER	MET	ASP	PRO	MET	LYS
ASN	GLU	ASN	VAL	ALA	ARG
PRO	PHE	CYS	ARG	ALA	GLY
SER	GLU	PRO	TRP	GLU	THR
ASP	ASP	GLU	MET	ILE	LYS
TYR	MET	ALA	ALA	ALA	CYS
LYS	GLU	VAL	PRO	ASP	THR
ASP	ASN	THR	GLU	GLY	LEU
ASP	VAL	ASP	SER	MET	ARG
ASP	PRO	LEU	LEU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

- Molecule 2: S961 Insulin receptor antagonist



- Molecule 2: S961 Insulin receptor antagonist



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	378182	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.631	Depositor
Minimum map value	-1.253	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0942	Depositor
Map size (\AA)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/6511	0.29	0/8828
1	C	0.14	0/6511	0.29	0/8828
2	B	0.11	0/311	0.26	0/419
2	D	0.15	0/325	0.29	0/438
All	All	0.14	0/13658	0.29	0/18513

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6355	6196	6193	142	0
1	C	6355	6194	6191	126	0
2	B	302	254	253	5	0
2	D	316	270	269	11	0
All	All	13328	12914	12906	266	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (266) 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:A:373:SER:OG	1:A:405:ASN:OD1	1.87	0.92
1:A:343:ASN:ND2	1:A:371:ARG:O	2.08	0.86
1:A:484:LYS:NZ	2:B:25:GLU:OE2	2.09	0.85
1:C:789:ASN:OD1	1:C:796:ARG:NH1	2.10	0.84
1:A:103:GLU:N	1:A:103:GLU:OE1	2.14	0.81
1:C:599:VAL:CG2	1:C:801:ALA:HB2	2.10	0.80
1:A:101:LEU:HD23	1:A:125:LEU:HD11	1.62	0.80
1:A:196:CYS:O	1:A:199:HIS:ND1	2.15	0.80
1:A:287:GLU:OE2	1:A:287:GLU:N	2.15	0.79
1:C:475:PHE:HB3	1:C:478:ILE:HD11	1.63	0.79
1:A:338:GLY:N	1:A:365:SER:OG	2.15	0.79
1:C:379:LEU:O	1:C:412:TRP:NE1	2.18	0.76
1:A:59:ASP:OD2	1:A:86:ARG:NE	2.18	0.76
1:A:372:ARG:NH2	1:C:504:MET:SD	2.59	0.76
1:A:3:TYR:OH	1:A:56:MET:SD	2.44	0.76
2:B:25:GLU:N	2:B:25:GLU:OE1	2.18	0.76
1:A:784:GLU:OE2	1:A:786:GLN:NE2	2.20	0.74
1:A:50:SER:OG	1:A:74:ASP:O	2.06	0.74
1:A:644:PHE:O	1:A:865:ARG:NE	2.22	0.72
1:A:533:ASP:OD2	1:C:371:ARG:NH1	2.23	0.72
1:C:266:CYS:SG	1:C:275:HIS:N	2.65	0.69
1:C:443:GLU:OE2	1:C:452:GLN:NE2	2.25	0.69
1:A:31:GLY:N	1:A:58:THR:OG1	2.26	0.68
1:C:66:VAL:HG12	1:C:69:LEU:HD23	1.74	0.68
1:C:470:ASN:OD1	1:C:471:GLU:N	2.27	0.68
1:C:599:VAL:HG22	1:C:801:ALA:HB2	1.77	0.67
1:A:378:SER:OG	1:A:410:GLN:O	2.11	0.66
1:A:465:GLN:N	1:A:465:GLN:OE1	2.30	0.65
1:A:607:SER:OG	1:A:808:MET:SD	2.50	0.64
1:C:487:LEU:HD12	1:C:505:LEU:HD11	1.79	0.63
1:C:408:LEU:CD2	1:C:434:LEU:HD12	2.29	0.63
1:A:79:LEU:O	1:A:109:LEU:N	2.31	0.63
1:A:762:GLU:OE1	1:A:763:LYS:N	2.31	0.63
1:A:418:ASN:OD1	1:A:419:LEU:N	2.33	0.62
1:A:146:VAL:HG23	1:A:147:LEU:HD12	1.81	0.62
1:A:383:ARG:O	1:A:417:HIS:NE2	2.32	0.62
1:A:485:ILE:CG2	1:A:487:LEU:HD21	2.30	0.62
1:C:488:ARG:NH2	2:D:31:ILE:HD13	2.15	0.61
1:C:129:ALA:O	1:C:181:ARG:NH2	2.33	0.61
1:A:509:GLU:N	1:A:509:GLU:OE1	2.34	0.61
1:A:298:ASN:OD1	1:A:298:ASN:O	2.17	0.61
1:A:587:ILE:O	1:A:587:ILE:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:MET:HE1	1:A:23:LEU:HD13	1.83	0.61
1:A:778:PHE:N	1:A:807:THR:OG1	2.34	0.60
1:C:630:TYR:O	1:C:632:VAL:HG23	2.01	0.60
1:C:494:PRO:HB3	1:C:580:THR:HG21	1.83	0.60
2:D:34:GLU:OE1	2:D:35:VAL:HG13	2.01	0.60
1:C:778:PHE:N	1:C:807:THR:OG1	2.35	0.60
1:A:595:THR:O	1:A:789:ASN:ND2	2.34	0.59
1:C:428:PHE:CG	1:C:439:ILE:HD11	2.36	0.59
1:A:314:LEU:HD11	1:A:336:ILE:HD11	1.85	0.59
1:A:453:GLU:N	1:A:456:ASP:OD2	2.35	0.59
1:A:475:PHE:CD2	1:A:588:ILE:HD13	2.38	0.58
1:C:465:GLN:N	1:C:465:GLN:OE1	2.36	0.58
1:A:557:GLY:C	1:A:558:LEU:HD22	2.28	0.58
1:C:59:ASP:OD2	1:C:86:ARG:NH2	2.37	0.58
1:C:890:ALA:O	1:C:897:GLY:N	2.37	0.57
1:C:775:LEU:HD12	1:C:781:TYR:CZ	2.39	0.57
1:A:808:MET:SD	1:A:808:MET:N	2.78	0.57
1:A:613:ILE:HG12	1:A:775:LEU:HD12	1.85	0.57
1:A:233:LEU:O	1:A:236:ARG:N	2.37	0.57
1:A:633:PHE:O	1:A:784:GLU:N	2.30	0.57
1:C:80:THR:HG22	1:C:108:ASN:OD1	2.04	0.56
1:C:287:GLU:N	1:C:287:GLU:OE1	2.38	0.56
1:A:94:VAL:HG22	1:A:118:ARG:HB3	1.87	0.56
1:A:486:LEU:C	1:A:487:LEU:HD23	2.31	0.56
1:C:494:PRO:CB	1:C:580:THR:HG21	2.36	0.56
1:C:192:CYS:SG	1:C:201:CYS:N	2.79	0.55
1:A:505:LEU:HG	1:A:568:VAL:HG22	1.88	0.55
1:A:20:LEU:HD12	1:A:20:LEU:O	2.06	0.55
1:A:23:LEU:HD21	1:A:54:LEU:HD22	1.88	0.55
1:A:534:ILE:HD12	1:A:553:TRP:CD2	2.41	0.55
1:A:192:CYS:SG	1:A:201:CYS:N	2.79	0.55
1:C:111:ASN:ND2	1:C:136:ILE:O	2.36	0.55
1:C:255:ASN:OD1	1:C:256:PHE:N	2.40	0.54
1:C:478:ILE:N	1:C:478:ILE:HD12	2.22	0.54
1:A:300:LEU:HD11	1:A:302:THR:HG23	1.89	0.54
1:C:339:SER:OG	1:C:340:LEU:N	2.37	0.54
1:C:580:THR:HG22	1:C:580:THR:O	2.08	0.54
1:C:798:SER:OG	1:C:799:VAL:N	2.40	0.54
1:A:18:THR:O	1:A:21:HIS:CD2	2.61	0.54
1:A:58:THR:O	1:A:84:GLY:N	2.40	0.54
1:C:30:GLU:OE2	1:C:251:TRP:NE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:SER:OG	1:C:577:GLU:OE2	2.26	0.54
1:A:506:PHE:HD1	1:A:531:VAL:HG22	1.73	0.54
1:A:890:ALA:O	1:A:897:GLY:N	2.41	0.53
1:C:631:LEU:HD23	1:C:632:VAL:N	2.23	0.53
1:A:629:HIS:ND1	1:A:791:ASP:OD1	2.41	0.53
1:C:888:ILE:H	1:C:900:THR:HG22	1.74	0.53
1:C:550:HIS:O	2:D:31:ILE:HD11	2.08	0.53
1:C:33:LEU:HD22	1:C:61:LEU:HD13	1.90	0.53
1:C:505:LEU:HD21	1:C:555:MET:HE1	1.91	0.52
1:A:658:ARG:NE	1:C:154:GLU:OE2	2.42	0.52
1:C:413:ASP:OD1	1:C:413:ASP:N	2.38	0.52
1:A:370:ILE:CD1	1:A:379:LEU:HD11	2.39	0.52
1:C:820:VAL:HG21	1:C:900:THR:HG21	1.92	0.52
1:C:338:GLY:N	1:C:365:SER:OG	2.43	0.52
1:C:353:GLU:O	1:C:357:ASN:ND2	2.43	0.51
1:A:379:LEU:O	1:A:412:TRP:NE1	2.43	0.51
1:A:613:ILE:HD11	1:A:807:THR:HG22	1.91	0.51
1:C:405:ASN:ND2	1:C:431:ASN:OD1	2.42	0.51
1:A:336:ILE:O	1:A:336:ILE:HG23	2.11	0.51
1:A:300:LEU:CD1	1:A:302:THR:HG23	2.41	0.51
2:B:27:GLU:OE1	2:B:30:GLN:NE2	2.44	0.50
1:A:532:VAL:HG12	1:A:533:ASP:N	2.26	0.50
1:C:533:ASP:OD1	1:C:534:ILE:N	2.44	0.50
1:C:532:VAL:HG11	1:C:553:TRP:NE1	2.26	0.50
1:A:33:LEU:HD21	1:A:76:PHE:CZ	2.47	0.50
1:A:365:SER:O	1:A:390:GLY:N	2.45	0.50
1:C:833:MET:HA	1:C:833:MET:HE3	1.92	0.50
1:A:486:LEU:O	1:A:487:LEU:HD23	2.11	0.50
1:C:614:ILE:HG22	1:C:771:VAL:HG22	1.94	0.50
1:A:355:GLU:OE1	1:A:356:ALA:N	2.45	0.49
1:C:772:ILE:HG22	1:C:775:LEU:HD21	1.94	0.49
1:A:3:TYR:O	1:A:3:TYR:CG	2.65	0.49
1:A:23:LEU:HD23	1:A:51:PHE:HD2	1.78	0.49
1:C:765:VAL:O	1:C:765:VAL:HG23	2.13	0.49
1:A:387:LEU:HD12	1:A:420:THR:O	2.13	0.49
1:A:480:THR:HG21	1:A:591:GLN:O	2.13	0.49
1:C:33:LEU:HD22	1:C:61:LEU:CD1	2.43	0.49
1:C:119:ILE:HG22	1:C:122:ASN:ND2	2.28	0.48
1:A:202:THR:OG1	1:A:203:ALA:N	2.47	0.48
1:C:119:ILE:HB	1:C:145:ILE:HG22	1.96	0.48
1:A:485:ILE:HG22	1:A:487:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ILE:HG23	1:C:207:CYS:SG	2.54	0.48
1:C:761:PHE:C	1:C:761:PHE:CD1	2.91	0.48
1:C:131:ILE:O	1:C:181:ARG:NH2	2.46	0.48
1:C:846:LEU:HD13	1:C:862:CYS:SG	2.54	0.48
1:C:16:ASN:C	1:C:38:MET:HE1	2.39	0.48
1:C:460:LYS:O	1:C:461:THR:HG22	2.13	0.48
1:A:370:ILE:HD13	1:A:379:LEU:HD21	1.95	0.48
1:C:788:CYS:SG	1:C:795:GLU:HB3	2.53	0.48
1:C:21:HIS:CD2	1:C:21:HIS:C	2.92	0.47
1:C:612:GLN:CD	1:C:773:SER:HG	2.11	0.47
1:C:833:MET:SD	1:C:833:MET:N	2.88	0.47
1:A:339:SER:OG	1:A:367:TYR:O	2.24	0.47
1:C:790:GLN:OE1	1:C:796:ARG:NH2	2.47	0.47
1:A:18:THR:HG23	1:A:19:ARG:N	2.29	0.47
1:A:13:ILE:HD13	1:A:20:LEU:HA	1.95	0.47
1:A:246:TYR:CG	1:A:279:ILE:HD11	2.49	0.47
1:A:363:GLU:OE1	1:A:387:LEU:HD23	2.15	0.47
1:C:278:VAL:CG1	1:C:294:MET:HE3	2.45	0.47
1:C:640:ASP:OD1	1:C:640:ASP:N	2.47	0.47
1:A:607:SER:HA	1:A:613:ILE:HD13	1.96	0.47
1:A:122:ASN:ND2	1:A:125:LEU:HD12	2.30	0.47
1:C:775:LEU:HD12	1:C:781:TYR:CE2	2.50	0.47
1:A:161:GLY:O	1:A:166:LYS:N	2.37	0.47
1:A:613:ILE:CG1	1:A:775:LEU:HD12	2.45	0.47
1:C:56:MET:SD	1:C:56:MET:C	2.98	0.47
1:A:394:GLU:OE1	1:A:395:ILE:N	2.39	0.46
1:C:605:SER:HA	1:C:615:LEU:HD12	1.96	0.46
1:C:831:HIS:CE1	1:C:833:MET:HE1	2.51	0.46
1:A:17:LEU:HD21	1:A:46:PHE:CE1	2.50	0.46
1:C:365:SER:O	1:C:390:GLY:N	2.49	0.46
1:A:463:GLY:HA2	1:A:466:ALA:HB2	1.98	0.46
1:A:764:VAL:HG13	1:A:767:LYS:CE	2.46	0.46
1:A:848:GLU:OE1	1:A:896:ASN:ND2	2.48	0.46
1:C:93:LEU:HB3	1:C:117:VAL:HG22	1.97	0.46
1:A:504:MET:HE2	1:A:571:LEU:HD23	1.98	0.46
1:C:402:ALA:HB3	1:C:428:PHE:CD1	2.51	0.46
1:A:154:GLU:O	1:C:658:ARG:NH2	2.48	0.46
1:A:270:ARG:CG	1:A:270:ARG:O	2.64	0.46
1:A:506:PHE:CD1	1:A:531:VAL:HG22	2.51	0.46
1:C:363:GLU:OE2	1:C:389:ARG:NE	2.39	0.46
1:C:500:LEU:HD11	1:C:570:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:O	1:A:146:VAL:HG13	2.17	0.45
1:A:297:SER:O	1:A:299:LEU:N	2.44	0.45
1:C:320:THR:O	1:C:320:THR:HG22	2.15	0.45
2:D:28:TRP:HA	2:D:31:ILE:HG22	1.98	0.45
1:C:196:CYS:O	1:C:199:HIS:ND1	2.49	0.45
1:A:156:GLY:O	1:A:157:ASP:C	2.60	0.45
1:A:353:GLU:OE1	1:A:353:GLU:N	2.44	0.45
1:C:779:THR:N	1:C:807:THR:OG1	2.46	0.45
1:C:836:GLU:OE1	1:C:836:GLU:N	2.45	0.45
1:A:204:GLU:OE1	1:A:204:GLU:N	2.48	0.45
1:A:414:TRP:CZ3	1:A:445:VAL:HG11	2.52	0.45
1:A:157:ASP:O	1:C:654:LYS:NZ	2.45	0.45
1:A:488:ARG:HD3	2:B:31:ILE:HD13	1.99	0.45
1:C:453:GLU:N	1:C:456:ASP:OD2	2.39	0.45
1:C:92:ALA:N	1:C:116:SER:O	2.48	0.44
1:C:66:VAL:HG12	1:C:69:LEU:CD2	2.46	0.44
1:C:550:HIS:O	2:D:35:VAL:HG11	2.17	0.44
1:C:868:PHE:O	1:C:872:ARG:N	2.50	0.44
1:A:89:PHE:HB3	2:D:3:LEU:HD13	2.00	0.44
1:A:100:HIS:N	1:A:124:GLU:OE2	2.43	0.44
1:C:887:ARG:NE	1:C:900:THR:O	2.41	0.44
1:A:370:ILE:O	1:A:402:ALA:HA	2.18	0.44
1:A:830:VAL:HG21	1:A:905:PHE:CE2	2.51	0.44
1:C:434:LEU:HD23	1:C:434:LEU:C	2.43	0.44
1:A:370:ILE:N	1:A:401:TYR:O	2.41	0.44
1:A:538:LEU:HD23	2:B:36:TRP:C	2.43	0.44
1:A:632:VAL:HG22	1:A:785:LEU:HD13	2.00	0.44
1:C:775:LEU:N	1:C:775:LEU:HD22	2.33	0.44
1:C:488:ARG:CZ	2:D:31:ILE:HD13	2.48	0.43
1:A:764:VAL:HG13	1:A:767:LYS:HE3	1.99	0.43
1:A:851:TYR:OH	1:A:859:LEU:HD23	2.18	0.43
1:C:294:MET:SD	1:C:295:ASN:N	2.91	0.43
1:A:63:LEU:HD13	1:A:72:LEU:HD21	2.00	0.43
1:A:459:LEU:O	1:A:460:LYS:HD3	2.18	0.43
1:A:422:THR:O	1:A:451:ARG:NH1	2.51	0.43
1:A:868:PHE:O	1:A:872:ARG:N	2.51	0.43
1:A:555:MET:HE2	1:A:558:LEU:HD11	2.01	0.43
1:C:335:VAL:HG13	1:C:363:GLU:HG2	2.00	0.43
1:A:815:ASP:OD1	1:A:898:SER:OG	2.35	0.43
1:A:596:ASN:O	1:A:624:ASN:ND2	2.43	0.43
1:C:69:LEU:HB2	1:C:101:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:SER:OG	1:A:103:GLU:OE2	2.29	0.43
1:A:506:PHE:CD1	1:A:531:VAL:HG13	2.54	0.42
1:C:479:ARG:HG3	2:D:24:LEU:HD21	2.01	0.42
1:A:408:LEU:HD23	1:A:434:LEU:HD13	2.00	0.42
1:A:792:THR:OG1	1:A:793:PRO:HD3	2.19	0.42
1:C:157:ASP:N	1:C:157:ASP:OD1	2.52	0.42
1:C:294:MET:HE2	1:C:294:MET:HA	2.00	0.42
1:C:452:GLN:NE2	1:C:457:ILE:HD11	2.34	0.42
1:C:775:LEU:HD12	1:C:781:TYR:CE1	2.54	0.42
1:A:794:GLU:O	1:A:796:ARG:N	2.52	0.42
2:D:31:ILE:O	2:D:35:VAL:HG22	2.20	0.42
1:A:555:MET:HE2	1:A:558:LEU:HD21	2.00	0.42
1:C:314:LEU:HD11	1:C:336:ILE:CG2	2.50	0.42
1:C:414:TRP:CZ2	1:C:442:MET:HE3	2.54	0.42
1:A:487:LEU:HD11	1:A:566:ILE:CD1	2.50	0.42
1:C:531:VAL:HG12	1:C:532:VAL:N	2.34	0.42
1:A:59:ASP:O	1:A:84:GLY:HA2	2.19	0.42
1:A:558:LEU:HD12	1:A:564:TYR:CE1	2.54	0.42
1:A:16:ASN:HB3	1:A:18:THR:HG22	2.01	0.42
1:A:157:ASP:OD1	1:A:157:ASP:N	2.52	0.42
1:C:57:ILE:HG22	1:C:82:ILE:HG12	2.02	0.42
1:C:866:LYS:O	1:C:867:HIS:C	2.63	0.42
1:A:12:ASP:OD1	1:A:12:ASP:N	2.52	0.41
1:A:66:VAL:O	1:A:98:MET:HE1	2.20	0.41
1:C:413:ASP:OD2	1:C:416:LYS:NZ	2.53	0.41
1:C:792:THR:N	1:C:793:PRO:CD	2.84	0.41
1:A:135:ARG:HD3	1:A:191:VAL:HG13	2.01	0.41
1:A:594:ALA:O	1:A:796:ARG:NH1	2.51	0.41
1:C:318:GLU:OE2	1:C:367:TYR:OH	2.34	0.41
1:A:294:MET:SD	1:A:295:ASN:N	2.94	0.41
1:C:500:LEU:HD11	1:C:570:THR:CG2	2.50	0.41
1:A:109:LEU:HD23	1:A:109:LEU:C	2.46	0.41
1:A:278:VAL:HG21	1:A:288:CYS:SG	2.61	0.41
1:A:322:ASP:C	1:A:322:ASP:OD1	2.63	0.41
1:A:481:SER:N	1:A:484:LYS:O	2.53	0.41
1:C:452:GLN:HE22	1:C:457:ILE:HD11	1.85	0.41
1:C:831:HIS:NE2	1:C:833:MET:HE1	2.36	0.41
1:A:342:ILE:O	1:A:343:ASN:ND2	2.53	0.41
1:C:243:PRO:N	1:C:244:PRO:HD2	2.35	0.41
1:C:428:PHE:CD1	1:C:439:ILE:HD11	2.56	0.41
1:C:479:ARG:CG	2:D:24:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:VAL:HG11	2:D:15:LEU:HD21	2.03	0.41
1:A:785:LEU:HD12	1:A:786:GLN:N	2.34	0.41
1:C:632:VAL:HG22	1:C:785:LEU:HD23	2.02	0.41
1:C:641:SER:O	1:C:644:PHE:N	2.48	0.41
1:A:492:TYR:CE2	1:A:570:THR:HG21	2.55	0.41
1:A:533:ASP:C	1:A:534:ILE:HD13	2.46	0.41
1:C:792:THR:OG1	1:C:793:PRO:HD3	2.21	0.41
1:C:39:PHE:O	1:C:42:ARG:NH1	2.54	0.41
1:A:55:ILE:HG21	1:A:226:VAL:HG22	2.03	0.40
1:C:492:TYR:CZ	1:C:583:ALA:HB2	2.55	0.40
1:C:422:THR:O	1:C:451:ARG:NH1	2.54	0.40
1:A:487:LEU:HD11	1:A:566:ILE:HD12	2.02	0.40
1:C:579:ARG:O	1:C:579:ARG:CG	2.69	0.40
1:A:402:ALA:N	1:A:427:PHE:O	2.51	0.40
1:A:531:VAL:HG12	1:A:532:VAL:N	2.35	0.40
1:A:646:LEU:HD11	1:C:158:ILE:CD1	2.51	0.40
1:C:233:LEU:HD23	1:C:233:LEU:HA	1.96	0.40
1:A:646:LEU:HD11	1:C:158:ILE:HD12	2.03	0.40
1:C:505:LEU:HD21	1:C:555:MET:CE	2.51	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	778/1371 (57%)	713 (92%)	64 (8%)	1 (0%)	48	78
1	C	778/1371 (57%)	705 (91%)	73 (9%)	0	100	100
2	B	36/43 (84%)	33 (92%)	3 (8%)	0	100	100
2	D	38/43 (88%)	38 (100%)	0	0	100	100
All	All	1630/2828 (58%)	1489 (91%)	140 (9%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASN

5.3.2 Protein sidechains [i](#)

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	714/1228 (58%)	712 (100%)	2 (0%)	86	83
1	C	714/1228 (58%)	712 (100%)	2 (0%)	86	83
2	B	30/34 (88%)	30 (100%)	0	100	100
2	D	32/34 (94%)	32 (100%)	0	100	100
All	All	1490/2524 (59%)	1486 (100%)	4 (0%)	84	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	CYS
1	A	550	HIS
1	C	426	LEU
1	C	439	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	108	ASN
1	A	111	ASN
1	A	122	ASN
1	A	185	HIS
1	A	230	ASN
1	A	249	GLN
1	A	264	HIS
1	A	440	HIS
1	A	786	GLN

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Mol	Chain	Res	Type
1	A	867	HIS
2	B	30	GLN
1	C	16	ASN
1	C	21	HIS
1	C	282	ASN
1	C	357	ASN
1	C	406	GLN
1	C	452	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.

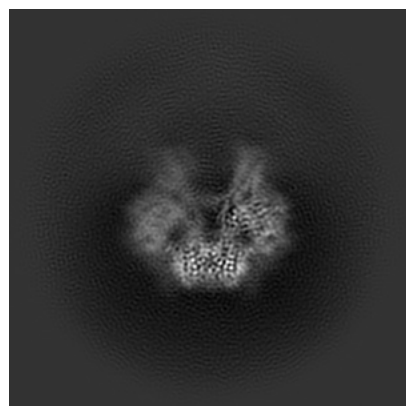
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71877. These allow visual inspection of the internal detail of the map and identification of artifacts.

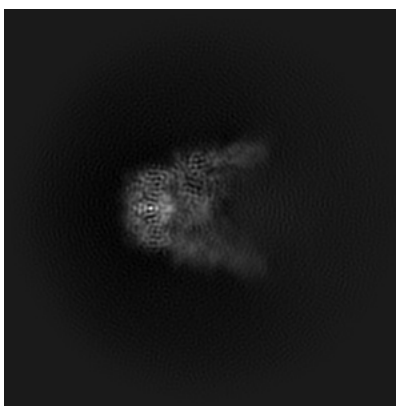
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

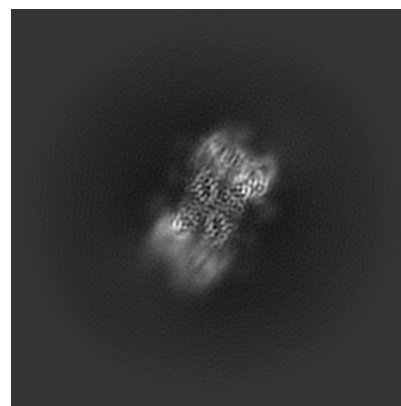
6.1.1 Primary map



X

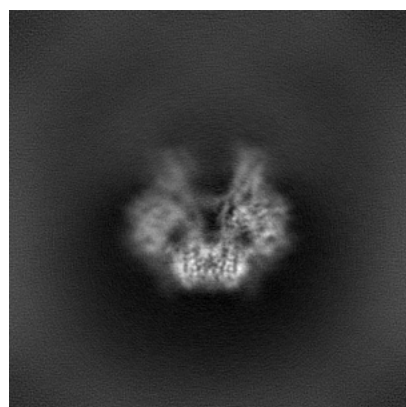


Y

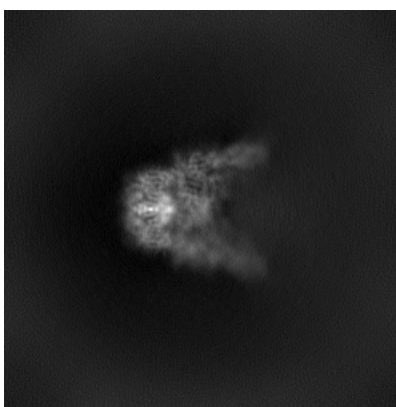


Z

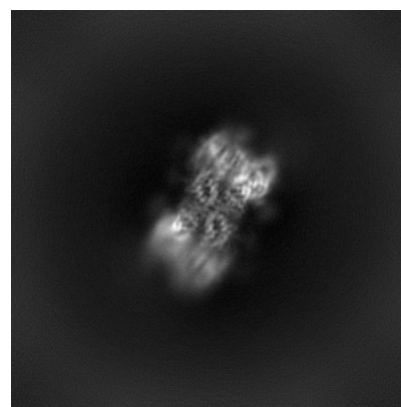
6.1.2 Raw map



X



Y

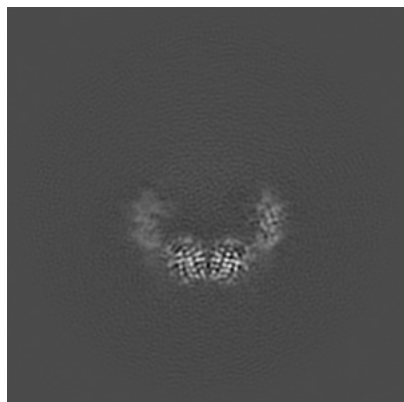


Z

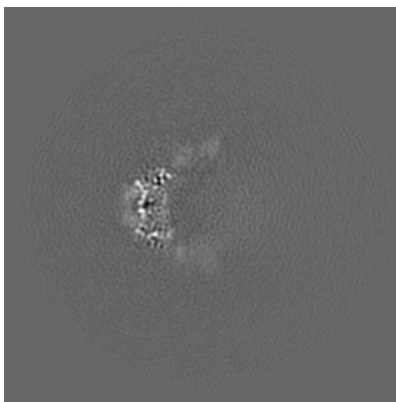
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

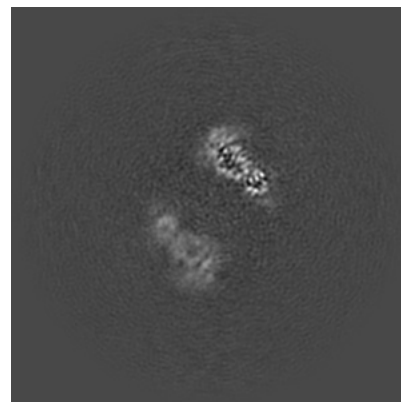
6.2.1 Primary map



X Index: 160

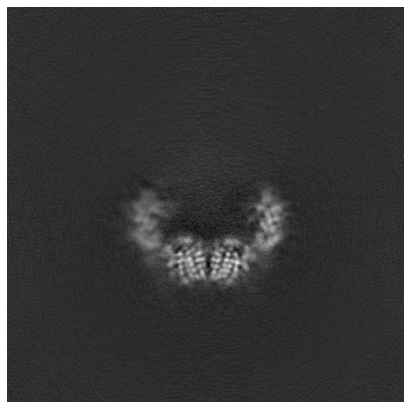


Y Index: 160

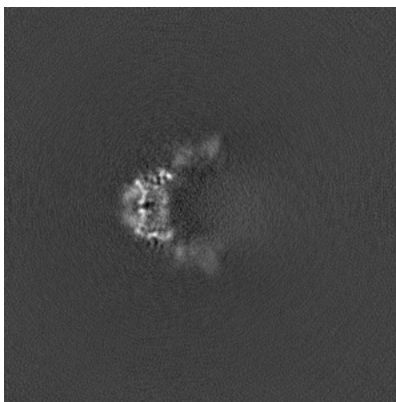


Z Index: 160

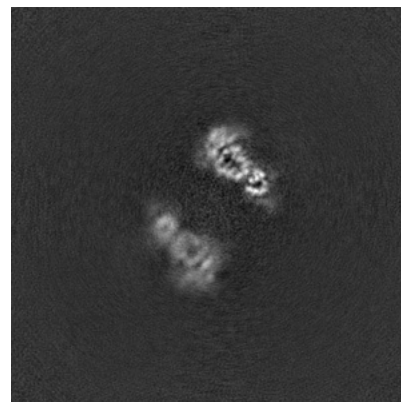
6.2.2 Raw map



X Index: 160



Y Index: 160

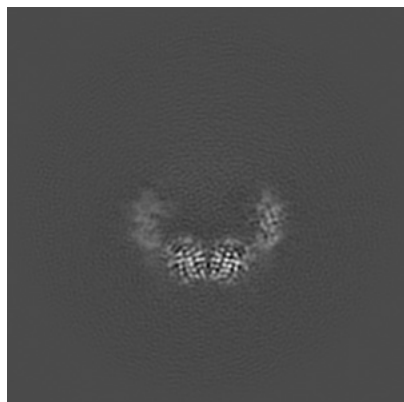


Z Index: 160

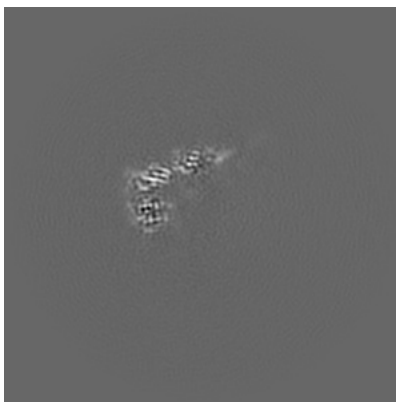
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

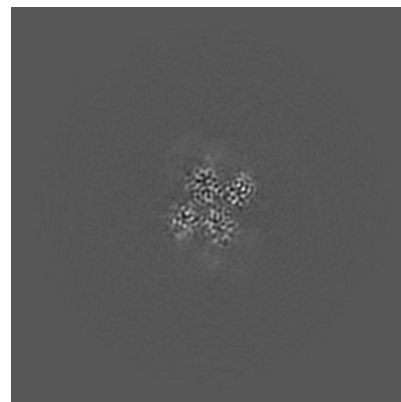
6.3.1 Primary map



X Index: 160

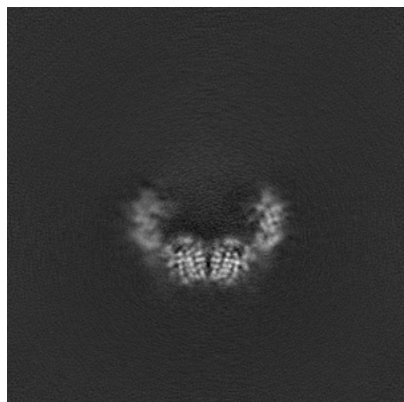


Y Index: 177

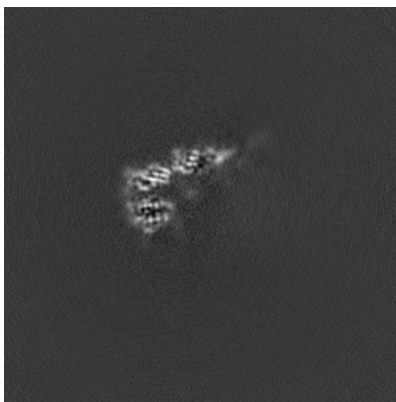


Z Index: 118

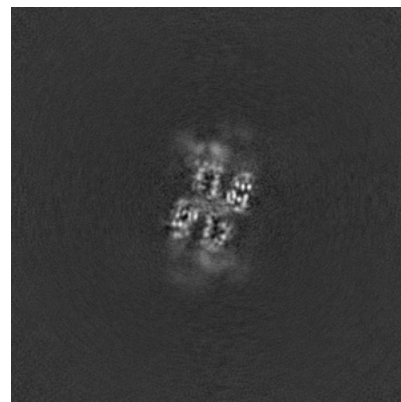
6.3.2 Raw map



X Index: 160



Y Index: 177

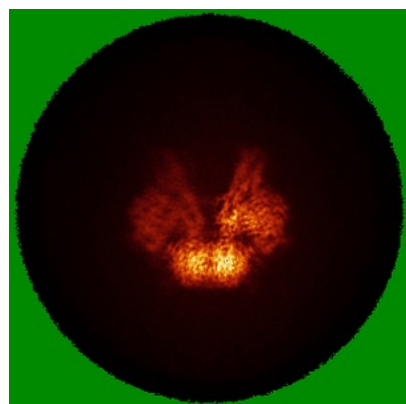


Z Index: 125

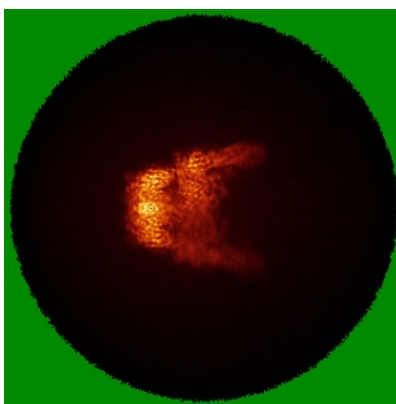
The images above show the largest variance slices of the map in three orthogonal directions.

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

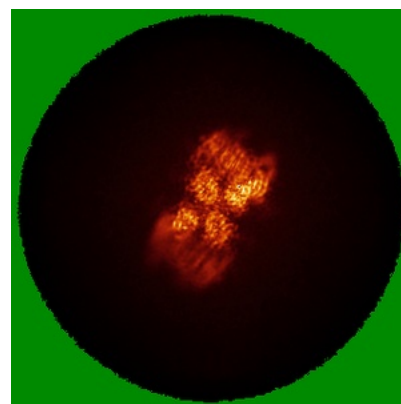
6.4.1 Primary map



X

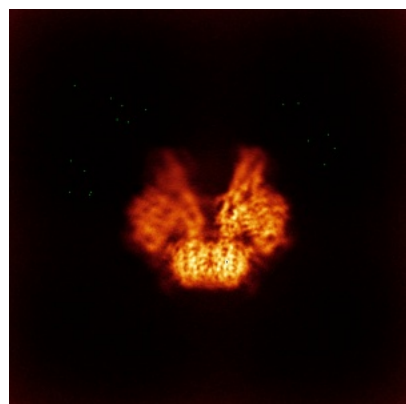


Y

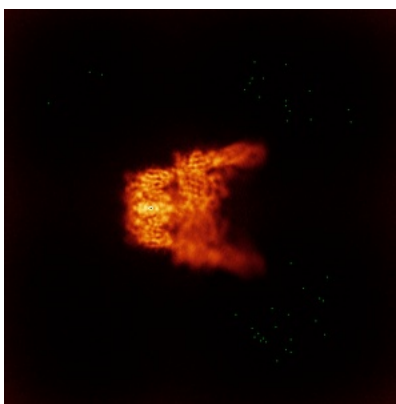


Z

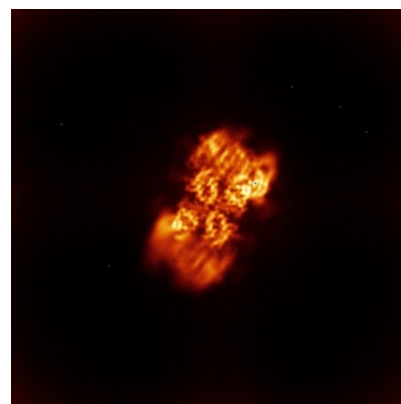
6.4.2 Raw map



X



Y

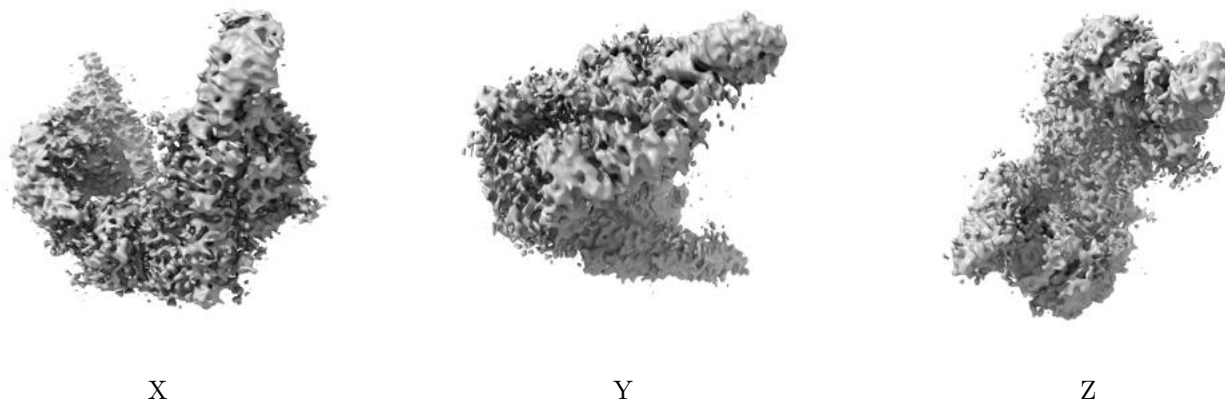


Z

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.

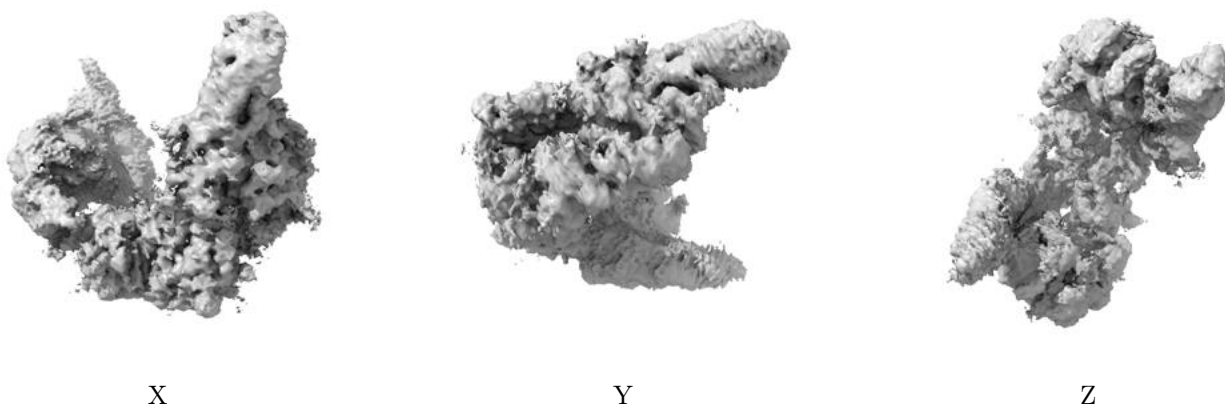
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0942. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

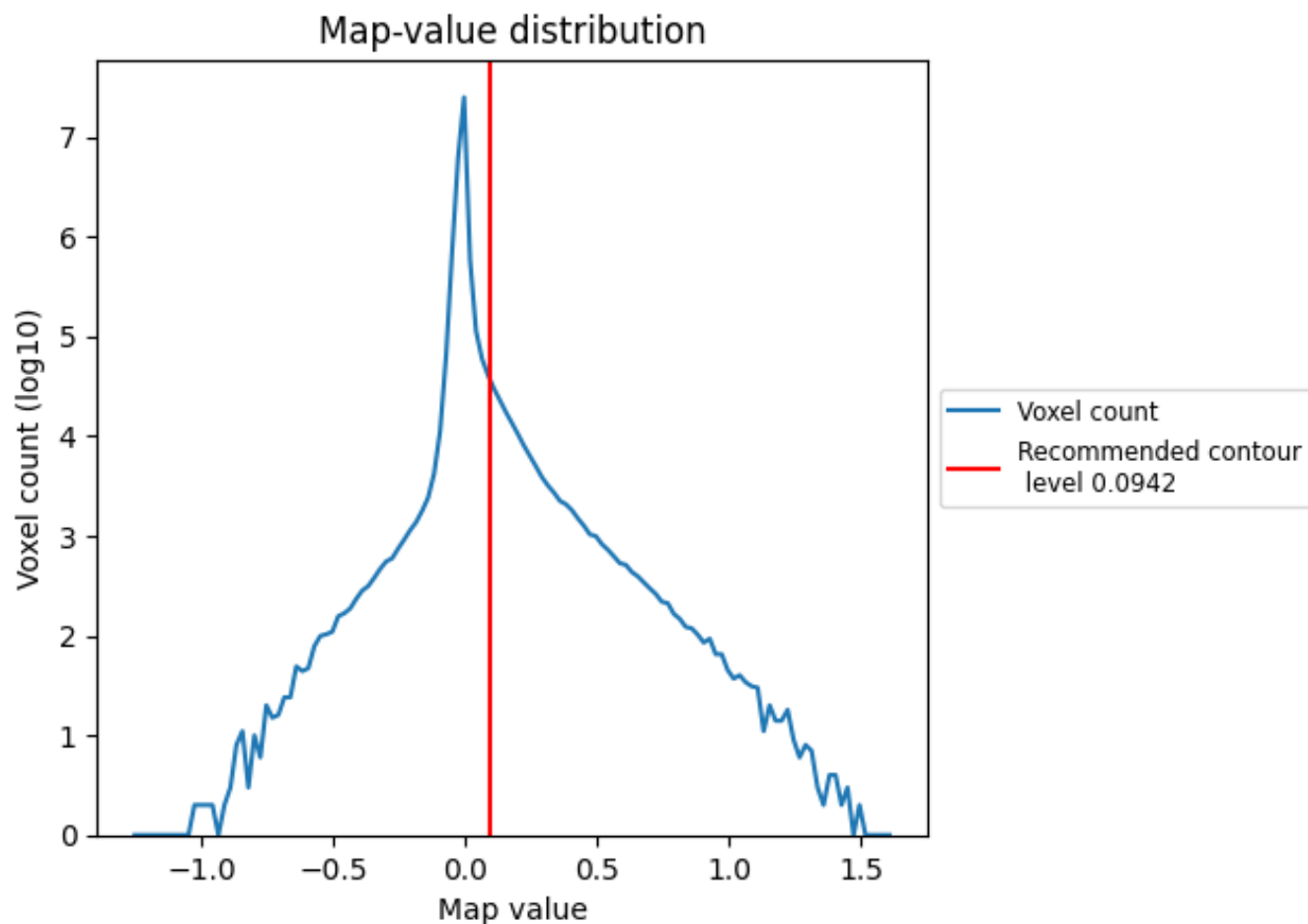
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

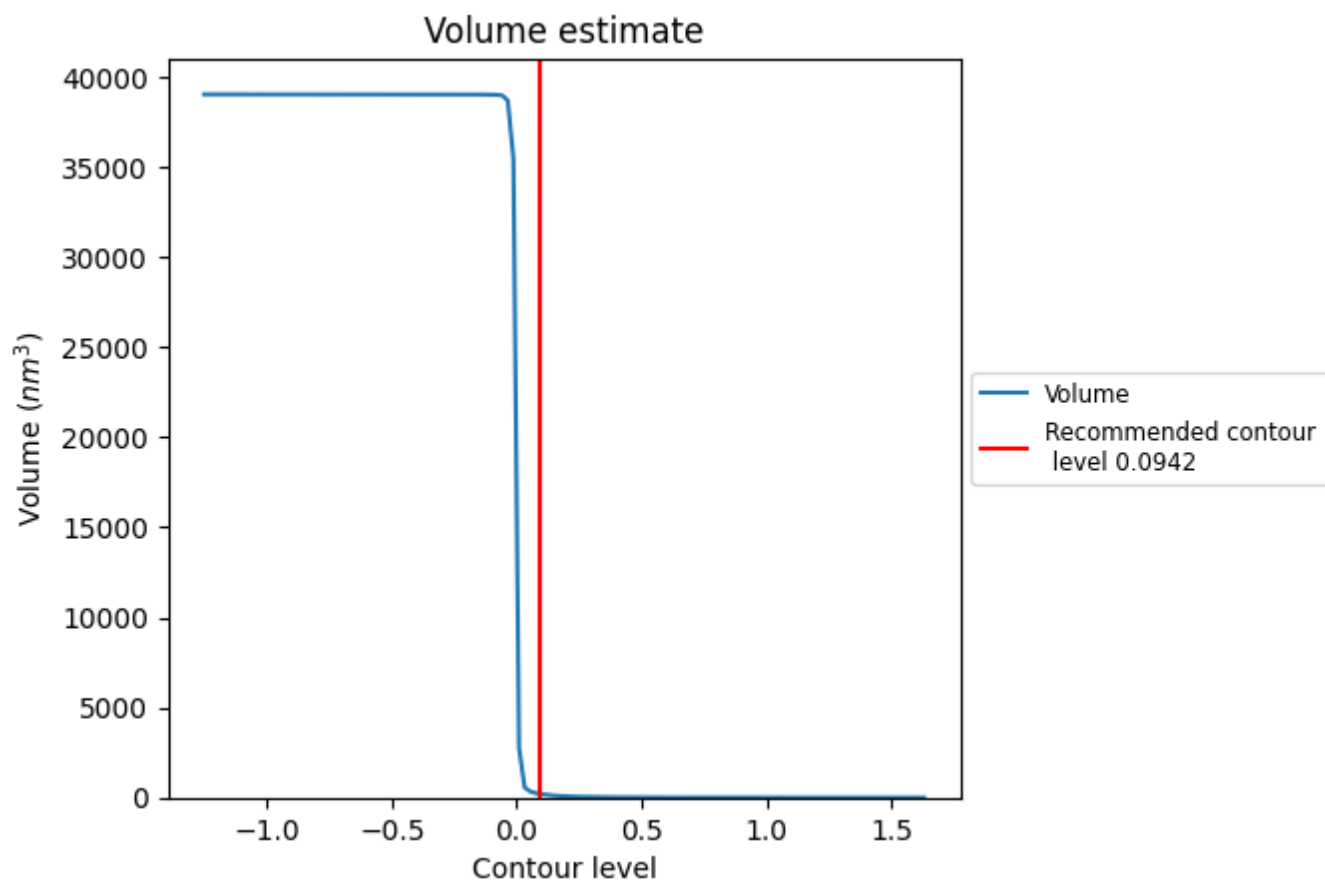
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

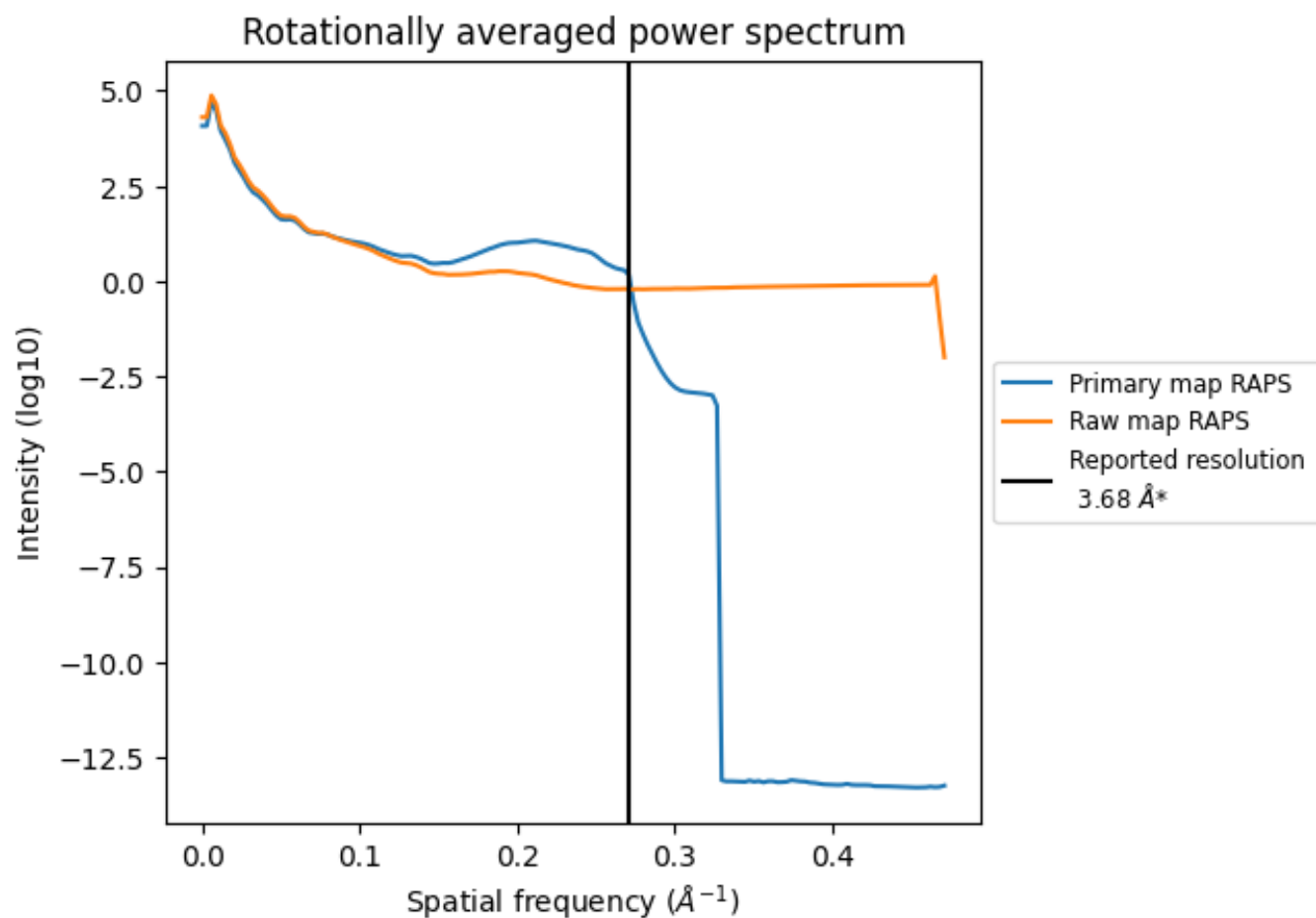
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 200 nm^3 ; this corresponds to an approximate mass of 180 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 ⓘ

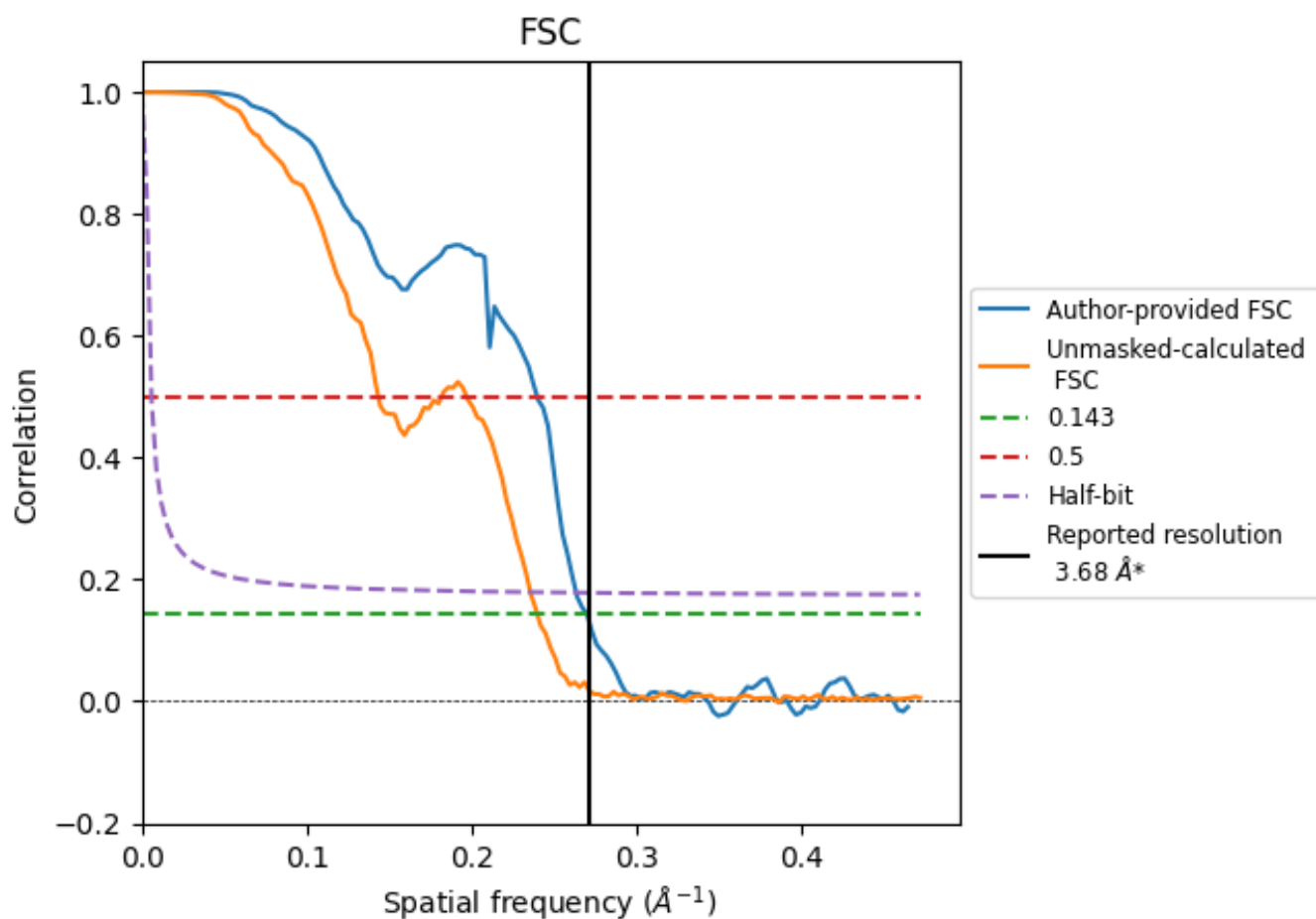


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 \AA^{-1}

8.2 Resolution estimates [i](#)

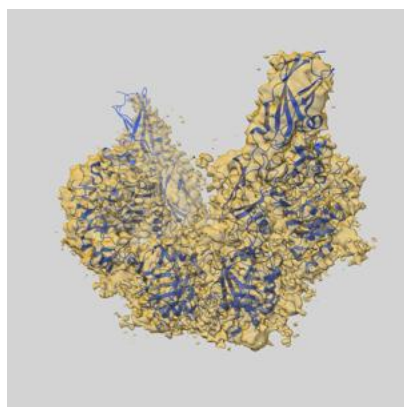
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.71	4.17	3.80
Unmasked-calculated*	4.17	6.98	4.25

*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 4.17 differs from the reported value 3.68 by more than 10 %

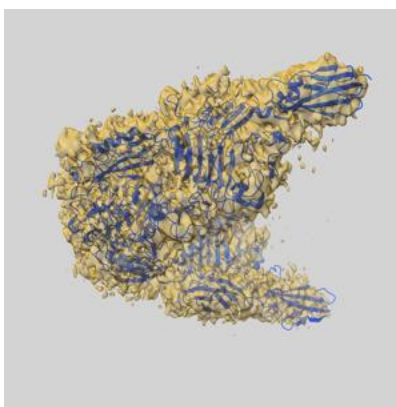
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71877 and PDB model 9PUV. Per-residue inclusion information can be found in section [3](#) on page [5](#).

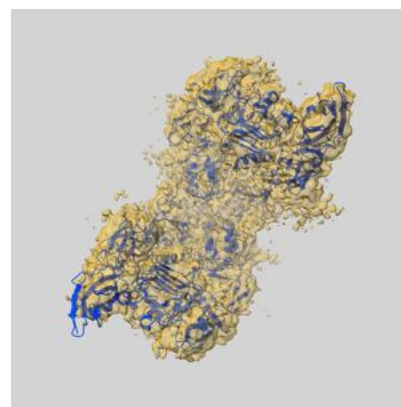
9.1 Map-model overlay [i](#)



X



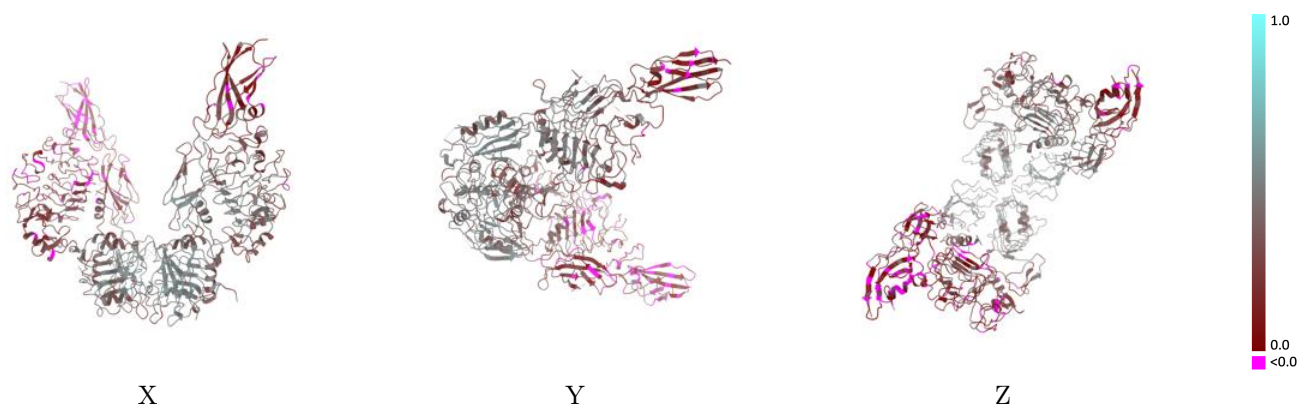
Y



Z

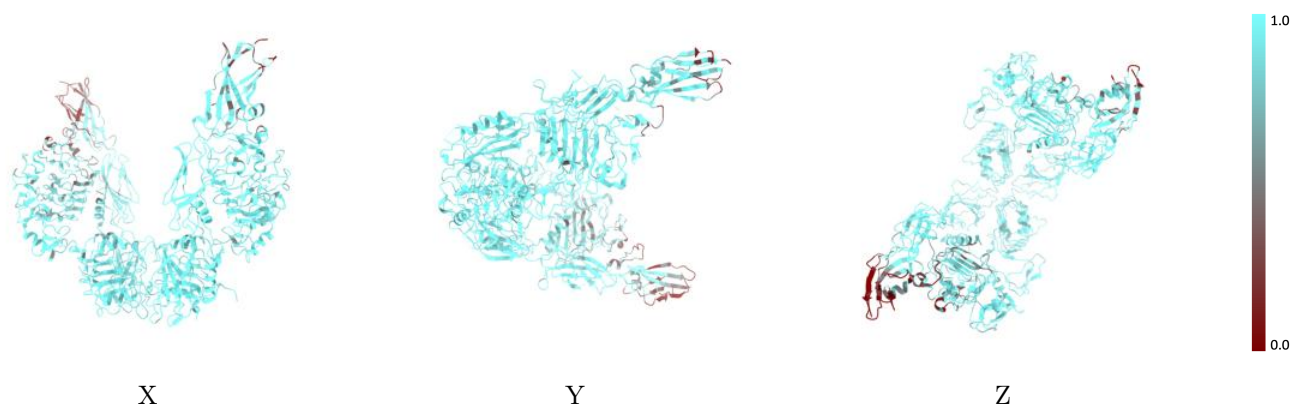
The images above show the 3D surface view of the map at the recommended contour level 0.0942 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



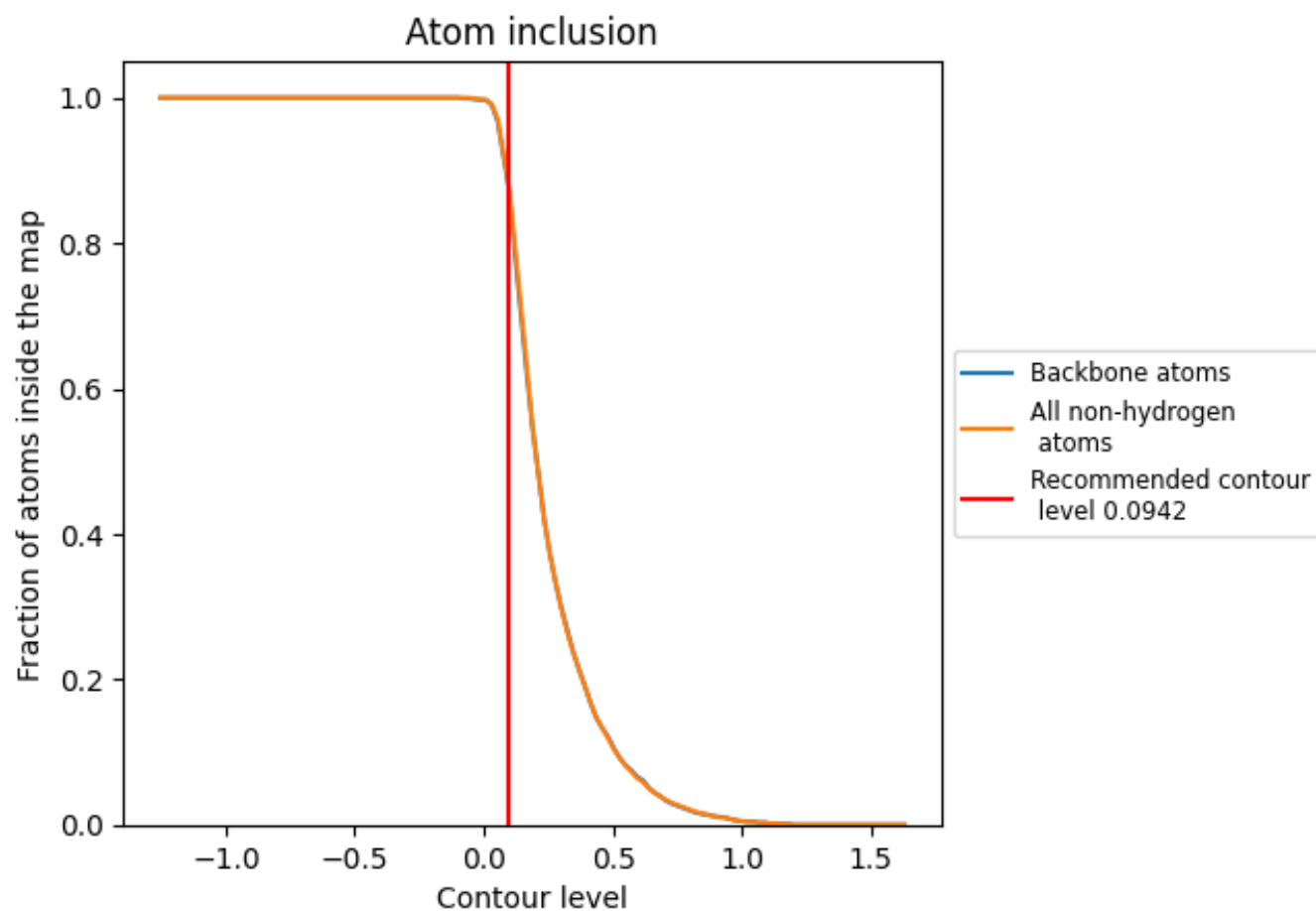
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0942).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 89% 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 (0.0942) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8870	<div></div> 0.3290
A	<div></div> 0.8770	<div></div> 0.3330
B	<div></div> 0.9120	<div></div> 0.3090
C	<div></div> 0.8960	<div></div> 0.3210
D	<div></div> 0.9580	<div></div> 0.4180

