



Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 04:48 PM JST

PDB ID : 7XQ8 / pdb_00007xq8
EMDB ID : EMD-33390
Title : Structure of human B-cell antigen receptor of the IgM isotype
Authors : Chen, M.Y.; Su, Q.; Shi, Y.G.
Deposited on : 2022-05-07
Resolution : 3.30 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

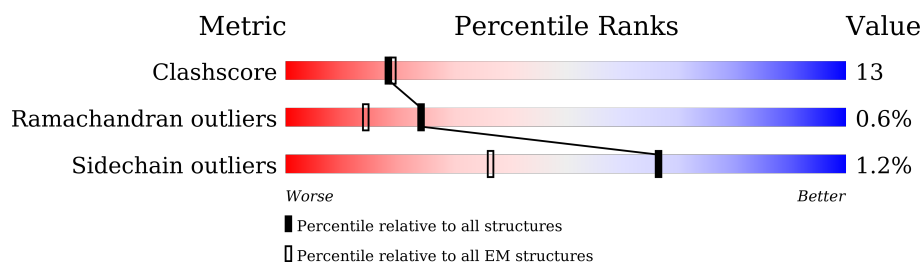
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	C	614	<div> <div>61%</div> <div>80% 16% .</div> </div>
1	v	614	<div> <div>56%</div> <div>78% 17% . .</div> </div>
2	L	250	<div> <div>84%</div> <div>83% . 16%</div> </div>
2	R	250	<div> <div>84%</div> <div>83% . 16%</div> </div>
3	A	257	<div> <div>5%</div> <div>41% 13% 46%</div> </div>
4	B	260	<div> <div>5%</div> <div>35% 18% 46%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12452 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 Chimera of Heavy chain of VRC01 antibody Fab and Isoform 2 of Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	595	Total	C	N	O	S	0	0
			3979	2471	710	786	12		
1	v	595	Total	C	N	O	S	0	0
			3968	2462	710	784	12		

- Molecule 2 is a protein called Light chain of Fab fragments of the VRC01 antibody, Immunoglobulin kappa constant.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	210	Total	C	N	O	0	0
			1035	614	210	211		
2	R	210	Total	C	N	O	0	0
			1035	614	210	211		

- Molecule 3 is a protein called B-cell antigen receptor complex-associated protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	139	Total	C	N	O	S	0	0
			1108	706	200	195	7		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	ALA	-	expression tag	UNP P11912
A	228	ALA	-	expression tag	UNP P11912
A	229	ALA	-	expression tag	UNP P11912
A	230	TRP	-	expression tag	UNP P11912
A	231	SER	-	expression tag	UNP P11912
A	232	HIS	-	expression tag	UNP P11912
A	233	PRO	-	expression tag	UNP P11912
A	234	GLN	-	expression tag	UNP P11912
A	235	PHE	-	expression tag	UNP P11912

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Chain	Residue	Modelled	Actual	Comment	Reference
A	236	GLU	-	expression tag	UNP P11912
A	237	LYS	-	expression tag	UNP P11912
A	238	GLY	-	expression tag	UNP P11912
A	239	GLY	-	expression tag	UNP P11912
A	240	GLY	-	expression tag	UNP P11912
A	241	SER	-	expression tag	UNP P11912
A	242	GLY	-	expression tag	UNP P11912
A	243	GLY	-	expression tag	UNP P11912
A	244	GLY	-	expression tag	UNP P11912
A	245	SER	-	expression tag	UNP P11912
A	246	GLY	-	expression tag	UNP P11912
A	247	GLY	-	expression tag	UNP P11912
A	248	SER	-	expression tag	UNP P11912
A	249	ALA	-	expression tag	UNP P11912
A	250	TRP	-	expression tag	UNP P11912
A	251	SER	-	expression tag	UNP P11912
A	252	HIS	-	expression tag	UNP P11912
A	253	PRO	-	expression tag	UNP P11912
A	254	GLN	-	expression tag	UNP P11912
A	255	PHE	-	expression tag	UNP P11912
A	256	GLU	-	expression tag	UNP P11912
A	257	LYS	-	expression tag	UNP P11912

- Molecule 4 is a protein called B-cell antigen receptor complex-associated protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	140	Total	C	N	O	S	0	0
			1131	719	197	204	11		

There are 31 discrepancies between the modelled and reference sequences:

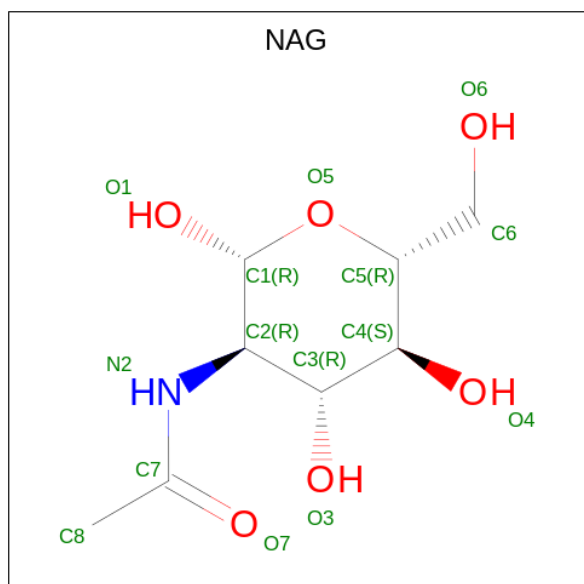
Chain	Residue	Modelled	Actual	Comment	Reference
B	230	ALA	-	expression tag	UNP P40259
B	231	ALA	-	expression tag	UNP P40259
B	232	ALA	-	expression tag	UNP P40259
B	233	TRP	-	expression tag	UNP P40259
B	234	SER	-	expression tag	UNP P40259
B	235	HIS	-	expression tag	UNP P40259
B	236	PRO	-	expression tag	UNP P40259
B	237	GLN	-	expression tag	UNP P40259
B	238	PHE	-	expression tag	UNP P40259
B	239	GLU	-	expression tag	UNP P40259

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Chain	Residue	Modelled	Actual	Comment	Reference
B	240	LYS	-	expression tag	UNP P40259
B	241	GLY	-	expression tag	UNP P40259
B	242	GLY	-	expression tag	UNP P40259
B	243	GLY	-	expression tag	UNP P40259
B	244	SER	-	expression tag	UNP P40259
B	245	GLY	-	expression tag	UNP P40259
B	246	GLY	-	expression tag	UNP P40259
B	247	GLY	-	expression tag	UNP P40259
B	248	SER	-	expression tag	UNP P40259
B	249	GLY	-	expression tag	UNP P40259
B	250	GLY	-	expression tag	UNP P40259
B	251	SER	-	expression tag	UNP P40259
B	252	ALA	-	expression tag	UNP P40259
B	253	TRP	-	expression tag	UNP P40259
B	254	SER	-	expression tag	UNP P40259
B	255	HIS	-	expression tag	UNP P40259
B	256	PRO	-	expression tag	UNP P40259
B	257	GLN	-	expression tag	UNP P40259
B	258	PHE	-	expression tag	UNP P40259
B	259	GLU	-	expression tag	UNP P40259
B	260	LYS	-	expression tag	UNP P40259

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

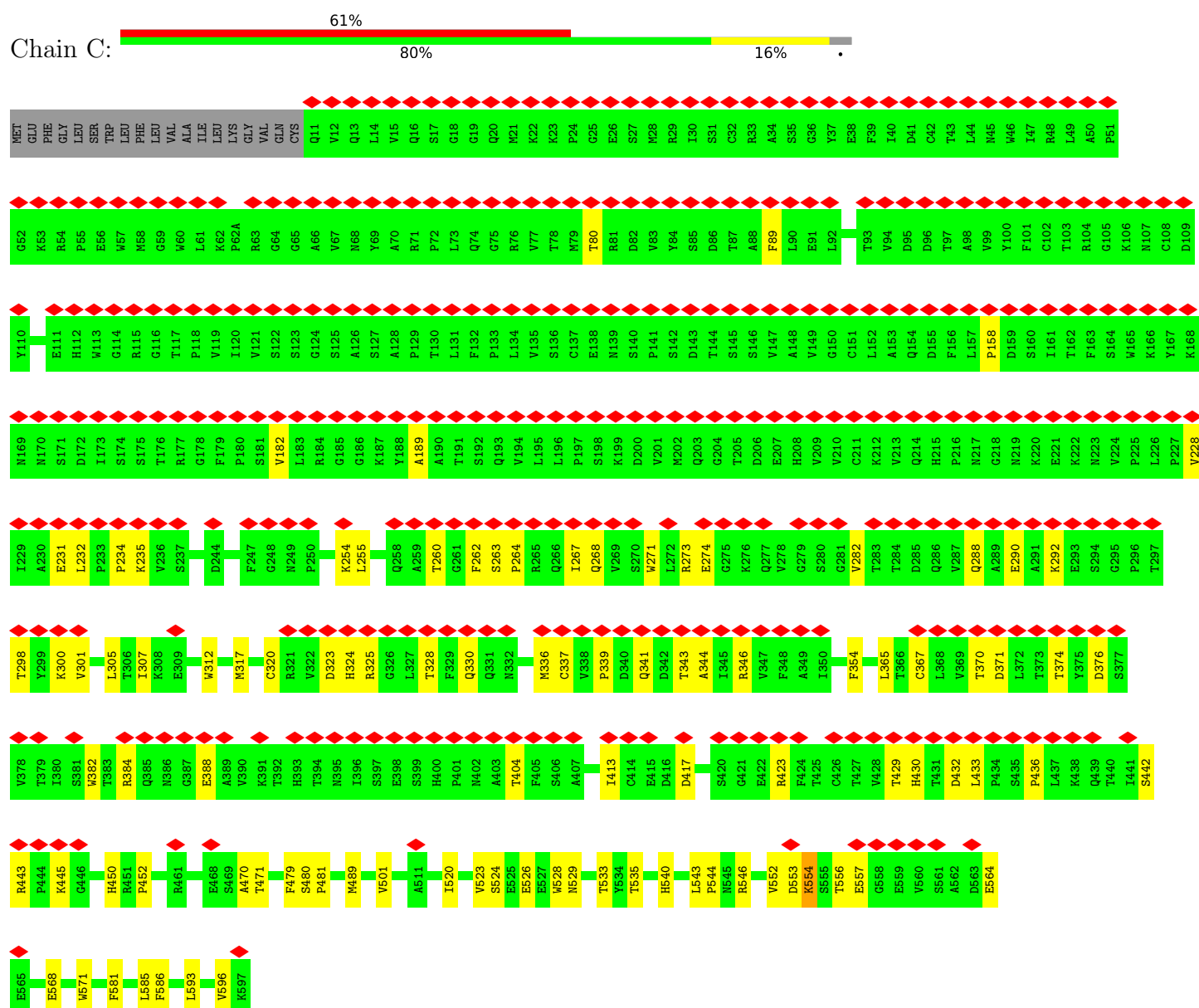


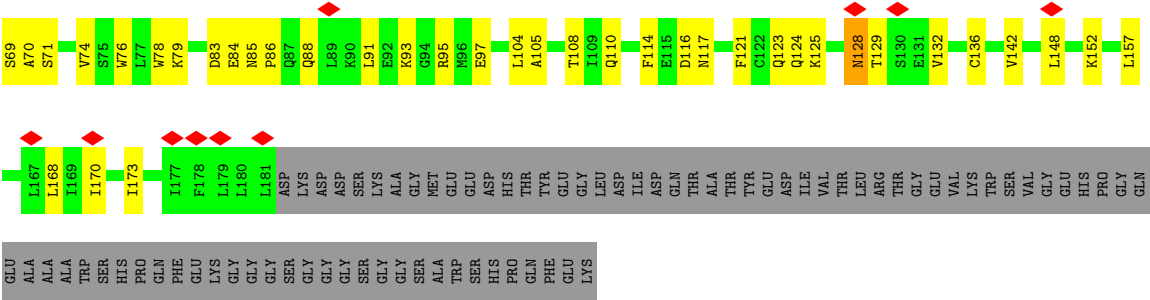
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	v	1	Total	C	N	O	0
			14	8	1	5	
5	v	1	Total	C	N	O	0
			14	8	1	5	
5	v	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

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: Chimera of Heavy chain of VRC01 antibody Fab and Isoform 2 of Immunoglobulin heavy constant mu





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	697919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.252	Depositor
Minimum map value	-4.534	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.904	Depositor
Map size (\AA)	387.72, 387.72, 387.72	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.077, 1.077, 1.077	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	C	0.17	0/4050	0.39	0/5556
1	v	0.31	1/4037 (0.0%)	0.52	4/5537 (0.1%)
2	L	0.15	0/1034	0.40	0/1436
2	R	0.13	0/1034	0.37	0/1436
3	A	0.24	0/1142	0.49	0/1557
4	B	0.27	0/1150	0.50	1/1546 (0.1%)
All	All	0.24	1/12447 (0.0%)	0.45	5/17068 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	v	485	PHE	CA-C	-5.28	1.47	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	v	531	GLY	N-CA-C	7.37	125.59	114.61
1	v	233	PRO	CA-C-N	-7.20	110.84	119.84
1	v	233	PRO	C-N-CA	-7.20	110.84	119.84
4	B	128	ASN	N-CA-C	-5.88	107.91	114.62
1	v	235	LYS	N-CA-C	5.11	117.97	109.94

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	C	3979	0	3288	64	0
1	v	3968	0	3265	172	0
2	L	1035	0	466	1	0
2	R	1035	0	466	1	0
3	A	1108	0	1070	27	0
4	B	1131	0	1143	37	0
5	A	84	0	78	2	0
5	B	28	0	26	0	0
5	C	42	0	38	1	0
5	v	42	0	39	6	0
All	All	12452	0	9879	289	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 13.

All (289) 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:v:233:PRO:CB	1:v:262:PHE:CD1	1.80	1.59
1:v:332:ASN:HD21	5:v:603:NAG:C1	1.31	1.43
1:v:233:PRO:CB	1:v:262:PHE:HD1	1.20	1.42
1:v:319:THR:HG23	1:v:332:ASN:CB	1.50	1.38
1:v:233:PRO:CB	1:v:262:PHE:HA	1.53	1.37
1:v:319:THR:CG2	1:v:332:ASN:HB3	1.52	1.37
1:v:332:ASN:ND2	5:v:603:NAG:C1	1.93	1.31
1:v:233:PRO:C	1:v:262:PHE:HE1	1.37	1.30
1:v:233:PRO:C	1:v:262:PHE:CE1	2.11	1.28
1:v:234:PRO:N	1:v:262:PHE:HE1	1.33	1.24
1:v:234:PRO:N	1:v:262:PHE:CE1	2.09	1.20
1:v:235:LYS:HG2	1:v:236:VAL:H	1.08	1.17
1:v:527:GLU:HA	1:v:530:THR:HG21	1.28	1.15
1:v:236:VAL:HG23	1:v:258:GLN:O	1.46	1.14
1:v:527:GLU:HA	1:v:530:THR:CG2	1.79	1.12
1:v:235:LYS:HG2	1:v:236:VAL:N	1.64	1.07
1:v:321:ARG:HB3	1:v:330:GLN:OE1	1.53	1.07
1:v:262:PHE:CE2	1:v:267:ILE:HG21	1.89	1.07
1:v:234:PRO:O	1:v:329:PHE:CG	2.09	1.05
1:v:233:PRO:CA	1:v:262:PHE:HD1	1.71	1.03
1:v:233:PRO:CA	1:v:262:PHE:CD1	2.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:233:PRO:CB	1:v:262:PHE:CA	2.45	0.95
1:C:528:TRP:O	1:C:554:LYS:HD2	1.66	0.95
1:C:529:ASN:HA	1:C:554:LYS:HE2	1.50	0.94
1:v:262:PHE:O	1:v:299:TYR:N	2.02	0.92
1:v:235:LYS:CG	1:v:236:VAL:N	2.32	0.92
1:v:236:VAL:HG23	1:v:258:GLN:C	1.96	0.90
1:v:262:PHE:CE2	1:v:267:ILE:CG2	2.55	0.90
1:v:319:THR:CB	1:v:332:ASN:HB3	2.02	0.89
1:v:234:PRO:O	1:v:329:PHE:CD2	2.27	0.86
1:v:236:VAL:CG2	1:v:258:GLN:O	2.25	0.85
1:v:527:GLU:CA	1:v:530:THR:CG2	2.54	0.85
1:v:262:PHE:HE2	1:v:267:ILE:HG21	1.39	0.84
1:v:321:ARG:HD2	1:v:330:GLN:HE22	1.42	0.84
1:v:234:PRO:CA	1:v:262:PHE:HE1	1.91	0.84
1:v:319:THR:HG23	1:v:332:ASN:CG	2.02	0.83
1:v:263:SER:CB	1:v:264:PRO:HD3	2.10	0.82
1:v:526:GLU:O	1:v:530:THR:HG21	1.79	0.82
3:A:33:LEU:HD21	3:A:36:HIS:HD2	1.45	0.81
1:C:529:ASN:HA	1:C:554:LYS:CE	2.12	0.80
1:v:233:PRO:HA	1:v:261:GLY:O	1.81	0.80
1:v:233:PRO:CB	1:v:262:PHE:CG	2.63	0.79
1:v:233:PRO:C	1:v:262:PHE:CD1	2.57	0.79
1:v:262:PHE:CD2	1:v:267:ILE:HG21	2.17	0.79
1:v:263:SER:HB3	1:v:264:PRO:HD3	1.65	0.79
1:v:319:THR:HA	1:v:332:ASN:HA	1.66	0.78
1:v:319:THR:HG23	1:v:332:ASN:HB3	0.79	0.77
1:v:487:GLN:HB3	1:v:537:VAL:HG13	1.65	0.77
1:v:234:PRO:CA	1:v:262:PHE:CE1	2.68	0.77
1:v:527:GLU:CA	1:v:530:THR:HG21	2.13	0.76
1:v:527:GLU:HA	1:v:530:THR:HG23	1.68	0.76
1:v:321:ARG:HB3	1:v:330:GLN:CD	2.10	0.75
1:v:375:TYR:HB2	1:v:396:ILE:HD13	1.68	0.74
1:v:496:SER:HB3	1:v:499:LYS:HG3	1.70	0.74
4:B:95:ARG:NH2	4:B:116:ASP:OD2	2.21	0.73
1:v:330:GLN:OE1	1:v:330:GLN:HA	1.87	0.73
1:v:286:GLN:HE21	1:v:288:GLN:HB3	1.55	0.70
1:v:529:ASN:HA	1:v:554:LYS:HD2	1.73	0.70
1:C:344:ALA:HA	1:C:371:ASP:HB3	1.74	0.69
1:v:491:ARG:NH2	1:v:532:GLU:OE2	2.24	0.69
3:A:86:ASP:HB3	3:A:87:PRO:HD3	1.73	0.69
1:v:255:LEU:HB2	1:v:307:ILE:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:262:PHE:HE2	1:v:267:ILE:CG2	2.02	0.69
1:v:320:CYS:N	1:v:331:GLN:O	2.25	0.68
1:v:433:LEU:HD13	1:v:437:LEU:HD13	1.74	0.68
1:v:234:PRO:C	1:v:329:PHE:CD1	2.71	0.68
1:C:343:THR:HG22	1:C:344:ALA:H	1.58	0.67
4:B:123:GLN:HE21	4:B:132:VAL:HG21	1.58	0.67
1:v:331:GLN:HA	1:v:331:GLN:NE2	2.10	0.67
1:v:321:ARG:CB	1:v:330:GLN:OE1	2.39	0.66
1:v:233:PRO:CA	1:v:261:GLY:O	2.43	0.66
3:A:36:HIS:ND1	4:B:136:CYS:HB3	2.12	0.65
1:C:234:PRO:HB3	1:C:262:PHE:HB3	1.79	0.65
1:v:487:GLN:HB3	1:v:537:VAL:CG1	2.25	0.65
1:v:332:ASN:HD22	5:v:603:NAG:C1	2.08	0.65
4:B:114:PHE:HA	4:B:142:VAL:HG11	1.77	0.64
3:A:131:ARG:CZ	3:A:135:ASP:HB2	2.28	0.64
1:C:271:TRP:CD1	1:C:305:LEU:HB2	2.33	0.63
1:v:319:THR:CA	1:v:332:ASN:HB3	2.29	0.63
3:A:85:GLU:HG3	3:A:92:ILE:HD12	1.81	0.63
1:v:234:PRO:C	1:v:329:PHE:CG	2.78	0.62
1:v:565:GLU:OE2	4:B:57:ARG:NH1	2.28	0.62
1:v:319:THR:HA	1:v:332:ASN:HB3	1.82	0.62
1:v:236:VAL:HG22	1:v:237:SER:N	2.15	0.62
1:C:429:THR:HG22	1:C:436:PRO:HB3	1.82	0.62
1:v:527:GLU:C	1:v:530:THR:HG23	2.23	0.62
1:v:319:THR:HA	1:v:332:ASN:CB	2.30	0.62
1:v:319:THR:HA	1:v:332:ASN:CA	2.29	0.61
1:C:288:GLN:HB2	1:C:300:LYS:HE3	1.81	0.61
1:v:265:ARG:O	1:v:265:ARG:NH1	2.31	0.61
1:v:452:PRO:HB3	1:v:479:PHE:HB3	1.82	0.61
1:v:234:PRO:HA	1:v:262:PHE:CE1	2.35	0.60
1:v:345:ILE:HG13	1:v:433:LEU:HD21	1.84	0.60
1:C:384:ARG:NH1	1:C:388:GLU:OE2	2.35	0.59
1:v:576:THR:HG21	3:A:146:THR:HG23	1.84	0.59
1:v:233:PRO:CB	1:v:262:PHE:CE1	2.69	0.59
1:v:235:LYS:HD3	1:v:235:LYS:C	2.28	0.59
1:C:234:PRO:HD3	1:C:324:HIS:HD1	1.68	0.59
1:v:289:ALA:HA	1:v:299:TYR:HD2	1.68	0.59
1:C:290:GLU:HB2	1:C:298:THR:HG23	1.83	0.58
1:C:533:THR:HA	1:C:553:ASP:HB3	1.84	0.58
1:v:319:THR:HG21	5:v:603:NAG:HN2	1.67	0.58
1:v:557:GLU:O	4:B:56:LYS:NZ	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:GLU:O	1:C:568:GLU:HG2	2.04	0.58
1:v:234:PRO:C	1:v:329:PHE:CE1	2.82	0.58
1:v:233:PRO:O	1:v:324:HIS:ND1	2.29	0.57
1:v:321:ARG:HD2	1:v:330:GLN:NE2	2.16	0.57
1:v:527:GLU:CA	1:v:530:THR:HG23	2.29	0.57
3:A:65:THR:OG1	3:A:67:TRP:NE1	2.34	0.57
1:v:562:ALA:O	4:B:57:ARG:NH2	2.38	0.57
1:C:480:SER:OG	1:C:481:PRO:HD3	2.05	0.57
1:v:263:SER:CB	1:v:264:PRO:CD	2.79	0.57
1:v:319:THR:HG22	1:v:331:GLN:O	2.04	0.57
4:B:60:THR:HG22	4:B:110:GLN:HA	1.87	0.57
1:v:526:GLU:O	1:v:530:THR:CG2	2.51	0.56
1:C:336:MET:HE3	1:C:336:MET:HA	1.87	0.56
1:C:384:ARG:NH2	1:C:417:ASP:OD2	2.37	0.56
3:A:158:VAL:HB	3:A:159:PRO:HD3	1.87	0.56
1:C:471:THR:HG23	1:C:520:ILE:HG23	1.87	0.56
1:v:312:TRP:NE1	1:v:336:MET:HE1	2.20	0.56
1:v:332:ASN:ND2	5:v:603:NAG:C2	2.66	0.56
1:v:540:HIS:CD2	1:v:542:ALA:H	2.24	0.55
1:C:268:GLN:HE21	1:C:323:ASP:HB2	1.72	0.55
1:v:384:ARG:NH1	1:v:417:ASP:OD2	2.40	0.55
1:C:367:CYS:HB2	1:C:382:TRP:CZ2	2.42	0.55
1:C:235:LYS:N	1:C:260:THR:O	2.40	0.54
4:B:93:LYS:HA	4:B:93:LYS:HE3	1.89	0.54
1:v:238:VAL:HB	1:v:333:ALA:HB2	1.90	0.54
3:A:64:VAL:HG22	3:A:108:VAL:HG22	1.90	0.54
1:C:271:TRP:HD1	1:C:282:VAL:HG23	1.71	0.53
3:A:88:ASN:HB2	5:A:304:NAG:H2	1.90	0.53
1:v:530:THR:O	1:v:530:THR:OG1	2.21	0.53
1:C:354:PHE:HE1	1:C:546:ARG:HH11	1.56	0.53
4:B:83:ASP:OD1	4:B:84:GLU:N	2.37	0.53
1:C:529:ASN:O	1:C:554:LYS:HE3	2.08	0.53
4:B:46:ILE:HD11	4:B:124:GLN:HB3	1.89	0.53
1:v:321:ARG:HB3	1:v:330:GLN:NE2	2.24	0.53
1:v:234:PRO:O	1:v:329:PHE:CD1	2.62	0.53
1:v:318:PHE:O	1:v:332:ASN:HA	2.09	0.52
3:A:66:TRP:NE1	3:A:89:GLY:O	2.36	0.52
1:v:308:LYS:HG3	1:v:310:SER:H	1.73	0.52
3:A:84:GLY:HA3	3:A:89:GLY:HA2	1.91	0.52
1:v:235:LYS:CA	1:v:329:PHE:CD1	2.93	0.52
1:v:560:VAL:HG23	1:v:562:ALA:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:PRO:HB3	1:C:479:PHE:HB3	1.91	0.51
1:v:262:PHE:CE2	1:v:267:ILE:HG22	2.44	0.51
1:v:233:PRO:O	1:v:262:PHE:CE1	2.59	0.51
1:C:586:PHE:HE2	4:B:168:LEU:HD21	1.75	0.51
1:v:262:PHE:O	1:v:298:THR:HA	2.11	0.51
1:C:374:THR:OG1	1:C:376:ASP:OD1	2.26	0.51
1:v:430:HIS:HB3	1:v:433:LEU:HG	1.93	0.51
1:C:556:THR:O	1:C:557:GLU:HG3	2.11	0.51
1:C:346:ARG:O	1:C:370:THR:OG1	2.29	0.50
1:v:270:SER:HB2	1:v:277:GLN:HE22	1.77	0.50
1:v:486:VAL:HB	1:v:538:VAL:HG22	1.92	0.50
4:B:91:LEU:HD12	4:B:91:LEU:O	2.12	0.50
1:C:543:LEU:HB3	1:C:544:PRO:HD2	1.94	0.50
1:v:262:PHE:CZ	1:v:324:HIS:CB	2.95	0.50
1:v:263:SER:OG	1:v:264:PRO:HD3	2.12	0.50
1:v:377:SER:OG	1:v:430:HIS:ND1	2.44	0.50
3:A:133:PHE:C	3:A:135:ASP:H	2.21	0.49
1:v:451:ARG:NH1	1:v:452:PRO:O	2.45	0.49
1:C:267:ILE:HG21	1:C:301:VAL:HG11	1.95	0.49
1:C:430:HIS:HB3	1:C:433:LEU:HG	1.94	0.49
1:C:470:ALA:HB3	1:C:523:VAL:HG13	1.93	0.49
1:v:235:LYS:CD	1:v:236:VAL:N	2.75	0.49
1:v:527:GLU:C	1:v:530:THR:CG2	2.83	0.49
1:C:307:ILE:HD12	1:C:312:TRP:HB2	1.94	0.49
1:v:345:ILE:HA	1:v:371:ASP:HB3	1.94	0.49
1:v:450:HIS:ND1	1:v:480:SER:HB2	2.27	0.49
1:C:586:PHE:CE2	4:B:168:LEU:HD21	2.48	0.49
1:v:235:LYS:HB2	1:v:329:PHE:HD1	1.78	0.49
1:C:371:ASP:HA	1:C:404:THR:HG21	1.94	0.49
3:A:135:ASP:O	3:A:137:GLY:N	2.46	0.48
1:v:319:THR:HG22	1:v:331:GLN:C	2.38	0.48
1:v:336:MET:HB2	1:v:339:PRO:HG3	1.96	0.48
3:A:34:TRP:CG	3:A:56:HIS:HA	2.48	0.48
1:C:533:THR:CB	1:C:553:ASP:HB3	2.43	0.48
1:v:251:ARG:HG2	1:v:309:GLU:HB3	1.94	0.48
1:v:332:ASN:HD22	5:v:603:NAG:C2	2.27	0.48
1:v:233:PRO:CB	1:v:324:HIS:CE1	2.96	0.48
1:v:318:PHE:O	1:v:332:ASN:CA	2.62	0.48
3:A:52:PHE:HB2	3:A:91:LEU:HB3	1.95	0.48
1:C:593:LEU:HA	1:C:596:VAL:HG12	1.94	0.48
1:C:481:PRO:HD2	1:C:540:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:317:MET:SD	1:v:317:MET:N	2.85	0.47
1:C:341:GLN:NE2	1:C:433:LEU:HD22	2.29	0.47
1:v:267:ILE:HG22	1:v:324:HIS:HB2	1.95	0.47
1:C:581:PHE:CZ	1:C:585:LEU:HD11	2.50	0.47
1:v:533:THR:OG1	4:B:55:ARG:NH2	2.47	0.47
4:B:68:ASN:OD1	4:B:71:SER:HB2	2.13	0.47
1:C:323:ASP:OD2	1:C:328:THR:OG1	2.31	0.47
1:v:324:HIS:CE1	1:v:325:ARG:HG2	2.49	0.47
4:B:117:ASN:OD1	4:B:142:VAL:HG12	2.14	0.47
4:B:79:LYS:HE3	4:B:121:PHE:CE2	2.50	0.47
1:C:343:THR:HG21	1:C:432:ASP:HB2	1.96	0.46
1:v:236:VAL:HG22	1:v:237:SER:H	1.79	0.46
3:A:130:PRO:O	4:B:152:LYS:NZ	2.41	0.46
4:B:125:LYS:HA	4:B:132:VAL:HG12	1.96	0.46
1:v:234:PRO:HA	1:v:262:PHE:CZ	2.51	0.46
1:v:460:ALA:HB3	1:v:464:LEU:H	1.81	0.46
4:B:88:GLN:HG3	4:B:88:GLN:O	2.15	0.46
1:C:571:TRP:CZ2	4:B:157:LEU:HD23	2.49	0.46
1:C:231:GLU:HB3	1:C:325:ARG:HH11	1.81	0.46
1:v:235:LYS:HA	1:v:329:PHE:CD1	2.51	0.46
1:C:423:ARG:HA	1:C:442:SER:OG	2.16	0.45
2:L:151:LYS:O	2:L:195:ALA:N	2.45	0.45
4:B:49:SER:HB3	4:B:50:PRO:HD3	1.97	0.45
4:B:69:SER:OG	4:B:70:ALA:N	2.50	0.45
1:v:251:ARG:HH12	1:v:310:SER:HA	1.82	0.45
1:v:469:SER:HA	1:v:523:VAL:O	2.16	0.45
1:v:234:PRO:C	1:v:329:PHE:CD2	2.92	0.45
1:v:342:ASP:OD1	1:v:342:ASP:N	2.50	0.45
1:C:232:LEU:N	1:C:263:SER:OG	2.50	0.45
4:B:74:VAL:HG12	4:B:124:GLN:HB2	1.98	0.45
4:B:78:TRP:O	4:B:86:PRO:HD2	2.17	0.45
1:v:485:PHE:O	1:v:485:PHE:CD2	2.70	0.45
1:v:235:LYS:HD3	1:v:236:VAL:N	2.32	0.44
3:A:97:ASN:HD22	5:A:302:NAG:H62	1.81	0.44
3:A:77:PRO:HA	3:A:78:PRO:HD3	1.90	0.44
4:B:97:GLU:OE1	4:B:110:GLN:NE2	2.36	0.44
1:C:271:TRP:CZ3	1:C:320:CYS:HB2	2.52	0.44
1:v:553:ASP:OD1	1:v:553:ASP:N	2.45	0.44
1:C:273:ARG:O	1:C:274:GLU:HG3	2.17	0.44
1:C:330:GLN:OE1	5:C:602:NAG:N2	2.51	0.44
1:v:249:ASN:HB3	1:v:250:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:490:GLN:HB2	1:v:495:LEU:HD13	2.00	0.44
4:B:66:TYR:CE2	4:B:104:LEU:HD12	2.52	0.44
4:B:128:ASN:OD1	4:B:129:THR:N	2.51	0.44
1:v:273:ARG:HB3	1:v:276:LYS:HE3	2.00	0.44
1:v:305:LEU:HD22	1:v:307:ILE:HG22	2.00	0.44
4:B:43:CYS:HA	4:B:68:ASN:HD22	1.83	0.43
2:R:86:TYR:O	2:R:102:THR:N	2.46	0.43
1:v:236:VAL:CG2	1:v:237:SER:N	2.80	0.43
1:v:262:PHE:CE1	1:v:324:HIS:ND1	2.87	0.43
3:A:51:HIS:CD2	3:A:92:ILE:HG12	2.54	0.43
1:v:235:LYS:N	1:v:329:PHE:CD1	2.87	0.43
1:v:488:TRP:NE1	1:v:519:SER:OG	2.31	0.43
1:v:268:GLN:HE21	1:v:268:GLN:HB2	1.69	0.42
1:v:556:THR:OG1	1:v:557:GLU:N	2.52	0.42
1:C:533:THR:CA	1:C:553:ASP:HB3	2.49	0.42
1:v:375:TYR:HB2	1:v:396:ILE:HG21	2.00	0.42
1:v:485:PHE:HD2	1:v:539:ALA:HB3	1.84	0.42
1:C:489:MET:HB2	1:C:535:THR:HB	2.00	0.42
1:v:331:GLN:NE2	1:v:331:GLN:CA	2.71	0.42
1:v:246:PHE:HA	1:v:253:SER:HB2	2.02	0.42
1:v:461:ARG:NH1	1:v:462:GLU:HB2	2.34	0.42
4:B:76:TRP:HH2	4:B:105:ALA:HB1	1.85	0.42
1:v:347:VAL:O	1:v:439:GLN:NE2	2.51	0.42
1:v:491:ARG:O	4:B:66:TYR:OH	2.26	0.42
1:C:533:THR:HA	1:C:553:ASP:CB	2.49	0.42
4:B:62:LYS:HG2	4:B:108:THR:HG22	2.01	0.42
1:v:255:LEU:HD22	1:v:271:TRP:HZ3	1.85	0.42
1:v:559:GLU:OE1	1:v:559:GLU:N	2.53	0.42
3:A:164:LEU:HD23	3:A:164:LEU:HA	1.83	0.42
1:v:296:PRO:HB2	1:v:298:THR:HG23	2.02	0.42
3:A:67:TRP:HE3	3:A:78:PRO:HB2	1.84	0.42
3:A:129:PRO:HG3	4:B:148:LEU:HD11	2.02	0.42
1:v:238:VAL:HG12	1:v:257:CYS:SG	2.60	0.41
1:v:456:LEU:HD11	1:v:488:TRP:HH2	1.85	0.41
3:A:128:PRO:HA	3:A:129:PRO:HD3	1.94	0.41
1:C:80:THR:O	1:C:89:PHE:N	2.43	0.41
1:C:182:VAL:O	1:C:189:ALA:N	2.41	0.41
1:C:254:LYS:O	1:C:255:LEU:HD23	2.20	0.41
4:B:170:ILE:HA	4:B:173:ILE:HG22	2.03	0.41
1:C:365:LEU:HD11	1:C:413:ILE:HD13	2.02	0.41
1:C:443:ARG:HG2	1:C:445:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:452:PRO:HD3	1:v:540:HIS:CD2	2.55	0.41
1:C:317:MET:HE2	1:C:317:MET:HB2	1.85	0.41
1:v:233:PRO:O	1:v:234:PRO:CB	2.65	0.41
1:v:262:PHE:CZ	1:v:324:HIS:HB2	2.56	0.41
1:v:311:ASP:OD1	1:v:311:ASP:N	2.53	0.41
3:A:67:TRP:CE3	3:A:78:PRO:HB2	2.56	0.41
3:A:33:LEU:HD21	3:A:36:HIS:CD2	2.36	0.41
4:B:85:ASN:OD1	4:B:85:ASN:N	2.48	0.41
4:B:95:ARG:HH22	4:B:116:ASP:CG	2.28	0.41
1:C:290:GLU:HB3	1:C:292:LYS:NZ	2.36	0.41
1:C:450:HIS:O	1:C:479:PHE:HA	2.21	0.41
1:v:527:GLU:O	1:v:532:GLU:HB2	2.21	0.41
1:v:317:MET:SD	1:v:334:SER:OG	2.78	0.40
1:v:359:LEU:HD23	1:v:359:LEU:HA	1.94	0.40
3:A:51:HIS:NE2	3:A:92:ILE:HG12	2.36	0.40
1:v:318:PHE:O	1:v:332:ASN:HB2	2.21	0.40
1:C:337:CYS:HB3	1:C:339:PRO:HG3	2.04	0.40
1:C:501:VAL:HG11	1:v:516:PHE:CE1	2.57	0.40
1:v:466:LEU:HD23	1:v:466:LEU:HA	1.90	0.40
1:C:524:SER:O	1:C:526:GLU:HG2	2.22	0.40
1:v:251:ARG:HH12	1:v:310:SER:CA	2.34	0.40
1:v:264:PRO:HD2	1:v:324:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	593/614 (97%)	559 (94%)	30 (5%)	4 (1%)	19	50
1	v	593/614 (97%)	532 (90%)	57 (10%)	4 (1%)	19	50
2	L	208/250 (83%)	205 (99%)	2 (1%)	1 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	208/250 (83%)	206 (99%)	2 (1%)	0	100	100
3	A	137/257 (53%)	124 (90%)	11 (8%)	2 (2%)	8	33
4	B	138/260 (53%)	118 (86%)	20 (14%)	0	100	100
All	All	1877/2245 (84%)	1744 (93%)	122 (6%)	11 (1%)	24	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	158	PRO
2	L	143	PRO
1	v	232	LEU
1	v	234	PRO
1	v	249	ASN
3	A	136	MET
3	A	86	ASP
1	C	228	VAL
1	C	554	LYS
1	C	264	PRO
1	v	263	SER

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	C	325/537 (60%)	324 (100%)	1 (0%)	91	94
1	v	321/537 (60%)	311 (97%)	10 (3%)	35	61
2	L	1/214 (0%)	1 (100%)	0	100	100
2	R	1/214 (0%)	1 (100%)	0	100	100
3	A	121/210 (58%)	121 (100%)	0	100	100
4	B	126/220 (57%)	126 (100%)	0	100	100
All	All	895/1932 (46%)	884 (99%)	11 (1%)	66	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	552	VAL
1	v	235	LYS
1	v	262	PHE
1	v	263	SER
1	v	266	GLN
1	v	268	GLN
1	v	317	MET
1	v	319	THR
1	v	330	GLN
1	v	486	VAL
1	v	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	268	GLN
1	C	331	GLN
1	v	286	GLN
1	v	331	GLN
1	v	332	ASN
1	v	393	HIS
1	v	400	HIS
1	v	465	ASN
1	v	487	GLN
4	B	64	HIS
4	B	123	GLN
4	B	165	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

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	304	3	14,14,15	1.55	1 (7%)	17,19,21	1.85	1 (5%)
5	NAG	B	301	4	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	v	603	-	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	A	301	3	14,14,15	0.24	0	17,19,21	0.55	0
5	NAG	B	302	4	14,14,15	0.19	0	17,19,21	0.51	0
5	NAG	A	305	3	14,14,15	0.22	0	17,19,21	0.51	0
5	NAG	v	602	1	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	C	603	1	14,14,15	1.01	1 (7%)	17,19,21	1.16	1 (5%)
5	NAG	A	303	3	14,14,15	0.28	0	17,19,21	0.48	0
5	NAG	C	601	1	14,14,15	0.23	0	17,19,21	0.34	0
5	NAG	C	602	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	A	302	3	14,14,15	0.97	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	v	601	1	14,14,15	0.19	0	17,19,21	0.36	0
5	NAG	A	306	3	14,14,15	0.20	0	17,19,21	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	304	3	-	2/6/23/26	0/1/1/1
5	NAG	B	301	4	-	0/6/23/26	0/1/1/1
5	NAG	v	603	-	-	4/6/23/26	0/1/1/1
5	NAG	A	301	3	-	4/6/23/26	0/1/1/1
5	NAG	B	302	4	-	2/6/23/26	0/1/1/1
5	NAG	A	305	3	-	2/6/23/26	0/1/1/1
5	NAG	v	602	1	-	3/6/23/26	0/1/1/1
5	NAG	C	603	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	303	3	-	3/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1
5	NAG	C	602	1	-	2/6/23/26	0/1/1/1
5	NAG	A	302	3	-	4/6/23/26	0/1/1/1
5	NAG	v	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	306	3	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	304	NAG	O5-C1	5.62	1.52	1.43
5	C	603	NAG	O5-C1	3.55	1.49	1.43
5	A	302	NAG	O5-C1	3.37	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304	NAG	C1-O5-C5	7.40	122.22	112.19
5	C	603	NAG	C1-O5-C5	4.54	118.34	112.19
5	A	302	NAG	C1-O5-C5	3.88	117.44	112.19

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	v	603	NAG	C8-C7-N2-C2
5	v	603	NAG	O7-C7-N2-C2
5	A	303	NAG	C4-C5-C6-O6
5	A	302	NAG	C4-C5-C6-O6
5	A	306	NAG	O5-C5-C6-O6
5	C	602	NAG	C4-C5-C6-O6
5	C	602	NAG	O5-C5-C6-O6
5	A	302	NAG	O5-C5-C6-O6
5	A	303	NAG	O5-C5-C6-O6
5	A	301	NAG	C4-C5-C6-O6
5	v	603	NAG	O5-C5-C6-O6
5	v	603	NAG	C4-C5-C6-O6
5	A	304	NAG	O5-C5-C6-O6
5	v	601	NAG	C8-C7-N2-C2
5	v	601	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	v	602	NAG	C8-C7-N2-C2
5	v	602	NAG	O7-C7-N2-C2
5	A	301	NAG	C8-C7-N2-C2
5	A	301	NAG	O7-C7-N2-C2
5	B	302	NAG	C4-C5-C6-O6
5	A	306	NAG	C4-C5-C6-O6
5	A	305	NAG	O5-C5-C6-O6
5	A	301	NAG	O5-C5-C6-O6
5	B	302	NAG	O5-C5-C6-O6
5	C	603	NAG	O5-C5-C6-O6
5	A	304	NAG	C4-C5-C6-O6
5	v	602	NAG	O5-C5-C6-O6
5	A	305	NAG	C4-C5-C6-O6
5	A	302	NAG	C1-C2-N2-C7
5	A	303	NAG	C1-C2-N2-C7
5	A	302	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	NAG	1	0
5	v	603	NAG	6	0
5	C	602	NAG	1	0
5	A	302	NAG	1	0

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.

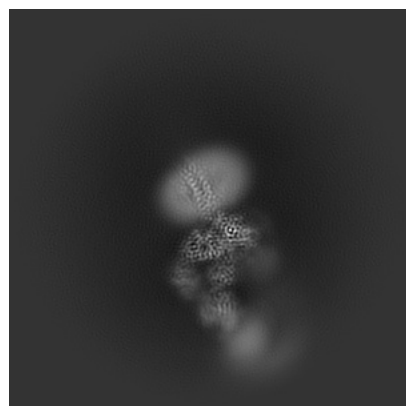
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33390. These allow visual inspection of the internal detail of the map and identification of artifacts.

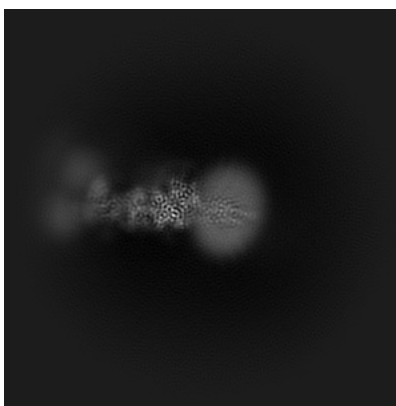
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

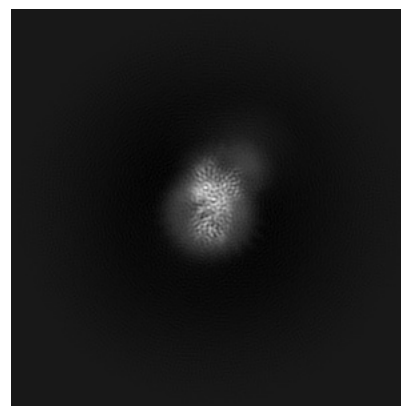
6.1.1 Primary map



X

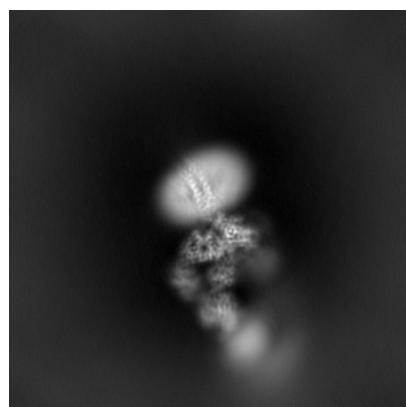


Y

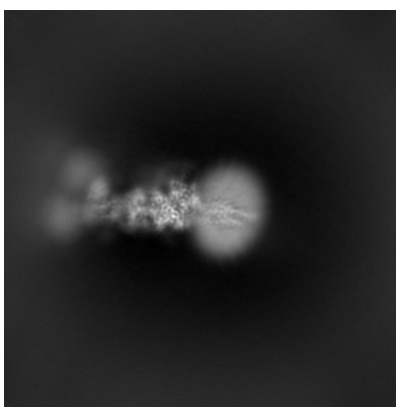


Z

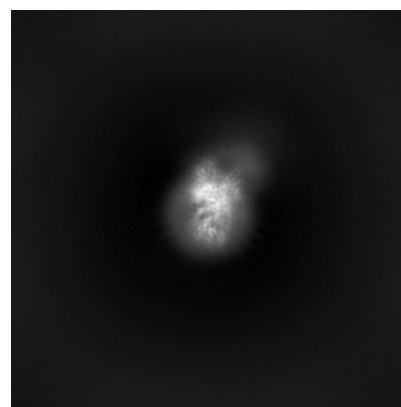
6.1.2 Raw map



X



Y

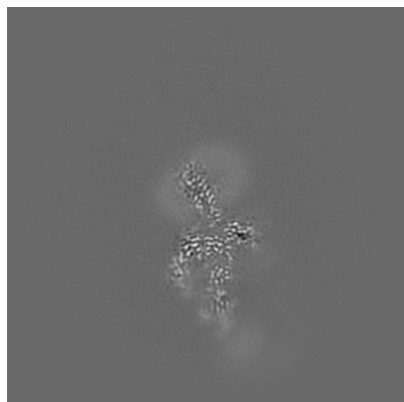


Z

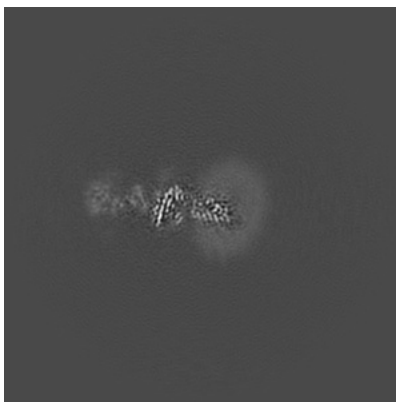
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

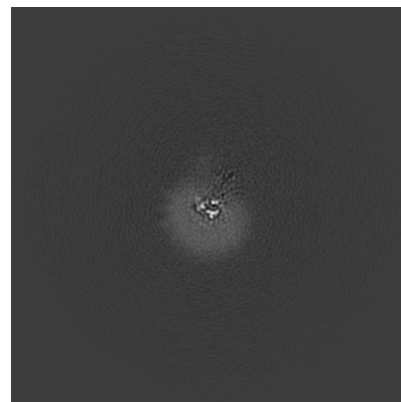
6.2.1 Primary map



X Index: 180

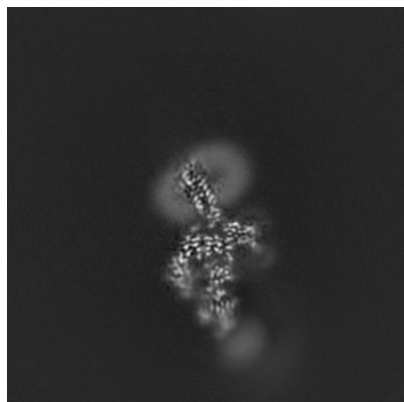


Y Index: 180

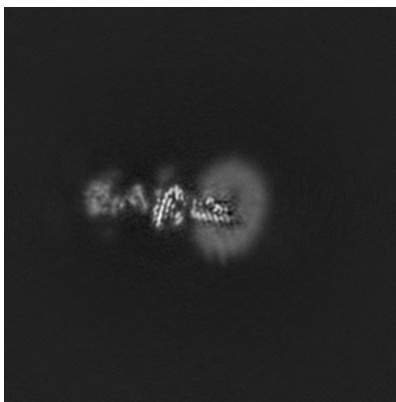


Z Index: 180

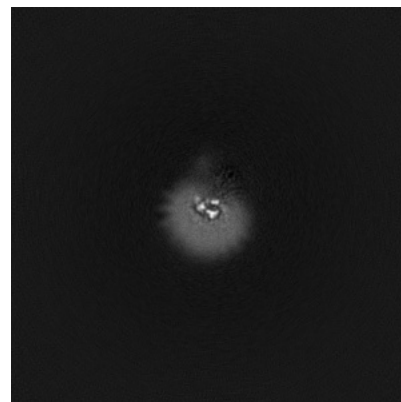
6.2.2 Raw map



X Index: 180



Y Index: 180

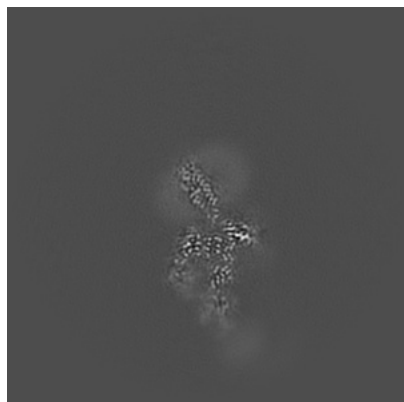


Z Index: 180

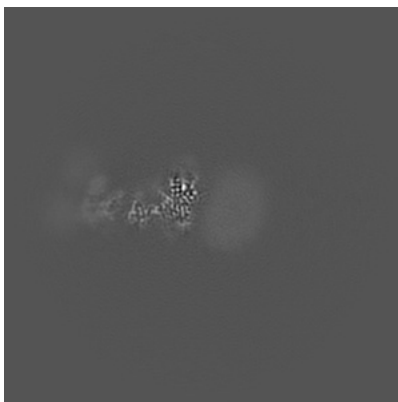
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 178

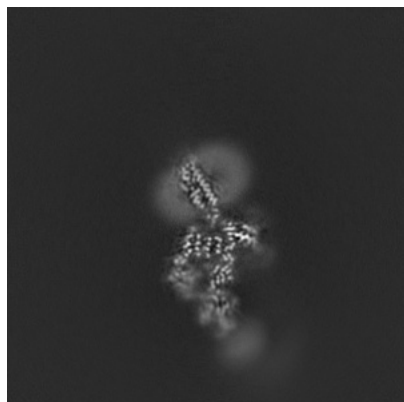


Y Index: 199

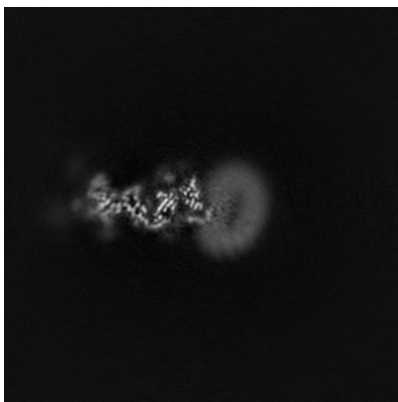


Z Index: 152

6.3.2 Raw map



X Index: 178



Y Index: 189

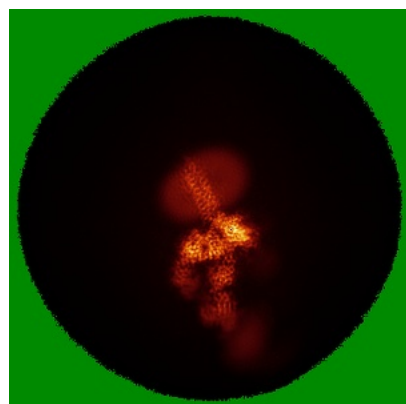


Z Index: 152

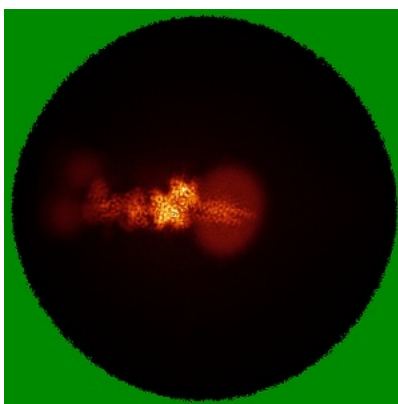
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X

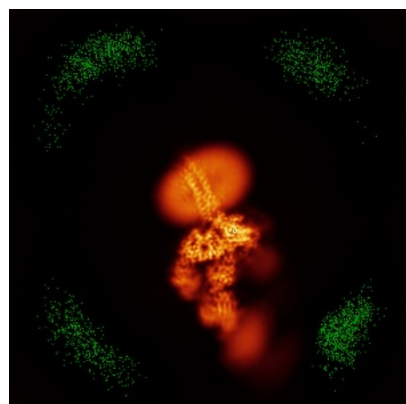


Y

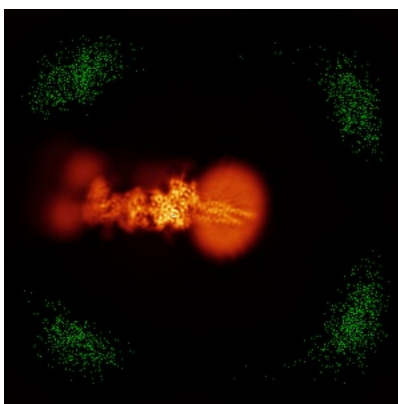


Z

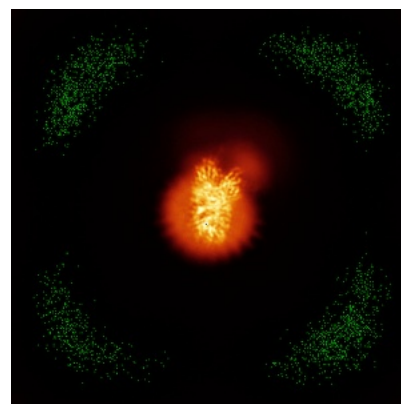
6.4.2 Raw map



X



Y

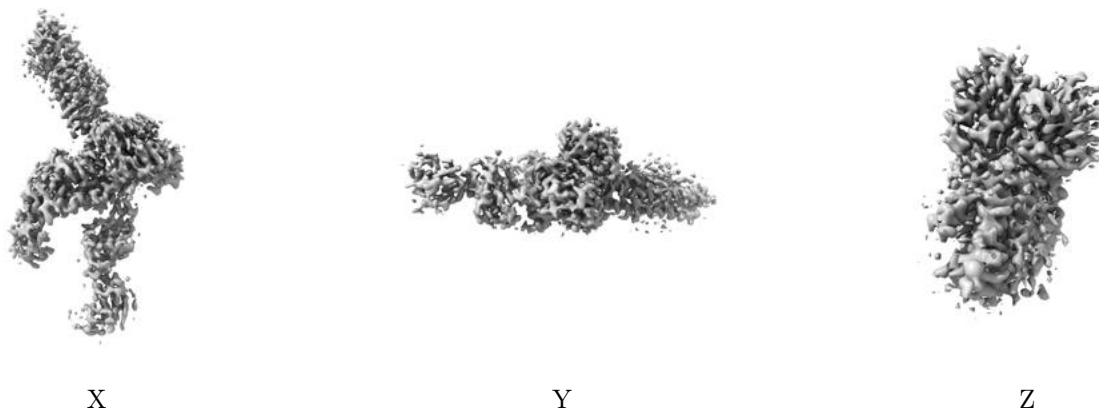


Z

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 0.904. 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.

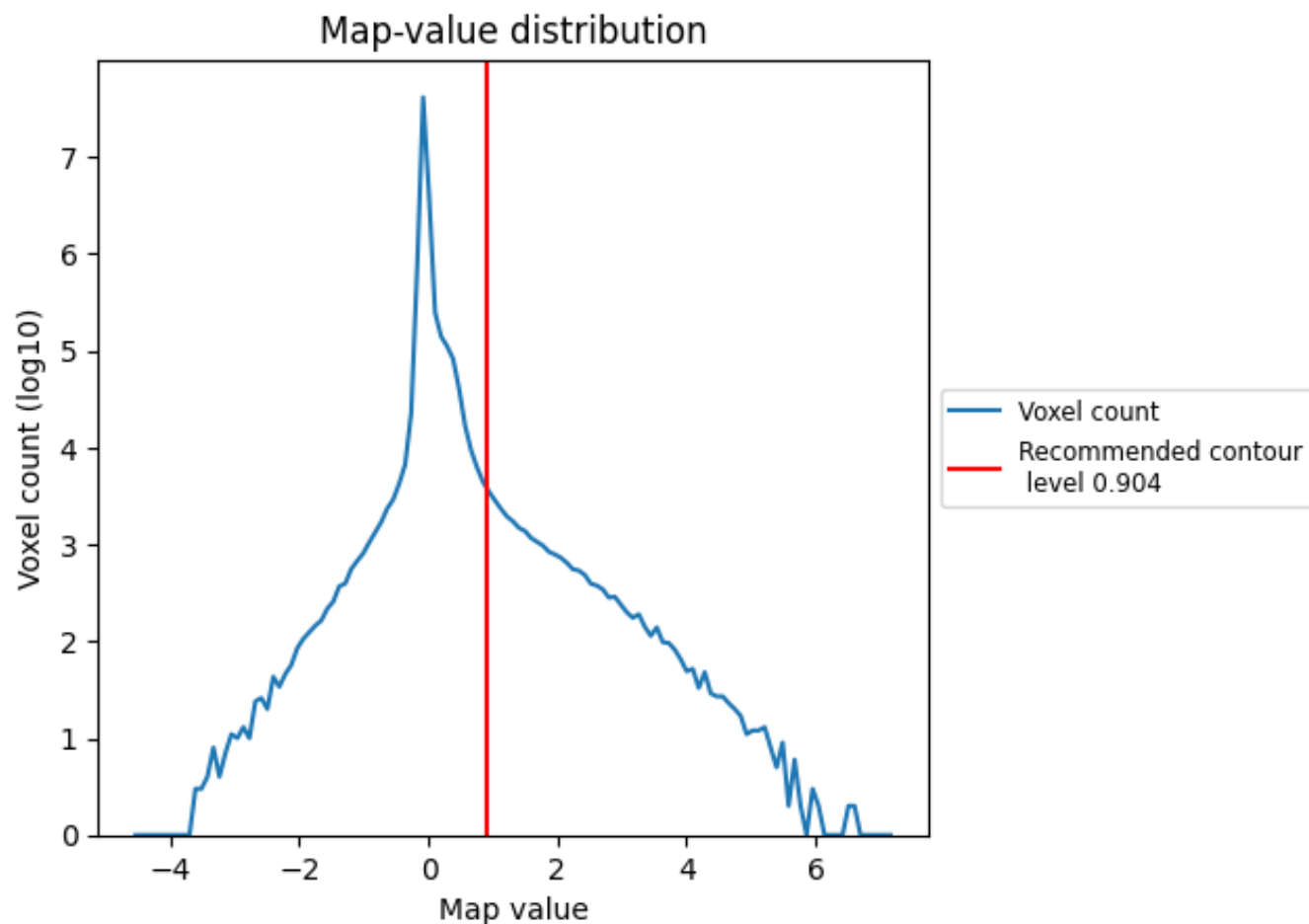
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

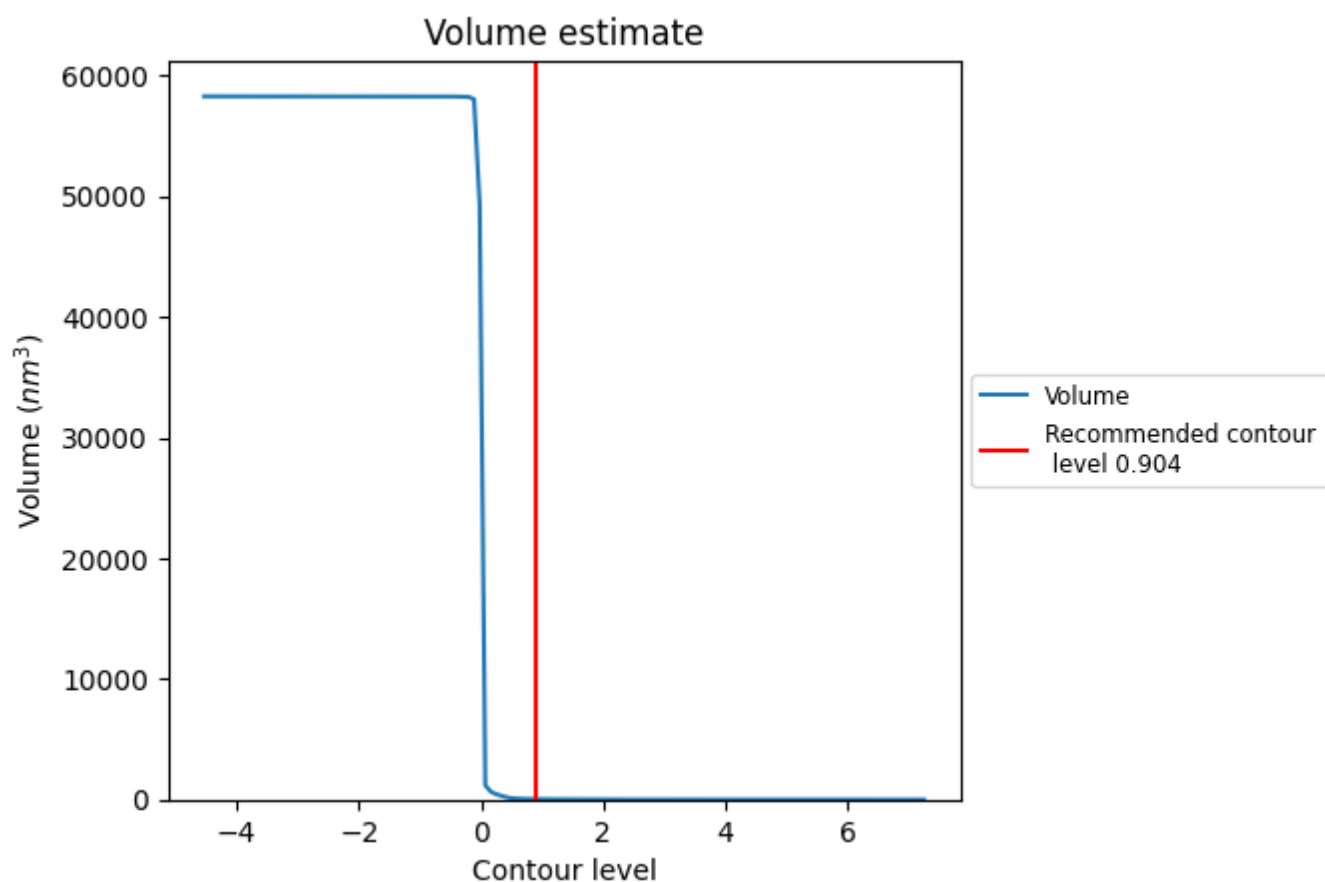
This section contains the results of statistical analysis of the map.

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.

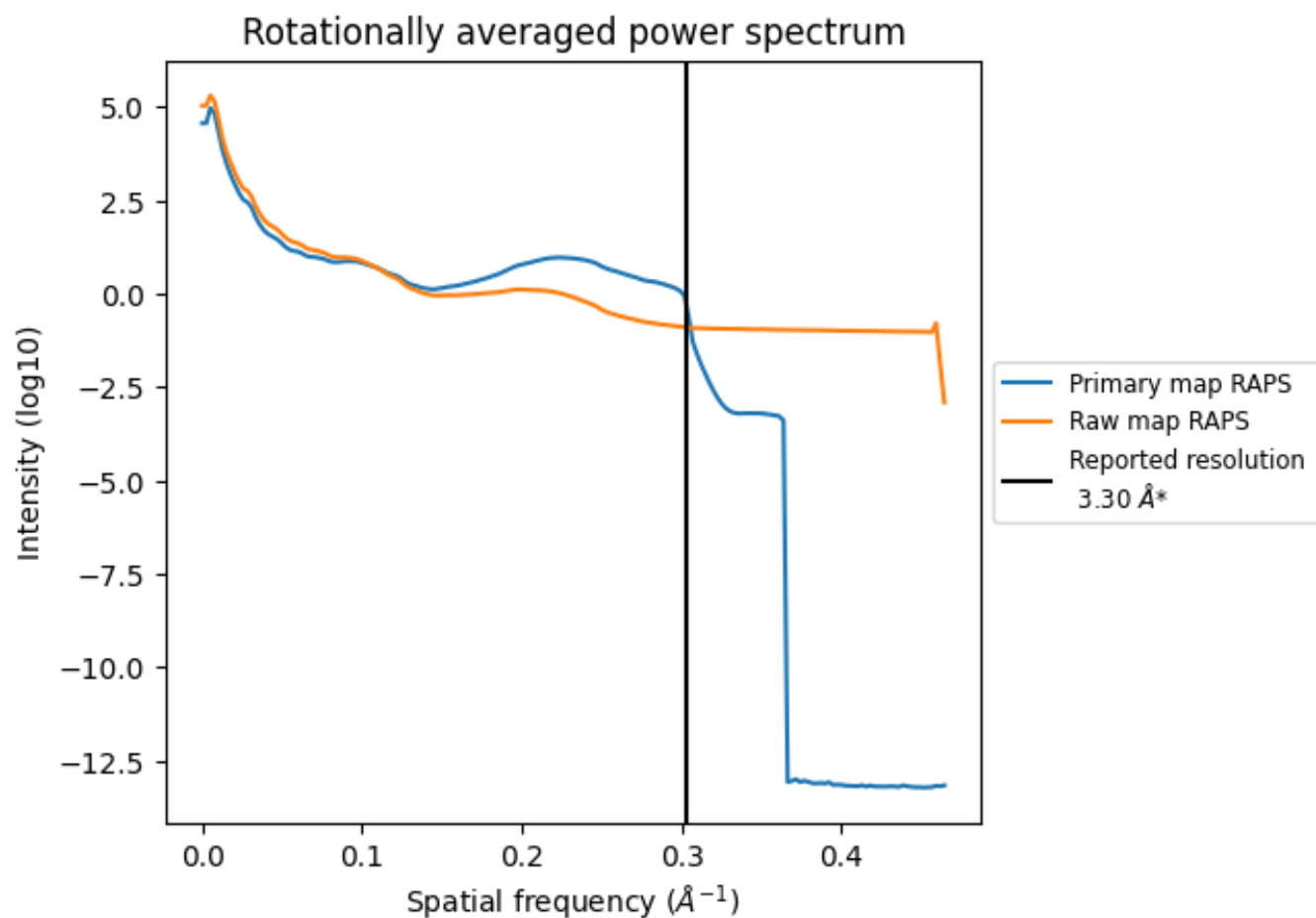
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 35 nm³; this corresponds to an approximate mass of 32 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 ⓘ

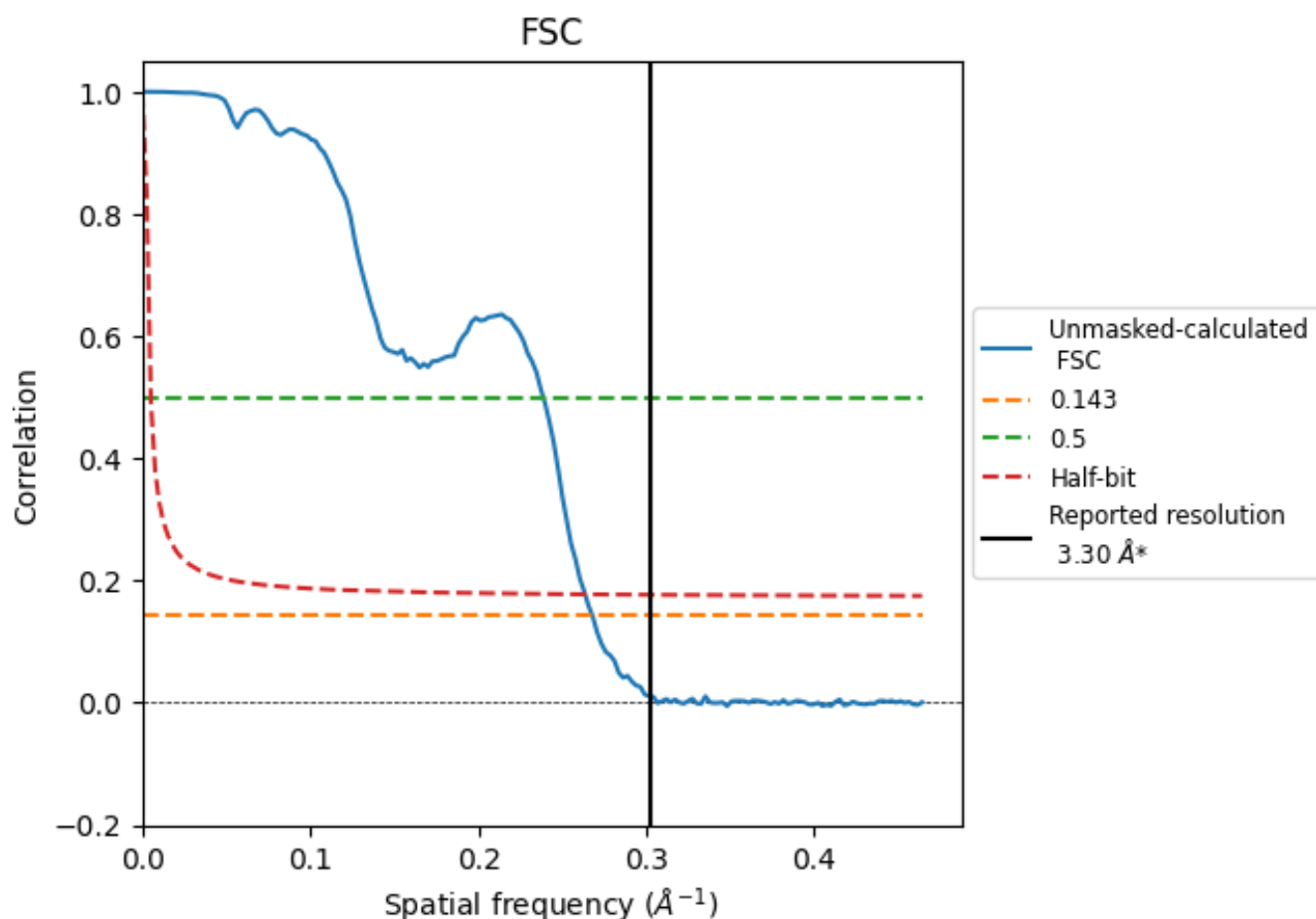


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

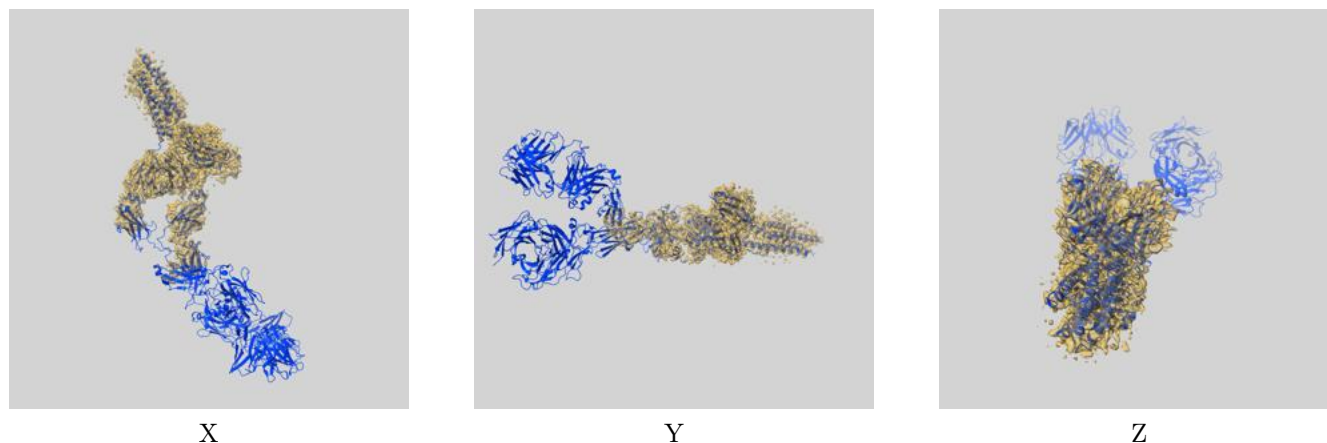
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.19	3.79

*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 3.73 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

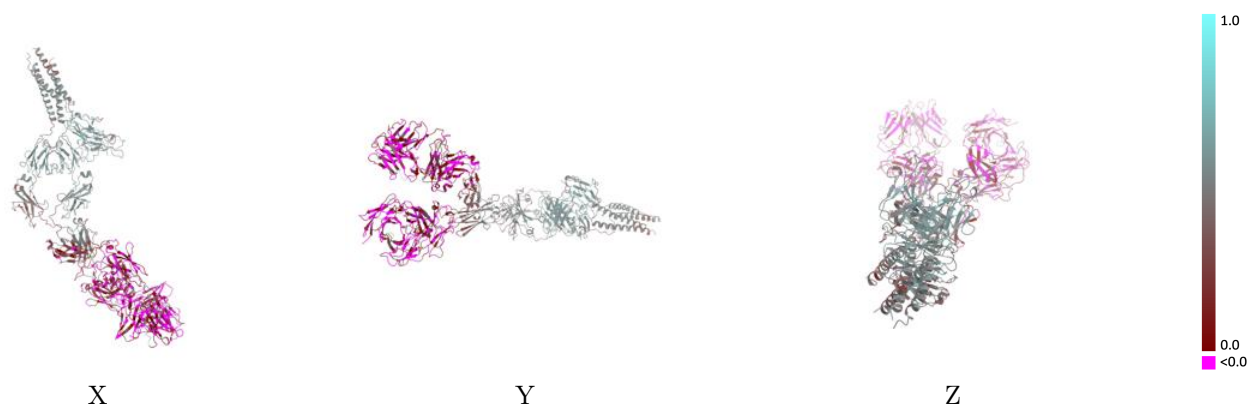
This section contains information regarding the fit between EMDB map EMD-33390 and PDB model 7XQ8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



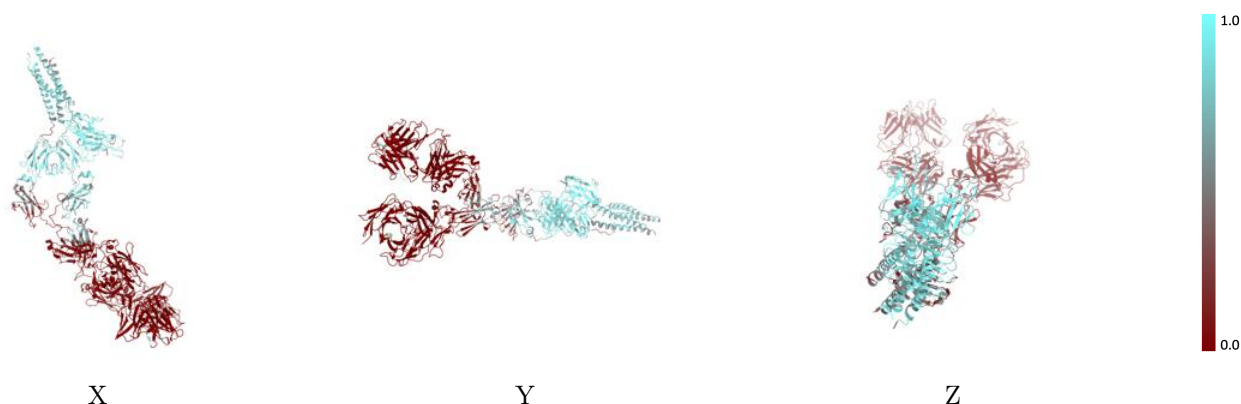
The images above show the 3D surface view of the map at the recommended contour level 0.904 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



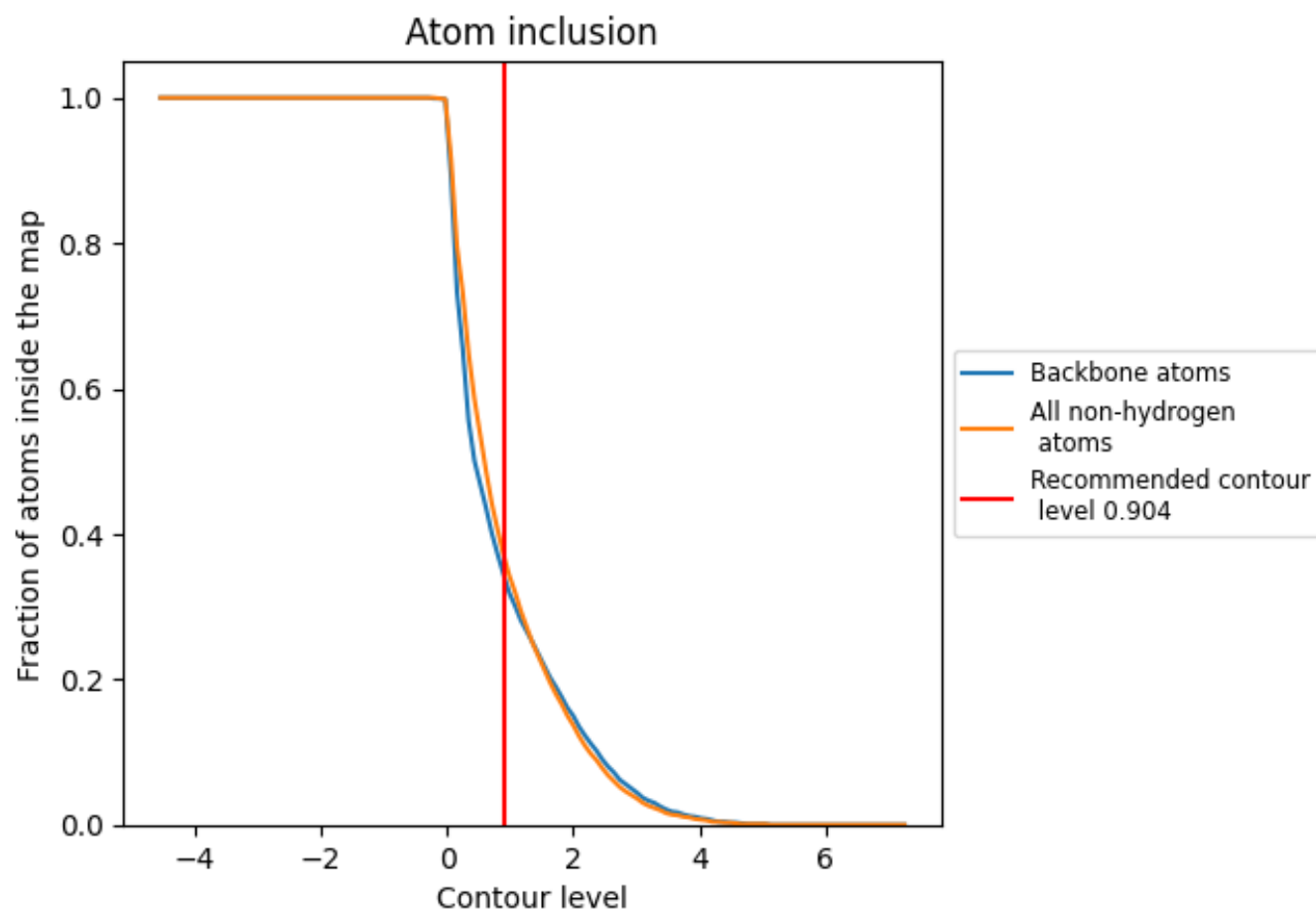
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.904).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 37% 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 (0.904) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3700	<div></div> 0.3130
A	<div></div> 0.7220	<div></div> 0.4950
B	<div></div> 0.7760	<div></div> 0.5140
C	<div></div> 0.3330	<div></div> 0.3240
L	<div></div> 0.0000	<div></div> 0.0320
R	<div></div> 0.0000	<div></div> 0.0640
v	<div></div> 0.3820	<div></div> 0.3260

1.0
0.0
-0.0