



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:43 PM UTC

PDB ID : 3J9D / pdb_00003j9d
EMDB ID : EMD-6239
Title : Atomic structure of a non-enveloped virus reveals pH sensors for a coordinated process of cell entry
Authors : Zhang, X.; Patel, A.; Celma, C.; Roy, P.; Zhou, Z.H.
Deposited on : 2015-01-09
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.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

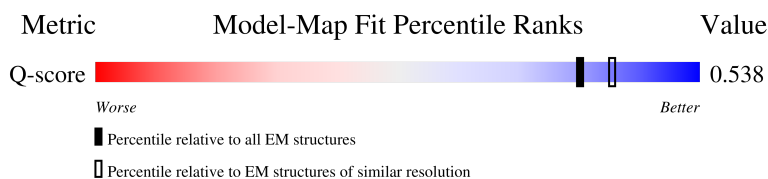
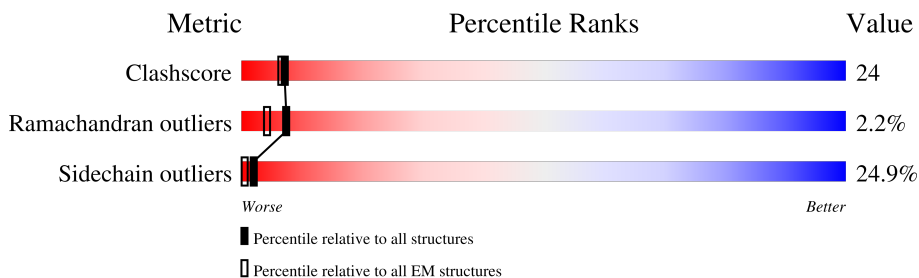
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	961	 34% 32% 11% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6086 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 Outer capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	746	Total	C	N	O	S	0	0
			6085	3891	1057	1105	32		

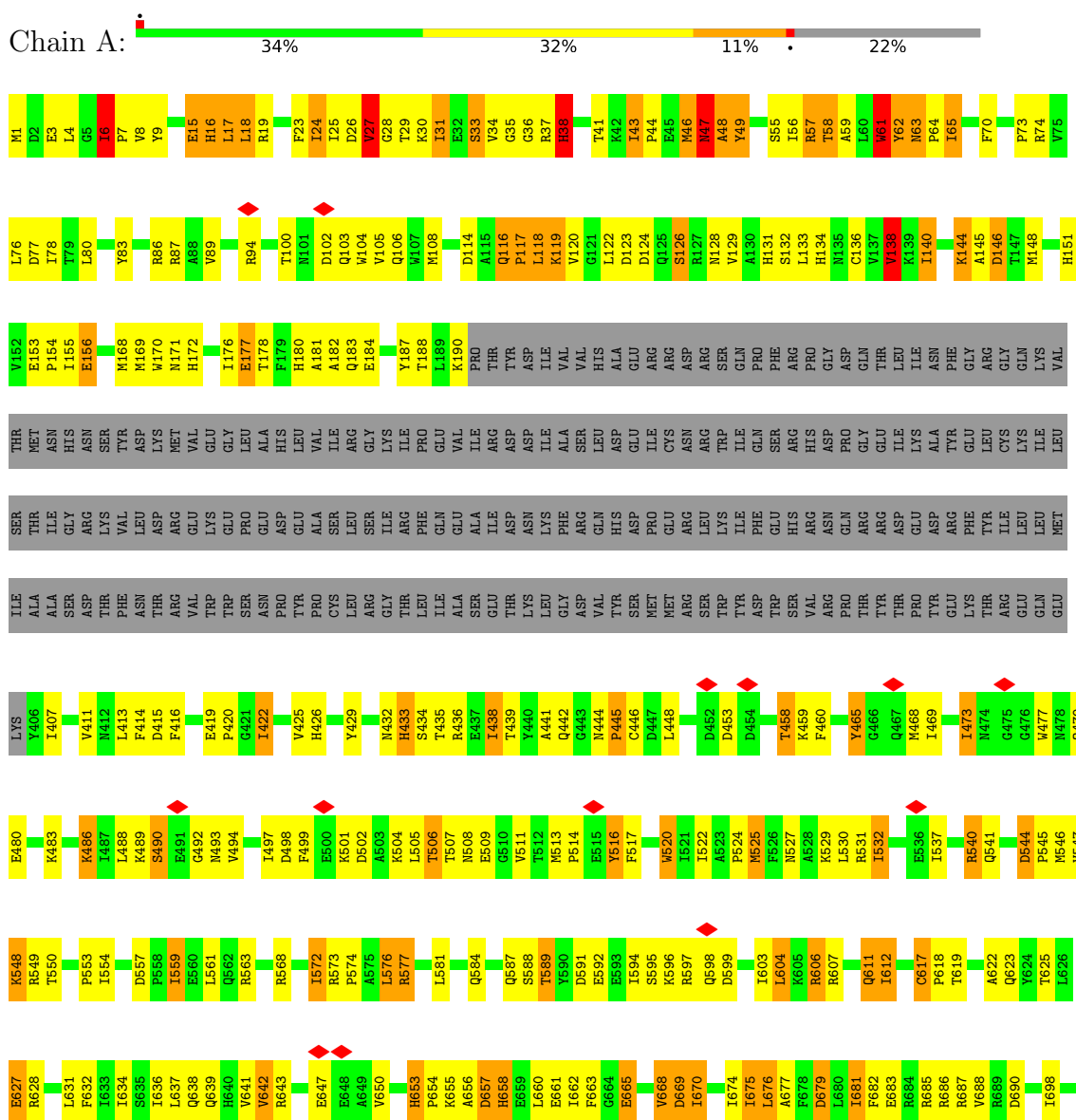
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	

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: Outer capsid protein VP2



L842	F915	T916	Y917	Y918	S919	Y923	S924	H925	R926	K929	K930	N931	L932	L933	K934	Y935	M936	G937	D938	L941	K943	F944	S945	V948	F949	G950	N951	D952	E953	M954	L955	T956	K957	L958	L959	N960	V961																	
L842	T845	Y846	L847	A848	S849	L850	C851	G852	G853	I854	S855	D856	G857	I858	V859	W860	Y861	L862	P863	I864	T865	C870	I871	V872	A873	I874	E875	W876	S877	R880	Y881	P882	I885	R886	I890	L892	R893	L896	S897	A898	R899	G903	V904	V905	I906	I907	G908	I909	D910	E914				
E769	V770	M771	V772	V773	P774	L775	E776	V777	G778	S779	Y780	N781	D782	R783	C784	G785	L786	I787	A788	Y789	L790	E791	Y792	M793	V794	F795	F796	P797	S798	K799	A800	I801	R802	F803	S804	K805	L806	I813	A814	L818	K819	Y820	A822	N823	G829	G830	V831	V835	V836	T837	T838	K839	Q840	L841
L701	R702	R703	M704	R705	E708	R709	L710	N711	V712	I713	A714	E715	T719	Y720	G721	G722	L723	L724	L727	N728	S729	V732	V733	Q734	N735	I736	M737	Y738	L739	N740	F741	L742	P743	L744	Y745	F746	L747	V748	G749	D750	Y754	S755	H756	R757	Q758	W759	S760	L763	L764	L765	Y766	T767	H768	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	24140	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	5.239	Depositor
Minimum map value	-3.042	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.220	Depositor
Recommended contour level	0.9	Depositor
Map size ($\text{\AA}$)	133.31999, 161.6, 147.45999	wwPDB
Map dimensions	160, 132, 146	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.26	11/6221 (0.2%)	1.32	59/8420 (0.7%)

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	A	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	771	MET	SD-CE	46.78	2.96	1.79
1	A	465	TYR	CD2-CE2	22.83	2.07	1.38
1	A	465	TYR	CD1-CE1	22.58	2.06	1.38
1	A	465	TYR	CE1-CZ	18.08	1.81	1.38
1	A	465	TYR	CE2-CZ	17.63	1.80	1.38
1	A	465	TYR	CG-CD2	15.14	1.71	1.39
1	A	465	TYR	CG-CD1	15.06	1.71	1.39
1	A	909	ILE	CA-CB	-5.56	1.47	1.54
1	A	138	VAL	CA-CB	-5.37	1.48	1.54
1	A	156	GLU	CB-CG	5.15	1.68	1.52
1	A	156	GLU	CG-CD	5.09	1.64	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	HIS	N-CA-C	-13.02	95.49	111.11
1	A	771	MET	CG-SD-CE	12.99	129.48	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	653	HIS	CA-C-N	-12.29	104.48	119.84
1	A	653	HIS	C-N-CA	-12.29	104.48	119.84
1	A	27	VAL	N-CA-C	10.40	122.06	112.29
1	A	715	GLU	N-CA-C	-9.99	99.89	113.18
1	A	713	ILE	N-CA-C	-9.09	99.94	110.21
1	A	877	SER	N-CA-C	8.08	120.40	108.60
1	A	520	TRP	N-CA-C	8.06	121.18	111.82
1	A	153	GLU	CA-C-N	8.02	128.04	119.78
1	A	153	GLU	C-N-CA	8.02	128.04	119.78
1	A	17	LEU	N-CA-C	7.92	122.04	112.38
1	A	923	VAL	CB-CA-C	-7.54	103.00	111.45
1	A	722	GLY	N-CA-C	-7.52	105.47	115.32
1	A	63	ASN	N-CA-C	7.49	126.36	109.81
1	A	63	ASN	C-N-CD	-7.43	104.25	120.60
1	A	917	VAL	CB-CA-C	-7.43	103.13	111.45
1	A	47	ASN	CA-C-N	7.41	135.04	121.70
1	A	47	ASN	C-N-CA	7.41	135.04	121.70
1	A	63	ASN	CA-C-N	7.26	144.42	127.00
1	A	63	ASN	C-N-CA	7.26	144.42	127.00
1	A	787	ILE	N-CA-C	-6.86	103.52	111.00
1	A	721	GLY	N-CA-C	-6.83	105.89	114.16
1	A	917	VAL	N-CA-C	6.72	117.81	110.21
1	A	43	ILE	CB-CA-C	-6.53	107.50	113.70
1	A	544	ASP	CA-C-N	-6.36	113.22	119.78
1	A	544	ASP	C-N-CA	-6.36	113.22	119.78
1	A	27	VAL	CB-CA-C	-6.32	103.23	111.88
1	A	657	ASP	N-CA-C	6.15	121.00	112.45
1	A	919	SER	N-CA-C	6.14	118.63	108.99
1	A	61	TRP	N-CA-C	-6.11	105.40	112.92
1	A	933	LEU	CB-CA-C	-6.02	109.65	116.63
1	A	6	ILE	CA-C-N	5.75	125.69	119.76
1	A	6	ILE	C-N-CA	5.75	125.69	119.76
1	A	445	PRO	CA-C-O	-5.71	114.46	121.31
1	A	778	GLY	N-CA-C	-5.70	96.77	113.30
1	A	128	ASN	N-CA-C	5.63	121.84	114.75
1	A	156	GLU	N-CA-C	-5.53	101.85	110.10
1	A	622	ALA	N-CA-C	-5.52	105.18	111.14
1	A	104	TRP	N-CA-C	-5.47	106.44	113.23
1	A	662	ILE	N-CA-C	5.46	117.49	109.63
1	A	951	ASN	N-CA-C	5.46	117.40	109.71
1	A	804	SER	N-CA-C	5.43	122.37	110.80
1	A	923	VAL	N-CA-C	5.42	116.34	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	GLN	CA-C-N	5.39	131.40	121.70
1	A	611	GLN	C-N-CA	5.39	131.40	121.70
1	A	931	ASN	N-CA-C	5.34	116.85	109.54
1	A	871	ILE	N-CA-C	5.33	116.47	109.21
1	A	881	VAL	CA-C-N	5.32	125.26	119.78
1	A	881	VAL	C-N-CA	5.32	125.26	119.78
1	A	46	MET	CA-C-N	-5.23	115.18	123.23
1	A	46	MET	C-N-CA	-5.23	115.18	123.23
1	A	831	VAL	CB-CA-C	-5.18	105.89	111.59
1	A	547	VAL	N-CA-C	-5.16	99.08	107.28
1	A	37	ARG	CA-C-N	-5.14	114.98	122.65
1	A	37	ARG	C-N-CA	-5.14	114.98	122.65
1	A	65	ILE	N-CA-C	5.06	117.25	111.88
1	A	675	ILE	N-CA-C	-5.06	105.45	110.62
1	A	748	VAL	N-CA-C	5.02	114.81	107.88

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	VAL	Peptide
1	A	34	VAL	Peptide
1	A	38	HIS	Peptide
1	A	49	TYR	Peptide
1	A	55	SER	Peptide
1	A	62	TYR	Peptide

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	6085	0	6087	288	0
2	A	1	0	0	0	0
All	All	6086	0	6087	288	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 24.

All (288) 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:465:TYR:CZ	1:A:465:TYR:CE2	1.80	1.65
1:A:465:TYR:CZ	1:A:465:TYR:CE1	1.81	1.60
1:A:465:TYR:CE1	1:A:465:TYR:CD1	2.06	1.43
1:A:465:TYR:CE2	1:A:465:TYR:CD2	2.07	1.39
1:A:465:TYR:CE2	1:A:771:MET:SD	2.35	1.19
1:A:465:TYR:CD2	1:A:771:MET:SD	2.36	1.18
1:A:465:TYR:CZ	1:A:771:MET:SD	2.39	1.16
1:A:465:TYR:CD1	1:A:771:MET:SD	2.39	1.15
1:A:465:TYR:CE1	1:A:771:MET:SD	2.41	1.14
1:A:465:TYR:CZ	1:A:771:MET:CE	2.33	1.12
1:A:465:TYR:CE1	1:A:771:MET:CE	2.32	1.12
1:A:465:TYR:CG	1:A:771:MET:SD	2.44	1.11
1:A:465:TYR:CE2	1:A:771:MET:CE	2.35	1.10
1:A:465:TYR:CD1	1:A:771:MET:CE	2.38	1.07
1:A:465:TYR:CD2	1:A:771:MET:CE	2.39	1.05
1:A:465:TYR:CG	1:A:771:MET:CE	2.46	0.98
1:A:559:ILE:HG12	1:A:628:ARG:HE	1.29	0.96
1:A:465:TYR:CZ	1:A:771:MET:HE3	2.03	0.94
1:A:607:ARG:HE	1:A:627:GLU:HG3	1.33	0.92
1:A:47:ASN:O	1:A:47:ASN:ND2	2.03	0.91
1:A:47:ASN:HB2	1:A:119:LYS:HG2	1.57	0.86
1:A:435:THR:HA	1:A:654:PRO:HD2	1.55	0.85
1:A:465:TYR:CD2	1:A:771:MET:HE1	2.07	0.85
1:A:465:TYR:CD1	1:A:771:MET:HE2	2.11	0.85
1:A:169:MET:HE1	1:A:623:GLN:HG3	1.60	0.83
1:A:544:ASP:HB3	1:A:577:ARG:HG3	1.62	0.82
1:A:714:ALA:HB2	1:A:721:GLY:HA3	1.62	0.81
1:A:803:PHE:O	1:A:805:LYS:N	2.13	0.81
1:A:465:TYR:CE1	1:A:771:MET:HE2	2.17	0.80
1:A:74:ARG:NE	1:A:114:ASP:OD2	2.16	0.78
1:A:516:TYR:HE1	1:A:532:ILE:HD11	1.49	0.78
1:A:465:TYR:CE2	1:A:771:MET:HE3	2.20	0.76
1:A:1:MET:HG2	1:A:948:VAL:HG13	1.68	0.75
1:A:177:GLU:HA	1:A:180:HIS:CE1	2.23	0.72
1:A:661:GLU:HB3	1:A:686:ARG:HD3	1.73	0.70
1:A:47:ASN:HA	1:A:48:ALA:CB	2.23	0.69
1:A:468:MET:HE1	1:A:774:PRO:HG3	1.74	0.69
1:A:617:CYS:SG	1:A:619:THR:OG1	2.50	0.69
1:A:483:LYS:HB2	1:A:486:LYS:HD3	1.75	0.68
1:A:131:HIS:CD2	1:A:148:MET:HE3	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:GLN:HA	1:A:737:MET:HE3	1.74	0.68
1:A:772:VAL:HG21	1:A:813:ILE:HG21	1.75	0.68
1:A:73:PRO:HD2	1:A:114:ASP:HB3	1.77	0.67
1:A:459:LYS:HB2	1:A:489:LYS:HD3	1.77	0.67
1:A:611:GLN:HB3	1:A:612:ILE:HB	1.76	0.67
1:A:6:ILE:HG21	1:A:23:PHE:HD2	1.60	0.67
1:A:458:THR:HG22	1:A:493:ASN:HA	1.76	0.66
1:A:465:TYR:OH	1:A:771:MET:HA	1.96	0.65
1:A:641:VAL:HG21	1:A:681:ILE:HG23	1.77	0.65
1:A:458:THR:CG2	1:A:493:ASN:HA	2.27	0.65
1:A:506:THR:OG1	1:A:507:THR:N	2.25	0.65
1:A:146:ASP:N	1:A:146:ASP:OD1	2.25	0.65
1:A:83:TYR:HB2	1:A:961:VAL:HG21	1.78	0.64
1:A:559:ILE:HD11	1:A:628:ARG:HH11	1.61	0.64
1:A:607:ARG:HE	1:A:627:GLU:CG	2.07	0.64
1:A:47:ASN:HA	1:A:48:ALA:HB2	1.79	0.64
1:A:687:ARG:HH11	1:A:687:ARG:HB2	1.63	0.64
1:A:425:VAL:HG21	1:A:499:PHE:CE1	2.33	0.63
1:A:923:VAL:HG13	1:A:944:PHE:CE1	2.34	0.63
1:A:559:ILE:HG12	1:A:628:ARG:NE	2.08	0.63
1:A:420:PRO:HD3	1:A:540:ARG:HB3	1.81	0.62
1:A:172:HIS:HE2	1:A:670:ILE:H	1.47	0.62
1:A:184:GLU:OE1	1:A:184:GLU:N	2.23	0.62
1:A:702:ARG:HA	1:A:709:ARG:HH12	1.65	0.61
1:A:465:TYR:CE1	1:A:771:MET:HG3	2.36	0.61
1:A:493:ASN:O	1:A:497:ILE:HG23	2.01	0.61
1:A:557:ASP:HB3	1:A:597:ARG:CZ	2.31	0.61
1:A:563:ARG:O	1:A:791:GLU:HG3	2.01	0.60
1:A:631:LEU:HD13	1:A:658:HIS:H	1.65	0.60
1:A:465:TYR:CE1	1:A:771:MET:CG	2.85	0.60
1:A:599:ASP:OD2	1:A:628:ARG:NH2	2.34	0.60
1:A:732:VAL:HA	1:A:805:LYS:HA	1.84	0.60
1:A:465:TYR:CG	1:A:771:MET:HE1	2.30	0.59
1:A:789:TYR:CE1	1:A:793:MET:HE3	2.37	0.59
1:A:446:CYS:HB3	1:A:795:PHE:CD1	2.37	0.59
1:A:155:ILE:HG12	1:A:853:GLY:O	2.04	0.58
1:A:859:VAL:HB	1:A:875:GLU:HG2	1.85	0.58
1:A:63:ASN:HA	1:A:835:VAL:HG22	1.86	0.58
1:A:763:LEU:HD13	1:A:775:LEU:HD21	1.84	0.58
1:A:737:MET:HE1	1:A:802:ARG:HG3	1.85	0.58
1:A:687:ARG:HB2	1:A:687:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ILE:HD11	1:A:676:LEU:HD13	1.86	0.57
1:A:176:ILE:HD13	1:A:670:ILE:HG13	1.86	0.57
1:A:419:GLU:HG3	1:A:420:PRO:HD2	1.85	0.57
1:A:448:LEU:HD11	1:A:767:THR:HG21	1.86	0.57
1:A:116:GLN:HG3	1:A:118:LEU:HD21	1.86	0.57
1:A:863:PRO:HG3	1:A:955:LEU:HD23	1.85	0.57
1:A:86:ARG:HG2	1:A:100:THR:HA	1.86	0.56
1:A:663:PHE:O	1:A:687:ARG:HA	2.05	0.56
1:A:64:PRO:HG3	1:A:838:THR:HG21	1.86	0.56
1:A:657:ASP:HB3	1:A:660:LEU:HB2	1.88	0.56
1:A:606:ARG:HH11	1:A:606:ARG:HB3	1.71	0.56
1:A:548:LYS:HG3	1:A:553:PRO:HB2	1.88	0.56
1:A:23:PHE:CD1	1:A:140:ILE:HG12	2.41	0.55
1:A:49:TYR:CD2	1:A:841:LEU:HD13	2.41	0.55
1:A:757:ARG:O	1:A:758:GLN:HB2	2.07	0.55
1:A:74:ARG:O	1:A:78:ILE:HG12	2.05	0.55
1:A:516:TYR:CE1	1:A:532:ILE:HD11	2.37	0.55
1:A:444:ASN:N	1:A:445:PRO:HD3	2.22	0.55
1:A:477:TRP:CH2	1:A:774:PRO:HB3	2.42	0.55
1:A:415:ASP:HA	1:A:541:GLN:HE21	1.72	0.54
1:A:3:GLU:HB3	1:A:943:LYS:HA	1.89	0.54
1:A:9:TYR:HE1	1:A:24:ILE:HG23	1.73	0.54
1:A:681:ILE:HG22	1:A:682:PHE:CD2	2.42	0.54
1:A:771:MET:SD	1:A:771:MET:CE	2.96	0.53
1:A:27:VAL:HG12	1:A:136:CYS:HB3	1.91	0.53
1:A:73:PRO:HB3	1:A:893:ARG:NH1	2.23	0.53
1:A:841:LEU:O	1:A:845:THR:HG23	2.09	0.53
1:A:798:SER:H	1:A:801:ILE:HD12	1.74	0.53
1:A:31:ILE:HG12	1:A:46:MET:HE2	1.91	0.53
1:A:446:CYS:HB3	1:A:795:PHE:CE1	2.43	0.53
1:A:598:GLN:O	1:A:599:ASP:HB3	2.09	0.53
1:A:102:ASP:O	1:A:106:GLN:HG2	2.09	0.53
1:A:184:GLU:HG3	1:A:426:HIS:ND1	2.24	0.53
1:A:23:PHE:HD1	1:A:140:ILE:HG12	1.73	0.53
1:A:740:ASN:O	1:A:743:PRO:HD2	2.09	0.53
1:A:62:TYR:CE2	1:A:64:PRO:HB3	2.44	0.52
1:A:527:ASN:HB2	1:A:795:PHE:HZ	1.74	0.52
1:A:683:GLU:HB3	1:A:685:ARG:HG3	1.91	0.52
1:A:737:MET:HG3	1:A:766:TYR:OH	2.09	0.52
1:A:57:ARG:H	1:A:57:ARG:HD2	1.73	0.52
1:A:78:ILE:HD12	1:A:108:MET:CG	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:TRP:HA	1:A:531:ARG:HB3	1.91	0.52
1:A:544:ASP:CG	1:A:544:ASP:O	2.53	0.52
1:A:885:ILE:HG13	1:A:886:ARG:N	2.21	0.52
1:A:460:PHE:CE2	1:A:525:MET:HG2	2.45	0.52
1:A:938:ASP:N	1:A:938:ASP:OD1	2.42	0.52
1:A:490:SER:O	1:A:492:GLY:HA2	2.10	0.51
1:A:524:PRO:HD2	1:A:525:MET:HE2	1.91	0.51
1:A:750:ASP:OD1	1:A:750:ASP:N	2.43	0.51
1:A:425:VAL:HG21	1:A:499:PHE:HE1	1.74	0.51
1:A:559:ILE:CG1	1:A:628:ARG:HE	2.12	0.51
1:A:438:ILE:HG12	1:A:444:ASN:H	1.76	0.51
1:A:170:TRP:HZ3	1:A:847:LEU:HB2	1.75	0.50
1:A:23:PHE:CE2	1:A:860:TRP:HZ3	2.29	0.50
1:A:429:TYR:CD1	1:A:429:TYR:C	2.90	0.50
1:A:639:GLN:HG3	1:A:653:HIS:NE2	2.27	0.50
1:A:864:ILE:HB	1:A:870:CYS:O	2.11	0.50
1:A:133:LEU:HD23	1:A:134:HIS:N	2.27	0.49
1:A:606:ARG:HD3	1:A:627:GLU:OE1	2.12	0.49
1:A:607:ARG:NE	1:A:627:GLU:HG3	2.14	0.49
1:A:23:PHE:CE1	1:A:138:VAL:HG13	2.47	0.49
1:A:755:SER:HA	1:A:829:GLY:HA3	1.94	0.49
1:A:655:LYS:HG2	1:A:656:ALA:O	2.12	0.49
1:A:861:TYR:HB3	1:A:871:ILE:HG23	1.93	0.49
1:A:187:TYR:HB2	1:A:425:VAL:CG2	2.42	0.49
1:A:438:ILE:HG12	1:A:444:ASN:N	2.27	0.49
1:A:544:ASP:OD2	1:A:589:THR:HG23	2.13	0.49
1:A:907:ILE:HD12	1:A:907:ILE:H	1.78	0.49
1:A:78:ILE:HD12	1:A:108:MET:HG3	1.94	0.49
1:A:746:PHE:N	1:A:746:PHE:CD1	2.80	0.49
1:A:747:LEU:HD21	1:A:777:VAL:HG11	1.95	0.48
1:A:62:TYR:CG	1:A:63:ASN:N	2.80	0.48
1:A:959:LEU:C	1:A:961:VAL:H	2.21	0.48
1:A:572:ILE:HG12	1:A:783:ARG:HH12	1.79	0.48
1:A:941:LEU:HD13	1:A:941:LEU:HA	1.61	0.48
1:A:441:ALA:N	1:A:647:GLU:HB3	2.29	0.48
1:A:676:LEU:HG	1:A:688:VAL:HG22	1.96	0.48
1:A:923:VAL:HG12	1:A:924:SER:N	2.28	0.48
1:A:26:ASP:C	1:A:28:GLY:HA3	2.38	0.48
1:A:433:HIS:CE1	1:A:436:ARG:HD3	2.49	0.48
1:A:411:VAL:HG21	1:A:416:PHE:CD1	2.49	0.48
1:A:777:VAL:HG23	1:A:777:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG12	1:A:131:HIS:CE1	2.49	0.48
1:A:133:LEU:HD23	1:A:134:HIS:H	1.78	0.48
1:A:182:ALA:HB1	1:A:554:ILE:HD11	1.96	0.48
1:A:522:ILE:HG12	1:A:529:LYS:HG3	1.95	0.47
1:A:568:ARG:HD3	1:A:780:TYR:HB3	1.96	0.47
1:A:70:PHE:CD1	1:A:70:PHE:N	2.82	0.47
1:A:711:ASN:O	1:A:715:GLU:HB2	2.14	0.47
1:A:596:LYS:HB2	1:A:596:LYS:HE3	1.42	0.47
1:A:7:PRO:HG2	1:A:24:ILE:HG12	1.96	0.47
1:A:78:ILE:HG23	1:A:108:MET:HG2	1.96	0.47
1:A:480:GLU:OE2	1:A:759:TRP:NE1	2.48	0.47
1:A:754:TYR:CE2	1:A:784:CYS:HB2	2.50	0.47
1:A:477:TRP:HH2	1:A:774:PRO:HB3	1.80	0.47
1:A:25:ILE:HG21	1:A:909:ILE:HD11	1.97	0.46
1:A:74:ARG:NH1	1:A:78:ILE:HD11	2.30	0.46
1:A:181:ALA:HB3	1:A:545:PRO:HB2	1.98	0.46
1:A:604:LEU:HD12	1:A:604:LEU:HA	1.63	0.46
1:A:123:ASP:OD1	1:A:124:ASP:N	2.48	0.46
1:A:743:PRO:HG3	1:A:821:TYR:OH	2.15	0.46
1:A:172:HIS:NE2	1:A:669:ASP:HA	2.30	0.46
1:A:498:ASP:O	1:A:502:ASP:HB2	2.16	0.46
1:A:19:ARG:HD3	1:A:126:SER:HB2	1.98	0.46
1:A:916:THR:O	1:A:916:THR:OG1	2.31	0.46
1:A:758:GLN:HA	1:A:776:GLU:CD	2.41	0.46
1:A:757:ARG:HG2	1:A:782:ASP:OD2	2.16	0.46
1:A:444:ASN:ND2	1:A:794:VAL:O	2.50	0.45
1:A:58:THR:HG22	1:A:61:TRP:NE1	2.32	0.45
1:A:414:PHE:HB2	1:A:573:ARG:HH11	1.81	0.45
1:A:587:GLN:NE2	1:A:591:ASP:OD2	2.49	0.45
1:A:416:PHE:HB3	1:A:549:ARG:NH2	2.31	0.45
1:A:708:GLU:H	1:A:708:GLU:HG3	1.52	0.45
1:A:587:GLN:NE2	1:A:618:PRO:HD3	2.32	0.45
1:A:677:ALA:O	1:A:681:ILE:HB	2.15	0.45
1:A:776:GLU:HG2	1:A:778:GLY:HA2	1.98	0.45
1:A:860:TRP:CD1	1:A:860:TRP:C	2.94	0.45
1:A:714:ALA:HB2	1:A:721:GLY:CA	2.41	0.45
1:A:905:VAL:CG2	1:A:923:VAL:HG11	2.47	0.45
1:A:514:PRO:O	1:A:516:TYR:N	2.47	0.45
1:A:62:TYR:CD1	1:A:63:ASN:N	2.78	0.44
1:A:422:ILE:O	1:A:422:ILE:HG13	2.17	0.44
1:A:434:SER:HB2	1:A:563:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:TYR:CZ	1:A:771:MET:CG	3.00	0.44
1:A:33:SER:HB2	1:A:38:HIS:HB3	2.00	0.44
1:A:35:GLY:HA2	1:A:36:GLY:HA2	1.66	0.44
1:A:181:ALA:HB1	1:A:546:MET:HB3	1.99	0.44
1:A:742:LEU:HA	1:A:742:LEU:HD23	1.65	0.44
1:A:755:SER:HA	1:A:829:GLY:CA	2.47	0.44
1:A:151:HIS:CG	1:A:151:HIS:O	2.70	0.44
1:A:956:THR:O	1:A:960:ASN:HB2	2.17	0.44
1:A:43:ILE:HA	1:A:46:MET:HG2	2.00	0.44
1:A:44:PRO:HD3	1:A:581:LEU:CD1	2.48	0.44
1:A:653:HIS:HB3	1:A:654:PRO:HD3	2.00	0.44
1:A:606:ARG:NH2	1:A:660:LEU:O	2.50	0.44
1:A:923:VAL:HG12	1:A:924:SER:H	1.83	0.44
1:A:488:LEU:HB2	1:A:493:ASN:HD22	1.83	0.43
1:A:701:ILE:HD13	1:A:713:ILE:HG12	2.00	0.43
1:A:607:ARG:NH1	1:A:623:GLN:HG2	2.33	0.43
1:A:757:ARG:H	1:A:757:ARG:HG3	1.47	0.43
1:A:862:LEU:HA	1:A:863:PRO:HD3	1.90	0.43
1:A:9:TYR:CD1	1:A:9:TYR:N	2.86	0.43
1:A:9:TYR:OH	1:A:26:ASP:HB2	2.19	0.43
1:A:59:ALA:O	1:A:62:TYR:HB3	2.18	0.43
1:A:140:ILE:HG21	1:A:145:ALA:HA	2.01	0.43
1:A:435:THR:O	1:A:435:THR:OG1	2.31	0.43
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.56	0.43
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.71	0.43
1:A:502:ASP:HB3	1:A:514:PRO:HG3	2.00	0.43
1:A:854:ILE:HG12	1:A:855:SER:N	2.34	0.43
1:A:505:LEU:HB2	1:A:506:THR:HA	1.99	0.43
1:A:508:ASN:HA	1:A:509:GLU:HA	1.74	0.43
1:A:527:ASN:HB2	1:A:795:PHE:CZ	2.53	0.43
1:A:799:LYS:HG2	1:A:803:PHE:CE1	2.53	0.43
1:A:432:ASN:HB3	1:A:527:ASN:OD1	2.19	0.43
1:A:890:ILE:HD13	1:A:890:ILE:HA	1.66	0.43
1:A:683:GLU:CD	1:A:719:THR:HG23	2.43	0.42
1:A:559:ILE:H	1:A:559:ILE:HG13	1.67	0.42
1:A:637:LEU:HD23	1:A:637:LEU:HA	1.70	0.42
1:A:642:VAL:HG13	1:A:734:GLN:OE1	2.19	0.42
1:A:155:ILE:HG22	1:A:156:GLU:O	2.19	0.42
1:A:607:ARG:HA	1:A:607:ARG:HD3	1.42	0.42
1:A:705:ARG:HD3	1:A:705:ARG:HA	1.87	0.42
1:A:479:GLN:HG3	1:A:480:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:PRO:HB2	1:A:576:LEU:HD22	2.01	0.42
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.92	0.42
1:A:74:ARG:HH12	1:A:78:ILE:HD11	1.85	0.42
1:A:144:LYS:HD2	1:A:144:LYS:HA	1.68	0.42
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.59	0.42
1:A:473:ILE:HG13	1:A:813:ILE:HD12	2.00	0.42
1:A:419:GLU:O	1:A:422:ILE:HG23	2.20	0.42
1:A:592:GLU:O	1:A:595:SER:HB3	2.20	0.42
1:A:116:GLN:HA	1:A:117:PRO:HD3	1.90	0.41
1:A:679:ASP:O	1:A:683:GLU:HB2	2.20	0.41
1:A:917:VAL:HG12	1:A:918:TYR:N	2.35	0.41
1:A:138:VAL:HB	1:A:858:ILE:HD11	2.01	0.41
1:A:865:THR:HB	1:A:954:MET:HE3	2.02	0.41
1:A:665:GLU:HG3	1:A:690:ASP:OD1	2.20	0.41
1:A:631:LEU:HD23	1:A:631:LEU:HA	1.69	0.41
1:A:736:ILE:HG12	1:A:814:ALA:CB	2.51	0.41
1:A:739:LEU:HD11	1:A:818:LEU:HB2	2.01	0.41
1:A:936:MET:HE3	1:A:936:MET:HB2	1.86	0.41
1:A:949:PHE:O	1:A:949:PHE:CD1	2.74	0.41
1:A:187:TYR:HB2	1:A:425:VAL:HG22	2.02	0.41
1:A:910:ASP:HB2	1:A:914:GLU:O	2.21	0.41
1:A:661:GLU:HB3	1:A:686:ARG:CD	2.47	0.41
1:A:674:ILE:HG12	1:A:744:LEU:HD22	2.02	0.41
1:A:70:PHE:CE2	1:A:117:PRO:HB3	2.56	0.41
1:A:78:ILE:HD12	1:A:108:MET:HG2	2.03	0.41
1:A:747:LEU:HD22	1:A:747:LEU:HA	1.85	0.41
1:A:760:SER:HB2	1:A:774:PRO:HB2	2.03	0.41
1:A:881:VAL:HG23	1:A:882:PRO:HD2	2.02	0.41
1:A:154:PRO:HB3	1:A:848:ALA:CA	2.51	0.41
1:A:154:PRO:HB3	1:A:848:ALA:HA	2.02	0.41
1:A:31:ILE:HA	1:A:31:ILE:HD12	1.60	0.40
1:A:574:PRO:HB2	1:A:576:LEU:CD2	2.51	0.40
1:A:802:ARG:O	1:A:802:ARG:HG2	2.19	0.40
1:A:952:ASP:N	1:A:952:ASP:OD1	2.52	0.40
1:A:701:ILE:HG12	1:A:712:VAL:HG23	2.03	0.40
1:A:872:VAL:HG13	1:A:903:GLY:O	2.21	0.40
1:A:6:ILE:HG22	1:A:23:PHE:HB3	2.04	0.40
1:A:6:ILE:H	1:A:6:ILE:HG12	1.80	0.40
1:A:632:PHE:CZ	1:A:636:ILE:HD11	2.57	0.40
1:A:737:MET:HE3	1:A:737:MET:HB2	1.67	0.40
1:A:766:TYR:CD1	1:A:797:PRO:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HD13	1:A:670:ILE:CG1	2.51	0.40
1:A:517:PHE:O	1:A:517:PHE:CG	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	742/961 (77%)	665 (90%)	61 (8%)	16 (2%)	5	26

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ALA
1	A	804	SER
1	A	15	GLU
1	A	540	ARG
1	A	897	SER
1	A	516	TYR
1	A	729	SER
1	A	668	VAL
1	A	960	ASN
1	A	117	PRO
1	A	442	GLN
1	A	781	ASN
1	A	806	LEU
1	A	129	VAL
1	A	511	VAL
1	A	770	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	666/863 (77%)	500 (75%)	166 (25%)	0 3

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	ILE
1	A	8	VAL
1	A	15	GLU
1	A	16	HIS
1	A	17	LEU
1	A	18	LEU
1	A	24	ILE
1	A	29	THR
1	A	30	LYS
1	A	31	ILE
1	A	33	SER
1	A	38	HIS
1	A	41	THR
1	A	47	ASN
1	A	56	ILE
1	A	57	ARG
1	A	58	THR
1	A	61	TRP
1	A	65	ILE
1	A	76	LEU
1	A	77	ASP
1	A	87	ARG
1	A	89	VAL
1	A	94	ARG
1	A	103	GLN
1	A	105	VAL
1	A	116	GLN
1	A	118	LEU
1	A	119	LYS

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Mol	Chain	Res	Type
1	A	122	LEU
1	A	126	SER
1	A	132	SER
1	A	138	VAL
1	A	140	ILE
1	A	144	LYS
1	A	146	ASP
1	A	168	MET
1	A	171	ASN
1	A	177	GLU
1	A	178	THR
1	A	183	GLN
1	A	188	THR
1	A	190	LYS
1	A	407	ILE
1	A	413	LEU
1	A	422	ILE
1	A	433	HIS
1	A	438	ILE
1	A	439	THR
1	A	453	ASP
1	A	458	THR
1	A	469	ILE
1	A	473	ILE
1	A	486	LYS
1	A	490	SER
1	A	494	VAL
1	A	501	LYS
1	A	504	LYS
1	A	506	THR
1	A	513	MET
1	A	525	MET
1	A	530	LEU
1	A	532	ILE
1	A	537	ILE
1	A	548	LYS
1	A	550	THR
1	A	559	ILE
1	A	561	LEU
1	A	572	ILE
1	A	576	LEU
1	A	577	ARG

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Mol	Chain	Res	Type
1	A	584	GLN
1	A	588	SER
1	A	589	THR
1	A	594	ILE
1	A	603	ILE
1	A	604	LEU
1	A	606	ARG
1	A	612	ILE
1	A	617	CYS
1	A	625	THR
1	A	627	GLU
1	A	638	GLN
1	A	642	VAL
1	A	643	ARG
1	A	650	VAL
1	A	658	HIS
1	A	665	GLU
1	A	668	VAL
1	A	669	ASP
1	A	670	ILE
1	A	675	ILE
1	A	676	LEU
1	A	679	ASP
1	A	681	ILE
1	A	698	ILE
1	A	704	MET
1	A	708	GLU
1	A	710	LEU
1	A	712	VAL
1	A	713	ILE
1	A	719	THR
1	A	723	LEU
1	A	724	LEU
1	A	727	LEU
1	A	733	VAL
1	A	736	ILE
1	A	739	LEU
1	A	747	LEU
1	A	750	ASP
1	A	755	SER
1	A	757	ARG
1	A	760	SER

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Mol	Chain	Res	Type
1	A	763	LEU
1	A	764	LEU
1	A	765	LEU
1	A	769	GLU
1	A	784	CYS
1	A	786	LEU
1	A	787	ILE
1	A	794	VAL
1	A	801	ILE
1	A	818	LEU
1	A	819	LYS
1	A	823	ASN
1	A	831	VAL
1	A	836	VAL
1	A	838	THR
1	A	839	LYS
1	A	842	LEU
1	A	845	THR
1	A	849	SER
1	A	851	CYS
1	A	856	ASP
1	A	858	ILE
1	A	860	TRP
1	A	862	LEU
1	A	865	THR
1	A	874	ILE
1	A	875	GLU
1	A	880	ARG
1	A	881	VAL
1	A	885	ILE
1	A	890	ILE
1	A	892	LEU
1	A	896	LEU
1	A	899	ARG
1	A	906	ILE
1	A	909	ILE
1	A	914	GLU
1	A	916	THR
1	A	917	VAL
1	A	923	VAL
1	A	926	ARG
1	A	929	LYS

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Mol	Chain	Res	Type
1	A	932	LEU
1	A	934	LYS
1	A	938	ASP
1	A	941	LEU
1	A	945	SER
1	A	955	LEU
1	A	956	THR
1	A	957	LYS
1	A	959	LEU
1	A	961	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	180	HIS
1	A	479	GLN
1	A	587	GLN
1	A	866	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

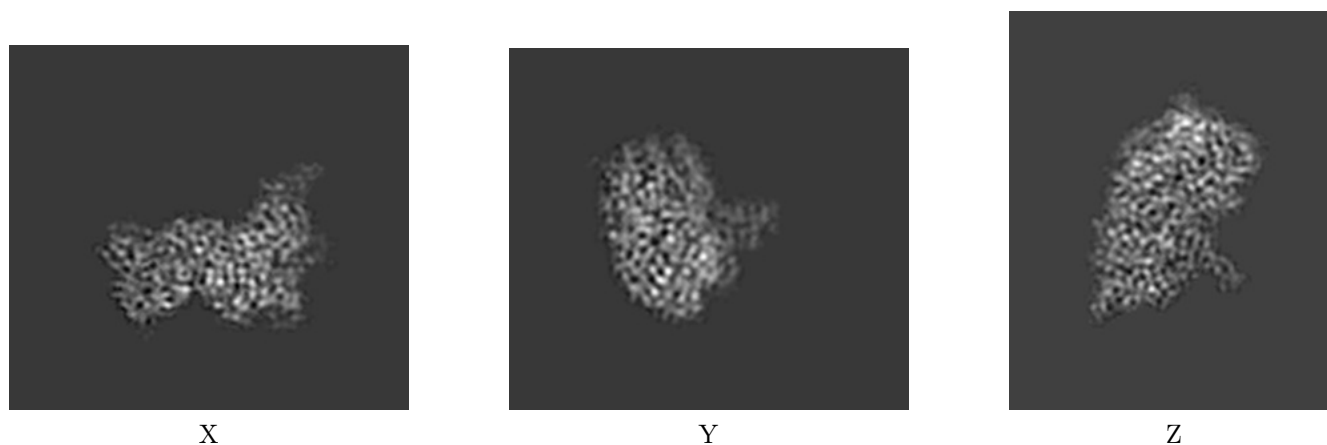
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6239. 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](#)

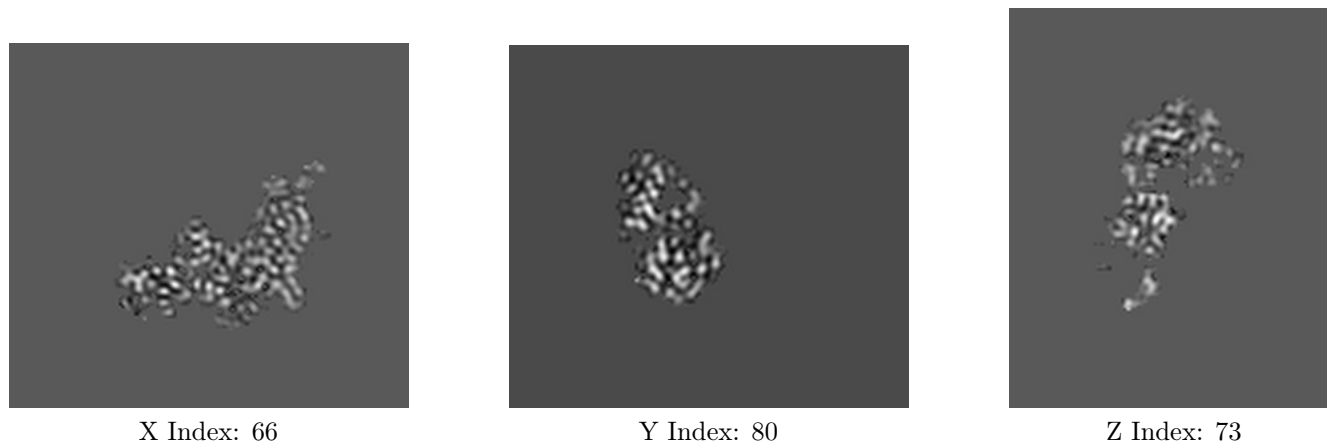
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



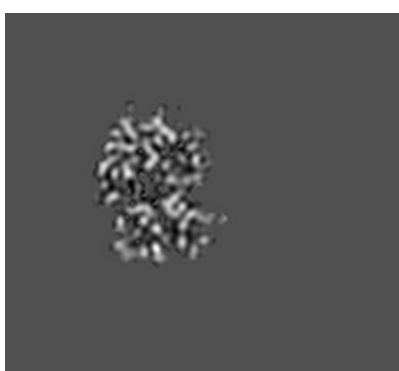
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 55



Y Index: 92



Z Index: 51

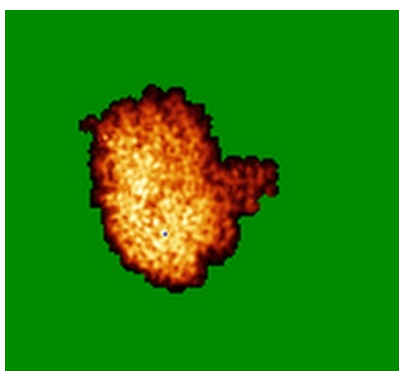
The images above show the largest variance slices of the map in three orthogonal directions.

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

This section was not generated.

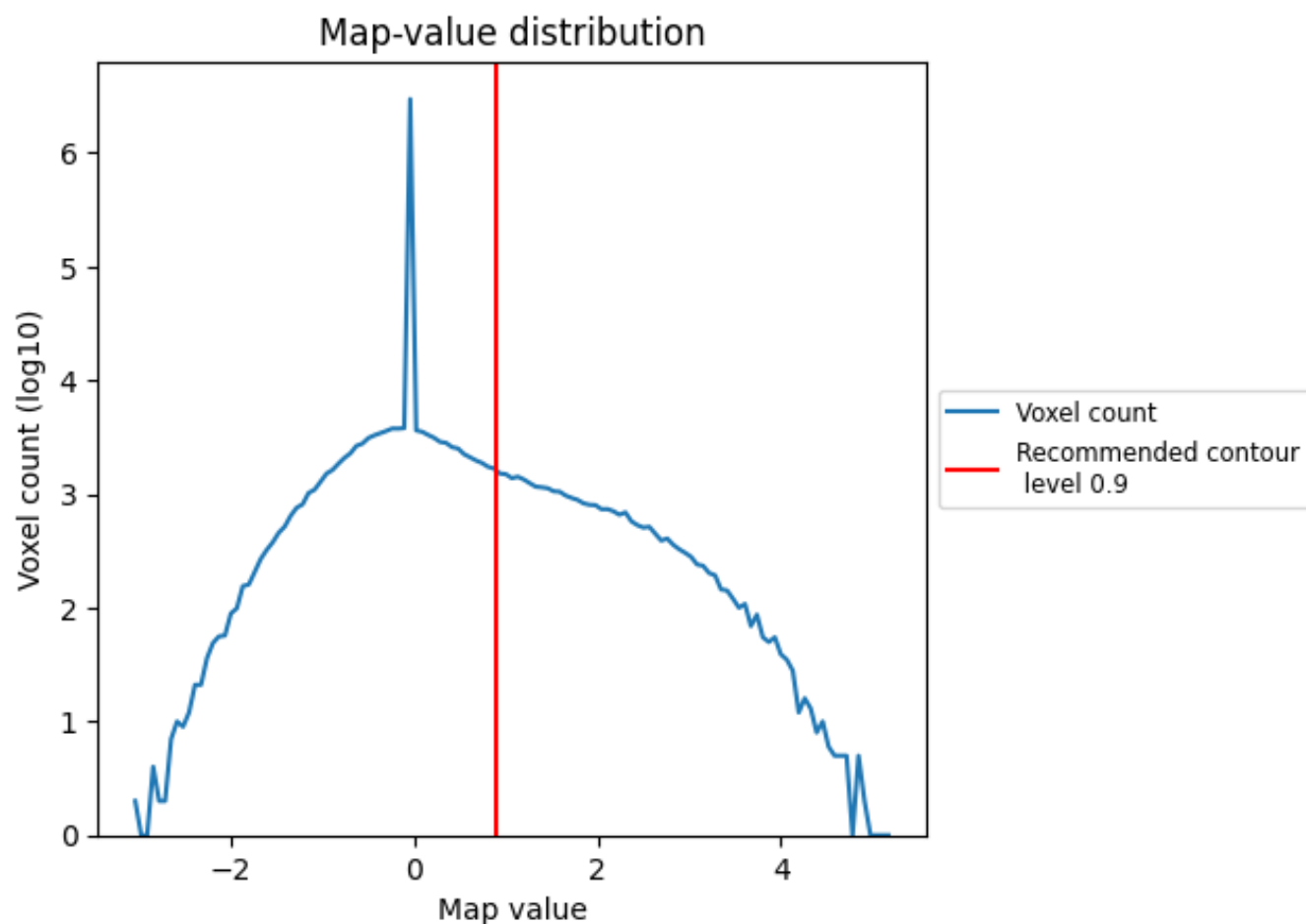
6.6 Mask visualisation

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

7 Map analysis [i](#)

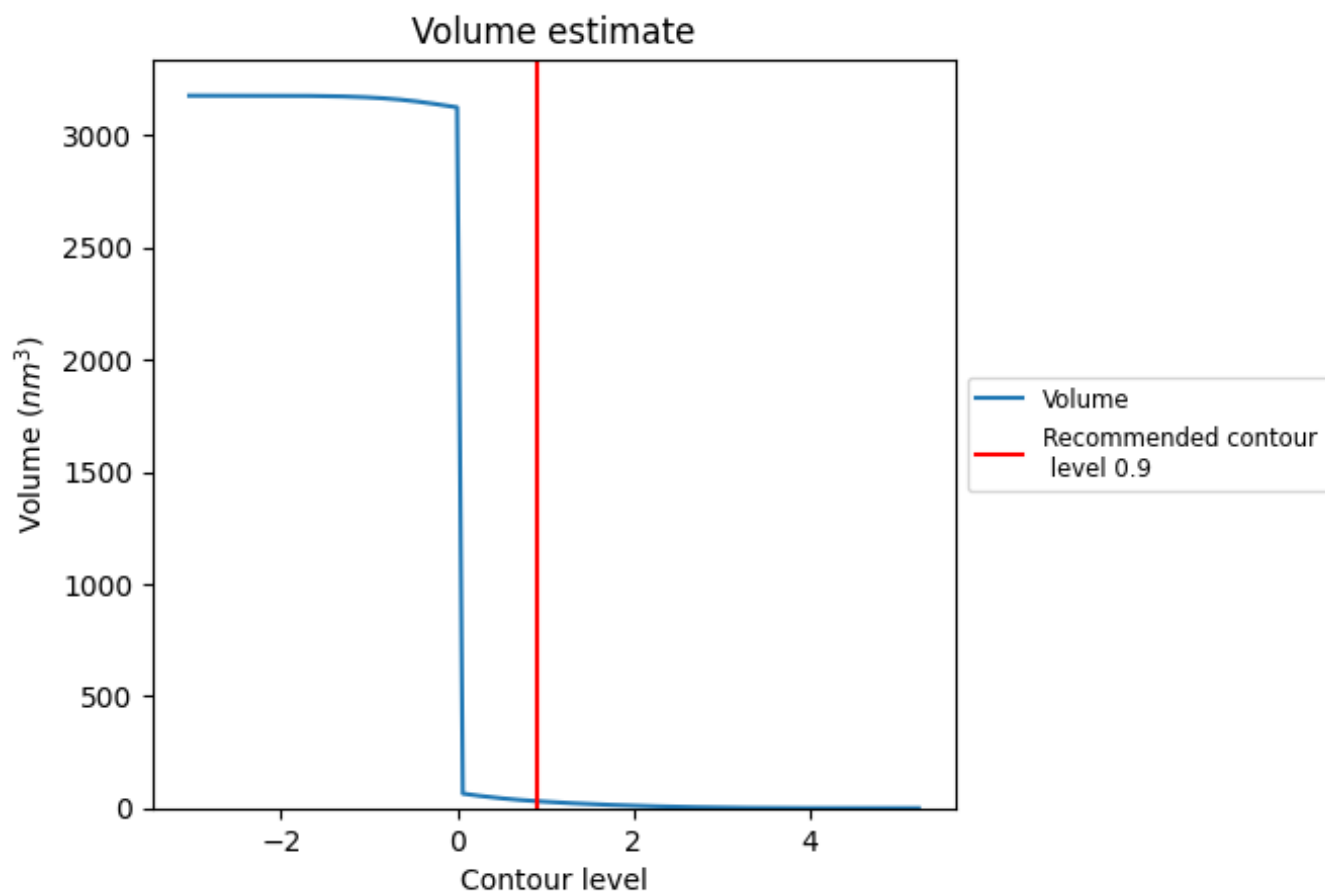
This section contains the results of statistical analysis of the map.

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 31 nm^3 ; this corresponds to an approximate mass of 28 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

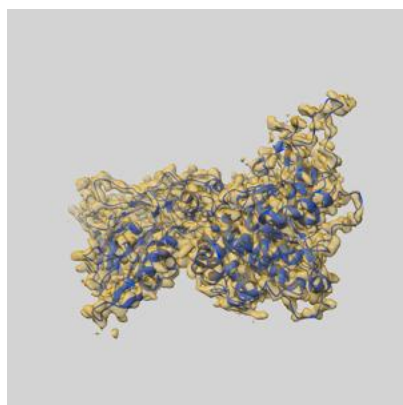
8 Fourier-Shell correlation ⓘ

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

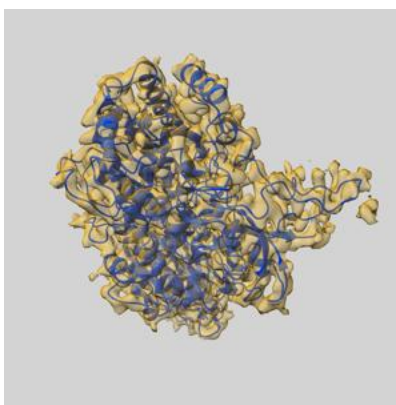
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6239 and PDB model 3J9D. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

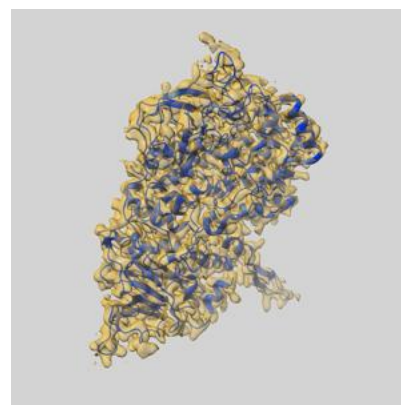
9.1 Map-model overlay [i](#)



X



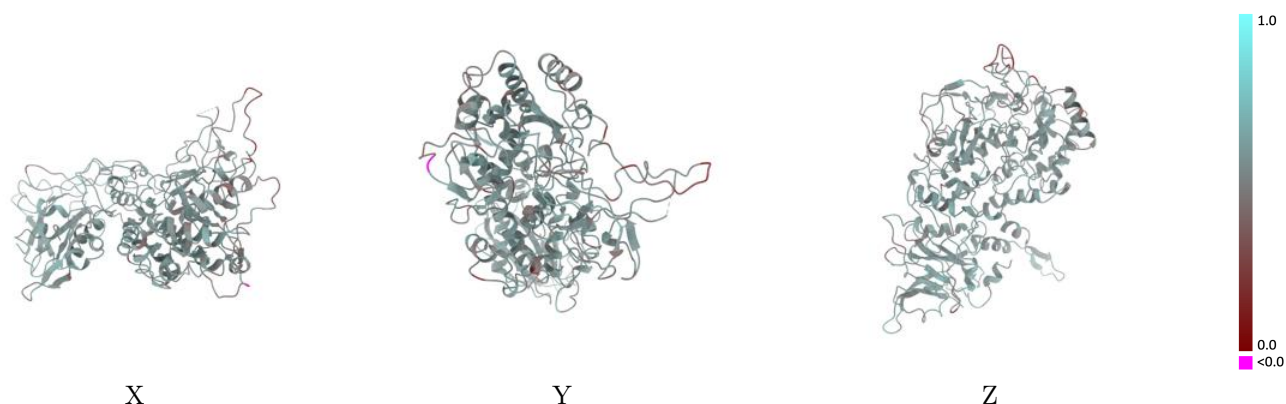
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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](#)

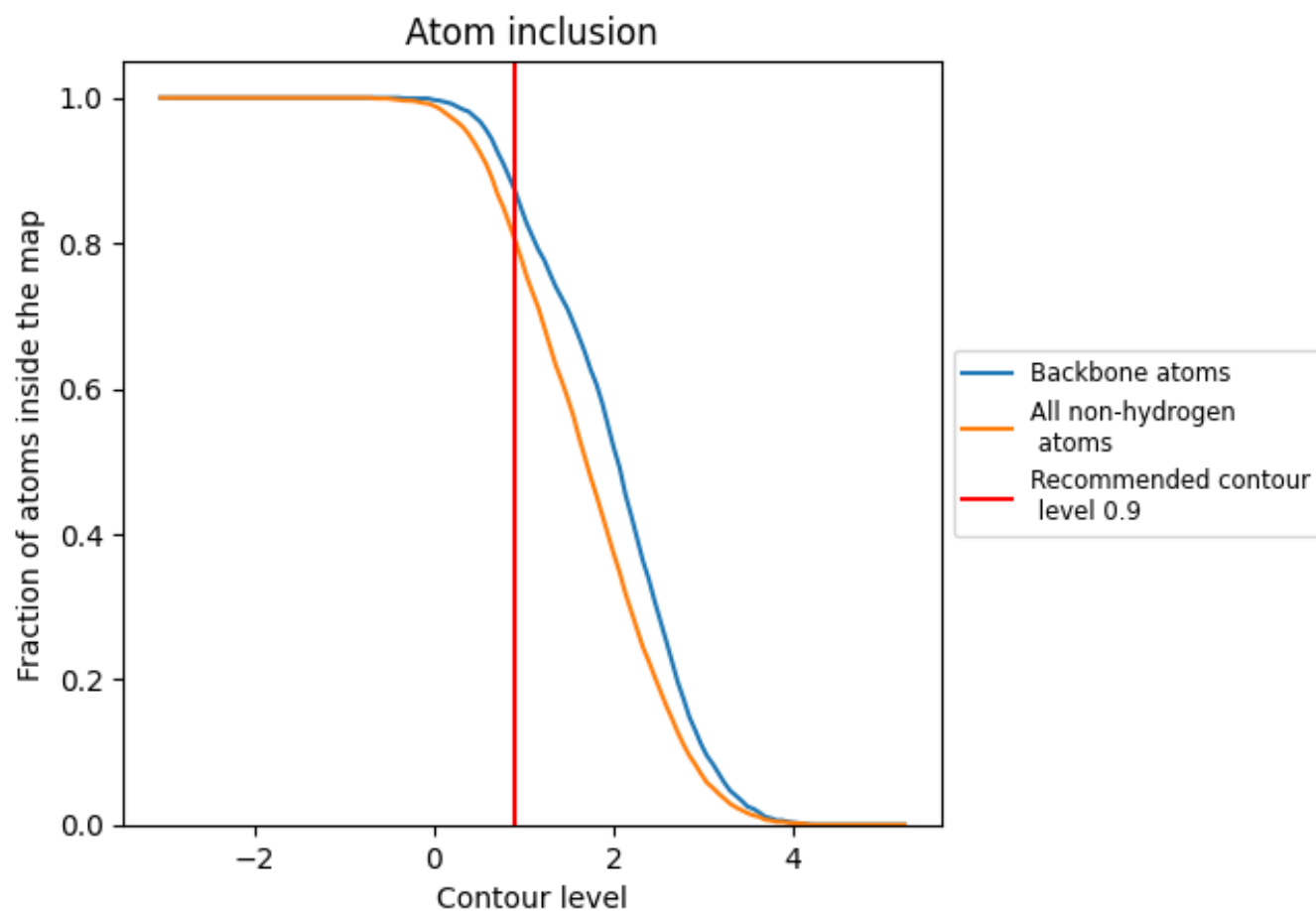


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.5380
A	0.8060	0.5380

