Full wwPDB EM Validation Report ⓘ

Feb 24, 2024 – 04:01 PM EST

PDB ID	:	6XQB
EMDB ID	:	EMD-22288
Title	:	SARS-CoV-2 RdRp/RNA complex
Authors	:	Liu, B.; Shi, W.; Yang, Y.
Deposited on	:	2020-07-09
Resolution	:	3.40 Å(reported)

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

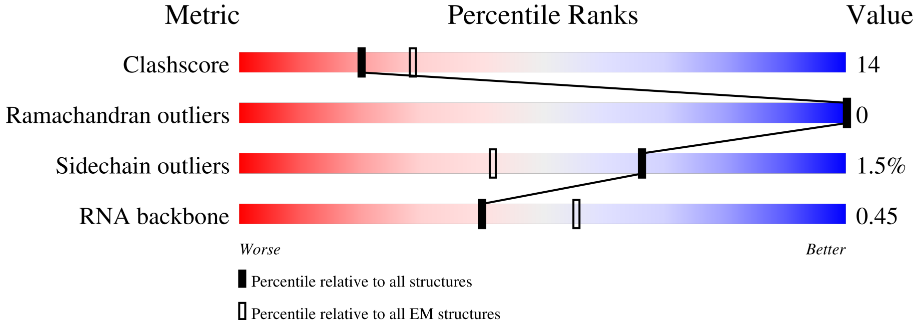
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

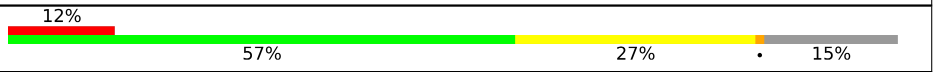
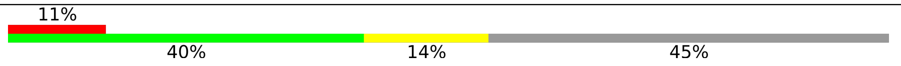
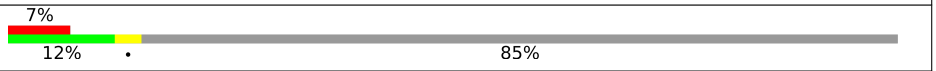
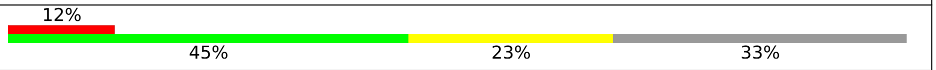
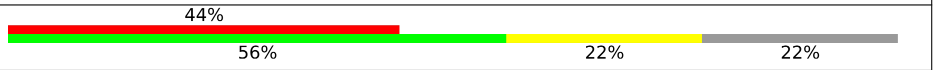
The reported resolution of this entry is 3.40 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	941	
2	B	207	
2	D	207	
3	C	92	
4	E	9	
4	F	9	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 16323 atoms, of which 7987 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	801	12682	4137	6236	1073	1191	45	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0DTD1
A	933	LEU	-	expression tag	UNP P0DTD1
A	934	GLU	-	expression tag	UNP P0DTD1
A	935	HIS	-	expression tag	UNP P0DTD1
A	936	HIS	-	expression tag	UNP P0DTD1
A	937	HIS	-	expression tag	UNP P0DTD1
A	938	HIS	-	expression tag	UNP P0DTD1
A	939	HIS	-	expression tag	UNP P0DTD1
A	940	HIS	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	114	1713	539	857	142	168	7	0	0
2	D	31	444	138	217	38	47	4	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P0DTD1
B	199	LEU	-	expression tag	UNP P0DTD1
B	200	GLU	-	expression tag	UNP P0DTD1
B	201	HIS	-	expression tag	UNP P0DTD1
B	202	HIS	-	expression tag	UNP P0DTD1
B	203	HIS	-	expression tag	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	204	HIS	-	expression tag	UNP P0DTD1
B	205	HIS	-	expression tag	UNP P0DTD1
B	206	HIS	-	expression tag	UNP P0DTD1
D	0	MET	-	initiating methionine	UNP P0DTD1
D	199	LEU	-	expression tag	UNP P0DTD1
D	200	GLU	-	expression tag	UNP P0DTD1
D	201	HIS	-	expression tag	UNP P0DTD1
D	202	HIS	-	expression tag	UNP P0DTD1
D	203	HIS	-	expression tag	UNP P0DTD1
D	204	HIS	-	expression tag	UNP P0DTD1
D	205	HIS	-	expression tag	UNP P0DTD1
D	206	HIS	-	expression tag	UNP P0DTD1

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	62	Total 993	C 305	H 512	N 79	O 92	S 5	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P0DTD1
C	84	LEU	-	expression tag	UNP P0DTD1
C	85	GLU	-	expression tag	UNP P0DTD1
C	86	HIS	-	expression tag	UNP P0DTD1
C	87	HIS	-	expression tag	UNP P0DTD1
C	88	HIS	-	expression tag	UNP P0DTD1
C	89	HIS	-	expression tag	UNP P0DTD1
C	90	HIS	-	expression tag	UNP P0DTD1
C	91	HIS	-	expression tag	UNP P0DTD1

- Molecule 4 is a RNA chain called RNA (5'-R(*GP*UP*GP*GP*GP*CP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	7	Total 229	C 67	H 78	N 29	O 48	P 7	0	0
4	F	8	Total 259	C 76	H 87	N 31	O 57	P 8	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

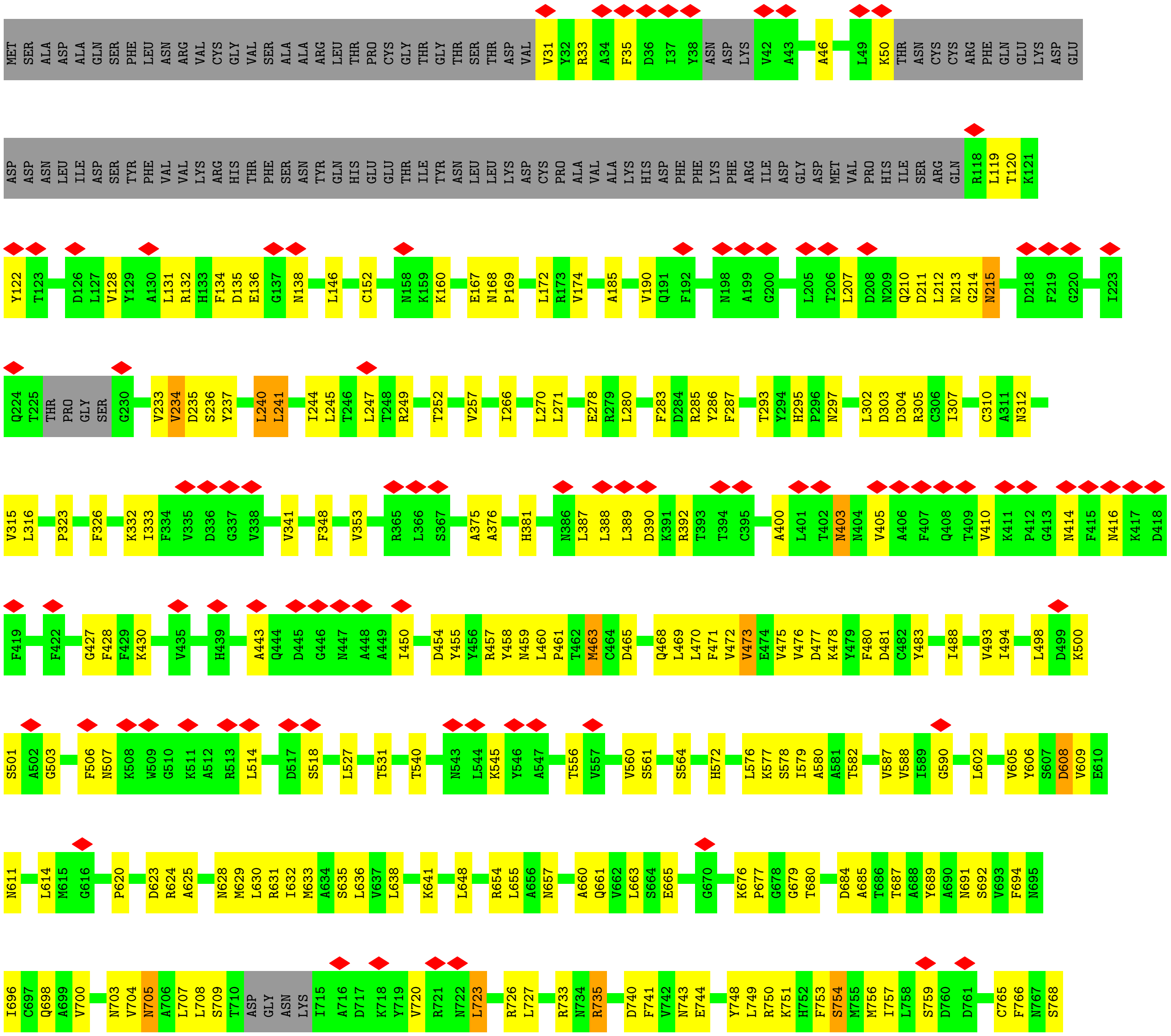
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0

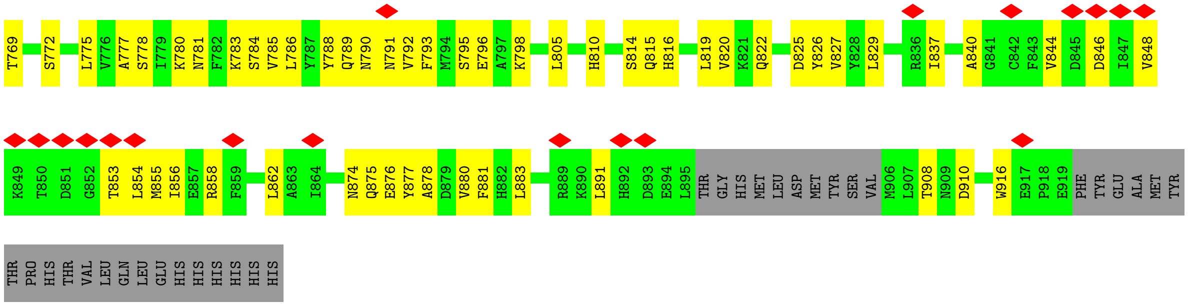
3 Residue-property plots ⓘ

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: RNA-directed RNA polymerase

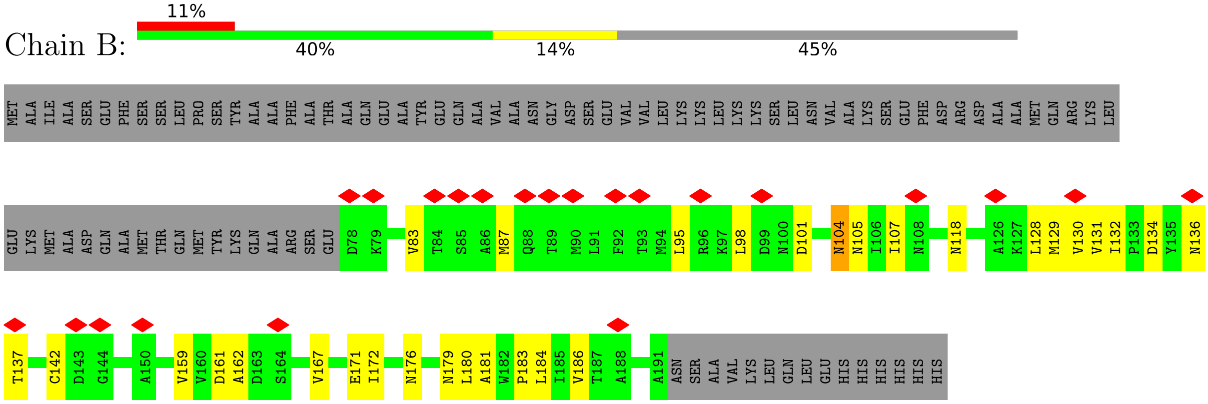
Chain A:





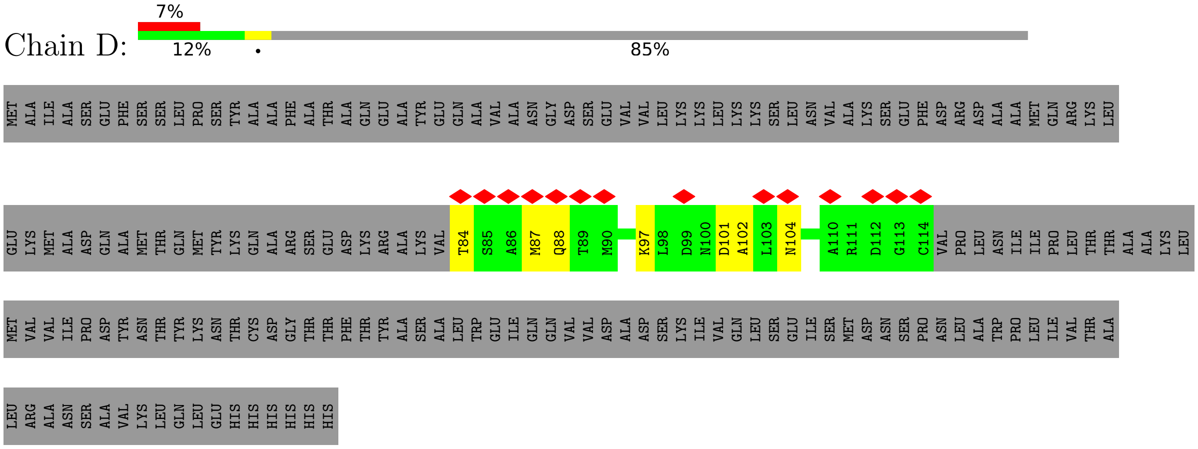
- Molecule 2: Non-structural protein 8

Chain B:



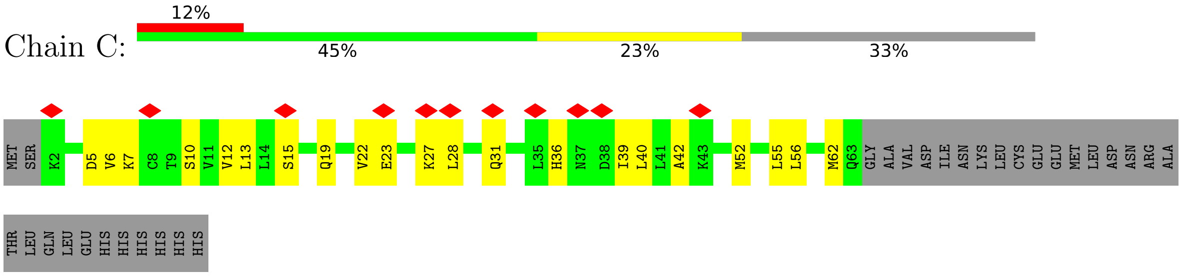
- Molecule 2: Non-structural protein 8

Chain D:



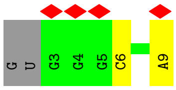
- Molecule 3: Non-structural protein 7

Chain C:



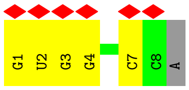
- Molecule 4: RNA (5’-R(*GP*UP*GP*GP*GP*CP*CP*CP*A)-3’)

Chain E:



- Molecule 4: RNA (5'-R(*GP*UP*GP*GP*GP*CP*CP*CP*A)-3')

Chain F:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	123246	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 ($e^-/\text{Å}^2$)	30, 30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.980	Depositor
Minimum map value	-0.490	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	192.23999, 192.23999, 192.23999	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8899999, 0.8899999, 0.8899999	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, MG

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	#$\lvert Z\rvert$ >5	RMSZ	#$\lvert Z\rvert$ >5
1	A	0.61	1/6605 (0.0%)	0.74	6/8961 (0.1%)
2	B	0.46	0/867	0.69	0/1186
2	D	0.32	0/227	0.58	0/306
3	C	0.47	0/484	0.66	0/652
4	E	0.55	0/168	1.35	3/260 (1.2%)
4	F	0.48	0/191	1.13	1/296 (0.3%)
All	All	0.58	1/8542 (0.0%)	0.76	10/11661 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	473	VAL	CB-CG2	-5.36	1.41	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	LEU	CA-CB-CG	7.80	133.24	115.30
1	A	247	LEU	CA-CB-CG	7.20	131.87	115.30
1	A	240	LEU	CA-CB-CG	5.93	128.93	115.30
4	E	6	C	N1-C2-O2	5.64	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	614	LEU	CA-CB-CG	5.49	127.94	115.30
4	E	6	C	C6-N1-C2	-5.49	118.10	120.30
1	A	723	LEU	CA-CB-CG	5.28	127.43	115.30
4	E	6	C	C2-N1-C1'	5.16	124.48	118.80
4	F	7	C	N3-C2-O2	-5.08	118.34	121.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ASN	Peptide
1	A	234	VAL	Peptide
1	A	465	ASP	Peptide
1	A	608	ASP	Peptide
1	A	705	ASN	Peptide
1	A	754	SER	Peptide
2	B	180	LEU	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	6446	6236	6237	189	0
2	B	856	857	857	24	0
2	D	227	217	217	5	0
3	C	481	512	512	14	0
4	E	151	78	78	1	0
4	F	172	87	88	5	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
All	All	8336	7987	7989	224	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 14.

All (224) 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:531:THR:OG1	1:A:654:ARG:NH2	2.07	0.87
1:A:207:LEU:HD12	1:A:240:LEU:HD13	1.57	0.84
1:A:556:THR:OG1	1:A:624:ARG:NH2	2.12	0.82
1:A:623:ASP:OD2	1:A:624:ARG:NH1	2.15	0.79
1:A:427:GLY:O	1:A:430:LYS:NZ	2.12	0.79
1:A:676:LYS:NZ	1:A:679:GLY:O	2.15	0.78
1:A:795:SER:OG	1:A:798:LYS:NZ	2.15	0.78
1:A:840:ALA:O	1:A:858:ARG:NH1	2.17	0.77
1:A:810:HIS:O	1:A:816:HIS:ND1	2.19	0.75
1:A:323:PRO:O	2:B:118:ASN:ND2	2.20	0.74
1:A:283:PHE:O	1:A:287:PHE:N	2.21	0.73
2:B:171:GLU:OE2	2:B:176:ASN:ND2	2.22	0.73
1:A:457:ARG:NH2	1:A:458:TYR:OH	2.22	0.72
1:A:503:GLY:O	1:A:507:ASN:N	2.22	0.72
1:A:822:GLN:NE2	1:A:916:TRP:O	2.22	0.71
1:A:759:SER:HG	4:E:9:A:HO2'	1.37	0.71
1:A:785:VAL:O	1:A:789:GLN:N	2.23	0.71
1:A:312:ASN:ND2	1:A:463:MET:SD	2.64	0.71
1:A:623:ASP:OD1	1:A:680:THR:OG1	2.09	0.70
1:A:636:LEU:HD21	1:A:655:LEU:HD22	1.71	0.70
1:A:326:PHE:O	2:B:118:ASN:ND2	2.27	0.68
1:A:483:TYR:O	1:A:641:LYS:NZ	2.24	0.68
1:A:31:VAL:N	1:A:50:LYS:O	2.27	0.67
1:A:700:VAL:O	1:A:704:VAL:HG23	1.94	0.66
1:A:211:ASP:OD2	1:A:213:ASN:ND2	2.28	0.66
1:A:611:ASN:ND2	1:A:769:THR:OG1	2.30	0.65
1:A:403:ASN:ND2	2:B:129:MET:SD	2.71	0.64
1:A:473:VAL:HA	1:A:476:VAL:HG12	1.77	0.64
1:A:472:VAL:HG22	1:A:700:VAL:HG11	1.78	0.64
1:A:501:SER:N	4:F:1:G:OP1	2.30	0.64
2:B:101:ASP:O	2:B:105:ASN:ND2	2.31	0.64
1:A:348:PHE:CZ	1:A:660:ALA:HB2	2.33	0.64
1:A:632:ILE:HG23	1:A:655:LEU:HD11	1.80	0.64
1:A:579:ILE:CG2	1:A:587:VAL:HG21	2.27	0.64
1:A:241:LEU:HD12	1:A:244:ILE:HD11	1.80	0.63
1:A:469:LEU:HD11	1:A:633:MET:HG2	1.78	0.63
2:B:167:VAL:HG21	2:B:172:ILE:HD11	1.79	0.63
1:A:332:LYS:O	1:A:333:ILE:HD13	1.99	0.63
1:A:500:LYS:NZ	4:F:2:U:OP2	2.30	0.62
1:A:136:GLU:N	1:A:136:GLU:OE1	2.33	0.62
3:C:27:LYS:O	3:C:31:GLN:NE2	2.33	0.62
2:B:161:ASP:O	2:B:181:ALA:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:HIS:N	1:A:310:CYS:SG	2.74	0.61
1:A:704:VAL:O	1:A:708:LEU:N	2.34	0.61
1:A:297:ASN:OD1	1:A:353:VAL:HG12	2.02	0.60
1:A:459:ASN:OD1	1:A:460:LEU:N	2.35	0.60
1:A:578:SER:O	1:A:582:THR:OG1	2.19	0.60
2:B:162:ALA:HB2	2:B:183:PRO:HB2	1.82	0.60
1:A:692:SER:O	1:A:696:ILE:HD12	2.01	0.60
1:A:46:ALA:HB2	1:A:709:SER:HA	1.84	0.60
2:B:159:VAL:HG22	2:B:186:VAL:HG13	1.84	0.59
1:A:704:VAL:HG13	1:A:727:LEU:HD21	1.83	0.59
3:C:10:SER:HB3	3:C:39:ILE:HD13	1.85	0.59
1:A:631:ARG:NH1	1:A:635:SER:OG	2.36	0.58
3:C:36:HIS:CE1	3:C:40:LEU:HD11	2.39	0.58
1:A:723:LEU:HD13	1:A:744:GLU:HG2	1.86	0.58
1:A:778:SER:OG	1:A:780:LYS:NZ	2.33	0.58
1:A:146:LEU:HD22	1:A:174:VAL:HG12	1.85	0.57
1:A:908:THR:HG23	1:A:910:ASP:H	1.69	0.57
1:A:389:LEU:HD23	2:B:130:VAL:HG22	1.86	0.57
2:B:134:ASP:OD1	2:B:137:THR:OG1	2.19	0.57
1:A:207:LEU:HD21	1:A:237:TYR:CE1	2.39	0.56
1:A:856:ILE:HD13	1:A:891:LEU:HD23	1.87	0.56
1:A:234:VAL:O	1:A:237:TYR:N	2.37	0.56
2:B:161:ASP:HA	2:B:184:LEU:HD23	1.87	0.56
1:A:134:PHE:O	1:A:784:SER:OG	2.20	0.56
1:A:705:ASN:ND2	1:A:708:LEU:HD12	2.20	0.56
2:D:84:THR:O	2:D:88:GLN:NE2	2.38	0.56
1:A:169:PRO:O	1:A:172:LEU:HD13	2.07	0.55
1:A:120:THR:OG1	1:A:211:ASP:OD1	2.09	0.55
1:A:483:TYR:HE1	1:A:582:THR:HG21	1.70	0.55
1:A:687:THR:O	1:A:691:ASN:ND2	2.40	0.55
1:A:241:LEU:CD1	1:A:244:ILE:HD11	2.37	0.54
1:A:388:LEU:HB2	1:A:400:ALA:HB2	1.89	0.54
1:A:608:ASP:OD2	1:A:751:LYS:NZ	2.35	0.54
3:C:12:VAL:O	3:C:15:SER:OG	2.21	0.54
1:A:876:GLU:O	1:A:880:VAL:HG23	2.08	0.54
3:C:36:HIS:HE1	3:C:40:LEU:HD11	1.73	0.53
1:A:477:ASP:OD1	1:A:478:LYS:N	2.42	0.53
1:A:628:ASN:ND2	1:A:677:PRO:O	2.42	0.53
1:A:152:CYS:HB2	1:A:174:VAL:HG13	1.91	0.53
1:A:278:GLU:OE1	1:A:278:GLU:N	2.41	0.53
3:C:5:ASP:OD1	3:C:6:VAL:N	2.41	0.53

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
3:C:19:GLN:NE2	2:D:84:THR:OG1	2.41	0.53
1:A:410:VAL:HG11	1:A:443:ALA:HA	1.92	0.52
1:A:531:THR:O	1:A:657:ASN:ND2	2.38	0.52
1:A:160:LYS:NZ	1:A:167:GLU:OE2	2.42	0.52
1:A:629:MET:HA	1:A:632:ILE:HD12	1.92	0.52
1:A:241:LEU:O	1:A:245:LEU:HD21	2.09	0.52
1:A:786:LEU:O	1:A:791:ASN:N	2.43	0.52
1:A:388:LEU:HD22	1:A:400:ALA:HB2	1.91	0.52
1:A:630:LEU:HD22	1:A:694:PHE:HE1	1.75	0.52
1:A:796:GLU:OE1	1:A:796:GLU:N	2.40	0.51
1:A:387:LEU:HD12	1:A:388:LEU:H	1.74	0.51
3:C:22:VAL:HG13	3:C:28:LEU:HD23	1.93	0.51
1:A:750:ARG:O	1:A:754:SER:OG	2.29	0.50
1:A:185:ALA:HB1	1:A:210:GLN:NE2	2.26	0.50
1:A:249:ARG:O	1:A:252:THR:HG23	2.10	0.50
1:A:454:ASP:OD1	1:A:455:TYR:N	2.43	0.50
1:A:210:GLN:NE2	1:A:214:GLY:O	2.35	0.50
1:A:428:PHE:CE2	1:A:883:LEU:HD22	2.46	0.50
2:D:101:ASP:OD1	2:D:102:ALA:N	2.44	0.50
1:A:625:ALA:HB1	1:A:790:ASN:O	2.11	0.50
2:B:142:CYS:SG	2:B:186:VAL:HG11	2.52	0.50
1:A:211:ASP:OD1	1:A:212:LEU:N	2.45	0.49
1:A:477:ASP:O	1:A:481:ASP:N	2.45	0.49
2:B:104:ASN:ND2	2:B:107:ILE:HD11	2.27	0.49
1:A:560:VAL:HG12	1:A:561:SER:H	1.77	0.49
1:A:689:TYR:OH	4:F:3:G:O2’	2.25	0.49
1:A:740:ASP:OD1	1:A:741:PHE:N	2.41	0.49
1:A:837:ILE:HG23	1:A:862:LEU:HB3	1.94	0.49
1:A:576:LEU:O	1:A:580:ALA:N	2.45	0.49
3:C:19:GLN:NE2	2:D:87:MET:SD	2.85	0.49
3:C:13:LEU:HD23	3:C:55:LEU:HD23	1.95	0.49
1:A:233:VAL:HG12	1:A:235:ASP:H	1.77	0.49
1:A:590:GLY:N	4:F:4:G:O2’	2.45	0.49
1:A:848:VAL:HG22	1:A:855:MET:HB3	1.95	0.49
1:A:241:LEU:HD12	1:A:244:ILE:CD1	2.43	0.48
1:A:908:THR:HG23	1:A:910:ASP:N	2.27	0.48
1:A:720:VAL:CG2	1:A:775:LEU:HD21	2.43	0.48
1:A:190:VAL:HG21	1:A:285:ARG:O	2.14	0.48
1:A:304:ASP:OD1	1:A:305:ARG:N	2.47	0.48
1:A:305:ARG:HE	1:A:735:ARG:HH12	1.62	0.48
1:A:494:ILE:HG22	1:A:494:ILE:O	2.14	0.48

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:749:LEU:HD23	1:A:750:ARG:N	2.28	0.48
1:A:814:SER:O	1:A:815:GLN:NE2	2.46	0.48
1:A:348:PHE:HZ	1:A:660:ALA:HB2	1.78	0.48
2:B:95:LEU:HA	2:B:98:LEU:HD12	1.95	0.48
1:A:332:LYS:HA	1:A:341:VAL:HG22	1.96	0.47
1:A:783:LYS:NZ	1:A:796:GLU:OE1	2.39	0.47
1:A:257:VAL:HG22	1:A:266:ILE:HG12	1.96	0.47
1:A:146:LEU:HD22	1:A:174:VAL:CG1	2.44	0.47
3:C:52:MET:O	3:C:56:LEU:HD13	2.14	0.47
1:A:498:LEU:H	1:A:498:LEU:HD23	1.79	0.47
1:A:119:LEU:H	1:A:119:LEU:HD23	1.79	0.47
1:A:470:LEU:O	1:A:473:VAL:HG12	2.15	0.47
1:A:704:VAL:O	1:A:707:LEU:N	2.48	0.47
1:A:820:VAL:HG21	1:A:829:LEU:HD12	1.97	0.47
1:A:514:LEU:O	1:A:518:SER:N	2.43	0.47
1:A:234:VAL:O	1:A:236:SER:N	2.48	0.47
1:A:387:LEU:HD21	2:B:128:LEU:HD13	1.98	0.46
1:A:270:LEU:C	1:A:271:LEU:HD12	2.36	0.46
1:A:450:ILE:HD12	1:A:450:ILE:H	1.81	0.46
1:A:241:LEU:HG	1:A:245:LEU:HD21	1.97	0.46
1:A:684:ASP:OD1	1:A:685:ALA:N	2.49	0.46
1:A:375:ALA:O	1:A:381:HIS:NE2	2.43	0.45
1:A:720:VAL:HG21	1:A:775:LEU:HD21	1.97	0.45
1:A:875:GLN:O	1:A:878:ALA:HB3	2.16	0.45
1:A:825:ASP:OD1	1:A:826:TYR:N	2.46	0.45
1:A:315:VAL:HG23	1:A:316:LEU:N	2.32	0.45
1:A:468:GLN:N	1:A:468:GLN:OE1	2.48	0.45
1:A:630:LEU:HD22	1:A:694:PHE:CE1	2.51	0.45
1:A:620:PRO:HG2	1:A:792:VAL:HG11	1.99	0.45
1:A:120:THR:OG1	1:A:122:TYR:O	2.35	0.45
1:A:781:ASN:O	1:A:785:VAL:HG23	2.16	0.45
1:A:293:THR:HG21	1:A:302:LEU:HD23	1.98	0.45
1:A:414:ASN:ND2	1:A:846:ASP:OD1	2.45	0.45
1:A:469:LEU:HD23	1:A:469:LEU:O	2.17	0.45
3:C:7:LYS:HE3	3:C:42:ALA:HB3	1.97	0.45
1:A:609:VAL:HG21	1:A:765:CYS:HB3	1.99	0.44
2:B:176:ASN:OD1	2:B:179:ASN:ND2	2.50	0.44
1:A:33:ARG:HB2	1:A:35:PHE:CE2	2.51	0.44
1:A:307:ILE:HG21	1:A:655:LEU:CD2	2.48	0.44
1:A:283:PHE:O	1:A:286:TYR:N	2.50	0.44
1:A:472:VAL:HG22	1:A:700:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:SER:HG	1:A:661:GLN:CD	2.20	0.44
1:A:579:ILE:HG22	1:A:587:VAL:HG21	1.99	0.44
1:A:768:SER:O	1:A:772:SER:N	2.48	0.44
1:A:878:ALA:O	1:A:881:PHE:N	2.50	0.44
1:A:270:LEU:O	1:A:271:LEU:HD12	2.18	0.44
1:A:753:PHE:CE1	1:A:777:ALA:HB3	2.53	0.44
1:A:307:ILE:HG21	1:A:655:LEU:HD23	2.00	0.43
1:A:572:HIS:CE1	1:A:638:LEU:HD23	2.53	0.43
3:C:23:GLU:OE1	3:C:23:GLU:N	2.46	0.43
1:A:348:PHE:CE1	1:A:660:ALA:HB2	2.53	0.43
1:A:280:LEU:HD13	1:A:280:LEU:O	2.17	0.43
1:A:560:VAL:HG12	1:A:561:SER:N	2.34	0.43
1:A:609:VAL:HG21	1:A:765:CYS:SG	2.59	0.43
1:A:704:VAL:HG13	1:A:727:LEU:CD2	2.49	0.43
1:A:135:ASP:O	1:A:138:ASN:N	2.47	0.43
1:A:698:GLN:HE21	1:A:786:LEU:HD11	1.84	0.43
1:A:297:ASN:CG	1:A:353:VAL:HG12	2.39	0.43
1:A:540:THR:N	1:A:665:GLU:OE1	2.52	0.43
2:B:159:VAL:HG13	2:B:186:VAL:HG22	2.01	0.43
1:A:128:VAL:HG13	1:A:244:ILE:HD13	2.00	0.42
1:A:480:PHE:O	1:A:641:LYS:NZ	2.50	0.42
1:A:488:ILE:HD11	1:A:493:VAL:HG22	2.01	0.42
1:A:332:LYS:C	1:A:333:ILE:HD13	2.40	0.42
1:A:405:VAL:HG21	2:B:131:VAL:HG21	2.01	0.42
1:A:572:HIS:CD2	1:A:638:LEU:HD23	2.55	0.42
2:B:167:VAL:CG2	2:B:172:ILE:HD11	2.48	0.42
1:A:233:VAL:HG11	1:A:733:ARG:HH21	1.84	0.42
1:A:390:ASP:HB2	1:A:392:ARG:HE	1.84	0.42
1:A:606:TYR:CD2	1:A:805:LEU:HD23	2.54	0.42
1:A:207:LEU:HD21	1:A:237:TYR:HE1	1.82	0.42
1:A:527:LEU:HD23	1:A:531:THR:CG2	2.49	0.42
1:A:628:ASN:HB3	1:A:663:LEU:HD11	2.02	0.42
2:B:83:VAL:HG22	2:B:87:MET:HE1	2.00	0.42
1:A:132:ARG:HA	1:A:788:TYR:CD1	2.55	0.42
1:A:494:ILE:HD12	1:A:577:LYS:HG3	2.02	0.42
2:B:132:ILE:HD11	2:B:184:LEU:HG	2.02	0.42
1:A:819:LEU:HD11	1:A:826:TYR:HB3	2.02	0.41
1:A:853:THR:OG1	1:A:854:LEU:N	2.53	0.41
1:A:376:ALA:HB2	1:A:506:PHE:HE2	1.86	0.41
1:A:792:VAL:HG12	1:A:793:PHE:N	2.36	0.41
1:A:460:LEU:HD23	1:A:461:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:O	1:A:475:VAL:HG23	2.21	0.41
1:A:483:TYR:CD2	1:A:579:ILE:HD11	2.56	0.41
1:A:588:VAL:HG22	1:A:757:ILE:O	2.21	0.41
1:A:609:VAL:HG11	1:A:766:PHE:N	2.36	0.41
3:C:5:ASP:OD2	2:D:97:LYS:NZ	2.50	0.41
4:F:1:G:O2’	4:F:2:U:O4’	2.32	0.41
1:A:606:TYR:O	1:A:609:VAL:HG23	2.20	0.40
2:B:83:VAL:HG22	2:B:87:MET:CE	2.51	0.40
2:B:132:ILE:O	2:B:183:PRO:HA	2.21	0.40
1:A:303:ASP:HA	1:A:648:LEU:HD11	2.02	0.40
1:A:602:LEU:HA	1:A:605:VAL:HG12	2.04	0.40
1:A:748:TYR:OH	1:A:775:LEU:HD23	2.22	0.40
1:A:257:VAL:HG22	1:A:266:ILE:CG1	2.51	0.40
1:A:460:LEU:HD23	1:A:461:PRO:N	2.35	0.40
1:A:588:VAL:HG11	1:A:756:MET:CE	2.52	0.40
1:A:874:ASN:HB3	1:A:877:TYR:CD2	2.57	0.40
1:A:416:ASN:OD1	1:A:844:VAL:HG23	2.22	0.40
1:A:819:LEU:HD12	1:A:827:VAL:O	2.22	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	789/941 (84%)	667 (84%)	122 (16%)	0	100	100
2	B	112/207 (54%)	87 (78%)	25 (22%)	0	100	100
2	D	29/207 (14%)	29 (100%)	0	0	100	100
3	C	60/92 (65%)	57 (95%)	3 (5%)	0	100	100
All	All	990/1447 (68%)	840 (85%)	150 (15%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	702/832 (84%)	693 (99%)	9 (1%)	69	84
2	B	95/176 (54%)	93 (98%)	2 (2%)	53	76
2	D	25/176 (14%)	24 (96%)	1 (4%)	31	60
3	C	59/86 (69%)	58 (98%)	1 (2%)	60	80
All	All	881/1270 (69%)	868 (98%)	13 (2%)	66	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	215	ASN
1	A	403	ASN
1	A	463	MET
1	A	545	LYS
1	A	703	ASN
1	A	726	ARG
1	A	735	ARG
1	A	743	ASN
2	B	104	ASN
2	B	136	ASN
3	C	62	MET
2	D	104	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	357	GLN
1	A	403	ASN
1	A	491	ASN
1	A	507	ASN
1	A	611	ASN

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Mol	Chain	Res	Type
1	A	691	ASN
1	A	698	GLN
1	A	705	ASN
2	B	104	ASN
2	B	105	ASN
2	B	118	ASN
2	B	179	ASN
3	C	19	GLN
3	C	31	GLN
3	C	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	6/9 (66%)	0	0
4	F	7/9 (77%)	0	0
All	All	13/18 (72%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are 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.

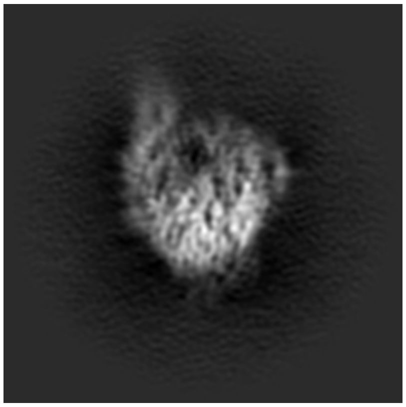
6 Map visualisation

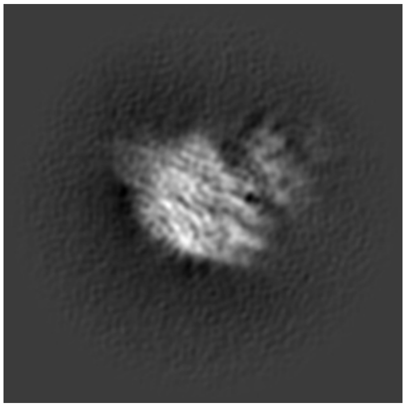
This section contains visualisations of the EMDB entry EMD-22288. These allow visual inspection of the internal detail of the map and identification of artifacts.

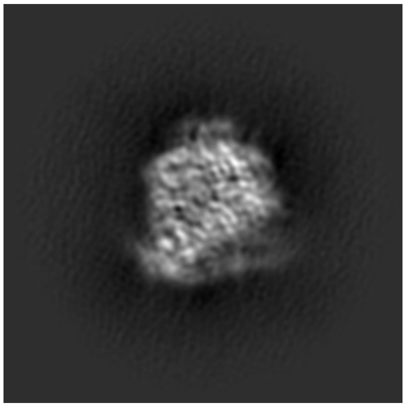
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

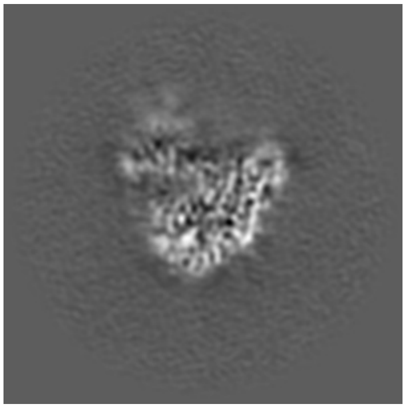

Y

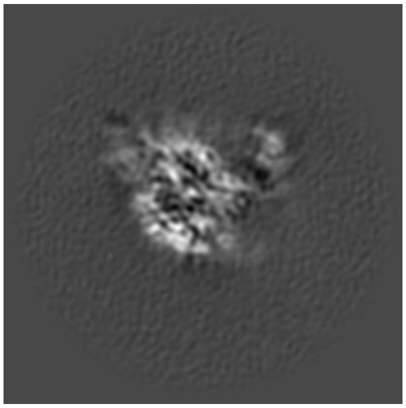

Z

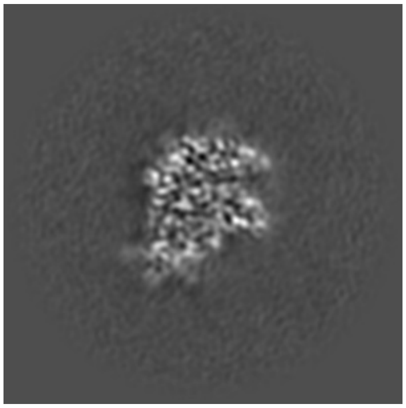
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 108

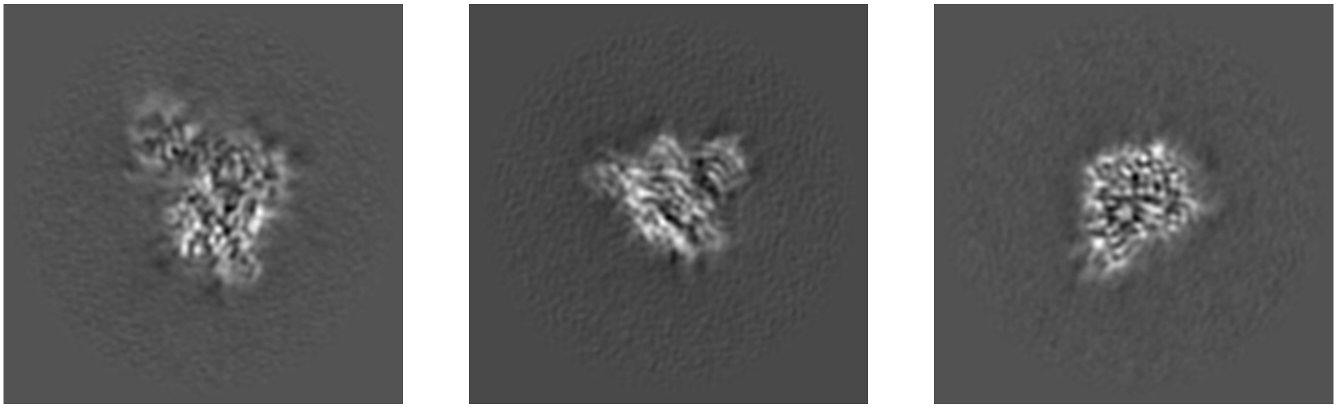

Y Index: 108


Z Index: 108

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

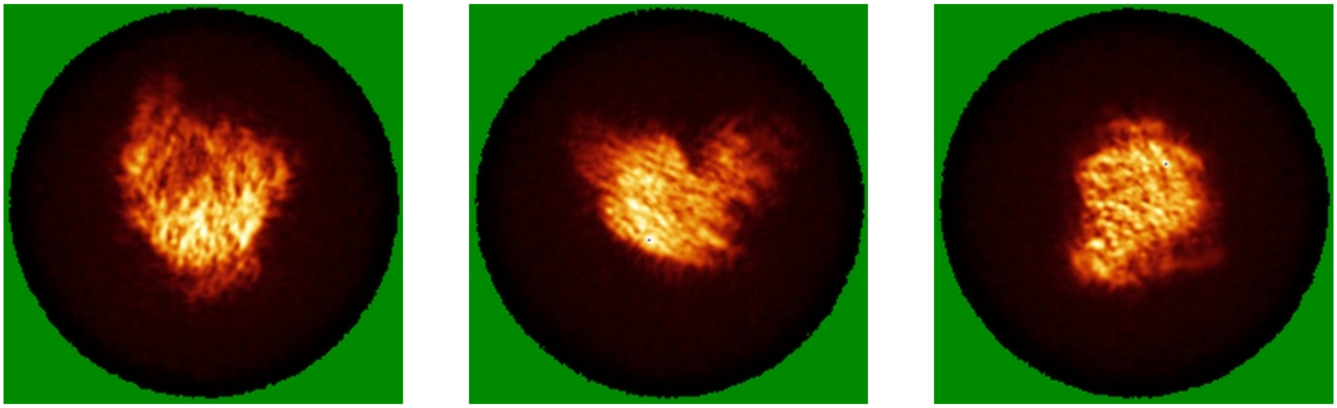


X Index: 119 Y Index: 131 Z Index: 97

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

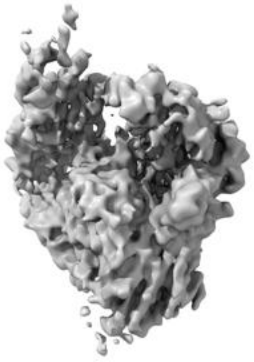


X Y Z

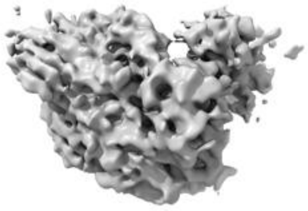
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

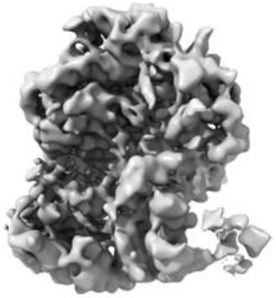
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

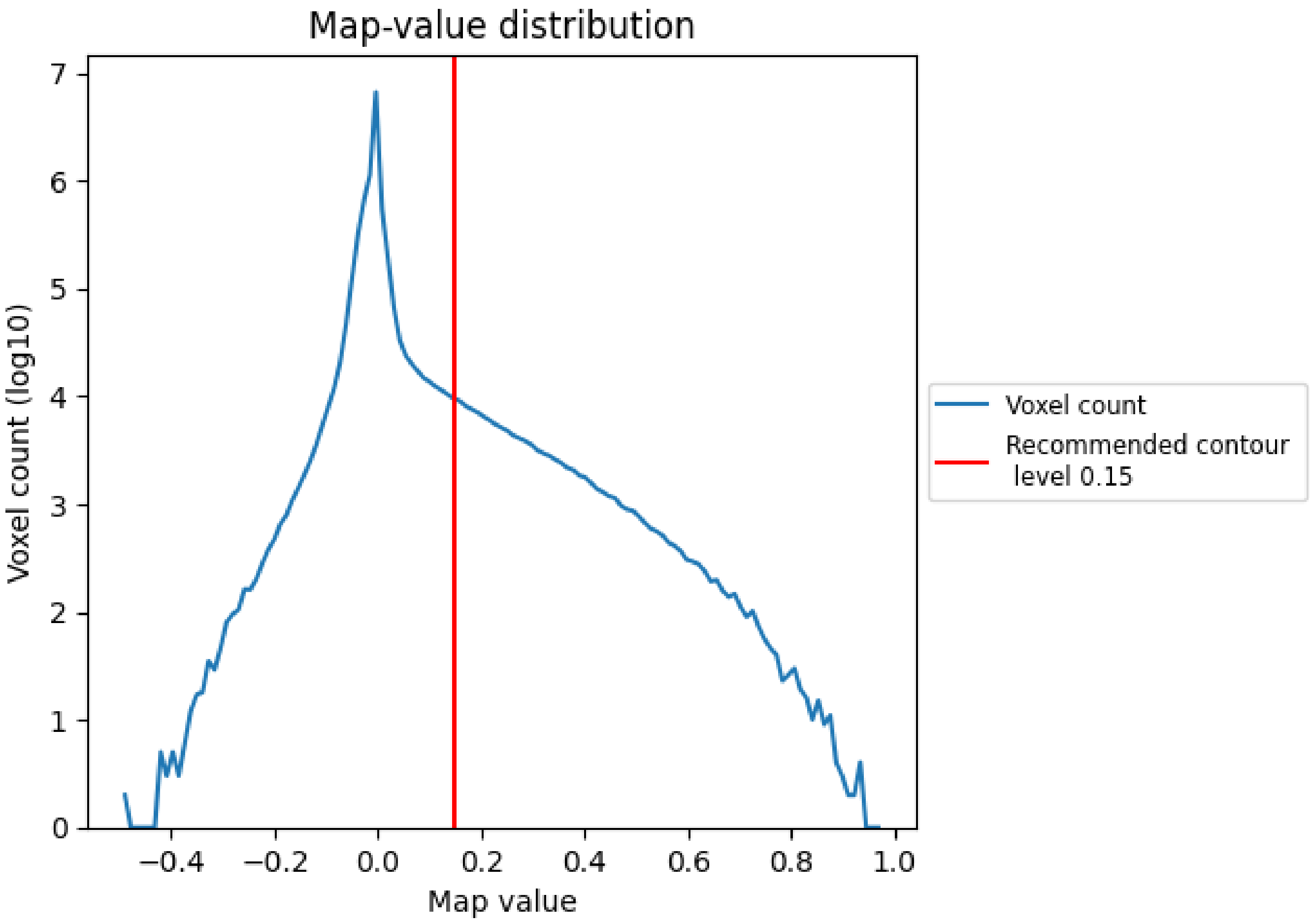
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

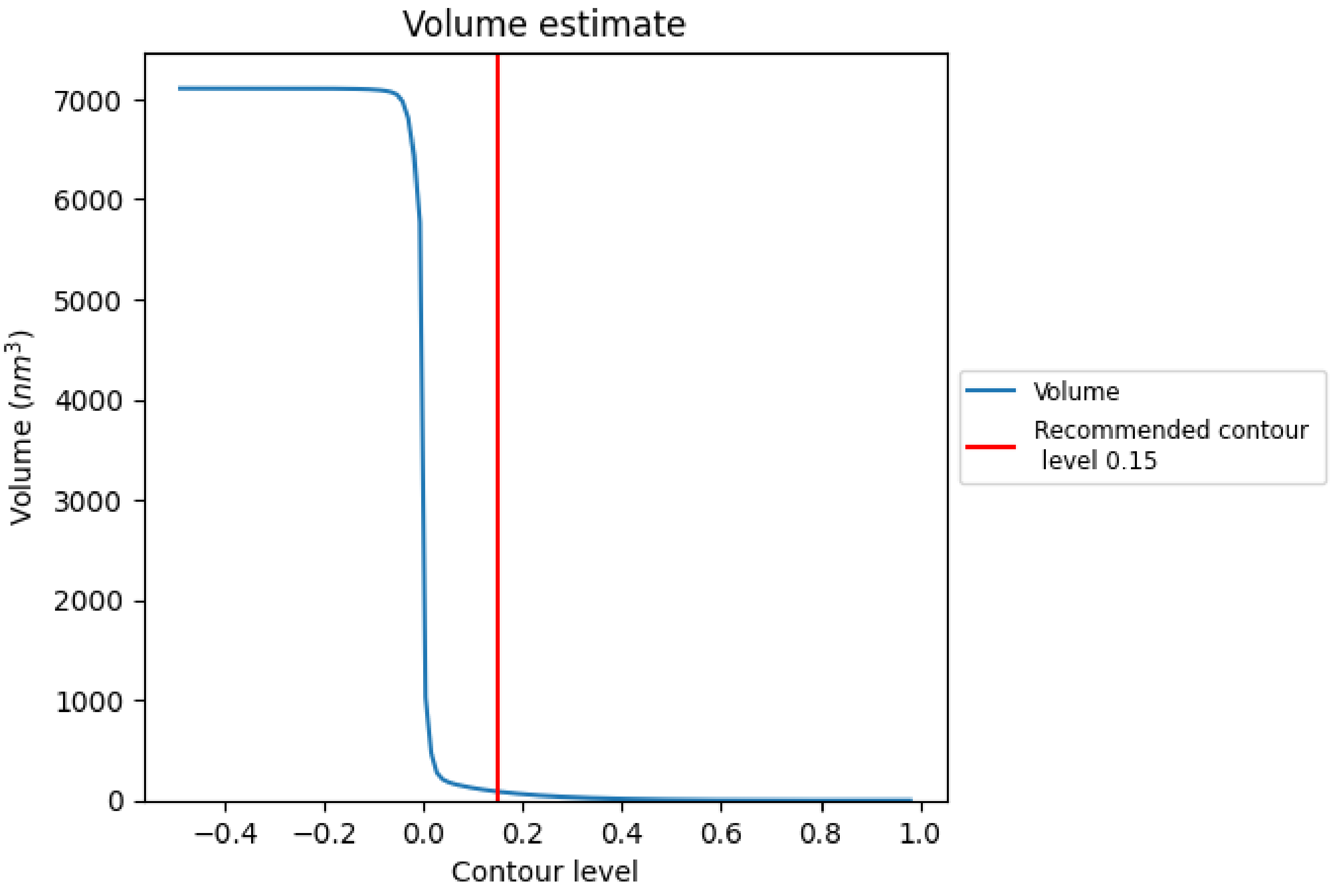
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

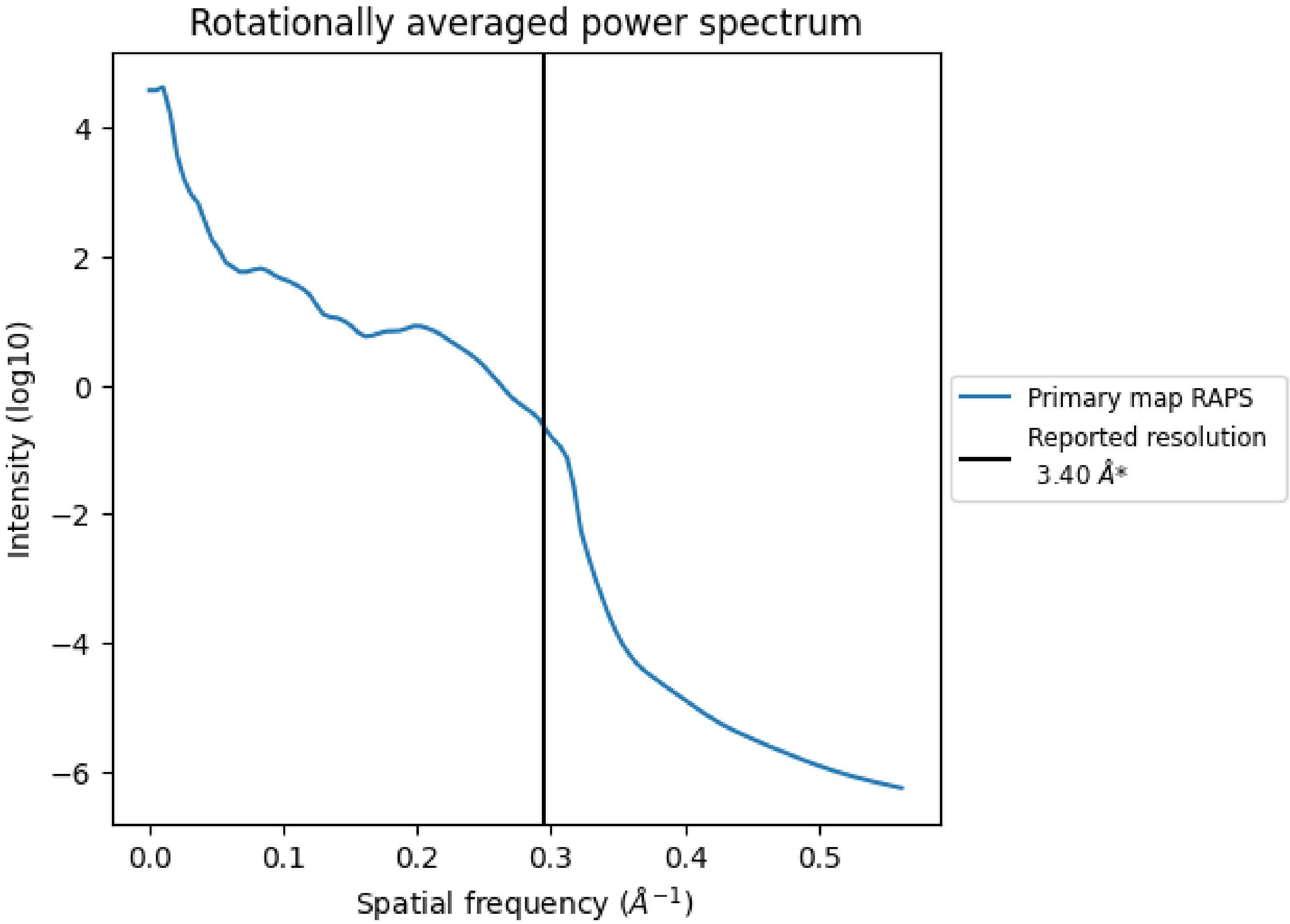
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 85 nm^3; this corresponds to an approximate mass of 77 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 0.294 Å^{-1}

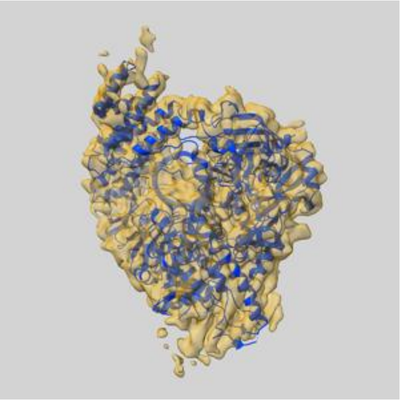
8 Fourier-Shell correlation ⓘ

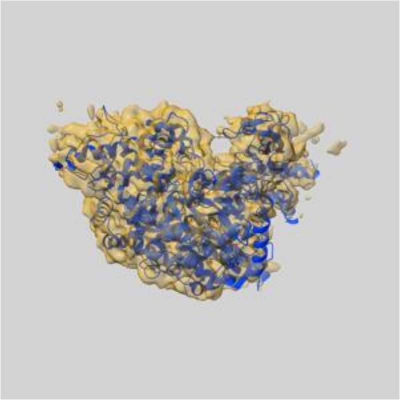
This section was not generated. No FSC curve or half-maps provided.

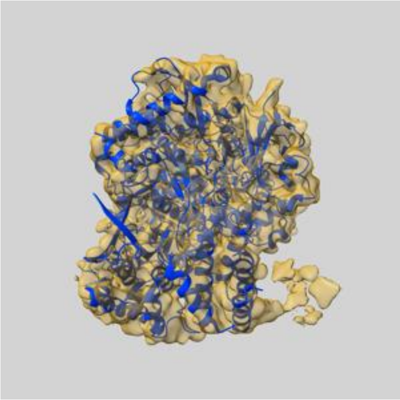
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-22288 and PDB model 6XQB. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

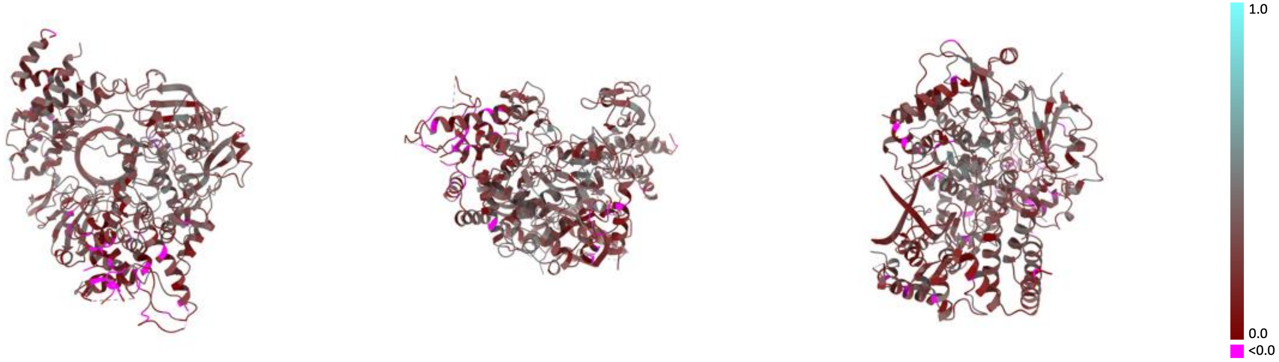

X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

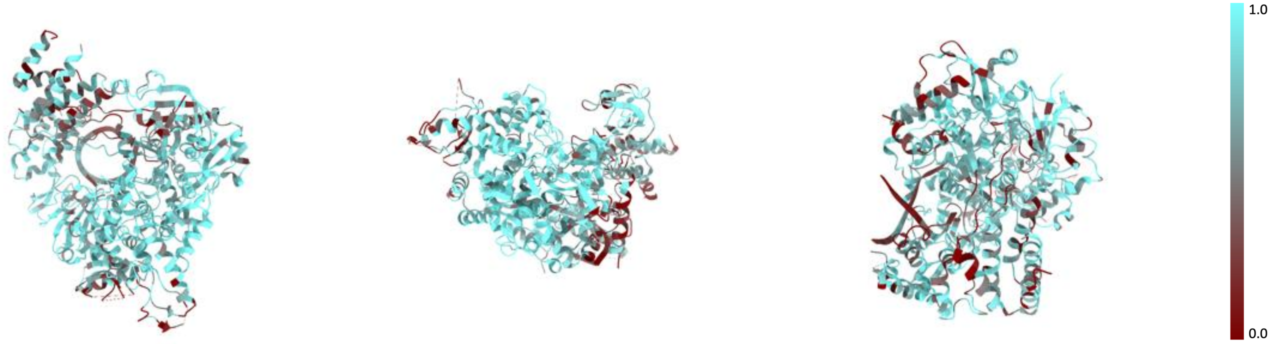
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according 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.

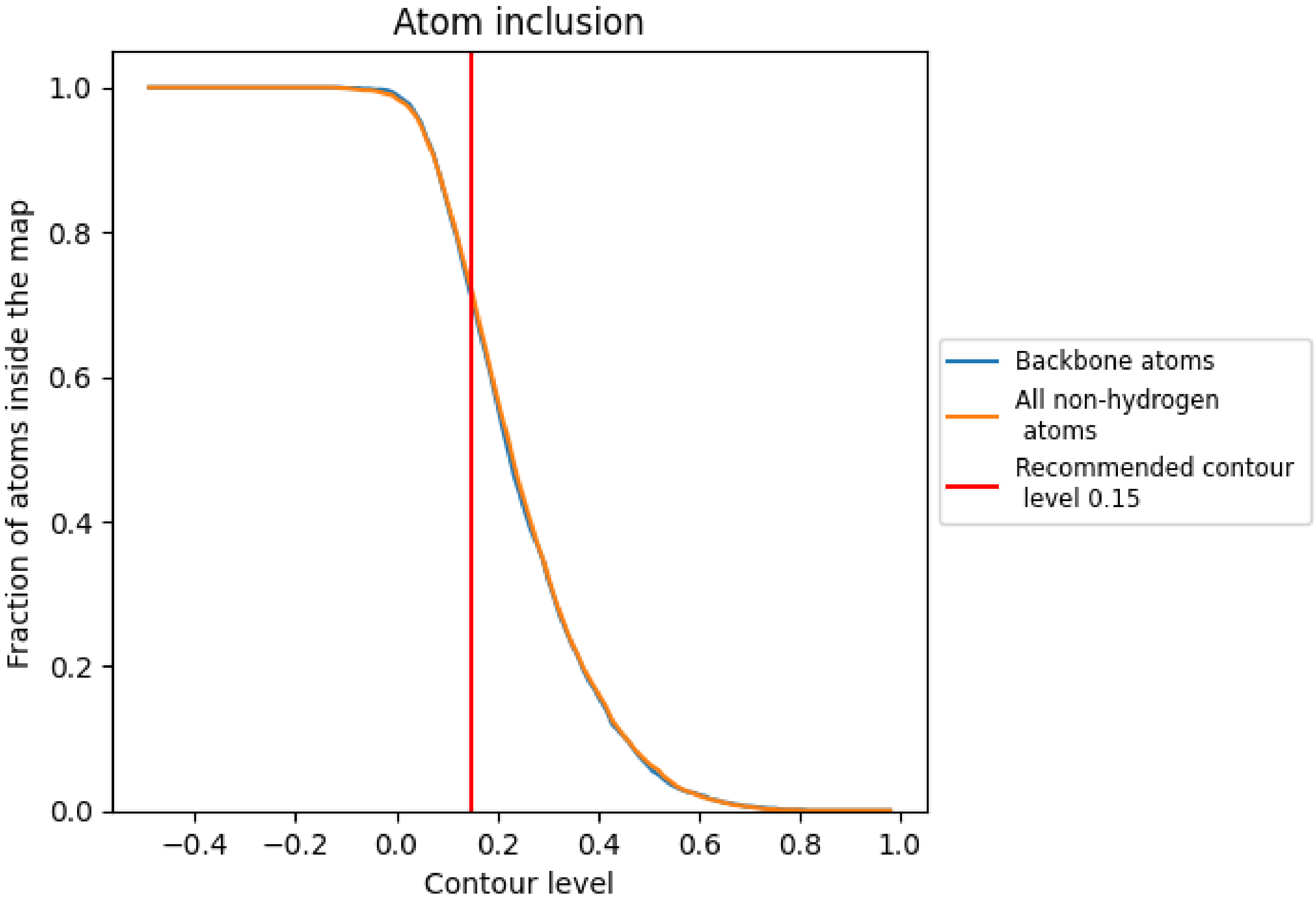
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 72% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	■ 0.7180	■ 0.2670
A	■ 0.7540	■ 0.2670
B	■ 0.6880	■ 0.2920
C	■ 0.6210	■ 0.3170
D	■ 0.4140	■ 0.2050
E	■ 0.3110	■ 0.1850
F	■ 0.3660	■ 0.1750