



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:19 AM UTC

PDB ID : 3J22 / pdb_00003j22
EMDB ID : EMD-5465
Title : The Enterovirus 71 A-particle
Authors : Shingler, K.L.
Deposited on : 2012-08-13
Resolution : 6.30 Å(reported)
Based on initial model : 3VBU

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

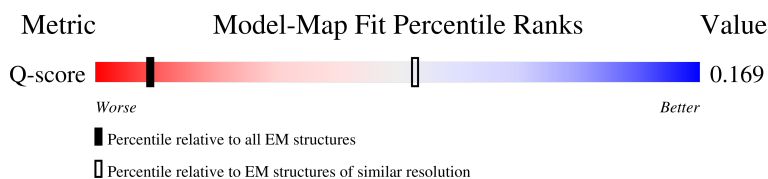
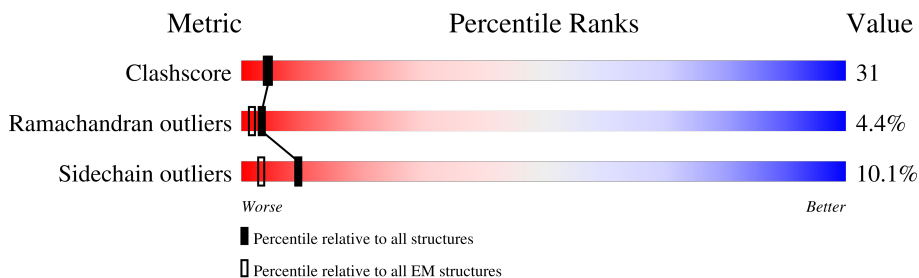
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 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	550 (5.80 - 6.80)

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	225	
2	B	237	
3	C	239	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5397 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 capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1724	1107	290	316	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	MET	CYS	SEE REMARK 999	UNP B2ZUN0

- Molecule 2 is a protein called capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	237	Total	C	N	O	S	0	0
			1834	1179	301	346	8		

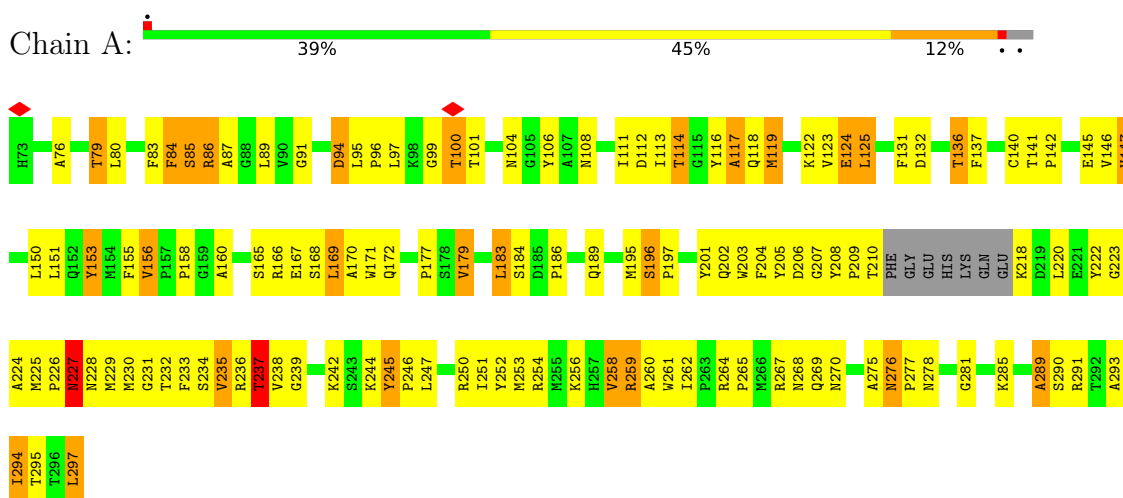
- Molecule 3 is a protein called capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	239	Total	C	N	O	S	0	0
			1839	1182	306	340	11		

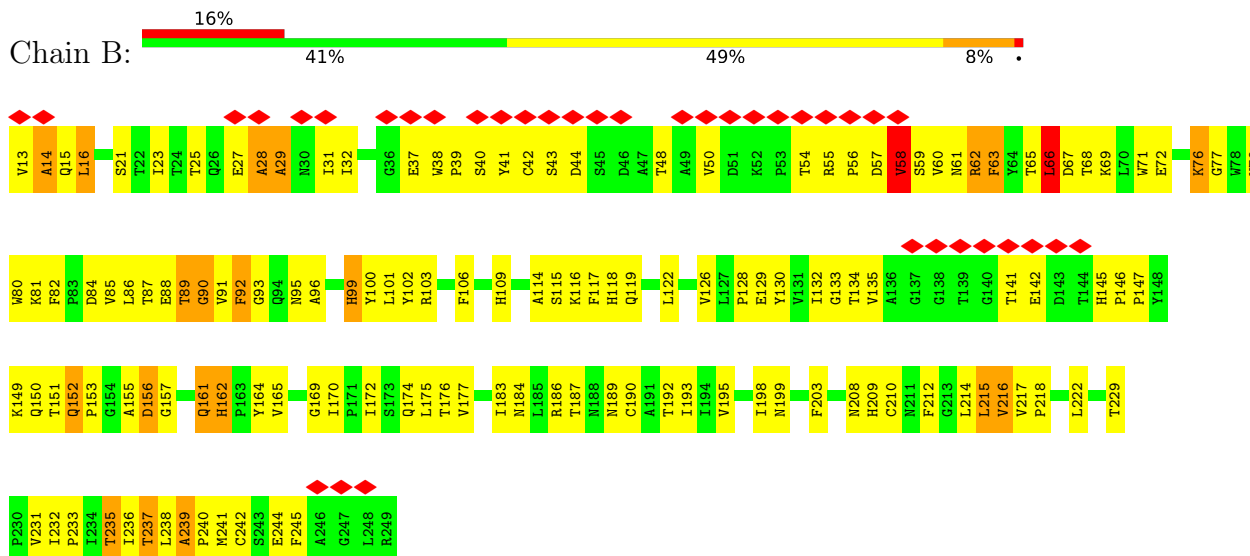
3 Residue-property plots

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: capsid protein VP1

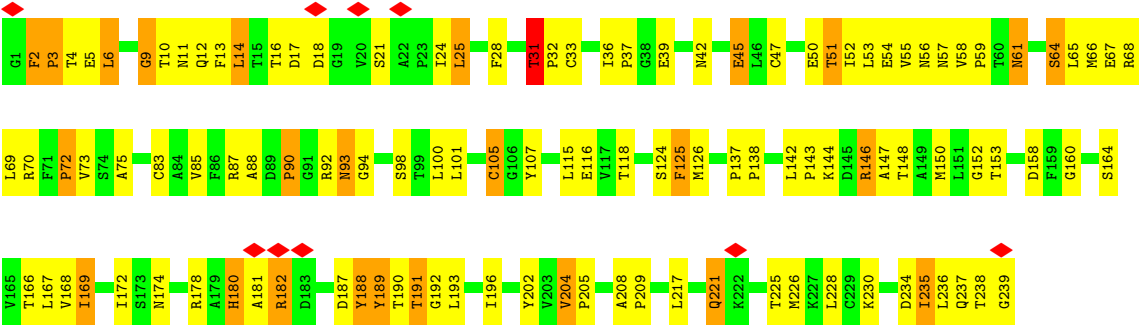


• Molecule 2: capsid protein VP0



• Molecule 3: capsid protein VP3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11436	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	auto3DEM	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1730	Depositor
Maximum defocus (nm)	4280	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	6.560	Depositor
Minimum map value	-4.726	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	445.77, 445.77, 445.77	wwPDB
Map dimensions	351, 351, 351	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.27, 1.27, 1.27	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/1776	1.21	16/2419 (0.7%)
2	B	0.73	0/1889	1.20	25/2592 (1.0%)
3	C	0.63	0/1891	1.12	14/2586 (0.5%)
All	All	0.67	0/5556	1.18	55/7597 (0.7%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	THR	N-CA-C	-9.07	102.34	113.41
2	B	92	PHE	N-CA-C	-8.34	103.29	113.97
3	C	9	GLY	N-CA-C	-8.29	104.62	114.48
1	A	201	TYR	N-CA-C	-8.10	97.82	109.96
1	A	84	PHE	N-CA-C	7.88	123.20	113.50
2	B	63	PHE	N-CA-C	7.83	120.81	108.67
2	B	152	GLN	CA-C-N	7.70	129.46	119.84
2	B	152	GLN	C-N-CA	7.70	129.46	119.84
2	B	239	ALA	CA-C-N	7.18	126.94	119.76
2	B	239	ALA	C-N-CA	7.18	126.94	119.76
3	C	64	SER	N-CA-C	-7.17	102.97	114.09
3	C	94	GLY	CA-C-N	7.17	127.49	119.32
3	C	94	GLY	C-N-CA	7.17	127.49	119.32
1	A	153	TYR	N-CA-C	-7.04	97.76	109.24
2	B	229	THR	CA-C-N	7.03	127.18	119.87
2	B	229	THR	C-N-CA	7.03	127.18	119.87
1	A	237	THR	N-CA-C	-7.02	100.61	110.50
2	B	161	GLN	N-CA-C	-6.86	105.44	113.88
2	B	106	PHE	N-CA-C	6.60	119.48	108.13
2	B	66	LEU	N-CA-C	6.59	119.79	110.50
2	B	141	THR	N-CA-C	6.48	120.19	112.93
3	C	31	THR	CA-C-N	6.41	127.86	119.84
3	C	31	THR	C-N-CA	6.41	127.86	119.84
2	B	44	ASP	N-CA-C	6.28	118.93	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	169	ILE	CA-C-N	6.26	127.67	119.84
3	C	169	ILE	C-N-CA	6.26	127.67	119.84
2	B	195	VAL	N-CA-C	6.21	114.66	107.89
2	B	89	THR	N-CA-C	6.07	119.47	110.48
3	C	192	GLY	N-CA-C	-5.99	103.34	112.51
3	C	2	PHE	CA-C-N	5.91	126.11	119.90
3	C	2	PHE	C-N-CA	5.91	126.11	119.90
1	A	275	ALA	N-CA-C	5.82	118.50	111.40
2	B	156	ASP	N-CA-C	-5.82	106.22	113.38
1	A	276	ASN	N-CA-C	5.78	119.28	110.50
1	A	125	LEU	N-CA-C	-5.75	104.98	112.23
2	B	212	PHE	N-CA-C	5.70	115.63	108.45
2	B	93	GLY	N-CA-C	-5.69	106.69	115.73
3	C	45	GLU	N-CA-C	-5.67	105.01	111.14
3	C	3	PRO	N-CA-C	5.65	119.33	110.80
3	C	28	PHE	N-CA-C	5.64	118.76	110.30
1	A	119	MET	N-CA-C	5.59	117.82	111.11
2	B	15	GLN	N-CA-C	5.53	118.26	109.24
1	A	258	VAL	N-CA-C	5.45	116.43	108.58
2	B	118	HIS	N-CA-C	-5.41	102.04	110.42
1	A	132	ASP	N-CA-C	-5.38	101.80	110.14
1	A	285	LYS	N-CA-C	5.35	117.70	110.31
2	B	100	TYR	N-CA-C	5.34	118.26	111.69
1	A	160	ALA	CA-C-N	5.34	126.51	119.84
1	A	160	ALA	C-N-CA	5.34	126.51	119.84
1	A	247	LEU	N-CA-C	5.27	118.15	109.72
1	A	99	GLY	N-CA-C	5.26	118.38	110.18
2	B	84	ASP	N-CA-C	5.24	117.67	111.33
2	B	162	HIS	CA-C-N	5.10	125.38	119.47
2	B	162	HIS	C-N-CA	5.10	125.38	119.47
2	B	43	SER	N-CA-C	5.04	117.03	110.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1724	0	1688	126	0
2	B	1834	0	1774	132	0
3	C	1839	0	1814	127	0
All	All	5397	0	5276	332	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 31.

All (332) 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:281:GLY:HA3	2:B:135:VAL:HG13	1.14	1.09
2:B:164:TYR:HA	3:C:66:MET:HE3	1.38	1.05
1:A:156:VAL:HG22	1:A:232:THR:HB	1.42	0.99
1:A:229:MET:HE2	1:A:231:GLY:H	1.26	0.97
2:B:134:THR:HG23	2:B:146:PRO:HG3	1.47	0.96
2:B:87:THR:HG22	2:B:96:ALA:HB1	1.51	0.92
2:B:55:ARG:HG2	2:B:244:GLU:HG2	1.56	0.87
1:A:76:ALA:O	1:A:79:THR:HG23	1.73	0.86
1:A:197:PRO:HA	3:C:31:THR:HG21	1.57	0.85
3:C:9:GLY:O	3:C:12:GLN:HG2	1.78	0.83
2:B:59:SER:O	2:B:62:ARG:HG2	1.78	0.83
2:B:172:ILE:HG21	3:C:66:MET:HE1	1.59	0.83
2:B:99:HIS:CD2	2:B:245:PHE:HB3	2.16	0.81
1:A:281:GLY:HA3	2:B:135:VAL:CG1	2.07	0.80
1:A:281:GLY:CA	2:B:135:VAL:HG13	2.04	0.79
2:B:56:PRO:HB3	2:B:60:VAL:HG21	1.63	0.78
2:B:164:TYR:CA	3:C:66:MET:HE3	2.14	0.78
1:A:112:ASP:OD1	1:A:114:THR:HG22	1.82	0.78
1:A:294:ILE:HD12	3:C:56:ASN:HA	1.67	0.77
2:B:103:ARG:HG2	2:B:244:GLU:HB2	1.67	0.76
2:B:16:LEU:HD21	2:B:25:THR:CG2	2.16	0.76
2:B:95:ASN:O	2:B:99:HIS:HB2	1.85	0.76
1:A:229:MET:HE3	1:A:230:MET:H	1.50	0.76
1:A:117:ALA:HB1	3:C:236:LEU:HB3	1.67	0.74
2:B:134:THR:HG22	2:B:150:GLN:HE22	1.53	0.74
2:B:198:ILE:HG12	3:C:37:PRO:HG2	1.67	0.74
3:C:105:CYS:HA	3:C:226:MET:HE1	1.68	0.73
2:B:87:THR:HG22	2:B:96:ALA:CB	2.18	0.73
3:C:188:TYR:O	3:C:189:TYR:HD2	1.72	0.73
3:C:142:LEU:HD23	3:C:143:PRO:O	1.91	0.70
1:A:229:MET:HE2	1:A:231:GLY:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:LEU:HD23	2:B:218:PRO:HA	1.72	0.70
3:C:180:HIS:CD2	3:C:181:ALA:H	2.09	0.70
3:C:158:ASP:C	3:C:160:GLY:H	1.99	0.69
3:C:92:ARG:HD3	3:C:188:TYR:HD2	1.58	0.68
3:C:10:THR:HG22	3:C:11:ASN:ND2	2.09	0.68
3:C:6:LEU:HD13	3:C:10:THR:HG21	1.74	0.68
3:C:92:ARG:HH22	3:C:191:THR:CG2	2.06	0.68
1:A:276:ASN:HB2	1:A:277:PRO:HD2	1.75	0.68
3:C:178:ARG:HH12	3:C:187:ASP:HB3	1.59	0.67
2:B:54:THR:O	2:B:56:PRO:HD3	1.95	0.67
1:A:80:LEU:HD21	1:A:260:ALA:HB3	1.75	0.66
3:C:42:ASN:O	3:C:45:GLU:HG3	1.95	0.66
3:C:58:VAL:HG23	3:C:59:PRO:HD3	1.78	0.66
2:B:119:GLN:NE2	3:C:209:PRO:HB2	2.11	0.65
1:A:270:ASN:HA	3:C:235:ILE:HG23	1.78	0.65
2:B:23:ILE:HG21	2:B:237:THR:HG21	1.79	0.65
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.32	0.64
2:B:21:SER:HB2	2:B:63:PHE:HB2	1.79	0.64
1:A:254:ARG:NH2	1:A:256:LYS:HD3	2.13	0.64
1:A:267:ARG:HD2	2:B:169:GLY:O	1.97	0.64
2:B:132:ILE:O	2:B:146:PRO:HG2	1.98	0.63
2:B:31:ILE:HG22	2:B:192:THR:HB	1.80	0.63
3:C:6:LEU:CD1	3:C:10:THR:HG21	2.28	0.63
1:A:165:SER:HB2	1:A:167:GLU:OE2	1.99	0.62
3:C:188:TYR:O	3:C:189:TYR:CD2	2.52	0.62
1:A:294:ILE:HD12	3:C:56:ASN:CA	2.29	0.62
1:A:153:TYR:HD1	1:A:235:VAL:HG13	1.65	0.62
1:A:156:VAL:HG23	1:A:156:VAL:O	2.00	0.62
2:B:172:ILE:CG2	3:C:66:MET:HE1	2.29	0.61
2:B:79:TYR:CB	2:B:215:LEU:HD12	2.30	0.61
1:A:94:ASP:C	1:A:96:PRO:HD3	2.24	0.61
1:A:206:ASP:OD1	2:B:81:LYS:HD2	2.01	0.61
3:C:2:PHE:CD1	3:C:3:PRO:HD2	2.35	0.61
1:A:150:LEU:O	1:A:151:LEU:HD23	2.01	0.61
2:B:48:THR:HG22	2:B:48:THR:O	2.00	0.61
1:A:294:ILE:HD11	3:C:55:VAL:HG12	1.82	0.61
1:A:104:ASN:O	1:A:166:ARG:HD2	2.01	0.60
2:B:69:LYS:HE3	2:B:156:ASP:O	2.02	0.60
2:B:32:ILE:HB	2:B:193:ILE:HG12	1.83	0.60
3:C:118:THR:HG23	3:C:166:THR:OG1	2.01	0.60
3:C:167:LEU:HD12	3:C:168:VAL:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:HB	1:A:142:PRO:HD2	1.84	0.59
3:C:180:HIS:CG	3:C:181:ALA:H	2.19	0.59
1:A:226:PRO:HG2	1:A:227:ASN:OD1	2.02	0.59
2:B:79:TYR:HB3	2:B:215:LEU:HD12	1.85	0.58
1:A:136:THR:HG23	1:A:189:GLN:HG3	1.85	0.58
1:A:156:VAL:O	1:A:156:VAL:CG2	2.50	0.58
2:B:56:PRO:HB3	2:B:60:VAL:CG2	2.30	0.58
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.69	0.58
3:C:90:PRO:CG	3:C:115:LEU:HD11	2.34	0.58
3:C:92:ARG:HH22	3:C:191:THR:HG21	1.68	0.58
3:C:4:THR:HG22	3:C:5:GLU:H	1.68	0.58
2:B:153:PRO:HB2	2:B:157:GLY:O	2.04	0.57
2:B:27:GLU:O	2:B:28:ALA:HB2	2.03	0.57
1:A:207:GLY:HA3	2:B:208:ASN:O	2.04	0.57
2:B:164:TYR:HA	3:C:66:MET:CE	2.24	0.57
1:A:156:VAL:CG2	1:A:232:THR:HB	2.25	0.56
2:B:231:VAL:O	2:B:232:ILE:HD13	2.05	0.56
2:B:149:LYS:H	2:B:149:LYS:HD2	1.70	0.56
2:B:184:ASN:HB3	2:B:187:THR:OG1	2.05	0.56
1:A:259:ARG:HG2	3:C:39:GLU:OE1	2.06	0.56
2:B:198:ILE:HG12	3:C:37:PRO:CG	2.35	0.56
2:B:177:VAL:HG22	2:B:177:VAL:O	2.04	0.56
1:A:277:PRO:HG2	2:B:133:GLY:HA3	1.88	0.56
2:B:149:LYS:HD2	2:B:149:LYS:N	2.20	0.56
3:C:6:LEU:HD13	3:C:10:THR:CG2	2.36	0.56
1:A:291:ARG:HD2	1:A:293:ALA:O	2.05	0.56
2:B:79:TYR:HA	2:B:214:LEU:O	2.06	0.56
3:C:92:ARG:NH2	3:C:191:THR:CG2	2.68	0.55
1:A:114:THR:HG23	3:C:237:GLN:HG2	1.89	0.55
1:A:202:GLN:HG2	1:A:225:MET:HE2	1.89	0.55
1:A:290:SER:OG	3:C:68:ARG:NH2	2.39	0.55
2:B:174:GLN:HA	3:C:51:THR:HG22	1.89	0.55
3:C:4:THR:HG22	3:C:5:GLU:N	2.21	0.55
3:C:167:LEU:HD12	3:C:168:VAL:H	1.71	0.55
1:A:117:ALA:HB1	3:C:236:LEU:HD23	1.89	0.55
2:B:92:PHE:CE1	2:B:245:PHE:HZ	2.25	0.55
2:B:172:ILE:C	2:B:174:GLN:H	2.14	0.54
1:A:295:THR:HA	3:C:85:VAL:HG12	1.89	0.54
3:C:146:ARG:O	3:C:146:ARG:HG2	2.06	0.54
2:B:164:TYR:HD1	3:C:66:MET:HE2	1.70	0.54
1:A:229:MET:HE3	1:A:230:MET:N	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ALA:HB1	3:C:172:ILE:HG21	1.89	0.54
2:B:41:TYR:CD1	2:B:55:ARG:HD3	2.43	0.54
3:C:105:CYS:CA	3:C:226:MET:HE1	2.37	0.54
1:A:202:GLN:HG2	1:A:225:MET:HG2	1.89	0.53
2:B:130:TYR:HE1	2:B:215:LEU:CD1	2.20	0.53
1:A:113:ILE:HG22	1:A:253:MET:HE1	1.89	0.53
1:A:208:TYR:CE1	1:A:222:TYR:HB2	2.44	0.53
2:B:71:TRP:CE2	2:B:222:LEU:HB2	2.44	0.53
3:C:105:CYS:SG	3:C:226:MET:HE1	2.48	0.53
1:A:224:ALA:O	1:A:226:PRO:HD3	2.09	0.53
2:B:82:PHE:O	2:B:210:CYS:HA	2.09	0.53
1:A:111:ILE:HD11	1:A:233:PHE:CE2	2.44	0.52
1:A:276:ASN:OD1	1:A:278:ASN:HB2	2.10	0.52
2:B:236:ILE:N	2:B:236:ILE:HD12	2.24	0.52
3:C:174:ASN:OD1	3:C:174:ASN:O	2.27	0.52
2:B:122:LEU:HB2	2:B:183:ILE:HB	1.92	0.52
3:C:83:CYS:HB3	3:C:196:ILE:HG22	1.90	0.52
1:A:84:PHE:O	1:A:85:SER:O	2.28	0.52
1:A:276:ASN:CB	1:A:277:PRO:HD2	2.40	0.52
2:B:134:THR:HG23	2:B:146:PRO:CG	2.29	0.52
3:C:90:PRO:HD2	3:C:188:TYR:OH	2.09	0.52
3:C:115:LEU:HB2	3:C:169:ILE:HB	1.92	0.52
1:A:155:PHE:O	1:A:177:PRO:HD2	2.10	0.52
1:A:245:TYR:CD1	1:A:245:TYR:N	2.78	0.52
1:A:254:ARG:NH1	3:C:18:ASP:HA	2.25	0.52
3:C:150:MET:O	3:C:150:MET:SD	2.67	0.51
1:A:140:CYS:HA	1:A:183:LEU:HD21	1.92	0.51
2:B:114:ALA:HB2	2:B:232:ILE:HD12	1.92	0.51
3:C:178:ARG:HH12	3:C:187:ASP:CB	2.23	0.51
1:A:104:ASN:HA	1:A:242:LYS:NZ	2.25	0.51
1:A:222:TYR:CE1	2:B:151:THR:HG23	2.45	0.51
3:C:178:ARG:NH1	3:C:187:ASP:HB3	2.25	0.51
2:B:119:GLN:HB3	3:C:124:SER:HA	1.92	0.50
1:A:220:LEU:HD23	2:B:145:HIS:HD2	1.77	0.50
2:B:16:LEU:HD21	2:B:25:THR:HG22	1.92	0.50
1:A:229:MET:CE	1:A:231:GLY:H	2.11	0.50
2:B:86:LEU:C	2:B:88:GLU:H	2.19	0.50
3:C:56:ASN:OD1	3:C:58:VAL:HG22	2.12	0.50
1:A:153:TYR:CD1	1:A:235:VAL:HG13	2.46	0.50
2:B:184:ASN:OD1	2:B:186:ARG:HG2	2.12	0.50
3:C:188:TYR:O	3:C:189:TYR:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HB	1:A:203:TRP:NE1	2.26	0.50
2:B:80:TRP:HZ3	2:B:216:VAL:CG1	2.25	0.50
3:C:61:ASN:ND2	3:C:64:SER:OG	2.44	0.49
1:A:123:VAL:C	1:A:125:LEU:H	2.21	0.49
2:B:161:GLN:O	2:B:162:HIS:HD2	1.95	0.49
3:C:105:CYS:HA	3:C:226:MET:CE	2.42	0.49
2:B:103:ARG:HD2	2:B:203:PHE:CE2	2.48	0.49
1:A:245:TYR:HB3	1:A:246:PRO:HD2	1.95	0.49
2:B:165:VAL:HA	2:B:170:ILE:O	2.12	0.49
1:A:123:VAL:HB	1:A:203:TRP:HE1	1.77	0.49
1:A:277:PRO:O	1:A:278:ASN:C	2.56	0.49
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.48	0.49
1:A:250:ARG:HG3	1:A:250:ARG:NH2	2.27	0.48
2:B:56:PRO:HB3	2:B:60:VAL:CB	2.44	0.48
2:B:116:LYS:HD3	3:C:125:PHE:CE1	2.48	0.48
3:C:66:MET:CE	3:C:69:LEU:HD11	2.42	0.48
1:A:168:SER:C	1:A:170:ALA:H	2.22	0.48
2:B:130:TYR:HE1	2:B:215:LEU:HD11	1.78	0.48
2:B:65:THR:OG1	2:B:237:THR:HG23	2.13	0.48
3:C:54:GLU:HG2	3:C:69:LEU:HD23	1.96	0.48
3:C:182:ARG:HH21	3:C:182:ARG:HG3	1.77	0.48
1:A:83:PHE:O	1:A:86:ARG:NH2	2.47	0.48
1:A:112:ASP:CG	1:A:114:THR:HG22	2.39	0.48
2:B:38:TRP:O	2:B:40:SER:N	2.46	0.48
2:B:41:TYR:CE1	2:B:55:ARG:HD3	2.49	0.48
3:C:236:LEU:N	3:C:236:LEU:HD12	2.29	0.47
2:B:86:LEU:C	2:B:88:GLU:N	2.72	0.47
1:A:116:TYR:CE2	1:A:118:GLN:HG3	2.48	0.47
2:B:28:ALA:O	2:B:29:ALA:O	2.33	0.47
2:B:99:HIS:HD2	2:B:245:PHE:HB3	1.70	0.47
2:B:241:MET:O	2:B:242:CYS:C	2.57	0.47
3:C:51:THR:HG21	3:C:100:LEU:HB2	1.95	0.47
3:C:144:LYS:HD3	3:C:148:THR:HG21	1.97	0.47
2:B:109:HIS:CE1	2:B:190:CYS:HB2	2.49	0.47
2:B:85:VAL:HG23	2:B:155:ALA:HA	1.96	0.47
3:C:182:ARG:HG3	3:C:182:ARG:NH2	2.29	0.47
2:B:71:TRP:HD1	2:B:72:GLU:N	2.13	0.47
3:C:105:CYS:SG	3:C:226:MET:CE	3.02	0.47
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.96	0.46
1:A:205:TYR:O	1:A:223:GLY:HA2	2.15	0.46
1:A:137:PHE:N	1:A:137:PHE:CD2	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:N	1:A:96:PRO:HD3	2.29	0.46
1:A:104:ASN:HB2	1:A:106:TYR:CD1	2.50	0.46
1:A:238:VAL:CG1	1:A:239:GLY:N	2.78	0.46
2:B:164:TYR:HD1	3:C:66:MET:CE	2.28	0.46
2:B:56:PRO:HG2	2:B:245:PHE:CD2	2.51	0.46
2:B:57:ASP:O	2:B:58:VAL:C	2.58	0.46
3:C:51:THR:HG21	3:C:100:LEU:CB	2.46	0.46
3:C:56:ASN:O	3:C:59:PRO:HD2	2.15	0.46
3:C:152:GLY:O	3:C:153:THR:C	2.57	0.46
2:B:103:ARG:HG3	2:B:103:ARG:HH11	1.80	0.46
1:A:220:LEU:HA	2:B:145:HIS:CD2	2.50	0.46
2:B:172:ILE:C	2:B:174:GLN:N	2.72	0.46
3:C:90:PRO:HG2	3:C:115:LEU:HD11	1.98	0.46
2:B:66:LEU:HD23	2:B:66:LEU:N	2.31	0.46
3:C:67:GLU:HG2	3:C:70:ARG:NH1	2.31	0.46
3:C:187:ASP:O	3:C:188:TYR:O	2.34	0.46
2:B:77:GLY:HA2	2:B:218:PRO:HD3	1.98	0.45
2:B:119:GLN:HB3	3:C:124:SER:CA	2.46	0.45
1:A:136:THR:HG21	3:C:13:PHE:CD2	2.52	0.45
3:C:75:ALA:HA	3:C:202:TYR:HB3	1.97	0.45
1:A:293:ALA:C	1:A:295:THR:H	2.24	0.45
1:A:179:VAL:HG22	1:A:179:VAL:O	2.15	0.45
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.52	0.45
1:A:85:SER:O	1:A:86:ARG:HB2	2.17	0.45
1:A:254:ARG:HH21	1:A:256:LYS:HB3	1.82	0.45
2:B:37:GLU:OE2	3:C:37:PRO:HA	2.16	0.45
3:C:24:ILE:HG23	3:C:25:LEU:HD22	1.99	0.45
2:B:13:VAL:O	2:B:14:ALA:HB2	2.17	0.45
2:B:13:VAL:HG22	2:B:14:ALA:N	2.32	0.45
3:C:58:VAL:HG23	3:C:59:PRO:CD	2.46	0.45
3:C:92:ARG:HD3	3:C:188:TYR:CD2	2.45	0.45
1:A:104:ASN:HB2	1:A:106:TYR:CE1	2.51	0.45
3:C:126:MET:HE2	3:C:205:PRO:HG3	1.98	0.45
1:A:117:ALA:CB	3:C:236:LEU:HD23	2.45	0.45
2:B:129:GLU:OE2	2:B:209:HIS:NE2	2.50	0.45
1:A:226:PRO:HG2	1:A:227:ASN:H	1.82	0.44
1:A:195:MET:O	1:A:196:SER:C	2.60	0.44
1:A:291:ARG:O	3:C:58:VAL:HG12	2.17	0.44
2:B:116:LYS:HB3	3:C:125:PHE:CD1	2.52	0.44
2:B:119:GLN:HB3	3:C:124:SER:N	2.32	0.44
1:A:114:THR:HG21	3:C:237:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:SER:C	1:A:167:GLU:H	2.25	0.44
2:B:79:TYR:HB2	2:B:215:LEU:HD12	1.98	0.44
2:B:161:GLN:O	2:B:162:HIS:CD2	2.71	0.44
3:C:31:THR:HA	3:C:32:PRO:HD3	1.85	0.44
3:C:54:GLU:HG3	3:C:98:SER:CB	2.48	0.44
3:C:66:MET:HE2	3:C:69:LEU:HD11	1.98	0.44
3:C:65:LEU:O	3:C:68:ARG:HG3	2.17	0.44
1:A:195:MET:O	1:A:196:SER:O	2.35	0.44
1:A:244:LYS:HB2	1:A:245:TYR:CE1	2.53	0.44
2:B:82:PHE:O	2:B:210:CYS:CA	2.66	0.44
2:B:176:THR:OG1	3:C:50:GLU:O	2.22	0.44
3:C:56:ASN:O	3:C:56:ASN:CG	2.59	0.44
1:A:87:ALA:HB1	1:A:252:TYR:HB3	1.99	0.44
1:A:291:ARG:HG3	3:C:58:VAL:HG12	2.00	0.44
2:B:151:THR:HG22	2:B:152:GLN:NE2	2.32	0.44
1:A:136:THR:HG21	3:C:13:PHE:CE2	2.52	0.44
2:B:28:ALA:C	2:B:29:ALA:O	2.60	0.44
2:B:238:LEU:HD12	2:B:238:LEU:C	2.43	0.44
1:A:113:ILE:HG22	1:A:253:MET:SD	2.58	0.44
1:A:140:CYS:HB2	1:A:145:GLU:O	2.18	0.44
2:B:101:LEU:HB3	2:B:203:PHE:HD1	1.83	0.44
1:A:116:TYR:O	1:A:117:ALA:C	2.61	0.43
1:A:197:PRO:CG	1:A:227:ASN:HB3	2.48	0.43
1:A:270:ASN:HA	3:C:235:ILE:CG2	2.46	0.43
1:A:297:LEU:HD12	1:A:297:LEU:H	1.83	0.43
2:B:57:ASP:O	2:B:58:VAL:O	2.36	0.43
1:A:89:LEU:HD11	1:A:91:GLY:O	2.18	0.43
3:C:56:ASN:O	3:C:68:ARG:HA	2.19	0.43
3:C:193:LEU:HA	3:C:193:LEU:HD23	1.80	0.43
3:C:204:VAL:HG22	3:C:208:ALA:HB3	2.00	0.43
2:B:71:TRP:HD1	2:B:72:GLU:H	1.65	0.43
1:A:131:PHE:HB3	1:A:258:VAL:HG22	2.01	0.43
1:A:168:SER:C	1:A:170:ALA:N	2.76	0.43
1:A:169:LEU:HD12	1:A:169:LEU:N	2.34	0.43
3:C:180:HIS:CG	3:C:181:ALA:N	2.87	0.43
2:B:130:TYR:C	2:B:130:TYR:CD2	2.96	0.43
1:A:276:ASN:HB2	1:A:277:PRO:CD	2.48	0.43
1:A:218:LYS:NZ	1:A:220:LEU:HD23	2.34	0.43
2:B:91:VAL:HG22	2:B:91:VAL:O	2.19	0.43
2:B:115:SER:C	2:B:117:PHE:H	2.25	0.43
1:A:158:PRO:HB3	1:A:229:MET:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:SER:CB	2:B:63:PHE:HB2	2.46	0.42
2:B:174:GLN:O	2:B:177:VAL:HG12	2.18	0.42
2:B:128:PRO:O	2:B:129:GLU:C	2.59	0.42
3:C:47:CYS:HB3	3:C:101:LEU:CD1	2.49	0.42
3:C:158:ASP:C	3:C:160:GLY:N	2.64	0.42
3:C:147:ALA:O	3:C:150:MET:HB3	2.19	0.42
1:A:86:ARG:NH1	1:A:86:ARG:HG3	2.35	0.42
3:C:178:ARG:HD3	3:C:180:HIS:HB3	2.01	0.42
1:A:209:PRO:O	1:A:210:THR:C	2.63	0.42
2:B:239:ALA:HA	2:B:240:PRO:HD3	1.80	0.42
3:C:54:GLU:OE2	3:C:68:ARG:NH1	2.49	0.42
3:C:138:PRO:HB3	3:C:190:THR:HA	2.01	0.42
2:B:117:PHE:CE2	3:C:126:MET:HG3	2.54	0.42
2:B:184:ASN:HB3	2:B:187:THR:HG1	1.85	0.42
2:B:232:ILE:HA	2:B:233:PRO:HD2	1.90	0.42
3:C:93:ASN:N	3:C:93:ASN:HD22	2.16	0.42
1:A:123:VAL:HG23	1:A:124:GLU:N	2.34	0.42
1:A:147:VAL:HG11	1:A:245:TYR:CD2	2.55	0.42
2:B:27:GLU:O	2:B:28:ALA:CB	2.67	0.42
2:B:122:LEU:CD2	2:B:218:PRO:HA	2.45	0.42
3:C:52:ILE:HA	3:C:217:LEU:HD23	2.02	0.42
3:C:158:ASP:OD1	3:C:160:GLY:CA	2.68	0.42
1:A:226:PRO:C	1:A:228:ASN:H	2.28	0.41
2:B:235:THR:C	2:B:236:ILE:HD12	2.45	0.41
2:B:13:VAL:N	2:B:27:GLU:HG3	2.35	0.41
3:C:172:ILE:O	3:C:172:ILE:HD12	2.20	0.41
3:C:238:THR:O	3:C:239:GLY:O	2.39	0.41
1:A:86:ARG:HG3	1:A:86:ARG:HH11	1.84	0.41
1:A:277:PRO:HG2	2:B:133:GLY:CA	2.51	0.41
2:B:61:ASN:OD1	2:B:240:PRO:HB2	2.20	0.41
2:B:89:THR:HG22	2:B:90:GLY:N	2.35	0.41
3:C:188:TYR:O	3:C:189:TYR:CB	2.68	0.41
2:B:189:ASN:CG	2:B:190:CYS:N	2.78	0.41
1:A:104:ASN:HA	1:A:242:LYS:HZ1	1.85	0.41
1:A:108:ASN:ND2	1:A:234:SER:OG	2.54	0.41
1:A:113:ILE:O	1:A:119:MET:HG2	2.21	0.41
1:A:122:LYS:HG2	3:C:107:TYR:CE1	2.56	0.41
1:A:289:ALA:HB3	3:C:93:ASN:HB3	2.02	0.41
2:B:76:LYS:HZ2	2:B:76:LYS:HB3	1.85	0.41
3:C:16:THR:O	3:C:17:ASP:C	2.64	0.41
1:A:268:ASN:ND2	1:A:269:GLN:HE21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:VAL:HA	2:B:218:PRO:HD3	1.88	0.41
3:C:54:GLU:OE2	3:C:68:ARG:HD3	2.21	0.41
1:A:204:PHE:CE1	1:A:264:ARG:HD3	2.56	0.40
3:C:178:ARG:NH1	3:C:187:ASP:CB	2.84	0.40
1:A:166:ARG:HH21	1:A:237:THR:HG23	1.85	0.40
2:B:68:THR:OG1	2:B:235:THR:HG23	2.20	0.40
2:B:86:LEU:HD23	2:B:89:THR:HB	2.03	0.40
2:B:199:ASN:OD1	2:B:209:HIS:CE1	2.75	0.40
1:A:97:LEU:HD11	1:A:246:PRO:HD3	2.03	0.40
2:B:132:ILE:HG21	2:B:150:GLN:HE21	1.86	0.40
1:A:89:LEU:HD12	1:A:251:ILE:O	2.22	0.40
1:A:171:TRP:CE2	1:A:236:ARG:HD2	2.57	0.40
2:B:68:THR:HG21	2:B:233:PRO:HB2	2.04	0.40
2:B:175:LEU:C	2:B:177:VAL:H	2.29	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	214/225 (95%)	188 (88%)	15 (7%)	11 (5%)	1	14
2	B	235/237 (99%)	196 (83%)	31 (13%)	8 (3%)	3	20
3	C	237/239 (99%)	202 (85%)	24 (10%)	11 (5%)	2	16
All	All	686/701 (98%)	586 (85%)	70 (10%)	30 (4%)	3	17

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER
2	B	28	ALA
2	B	29	ALA

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Mol	Chain	Res	Type
2	B	58	VAL
3	C	93	ASN
3	C	188	TYR
1	A	86	ARG
1	A	196	SER
1	A	227	ASN
2	B	14	ALA
2	B	90	GLY
3	C	180	HIS
3	C	182	ARG
3	C	189	TYR
1	A	124	GLU
1	A	289	ALA
2	B	39	PRO
3	C	221	GLN
1	A	117	ALA
1	A	169	LEU
3	C	72	PRO
3	C	137	PRO
2	B	67	ASP
3	C	57	ASN
3	C	105	CYS
3	C	191	THR
1	A	186	PRO
1	A	294	ILE
2	B	147	PRO
1	A	262	ILE

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	187/193 (97%)	167 (89%)	20 (11%)	6	21
2	B	201/201 (100%)	186 (92%)	15 (8%)	12	33
3	C	199/199 (100%)	175 (88%)	24 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	587/593 (99%)	528 (90%)	59 (10%)	9 23

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	94	ASP
1	A	100	THR
1	A	101	THR
1	A	114	THR
1	A	136	THR
1	A	146	VAL
1	A	147	VAL
1	A	156	VAL
1	A	172	GLN
1	A	179	VAL
1	A	183	LEU
1	A	184	SER
1	A	227	ASN
1	A	235	VAL
1	A	237	THR
1	A	245	TYR
1	A	259	ARG
1	A	265	PRO
1	A	297	LEU
2	B	16	LEU
2	B	42	CYS
2	B	50	VAL
2	B	58	VAL
2	B	62	ARG
2	B	66	LEU
2	B	76	LYS
2	B	99	HIS
2	B	102	TYR
2	B	126	VAL
2	B	142	GLU
2	B	215	LEU
2	B	216	VAL
2	B	235	THR
2	B	237	THR
3	C	6	LEU
3	C	14	LEU

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Mol	Chain	Res	Type
3	C	21	SER
3	C	25	LEU
3	C	31	THR
3	C	33	CYS
3	C	51	THR
3	C	53	LEU
3	C	61	ASN
3	C	72	PRO
3	C	73	VAL
3	C	87	ARG
3	C	90	PRO
3	C	116	GLU
3	C	125	PHE
3	C	146	ARG
3	C	164	SER
3	C	204	VAL
3	C	221	GLN
3	C	225	THR
3	C	228	LEU
3	C	230	LYS
3	C	234	ASP
3	C	235	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	152	GLN
1	A	228	ASN
1	A	268	ASN
1	A	278	ASN
2	B	99	HIS
2	B	111	GLN
2	B	113	ASN
2	B	119	GLN
2	B	145	HIS
2	B	150	GLN
2	B	152	GLN
2	B	162	HIS
2	B	208	ASN
3	C	48	GLN
3	C	61	ASN

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Mol	Chain	Res	Type
3	C	93	ASN
3	C	154	HIS
3	C	162	GLN
3	C	174	ASN
3	C	180	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

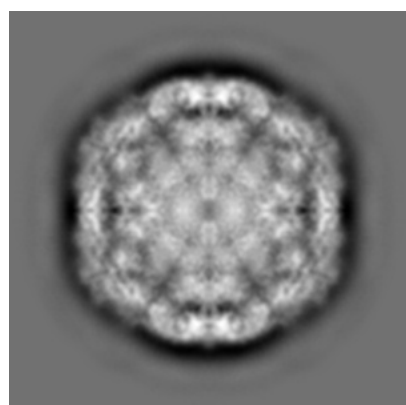
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5465. These allow visual inspection of the internal detail of the map and identification of artifacts.

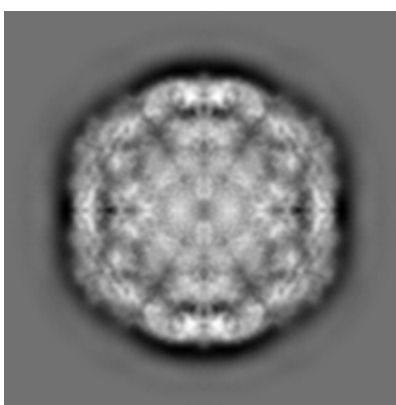
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

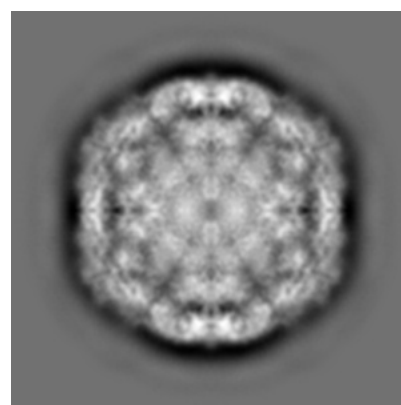
6.1.1 Primary map



X



Y

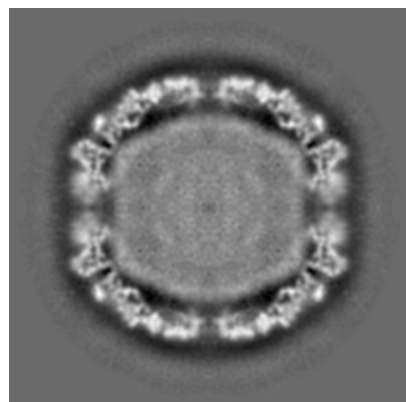


Z

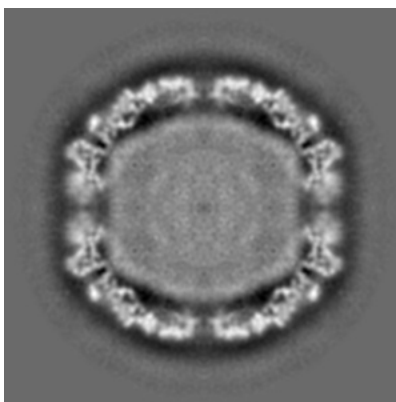
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

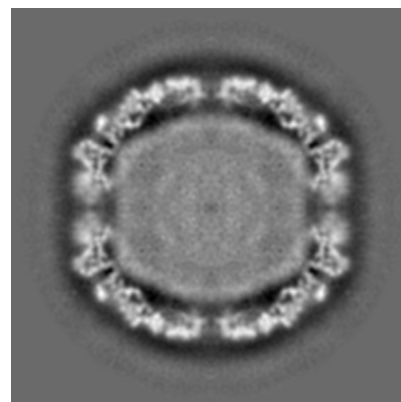
6.2.1 Primary map



X Index: 175



Y Index: 175

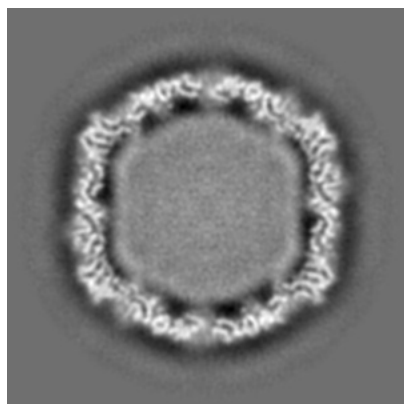


Z Index: 175

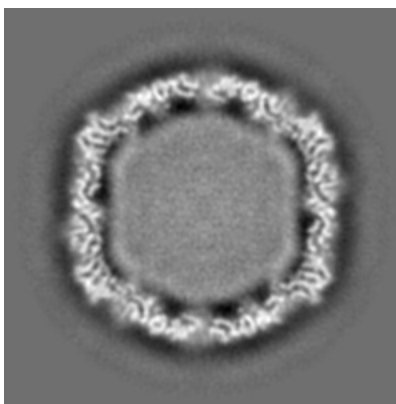
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

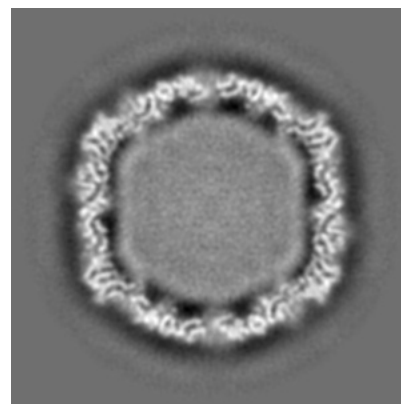
6.3.1 Primary map



X Index: 189



Y Index: 189

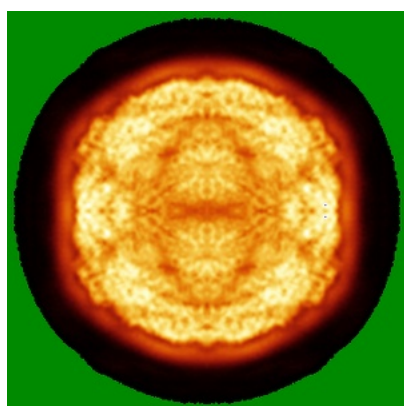


Z Index: 161

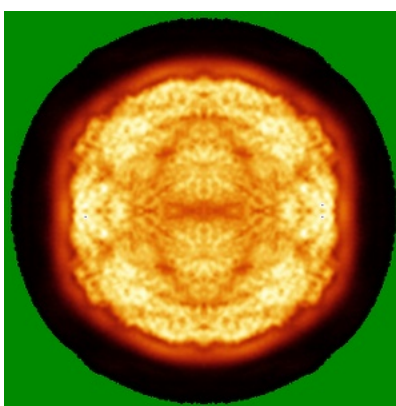
The images above show the largest variance slices of the map in three orthogonal directions.

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

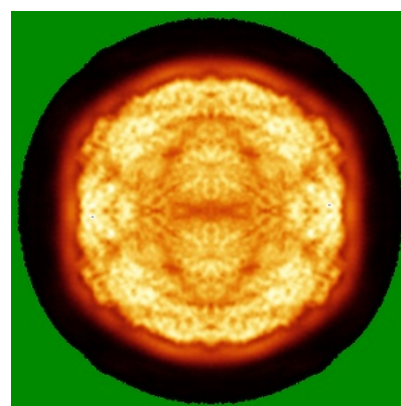
6.4.1 Primary map



X



Y

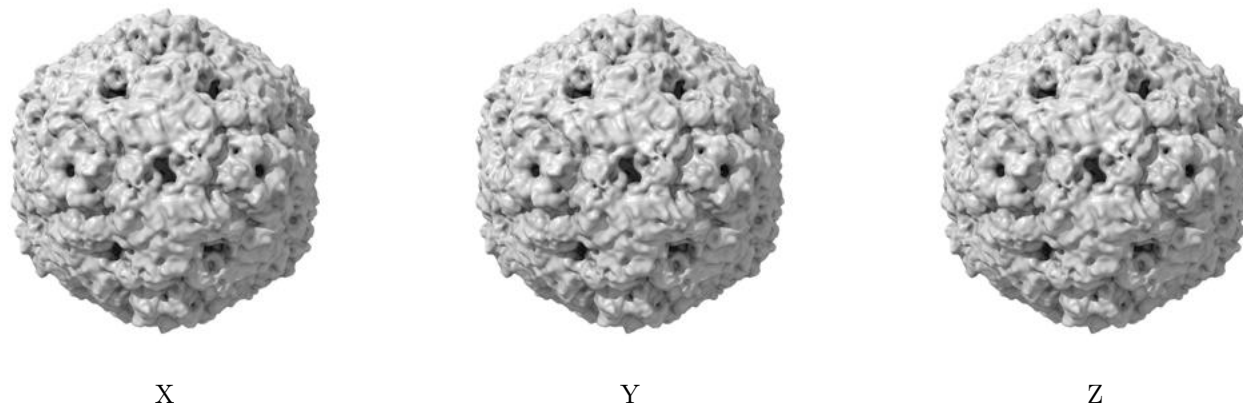


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

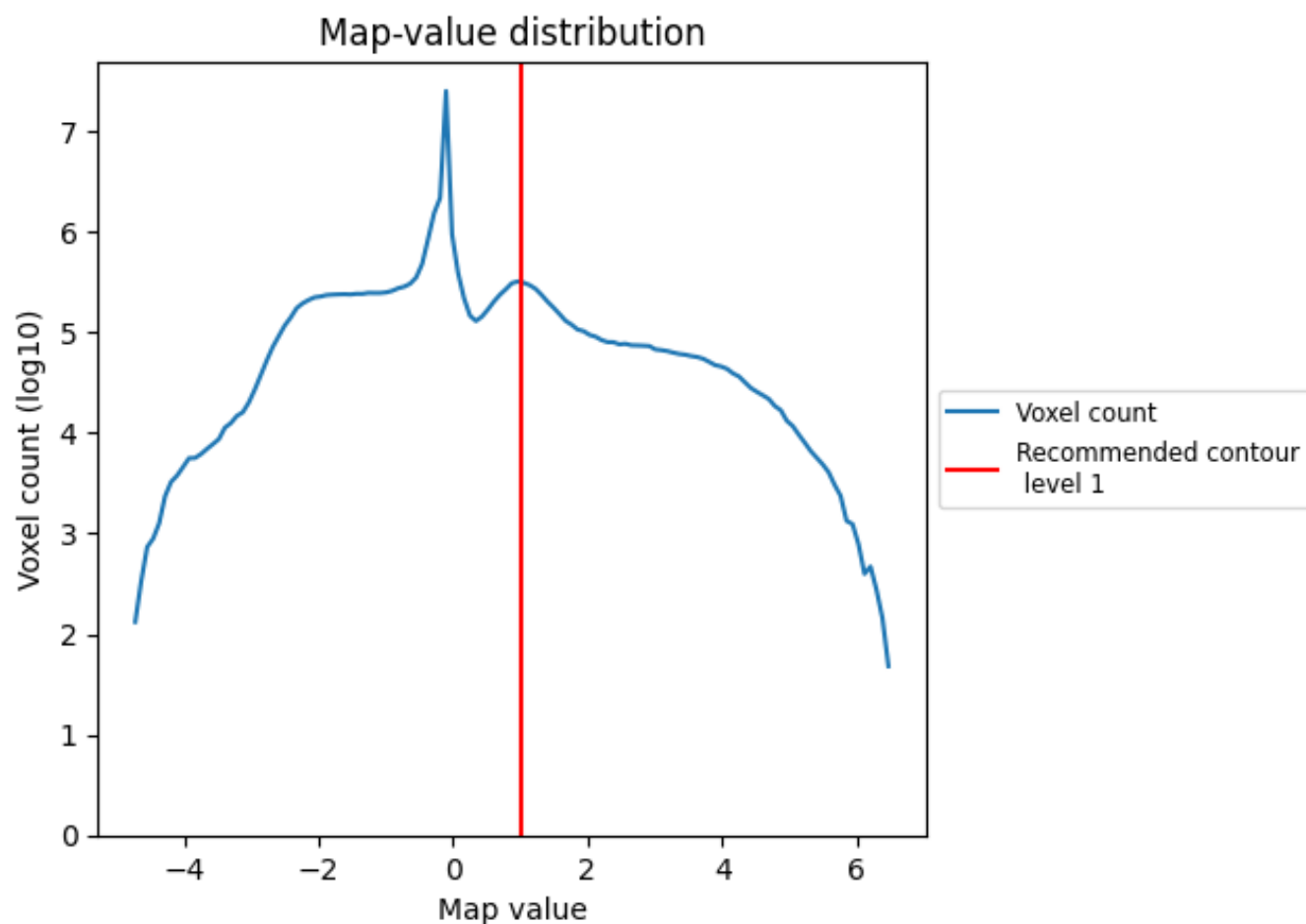
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

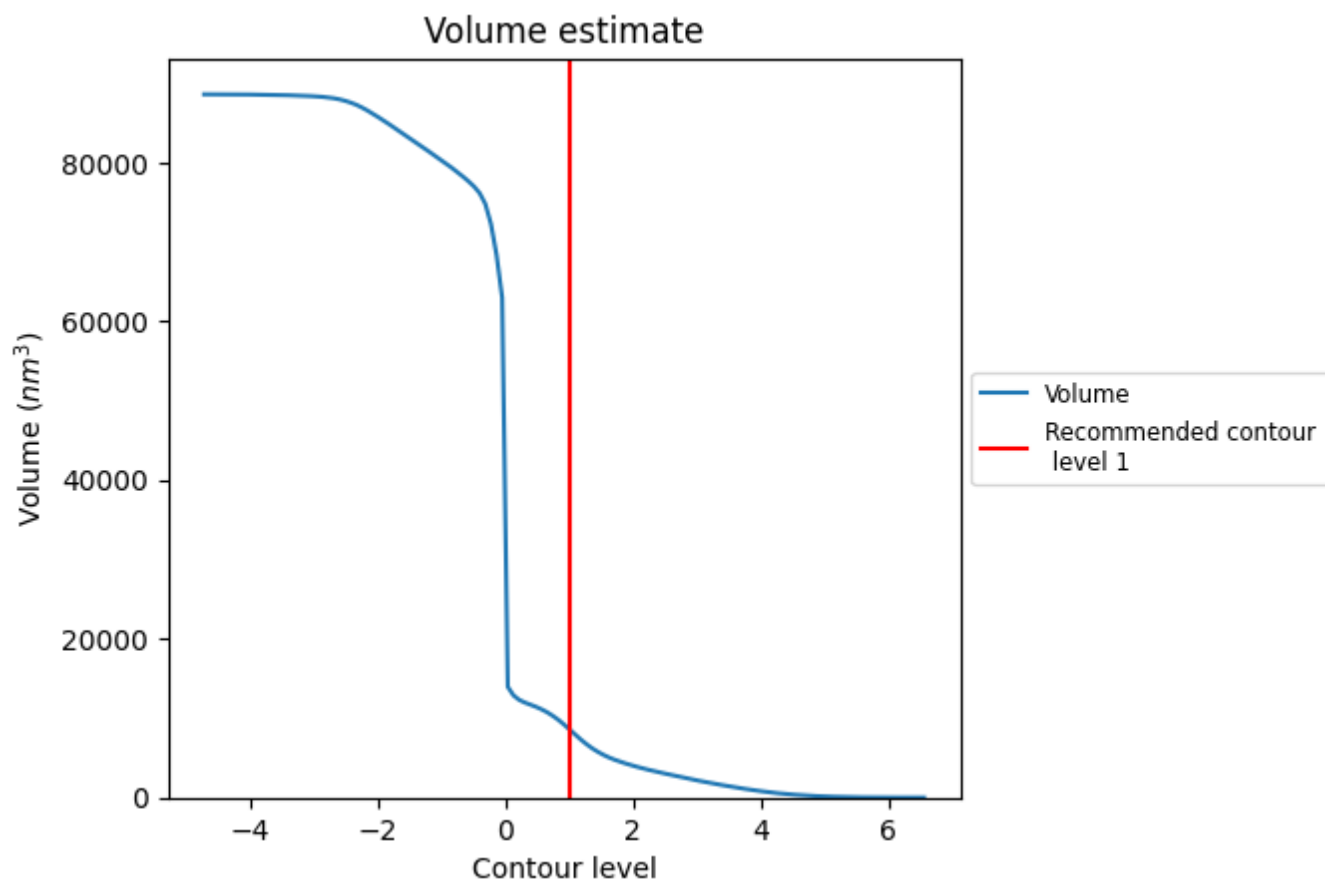
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

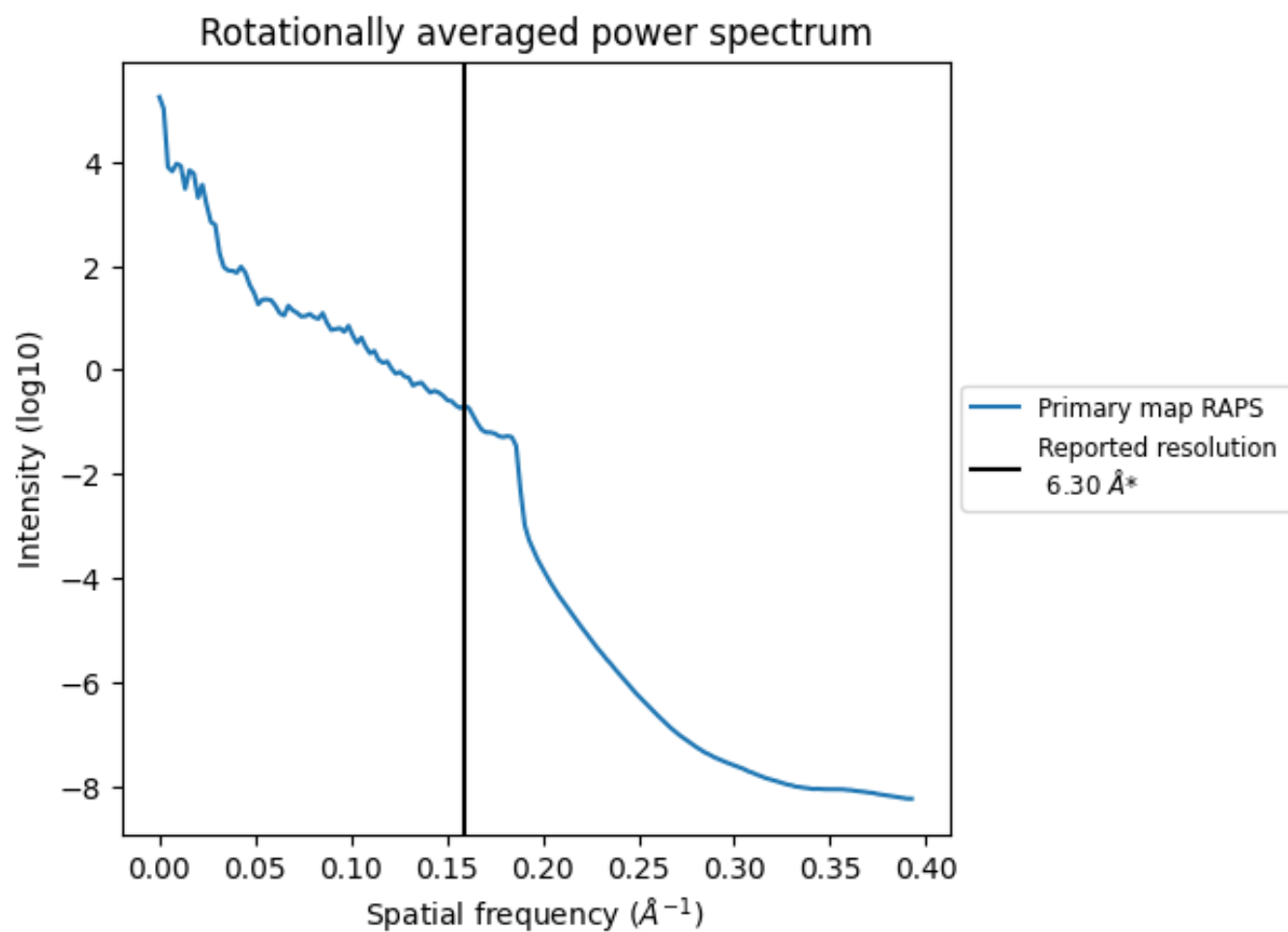
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8595 nm³; this corresponds to an approximate mass of 7764 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 0.159 Å⁻¹

8 Fourier-Shell correlation

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

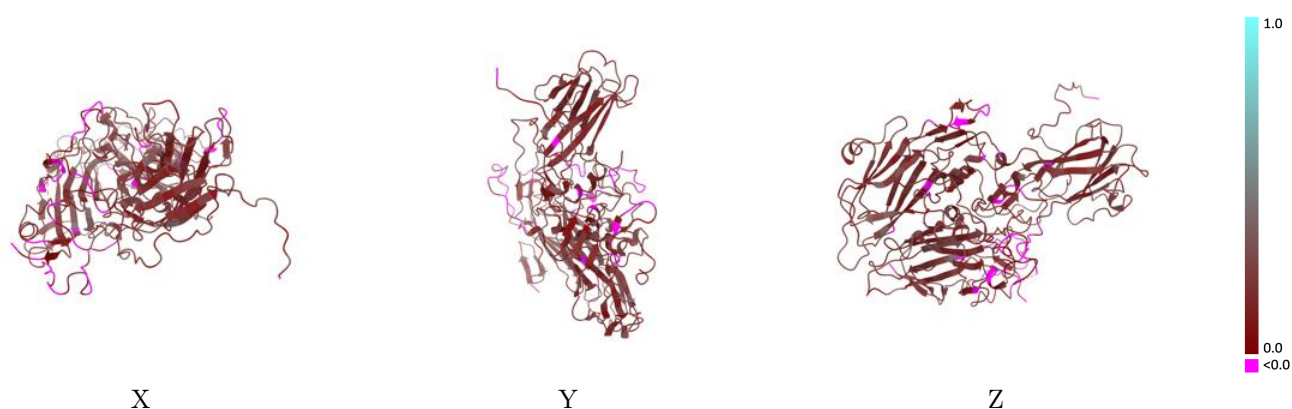
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5465 and PDB model 3J22. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

This section was not generated.

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

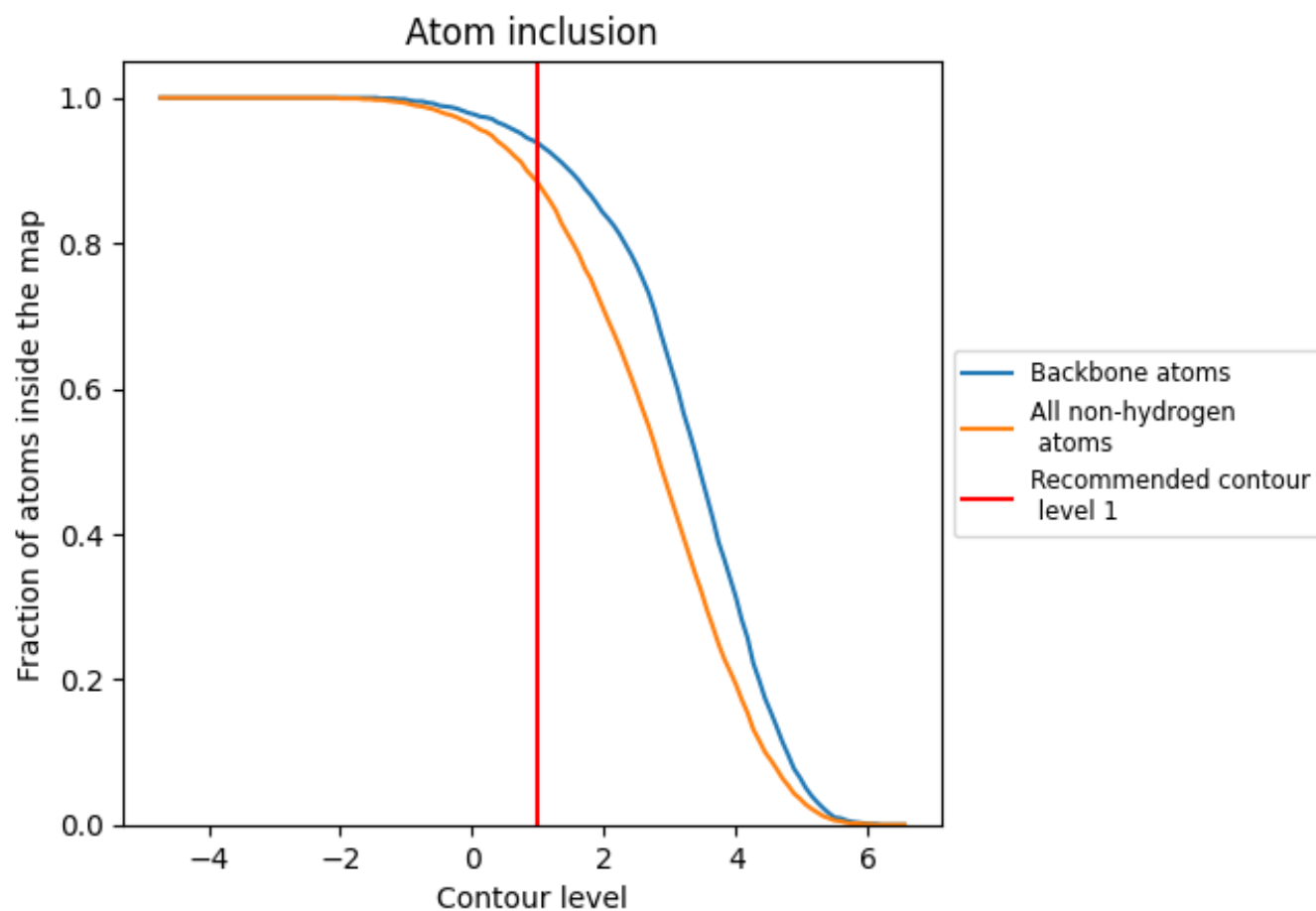


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 94% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.1690
A	0.9350	0.1820
B	0.8150	0.1450
C	0.9030	0.1820

