



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 01:13 AM UTC

PDB ID : 6Y9X / pdb_00006y9x
EMDB ID : EMD-10740
Title : Structure of the native full-length HIV-1 capsid protein in complex with Cy-
clophilin A from helical assembly (-13,7)
Authors : Ni, T.; Gerard, S.; Zhao, G.; Ning, J.; Zhang, P.
Deposited on : 2020-03-10
Resolution : 4.40 Å(reported)
Based on initial models : 4XFX, 1AK4

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:

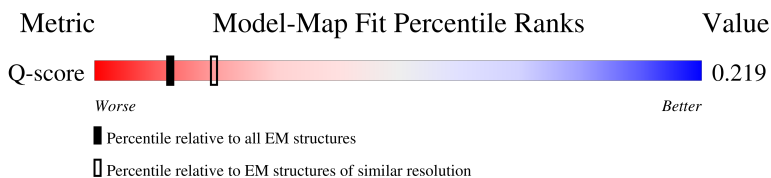
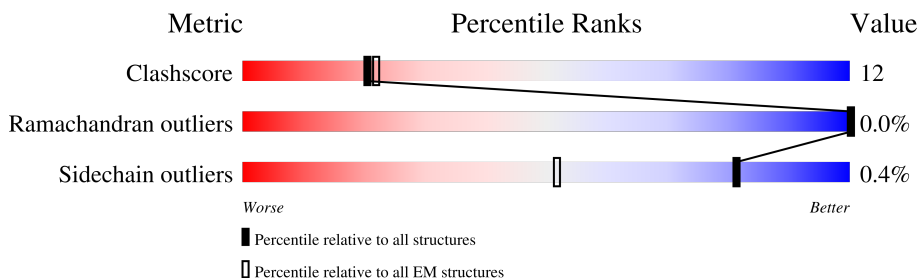
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	220	12% 55% 11% 34%
1	B	220	7% 78% 22%
1	C	220	15% 73% 26% .
1	D	220	23% 80% 20%

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Mol	Chain	Length	Quality of chain
1	G	220	
1	H	220	
1	N	220	
1	Y	220	
1	d	220	
1	e	220	
1	j	220	
1	k	220	
2	J	164	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18418 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 Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	146	Total	C	N	O	S	0	0
			1132	715	199	210	8		
1	B	220	Total	C	N	O	S	0	0
			1716	1081	299	323	13		
1	C	220	Total	C	N	O	S	0	0
			1716	1081	299	323	13		
1	D	220	Total	C	N	O	S	0	0
			1716	1081	299	323	13		
1	G	220	Total	C	N	O	S	0	0
			1716	1081	299	323	13		
1	H	220	Total	C	N	O	S	0	0
			1716	1081	299	323	13		
1	N	74	Total	C	N	O	S	0	0
			584	366	100	113	5		
1	Y	146	Total	C	N	O	S	0	0
			1132	715	199	210	8		
1	d	220	Total	C	N	O	S	0	0
			1716	1081	299	323	13		
1	e	220	Total	C	N	O	S	0	0
			1716	1081	299	323	13		
1	j	74	Total	C	N	O	S	0	0
			584	366	100	113	5		
1	k	220	Total	C	N	O	S	0	0
			1716	1081	299	323	13		

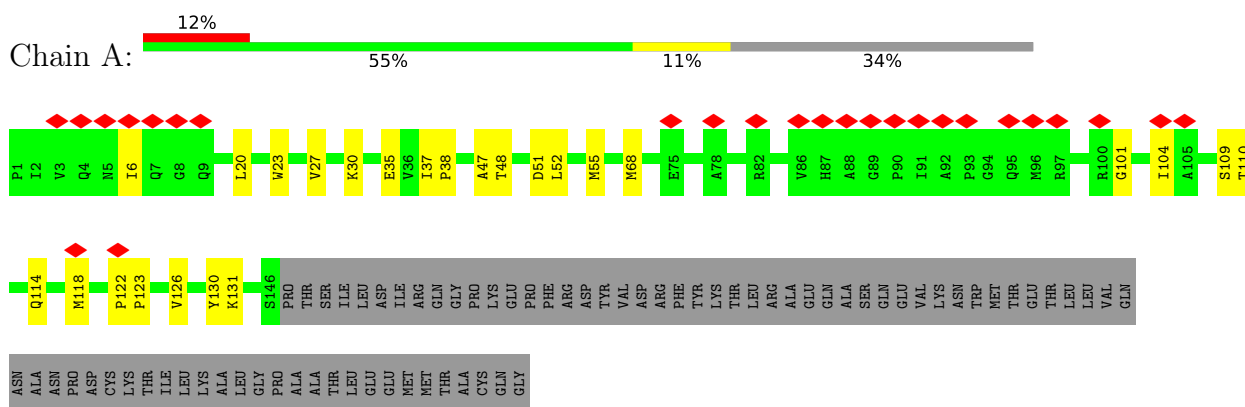
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	164	Total	C	N	O	S	0	0
			1258	797	217	236	8		

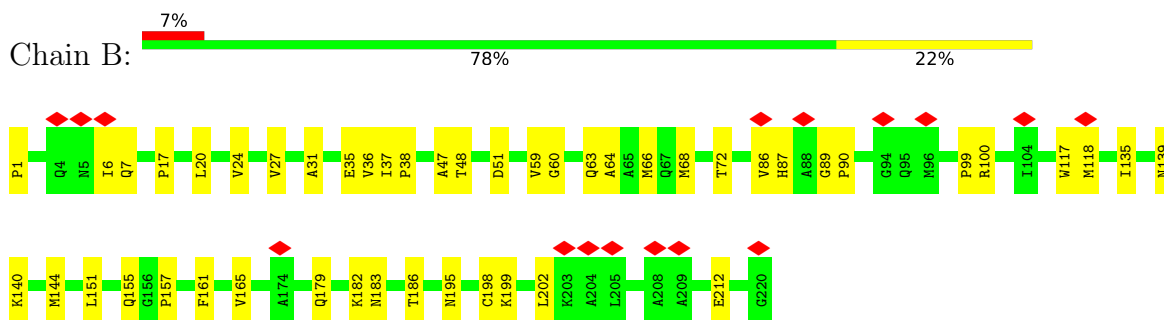
3 Residue-property plots

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.

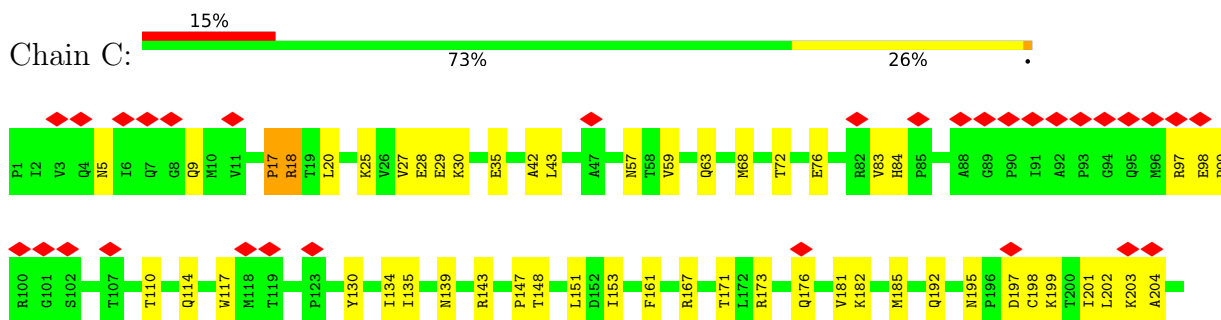
- Molecule 1: Gag-Pol polyprotein



- Molecule 1: Gag-Pol polyprotein

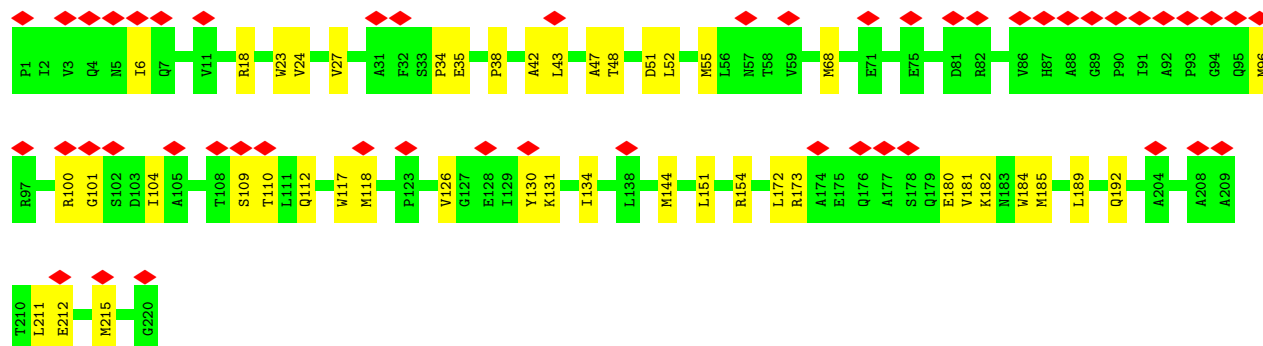
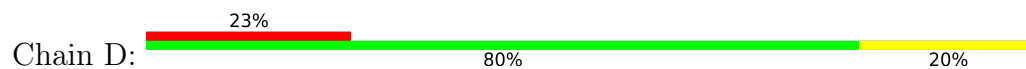


- Molecule 1: Gag-Pol polyprotein

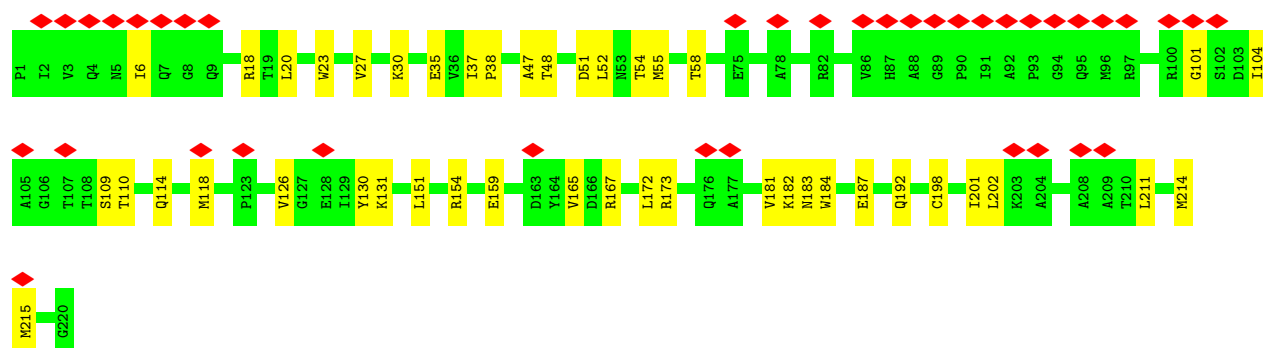
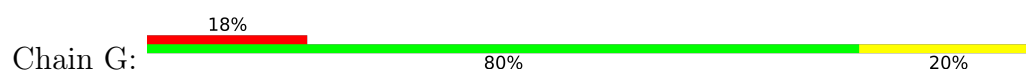




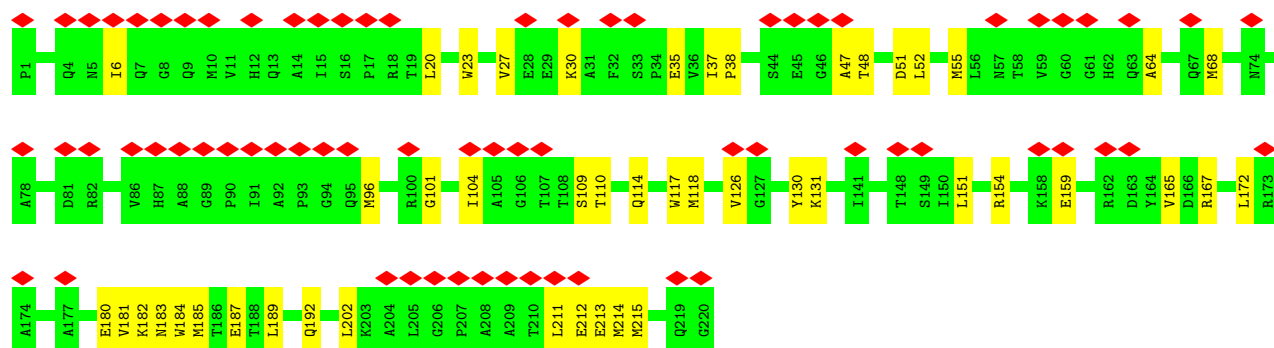
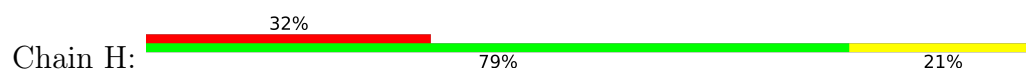
• Molecule 1: Gag-Pol polyprotein



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

ASN PRO PRO ILE VAL GLY GLY TYR LYS THR ARG ILE ILE LEU GLY ALA LEU ASN LYS ILE VAL ARG MET TYR SER P147 L151 R154 Q155 G156 P157 K158 E159 F160 R162 D163 Y164 V165 A174 A177 S178 Q179 V180 V181 K182 N183 I184 M185 T186 N195 C196 K199

L202 R203 A204 P207 L211 E212 W214 G220

• Molecule 1: Gag-Pol polyprotein

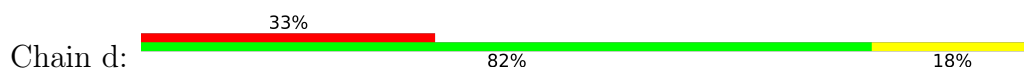


P1 I2 V3 Q4 N5 I6 Q7 Q8 Q9 M10 V11 L20 W23 V24 V27 E35 P38 A47 T48 D51 L52 M55 M68 A78 D81 R82 V86 H87 G89 P90 I91 P93 Q94 Q95 N96 R97 R100 G101 S102 D103 I104 A105 T106 S109

T110 L111 Q112 W117 M118 V126 G127 E128 I129 Y130 K131 I134 M144 Y145 S146 PRO THR SER ILE LEU ASP ILE ARG GLN GLY PRO LYS GLU PHE ARG TYR VAL ASP ARG PHE TYR LYS THR LEU ARG ALA GLN ALA SER A92 P93 Q94 Q95 N96 R97 R100 G101 S102 D103 I104 A105 T106 S109

THR LEU VAL ASN ALA ASN PRO ASP CYS THR ILE LEU LYS ALA LEU GLY PRO ALA THR SER ILE LEU ASP ILE ARG GLN GLY PRO LYS GLU PHE ARG TYR VAL ASP ARG PHE TYR LYS THR LEU ARG ALA GLN ALA SER A92 P93 Q94 Q95 N96 R97 R100 G101 S102 D103 I104 A105 T106 S109

• Molecule 1: Gag-Pol polyprotein



P1 Q4 N5 I6 Q7 Q8 Q9 M10 V11 H12 Q13 Q14 I15 P17 P18 W23 V24 V27 E28 E29 K30 A31 F32 F33 P34 E35 P38 S44 E45 G46 A47 T48 D51 L52 M55 L56 N57 G60 Q63 M68 N74 A78 D81 R82 P85

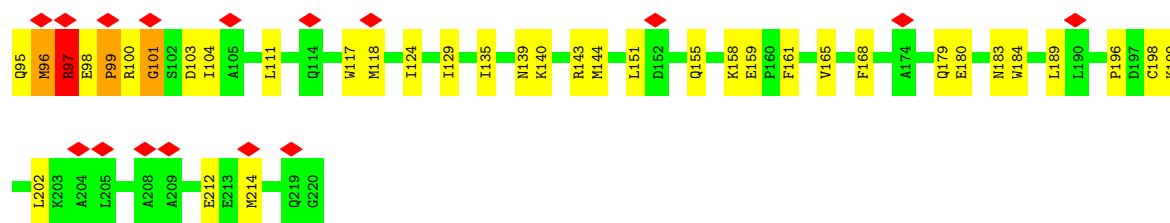
V86 H87 A88 G89 P90 I91 P93 Q94 Q95 N96 R100 G101 S102 D103 I104 A105 G106 T107 S109 T110 L111 Q112 W117 M118 N121 P125 V126 G127 E128 I129 Y130 K131 I134 I141 M144 T148 S149 I150 L151 R154 A158 E159 R162 L172 R173

A177 V181 K182 W184 M185 L189 Q192 N193 A204 L205 G206 P207 A208 T210 L211 E212 W215 Q219 G220

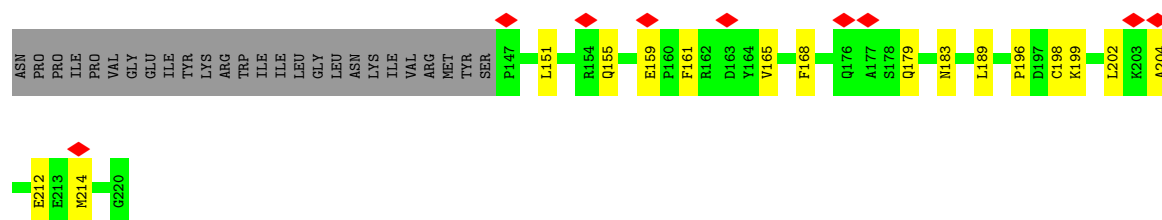
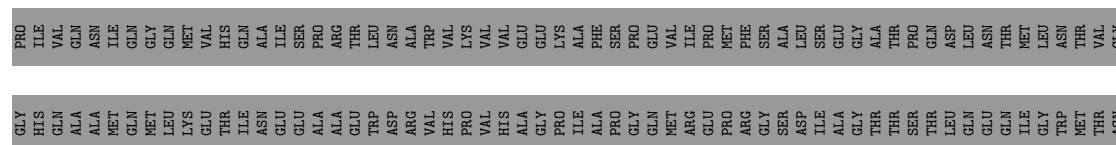
• Molecule 1: Gag-Pol polyprotein



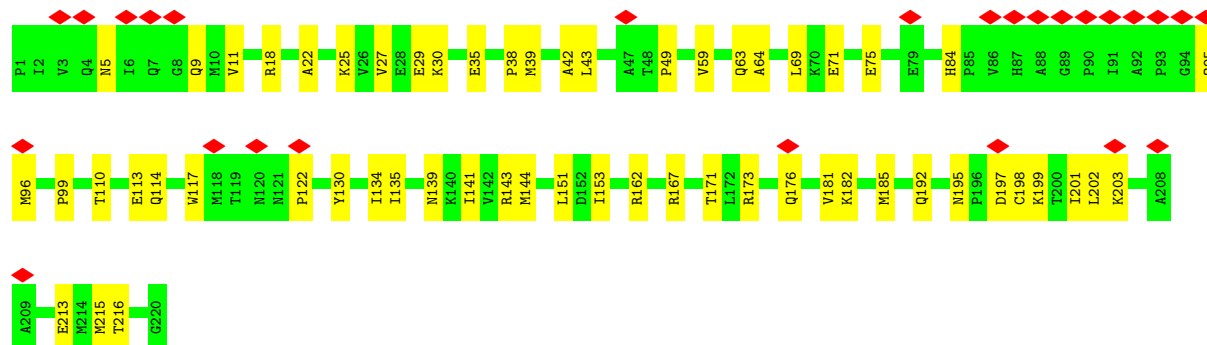
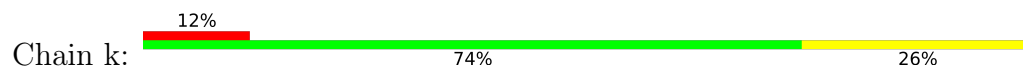
P1 Q4 N5 I6 Q7 Q8 H12 P17 L20 N21 V24 V27 F32 E35 P38 A42 A47 T48 D51 N57 T58 V59 Q60 Q63 A64 M68 T72 E79 H80 D81 R82 V83 H84 P85 V86 H87 A88 G89 P90 I91 P93 Q94



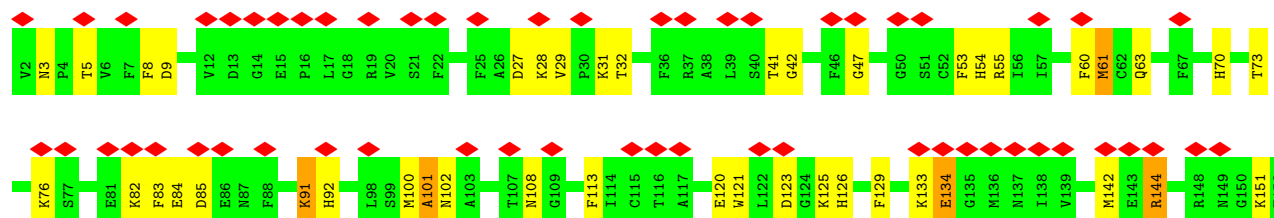
• Molecule 1: Gag-Pol polyprotein



• Molecule 1: Gag-Pol polyprotein



• Molecule 2: Peptidyl-prolyl cis-trans isomerase A



S153	K154	K155	I156	I157	I158	A159	D160	C161	G162	Q163	L164	E165
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136330	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	152.63998, 152.63998, 152.63998	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.24	0/1159	0.39	0/1578
1	B	0.27	0/1754	0.44	0/2385
1	C	2.12	3/1753 (0.2%)	1.15	7/2382 (0.3%)
1	D	0.28	0/1754	0.44	0/2385
1	G	0.21	0/1754	0.36	0/2385
1	H	0.21	0/1754	0.37	0/2385
1	N	0.13	0/594	0.29	0/803
1	Y	0.32	0/1159	0.48	0/1578
1	d	0.28	0/1754	0.44	0/2385
1	e	0.55	1/1754 (0.1%)	0.80	11/2385 (0.5%)
1	j	0.18	0/594	0.37	0/803
1	k	0.22	0/1754	0.40	0/2385
2	J	1.02	5/1286 (0.4%)	1.71	21/1723 (1.2%)
All	All	0.75	9/18823 (0.0%)	0.71	39/25562 (0.2%)

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	e	0	1
2	J	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	ARG	CA-C	61.63	2.37	1.52
1	C	18	ARG	N-CA	61.48	2.27	1.46
1	e	84	HIS	C-N	15.11	1.51	1.33
2	J	54	HIS	CD2-NE2	-7.11	1.30	1.37
2	J	70	HIS	CD2-NE2	-6.10	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	92	HIS	CD2-NE2	-6.07	1.31	1.37
1	C	98	GLU	C-N	5.48	1.40	1.33
2	J	54	HIS	CG-ND1	-5.36	1.32	1.38
2	J	126	HIS	CD2-NE2	-5.11	1.32	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ARG	N-CA-C	-39.57	64.16	113.23
1	C	18	ARG	CA-C-O	-23.31	92.00	119.27
1	e	97	ARG	CB-CA-C	9.83	133.23	111.30
1	e	84	HIS	CA-C-N	9.82	129.75	120.03
1	e	84	HIS	C-N-CA	9.82	129.75	120.03
1	e	83	VAL	CA-C-N	-9.43	112.67	122.28
1	e	83	VAL	C-N-CA	-9.43	112.67	122.28
1	e	96	MET	CA-C-N	-9.17	105.33	121.29
1	e	96	MET	C-N-CA	-9.17	105.33	121.29
1	C	17	PRO	CA-C-N	-8.35	106.97	121.66
1	C	17	PRO	C-N-CA	-8.35	106.97	121.66
1	C	97	ARG	N-CA-C	8.15	122.04	110.23
1	C	98	GLU	N-CA-C	7.02	120.32	110.07
1	C	18	ARG	N-CA-CB	-6.78	99.87	110.44
2	J	31	LYS	N-CA-CB	-6.58	100.40	110.20
1	e	84	HIS	CA-C-O	-6.56	114.77	121.07
2	J	8	PHE	CA-CB-CG	6.52	120.32	113.80
2	J	102	ASN	CA-CB-CG	6.21	118.81	112.60
2	J	83	PHE	CA-CB-CG	6.20	120.00	113.80
2	J	85	ASP	N-CA-C	-6.14	99.86	109.25
2	J	3	ASN	CA-C-N	6.09	126.44	119.92
2	J	3	ASN	C-N-CA	6.09	126.44	119.92
1	e	89	GLY	CA-C-N	-5.93	113.65	119.76
1	e	89	GLY	C-N-CA	-5.93	113.65	119.76
2	J	134	GLU	O-C-N	-5.72	115.75	123.19
2	J	53	PHE	CA-CB-CG	-5.71	108.09	113.80
2	J	134	GLU	CB-CG-CD	5.70	122.30	112.60
2	J	133	LYS	N-CA-C	-5.67	104.37	112.13
1	e	101	GLY	N-CA-C	-5.49	106.14	112.73
2	J	101	ALA	N-CA-C	-5.47	102.43	110.52
2	J	9	ASP	N-CA-C	-5.39	99.95	108.73
2	J	158	ILE	N-CA-CB	-5.35	106.87	112.06
2	J	144	ARG	CB-CG-CD	-5.34	99.02	111.30
2	J	113	PHE	CA-CB-CG	5.26	119.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	32	THR	CA-CB-OG1	-5.12	101.92	109.60
2	J	47	GLY	N-CA-C	5.12	117.75	110.74
2	J	31	LYS	CA-CB-CG	5.11	124.31	114.10
2	J	31	LYS	N-CA-C	-5.05	105.48	111.69
2	J	42	GLY	N-CA-C	-5.00	108.35	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	60	PHE	Sidechain
1	e	97	ARG	Mainchain

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	1132	0	1132	18	0
1	B	1716	0	1715	59	0
1	C	1716	0	1714	68	0
1	D	1716	0	1715	63	0
1	G	1716	0	1715	58	0
1	H	1716	0	1715	53	0
1	N	584	0	583	25	0
1	Y	1132	0	1132	24	0
1	d	1716	0	1715	47	0
1	e	1716	0	1715	73	0
1	j	584	0	583	17	0
1	k	1716	0	1713	76	0
2	J	1258	0	1225	32	0
All	All	18418	0	18372	446	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 12.

All (446) 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:B:151:LEU:HD11	1:j:151:LEU:CD1	1.37	1.54
1:B:151:LEU:CD1	1:j:151:LEU:HD12	1.49	1.42
1:G:192:GLN:OE1	1:d:151:LEU:CD1	1.75	1.32
1:B:151:LEU:CD1	1:j:151:LEU:CD1	2.03	1.28
1:D:68:MET:SD	1:D:144:MET:HE1	1.75	1.26
1:Y:68:MET:SD	1:Y:144:MET:HE1	1.75	1.26
1:G:6:ILE:HG13	1:k:11:VAL:CG1	1.66	1.25
1:d:68:MET:SD	1:d:144:MET:HE1	1.75	1.25
1:N:151:LEU:HD11	1:e:151:LEU:CD1	1.70	1.20
1:G:192:GLN:OE1	1:d:151:LEU:HD12	1.05	1.18
1:d:68:MET:HE3	1:j:212:GLU:HB3	1.26	1.17
1:N:151:LEU:HD12	1:e:151:LEU:HD12	1.22	1.17
1:N:151:LEU:CD1	1:e:151:LEU:CD1	2.22	1.16
1:G:6:ILE:HG13	1:k:11:VAL:HG11	1.17	1.12
1:e:35:GLU:O	1:e:38:PRO:HD2	1.50	1.11
1:B:151:LEU:HD12	1:j:151:LEU:HD12	1.11	1.09
1:N:151:LEU:CD1	1:e:151:LEU:HD12	1.82	1.07
1:B:87:HIS:ND1	2:J:73:THR:CG2	2.17	1.06
1:N:151:LEU:CD1	1:e:151:LEU:HD11	1.87	1.01
1:G:151:LEU:HD21	1:d:184:TRP:HH2	1.22	1.00
1:N:151:LEU:HD11	1:e:151:LEU:HD11	1.02	0.99
1:C:18:ARG:C	1:C:18:ARG:CA	2.37	0.98
1:D:184:TRP:CG	1:H:181:VAL:HG11	1.98	0.98
2:J:76:LYS:NZ	1:k:84:HIS:HE1	1.61	0.97
1:C:18:ARG:CA	1:C:18:ARG:N	2.27	0.96
2:J:76:LYS:HZ1	1:k:84:HIS:HE1	0.99	0.96
1:C:147:PRO:C	1:C:148:THR:N	2.24	0.96
1:G:192:GLN:CD	1:d:151:LEU:HD12	1.91	0.96
2:J:41:THR:O	1:k:122:PRO:HG3	1.64	0.96
1:B:90:PRO:CG	2:J:61:MET:HE2	1.94	0.95
1:d:35:GLU:O	1:d:38:PRO:HD2	1.66	0.95
1:B:90:PRO:HD2	2:J:63:GLN:OE1	1.66	0.95
1:D:35:GLU:O	1:D:38:PRO:HD2	1.66	0.94
1:Y:35:GLU:O	1:Y:38:PRO:HD2	1.66	0.94
1:e:63:GLN:HE22	1:k:173:ARG:HH11	1.16	0.92
1:B:90:PRO:HG3	2:J:61:MET:HE2	1.49	0.92
1:B:144:MET:HE1	1:C:215:MET:SD	2.09	0.92
1:B:87:HIS:ND1	2:J:73:THR:HG22	1.85	0.91
1:G:151:LEU:HD21	1:d:184:TRP:CH2	2.05	0.91
1:B:151:LEU:CD1	1:j:151:LEU:HD11	1.86	0.91
1:Y:35:GLU:C	1:Y:38:PRO:HD2	1.96	0.91
1:D:35:GLU:C	1:D:38:PRO:HD2	1.96	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HD11	1:j:151:LEU:HD11	0.91	0.90
1:D:151:LEU:HD21	1:H:184:TRP:CH2	2.07	0.90
1:d:35:GLU:C	1:d:38:PRO:HD2	1.96	0.90
1:D:154:ARG:HH22	1:H:154:ARG:NH2	1.71	0.89
1:Y:68:MET:SD	1:Y:144:MET:CE	2.61	0.89
1:d:68:MET:SD	1:d:144:MET:CE	2.61	0.89
1:D:184:TRP:CD1	1:H:181:VAL:HG11	2.07	0.88
1:C:25:LYS:O	1:C:29:GLU:HG3	1.74	0.88
1:D:68:MET:SD	1:D:144:MET:CE	2.61	0.88
1:G:151:LEU:HD12	1:d:192:GLN:OE1	1.73	0.88
1:N:181:VAL:HG21	1:e:180:GLU:OE1	1.73	0.87
1:G:6:ILE:HG13	1:k:11:VAL:HG12	1.55	0.87
1:G:104:ILE:HG13	1:G:126:VAL:HG23	1.57	0.86
2:J:76:LYS:HZ1	1:k:84:HIS:CE1	1.90	0.86
1:H:104:ILE:HG13	1:H:126:VAL:HG23	1.57	0.86
1:A:104:ILE:HG13	1:A:126:VAL:HG23	1.57	0.86
1:D:154:ARG:NH2	1:H:154:ARG:HH22	1.72	0.86
1:H:68:MET:SD	1:N:212:GLU:HB3	2.16	0.85
1:C:18:ARG:HH21	1:D:18:ARG:NH1	1.75	0.85
1:D:154:ARG:NH2	1:H:154:ARG:NH2	2.25	0.84
1:G:30:LYS:HD3	1:G:35:GLU:OE2	1.77	0.83
1:H:30:LYS:HD3	1:H:35:GLU:OE2	1.77	0.83
1:A:30:LYS:HD3	1:A:35:GLU:OE2	1.77	0.82
1:D:151:LEU:HD21	1:H:184:TRP:HH2	1.44	0.82
1:C:143:ARG:NH2	1:C:176:GLN:O	2.12	0.81
1:C:25:LYS:HB3	1:C:29:GLU:OE2	1.81	0.81
1:G:173:ARG:NH1	1:k:63:GLN:HE22	1.78	0.81
1:N:181:VAL:CG2	1:e:180:GLU:OE1	2.28	0.81
1:G:151:LEU:CD1	1:d:192:GLN:OE1	2.28	0.80
1:G:192:GLN:OE1	1:d:151:LEU:HD13	1.82	0.80
2:J:5:THR:HB	2:J:165:GLU:HG2	1.65	0.78
2:J:76:LYS:NZ	1:k:84:HIS:CE1	2.49	0.78
1:e:144:MET:HE1	1:k:215:MET:SD	2.23	0.78
1:C:151:LEU:HD21	1:k:192:GLN:OE1	1.85	0.77
1:N:181:VAL:HG23	1:e:180:GLU:OE2	1.85	0.77
1:D:151:LEU:HD12	1:H:192:GLN:OE1	1.85	0.77
1:e:35:GLU:C	1:e:38:PRO:HD2	2.10	0.77
1:D:180:GLU:OE2	1:H:180:GLU:HB3	1.85	0.76
1:B:90:PRO:HG2	2:J:61:MET:HE2	1.65	0.76
1:d:68:MET:CE	1:j:212:GLU:HB3	2.13	0.76
1:e:100:ARG:H	1:e:103:ASP:HB2	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LEU:CD2	1:k:192:GLN:OE1	2.34	0.75
1:D:180:GLU:OE1	1:H:181:VAL:HG23	1.85	0.74
1:D:180:GLU:OE1	1:H:181:VAL:CG2	2.35	0.73
1:C:18:ARG:C	1:C:18:ARG:N	2.47	0.73
1:B:90:PRO:HG2	2:J:61:MET:CE	2.18	0.73
1:C:18:ARG:NH2	1:D:18:ARG:NH1	2.37	0.73
1:D:151:LEU:CD1	1:H:192:GLN:OE1	2.37	0.73
1:B:87:HIS:ND1	2:J:73:THR:HG23	2.04	0.72
1:G:6:ILE:CG1	1:k:11:VAL:CG1	2.60	0.72
1:H:211:LEU:HG	1:H:215:MET:HE2	1.72	0.72
1:G:211:LEU:HG	1:G:215:MET:HE2	1.72	0.71
1:e:17:PRO:HB3	1:k:43:LEU:HD23	1.71	0.70
1:k:25:LYS:O	1:k:29:GLU:HG3	1.91	0.70
1:G:173:ARG:HD2	1:k:63:GLN:NE2	2.06	0.69
1:j:202:LEU:HD22	1:j:214:MET:HB3	1.74	0.69
1:e:202:LEU:HD22	1:e:214:MET:HB3	1.74	0.69
1:B:48:THR:HG22	1:B:118:MET:HE1	1.75	0.68
1:G:173:ARG:HH11	1:k:63:GLN:NE2	1.92	0.68
1:G:173:ARG:HH11	1:k:63:GLN:HE22	1.39	0.68
1:B:63:GLN:HE22	1:C:173:ARG:HH11	1.41	0.68
1:C:68:MET:HE3	1:D:212:GLU:HB3	1.76	0.68
1:e:97:ARG:C	1:e:117:TRP:HE1	2.02	0.68
1:B:90:PRO:HG2	2:J:55:ARG:HH12	1.58	0.67
1:D:211:LEU:HG	1:D:215:MET:HE2	1.77	0.67
1:d:211:LEU:HG	1:d:215:MET:HE2	1.77	0.66
1:C:192:GLN:HE22	1:k:151:LEU:HD21	1.61	0.66
1:e:48:THR:HG22	1:e:118:MET:HE1	1.75	0.66
1:e:100:ARG:N	1:e:103:ASP:HB2	2.11	0.65
1:C:192:GLN:NE2	1:k:151:LEU:HD21	2.12	0.65
1:C:99:PRO:HG3	1:C:117:TRP:CE2	2.30	0.65
1:B:90:PRO:HG2	2:J:55:ARG:NH1	2.12	0.65
1:C:57:ASN:O	1:D:173:ARG:NH2	2.29	0.64
2:J:41:THR:O	1:k:122:PRO:CG	2.42	0.64
1:C:198:CYS:O	1:C:202:LEU:HG	1.97	0.64
1:G:6:ILE:CG1	1:k:11:VAL:HG12	2.27	0.64
1:d:68:MET:HE3	1:j:212:GLU:CB	2.16	0.64
1:e:63:GLN:HE22	1:k:173:ARG:NH1	1.92	0.64
1:D:151:LEU:HD13	1:H:189:LEU:HD23	1.80	0.63
1:C:213:GLU:HA	1:C:216:THR:HG22	1.79	0.63
1:k:198:CYS:O	1:k:202:LEU:HG	1.99	0.62
1:d:34:PRO:HB2	1:d:173:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:PRO:HB2	1:D:173:ARG:HD3	1.82	0.62
1:k:213:GLU:HA	1:k:216:THR:HG22	1.80	0.62
1:N:181:VAL:CG2	1:e:180:GLU:CD	2.72	0.62
1:C:18:ARG:NH2	1:D:18:ARG:HH12	1.98	0.62
1:G:154:ARG:HH22	1:d:154:ARG:NH2	1.97	0.62
1:C:18:ARG:HH21	1:D:18:ARG:HH11	1.48	0.62
1:C:204:ALA:HB1	1:j:204:ALA:HB1	1.81	0.61
1:G:211:LEU:HD21	1:k:64:ALA:HB1	1.80	0.61
1:C:17:PRO:HB3	1:D:43:LEU:CD2	2.31	0.61
1:e:98:GLU:N	1:e:117:TRP:HE1	1.99	0.61
1:G:154:ARG:NH2	1:d:154:ARG:NH2	2.49	0.60
1:H:64:ALA:HB1	1:N:211:LEU:HD21	1.82	0.60
2:J:142:MET:HE3	2:J:156:ILE:HG21	1.83	0.60
1:k:198:CYS:HA	1:k:201:ILE:HD12	1.84	0.60
1:C:198:CYS:HA	1:C:201:ILE:HD12	1.82	0.60
1:G:154:ARG:NH2	1:d:154:ARG:HH22	1.99	0.60
1:G:215:MET:HE1	1:k:144:MET:SD	2.42	0.59
1:C:28:GLU:HA	1:C:28:GLU:OE1	2.03	0.59
1:D:154:ARG:HH22	1:H:154:ARG:HH21	1.50	0.59
1:D:151:LEU:HD21	1:H:184:TRP:CZ2	2.37	0.59
1:G:215:MET:CE	1:k:144:MET:SD	2.91	0.58
1:G:6:ILE:CG1	1:k:11:VAL:HG11	2.12	0.58
1:k:110:THR:O	1:k:114:GLN:NE2	2.37	0.58
1:B:37:ILE:HB	1:B:38:PRO:HD3	1.85	0.58
1:e:27:VAL:HG11	1:e:59:VAL:HG23	1.85	0.57
1:D:189:LEU:HD23	1:H:151:LEU:HD13	1.85	0.57
1:C:181:VAL:HG22	1:k:181:VAL:HG22	1.85	0.57
1:k:135:ILE:O	1:k:139:ASN:ND2	2.37	0.57
1:C:135:ILE:O	1:C:139:ASN:ND2	2.36	0.57
1:e:1:PRO:HB3	1:e:47:ALA:HA	1.86	0.57
1:B:90:PRO:CG	2:J:55:ARG:HH12	2.17	0.57
1:C:63:GLN:NE2	1:D:173:ARG:HD2	2.19	0.57
1:B:1:PRO:HB3	1:B:47:ALA:HA	1.87	0.56
1:j:198:CYS:O	1:j:202:LEU:HG	2.05	0.56
1:B:89:GLY:HA2	2:J:101:ALA:HB1	1.86	0.56
1:d:181:VAL:O	1:d:185:MET:HG2	2.06	0.56
1:e:155:GLN:NE2	1:e:159:GLU:O	2.35	0.56
1:j:155:GLN:NE2	1:j:159:GLU:O	2.35	0.56
1:G:151:LEU:HD12	1:d:192:GLN:CD	2.29	0.56
1:B:17:PRO:HB3	1:C:43:LEU:HD23	1.88	0.56
1:C:202:LEU:HD13	1:C:214:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:198:CYS:O	1:e:202:LEU:HG	2.05	0.55
1:B:179:GLN:NE2	1:B:183:ASN:OD1	2.40	0.55
1:e:21:ASN:HD21	1:k:22:ALA:HB1	1.71	0.55
1:B:24:VAL:HG11	1:C:30:LYS:HZ2	1.71	0.55
1:C:5:ASN:CB	1:D:6:ILE:HG21	2.36	0.55
1:D:181:VAL:O	1:D:185:MET:HG2	2.06	0.55
1:B:90:PRO:HD2	2:J:55:ARG:NH1	2.22	0.54
1:k:197:ASP:O	1:k:201:ILE:HG13	2.07	0.54
1:B:144:MET:HE1	1:C:215:MET:CE	2.38	0.54
1:C:110:THR:O	1:C:114:GLN:NE2	2.40	0.54
1:N:179:GLN:NE2	1:N:183:ASN:OD1	2.40	0.54
1:d:104:ILE:HG13	1:d:126:VAL:HG23	1.89	0.54
1:D:104:ILE:HG13	1:D:126:VAL:HG23	1.90	0.54
1:k:199:LYS:O	1:k:203:LYS:HG2	2.08	0.54
1:D:100:ARG:O	1:D:104:ILE:N	2.33	0.54
1:N:181:VAL:HG23	1:e:180:GLU:CD	2.33	0.54
1:e:179:GLN:OE1	1:e:183:ASN:ND2	2.38	0.54
1:e:196:PRO:HA	1:e:199:LYS:HB3	1.90	0.54
1:N:181:VAL:CG2	1:e:180:GLU:OE2	2.55	0.53
1:Y:104:ILE:HG13	1:Y:126:VAL:HG23	1.90	0.53
1:C:197:ASP:O	1:C:201:ILE:HG13	2.08	0.53
1:j:196:PRO:HA	1:j:199:LYS:HB3	1.90	0.53
1:D:151:LEU:HD12	1:H:192:GLN:CD	2.33	0.53
1:e:135:ILE:O	1:e:139:ASN:ND2	2.41	0.53
1:k:95:GLN:HE21	1:k:96:MET:H	1.56	0.53
1:B:60:GLY:HA3	1:C:35:GLU:CD	2.33	0.53
1:B:90:PRO:CD	2:J:55:ARG:HH12	2.22	0.53
1:D:184:TRP:CD2	1:H:181:VAL:HG11	2.42	0.53
1:e:96:MET:SD	1:e:96:MET:N	2.81	0.53
1:D:184:TRP:CG	1:H:181:VAL:CG1	2.83	0.53
1:N:185:MET:HE2	1:e:184:TRP:CH2	2.44	0.53
1:e:100:ARG:HG2	1:e:101:GLY:N	2.24	0.53
1:G:151:LEU:HD13	1:d:192:GLN:OE1	2.07	0.52
1:Y:100:ARG:O	1:Y:104:ILE:N	2.33	0.52
1:d:48:THR:HG22	1:d:118:MET:HE1	1.92	0.52
1:D:48:THR:HG22	1:D:118:MET:HE1	1.92	0.52
1:D:68:MET:HE1	1:D:144:MET:CE	2.40	0.52
1:H:68:MET:CE	1:N:212:GLU:HB3	2.39	0.52
1:Y:48:THR:HG22	1:Y:118:MET:HE1	1.92	0.52
1:Y:68:MET:HE1	1:Y:144:MET:CE	2.40	0.52
1:e:60:GLY:HA2	1:k:35:GLU:CD	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PRO:HG3	1:B:117:TRP:CE2	2.45	0.52
1:d:68:MET:HE1	1:d:144:MET:CE	2.40	0.52
1:j:179:GLN:OE1	1:j:183:ASN:ND2	2.38	0.52
1:Y:20:LEU:CD1	1:e:42:ALA:HB1	2.40	0.51
1:Y:68:MET:CE	1:Y:144:MET:CE	2.88	0.51
1:d:68:MET:CE	1:d:144:MET:CE	2.89	0.51
1:G:173:ARG:NH1	1:k:63:GLN:NE2	2.50	0.51
1:k:99:PRO:HG3	1:k:117:TRP:CE2	2.46	0.51
1:D:68:MET:CE	1:D:144:MET:CE	2.89	0.51
1:e:99:PRO:HG3	1:e:124:ILE:HG21	1.93	0.51
1:k:143:ARG:NH2	1:k:176:GLN:O	2.41	0.51
1:e:95:GLN:C	1:e:96:MET:SD	2.94	0.51
1:B:195:ASN:O	1:B:199:LYS:N	2.40	0.51
1:Y:68:MET:HE3	1:e:212:GLU:HB3	1.93	0.51
1:e:24:VAL:HG13	1:k:30:LYS:HZ1	1.76	0.51
1:B:90:PRO:CD	2:J:63:GLN:OE1	2.48	0.50
1:G:151:LEU:HD13	1:d:189:LEU:HD23	1.92	0.50
1:C:151:LEU:HD22	1:k:192:GLN:OE1	2.10	0.50
1:B:60:GLY:CA	1:C:35:GLU:CD	2.85	0.50
1:d:100:ARG:O	1:d:104:ILE:N	2.33	0.50
1:D:189:LEU:HA	1:D:192:GLN:HB2	1.94	0.50
1:N:151:LEU:HD12	1:e:151:LEU:CD1	1.99	0.50
1:e:80:TRP:CZ3	1:e:129:ILE:HD13	2.47	0.50
1:H:183:ASN:O	1:H:187:GLU:HG3	2.12	0.50
1:B:157:PRO:O	1:B:195:ASN:ND2	2.45	0.49
1:Y:47:ALA:HB1	1:Y:51:ASP:HB2	1.94	0.49
1:d:35:GLU:O	1:d:38:PRO:CD	2.51	0.49
1:H:109:SER:OG	1:H:110:THR:N	2.45	0.49
1:k:25:LYS:HB3	1:k:29:GLU:OE2	2.13	0.49
1:D:47:ALA:HB1	1:D:51:ASP:HB2	1.94	0.49
1:d:47:ALA:HB1	1:d:51:ASP:HB2	1.94	0.49
1:G:184:TRP:CG	1:d:181:VAL:HG11	2.47	0.49
1:d:189:LEU:HA	1:d:192:GLN:HB2	1.94	0.49
1:N:157:PRO:O	1:N:195:ASN:ND2	2.45	0.49
1:e:83:VAL:HG12	1:e:83:VAL:O	2.12	0.49
1:e:168:PHE:HE1	1:e:189:LEU:HD23	1.78	0.49
1:k:5:ASN:OD1	1:k:9:GLN:N	2.46	0.49
1:C:72:THR:O	1:C:76:GLU:HG2	2.12	0.49
1:e:24:VAL:HG13	1:k:30:LYS:NZ	2.28	0.49
1:k:153:ILE:HD11	1:k:171:THR:HG21	1.93	0.49
1:G:202:LEU:HD22	1:G:214:MET:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:LEU:HD22	1:H:214:MET:HG2	1.95	0.49
1:C:181:VAL:HG13	1:k:181:VAL:HG13	1.93	0.49
1:G:109:SER:OG	1:G:110:THR:N	2.45	0.48
1:e:24:VAL:HG11	1:k:30:LYS:HZ2	1.77	0.48
1:C:27:VAL:HG11	1:C:59:VAL:HG13	1.95	0.48
1:e:97:ARG:CA	1:e:117:TRP:HE1	2.26	0.48
1:k:69:LEU:HB2	1:k:141:ILE:HD11	1.96	0.48
1:B:24:VAL:CG1	1:C:30:LYS:NZ	2.76	0.48
1:e:20:LEU:CD1	1:k:42:ALA:CB	2.91	0.48
1:G:183:ASN:O	1:G:187:GLU:HG3	2.12	0.48
1:j:168:PHE:HE1	1:j:189:LEU:HD23	1.78	0.48
1:B:135:ILE:O	1:B:139:ASN:ND2	2.46	0.48
1:A:109:SER:OG	1:A:110:THR:N	2.45	0.48
1:e:17:PRO:HB3	1:k:43:LEU:CD2	2.40	0.48
1:e:72:THR:HG21	1:e:140:LYS:HD2	1.95	0.48
1:H:47:ALA:HB1	1:H:51:ASP:HB2	1.95	0.47
1:A:47:ALA:HB1	1:A:51:ASP:HB2	1.95	0.47
1:d:24:VAL:HA	1:d:27:VAL:HG12	1.96	0.47
1:D:24:VAL:HA	1:D:27:VAL:HG12	1.96	0.47
1:e:144:MET:HE2	1:k:162:ARG:HH21	1.79	0.47
1:C:153:ILE:HD11	1:C:171:THR:HG21	1.96	0.47
1:H:48:THR:HG22	1:H:118:MET:HE1	1.96	0.47
1:Y:131:LYS:HB2	1:Y:131:LYS:HE3	1.67	0.47
1:C:195:ASN:O	1:C:199:LYS:N	2.41	0.47
1:C:216:THR:HA	1:C:219:GLN:HE21	1.79	0.47
1:G:165:VAL:HG21	1:G:211:LEU:HD11	1.97	0.47
1:G:23:TRP:NE1	1:G:55:MET:O	2.47	0.47
1:G:47:ALA:HB1	1:G:51:ASP:HB2	1.96	0.47
1:H:165:VAL:HG21	1:H:211:LEU:HD11	1.97	0.47
1:B:24:VAL:HG11	1:C:30:LYS:NZ	2.29	0.47
1:B:47:ALA:HB1	1:B:51:ASP:HB2	1.97	0.47
1:A:48:THR:HG22	1:A:118:MET:HE1	1.96	0.46
1:G:48:THR:HG22	1:G:118:MET:HE1	1.96	0.46
1:H:30:LYS:CD	1:H:35:GLU:OE2	2.58	0.46
1:Y:24:VAL:HA	1:Y:27:VAL:HG12	1.96	0.46
1:e:24:VAL:CG1	1:k:30:LYS:NZ	2.78	0.46
1:B:20:LEU:CD1	1:C:42:ALA:CB	2.93	0.46
1:C:151:LEU:HD21	1:k:192:GLN:CD	2.39	0.46
1:D:131:LYS:HE3	1:D:131:LYS:HB2	1.66	0.46
1:B:86:VAL:HG21	1:B:100:ARG:HA	1.98	0.46
1:A:23:TRP:NE1	1:A:55:MET:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:THR:HG21	1:B:140:LYS:HD2	1.96	0.46
1:B:90:PRO:CD	2:J:55:ARG:NH1	2.78	0.46
1:e:95:GLN:HA	1:e:95:GLN:OE1	2.14	0.46
1:G:184:TRP:CD2	1:d:181:VAL:HG11	2.51	0.46
1:N:195:ASN:O	1:N:199:LYS:N	2.40	0.46
1:D:110:THR:HG23	1:D:112:GLN:H	1.81	0.46
1:G:18:ARG:NH1	1:k:18:ARG:HD3	2.30	0.46
1:e:47:ALA:HB1	1:e:51:ASP:HB2	1.97	0.46
1:e:58:THR:HG22	1:k:39:MET:HG3	1.97	0.46
1:k:27:VAL:HG11	1:k:59:VAL:HG13	1.97	0.46
1:C:197:ASP:OD1	1:C:198:CYS:N	2.45	0.46
2:J:121:TRP:O	2:J:125:LYS:NZ	2.47	0.46
1:B:59:VAL:HG11	1:B:66:MET:HE3	1.97	0.46
1:G:110:THR:O	1:G:114:GLN:HG2	2.16	0.46
1:Y:110:THR:HG23	1:Y:112:GLN:H	1.81	0.46
1:d:110:THR:HG23	1:d:112:GLN:H	1.81	0.46
1:D:151:LEU:HD13	1:H:192:GLN:OE1	2.16	0.46
1:H:131:LYS:HB2	1:H:131:LYS:HE3	1.68	0.45
1:k:130:TYR:CE2	1:k:134:ILE:HD11	2.51	0.45
1:A:110:THR:O	1:A:114:GLN:HG2	2.16	0.45
1:C:199:LYS:O	1:C:203:LYS:HG3	2.16	0.45
1:G:30:LYS:CD	1:G:35:GLU:OE2	2.58	0.45
1:e:85:PRO:HG2	1:e:87:HIS:NE2	2.31	0.45
1:A:30:LYS:CD	1:A:35:GLU:OE2	2.58	0.45
1:D:151:LEU:HD13	1:H:189:LEU:CD2	2.46	0.45
2:J:100:MET:HG2	2:J:129:PHE:CE1	2.51	0.45
1:G:18:ARG:NH1	1:k:18:ARG:HH21	2.14	0.45
1:H:110:THR:O	1:H:114:GLN:HG2	2.16	0.45
1:d:101:GLY:O	1:d:104:ILE:HG22	2.17	0.45
1:D:184:TRP:CZ3	1:H:184:TRP:CZ3	3.05	0.45
1:H:23:TRP:NE1	1:H:55:MET:O	2.47	0.45
1:e:58:THR:HG22	1:k:39:MET:CG	2.47	0.44
2:J:27:ASP:OD2	2:J:28:LYS:NZ	2.51	0.44
1:N:155:GLN:OE1	1:N:195:ASN:N	2.48	0.44
1:C:167:ARG:O	1:C:171:THR:HG22	2.17	0.44
1:H:23:TRP:O	1:H:27:VAL:HG23	2.17	0.44
1:Y:101:GLY:O	1:Y:104:ILE:HG22	2.17	0.44
1:B:87:HIS:CE1	2:J:73:THR:CG2	2.95	0.44
1:G:181:VAL:HG11	1:d:184:TRP:CG	2.52	0.44
1:H:64:ALA:CB	1:N:211:LEU:HD21	2.48	0.44
1:k:49:PRO:HD2	1:k:114:GLN:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:HH21	1:C:176:GLN:C	2.24	0.44
1:D:101:GLY:O	1:D:104:ILE:HG22	2.17	0.44
1:C:25:LYS:O	1:C:29:GLU:CG	2.55	0.44
1:G:23:TRP:O	1:G:27:VAL:HG23	2.17	0.44
1:G:172:LEU:HG	1:G:182:LYS:HE3	2.00	0.44
1:H:159:GLU:OE1	1:H:167:ARG:NH1	2.51	0.43
1:e:24:VAL:CG1	1:k:30:LYS:HZ2	2.31	0.43
1:A:23:TRP:O	1:A:27:VAL:HG23	2.17	0.43
1:C:83:VAL:HG13	1:C:84:HIS:ND1	2.34	0.43
1:G:159:GLU:OE1	1:G:167:ARG:NH1	2.51	0.43
1:d:131:LYS:HE3	1:d:131:LYS:HB2	1.67	0.43
1:e:64:ALA:O	1:e:68:MET:HG3	2.19	0.43
1:B:63:GLN:HE22	1:C:173:ARG:NH1	2.13	0.43
1:D:184:TRP:CD2	1:H:181:VAL:CG1	3.02	0.43
1:e:6:ILE:HA	1:e:7:GLN:HA	1.47	0.43
1:B:155:GLN:OE1	1:B:195:ASN:N	2.48	0.43
1:C:17:PRO:HB3	1:D:43:LEU:HD21	2.00	0.43
1:C:192:GLN:CD	1:k:151:LEU:HD21	2.43	0.43
1:G:181:VAL:HG11	1:d:184:TRP:CD1	2.54	0.43
1:d:172:LEU:HG	1:d:182:LYS:HE3	2.00	0.43
1:k:182:LYS:HA	1:k:185:MET:HE3	2.01	0.43
2:J:41:THR:O	1:k:122:PRO:CB	2.66	0.43
1:A:37:ILE:HB	1:A:38:PRO:HD3	2.01	0.43
1:B:24:VAL:CG1	1:C:30:LYS:HZ1	2.32	0.43
1:G:131:LYS:HB2	1:G:131:LYS:HE3	1.69	0.43
1:H:172:LEU:HG	1:H:182:LYS:HE3	2.01	0.43
1:k:110:THR:HG23	1:k:113:GLU:H	1.84	0.43
1:A:52:LEU:HD12	1:A:130:TYR:HD2	1.84	0.42
1:D:172:LEU:HG	1:D:182:LYS:HE3	2.01	0.42
1:G:37:ILE:HB	1:G:38:PRO:HD3	2.01	0.42
1:B:31:ALA:O	1:B:36:VAL:HG11	2.19	0.42
1:G:52:LEU:HD12	1:G:130:TYR:HD2	1.84	0.42
1:D:184:TRP:CZ2	1:H:185:MET:SD	3.12	0.42
1:e:57:ASN:HB3	1:k:38:PRO:CG	2.49	0.42
1:e:144:MET:HG2	1:k:162:ARG:NH2	2.34	0.42
1:e:20:LEU:HD23	1:e:20:LEU:HA	1.89	0.42
1:e:99:PRO:HB2	1:e:104:ILE:CG1	2.49	0.42
1:C:161:PHE:HE2	1:C:215:MET:HG2	1.84	0.42
1:G:35:GLU:C	1:G:38:PRO:HD2	2.45	0.42
1:H:37:ILE:HB	1:H:38:PRO:HD3	2.01	0.42
1:H:52:LEU:HD12	1:H:130:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:198:CYS:O	1:N:202:LEU:HG	2.19	0.42
1:C:76:GLU:HA	1:C:76:GLU:OE1	2.20	0.42
1:k:197:ASP:OD1	1:k:198:CYS:N	2.45	0.42
1:A:35:GLU:C	1:A:38:PRO:HD2	2.45	0.42
1:B:161:PHE:O	1:B:165:VAL:HG12	2.20	0.42
1:D:180:GLU:OE1	1:H:181:VAL:HG22	2.18	0.42
2:J:91:LYS:HZ3	2:J:123:ASP:HB3	1.85	0.42
1:e:100:ARG:NH1	1:e:103:ASP:OD2	2.51	0.42
1:B:198:CYS:O	1:B:202:LEU:HG	2.19	0.42
1:N:161:PHE:O	1:N:165:VAL:HG12	2.20	0.42
1:A:6:ILE:HD12	1:A:6:ILE:H	1.84	0.42
1:D:96:MET:HB3	1:D:117:TRP:HE1	1.85	0.42
1:H:6:ILE:HD12	1:H:6:ILE:H	1.84	0.42
1:Y:35:GLU:O	1:Y:38:PRO:CD	2.52	0.42
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.80	0.41
1:B:6:ILE:HA	1:B:7:GLN:HA	1.47	0.41
1:B:35:GLU:C	1:B:38:PRO:HD2	2.44	0.41
1:H:20:LEU:HA	1:H:20:LEU:HD23	1.80	0.41
1:H:35:GLU:C	1:H:38:PRO:HD2	2.44	0.41
1:Y:96:MET:HB3	1:Y:117:TRP:HE1	1.85	0.41
1:k:167:ARG:O	1:k:171:THR:HG22	2.19	0.41
1:G:6:ILE:HD12	1:G:6:ILE:H	1.84	0.41
1:B:24:VAL:HG13	1:C:30:LYS:HZ1	1.85	0.41
1:C:130:TYR:CE2	1:C:134:ILE:HD11	2.55	0.41
1:Y:23:TRP:NE1	1:Y:55:MET:O	2.53	0.41
1:Y:130:TYR:CE2	1:Y:134:ILE:HD11	2.56	0.41
1:e:12:HIS:CE1	1:e:111:LEU:HD21	2.55	0.41
1:e:60:GLY:HA2	1:k:35:GLU:OE2	2.21	0.41
1:e:158:LYS:HD2	1:e:158:LYS:HA	1.83	0.41
1:k:71:GLU:O	1:k:75:GLU:HG2	2.19	0.41
1:k:195:ASN:O	1:k:199:LYS:N	2.41	0.41
2:J:82:LYS:HA	2:J:108:ASN:O	2.21	0.41
1:e:161:PHE:O	1:e:165:VAL:HG12	2.19	0.41
1:Y:52:LEU:HD12	1:Y:130:TYR:HD2	1.85	0.41
1:d:130:TYR:CE2	1:d:134:ILE:HD11	2.56	0.41
1:e:100:ARG:HG2	1:e:101:GLY:H	1.84	0.41
1:j:161:PHE:O	1:j:165:VAL:HG12	2.19	0.41
1:C:182:LYS:HA	1:C:185:MET:HE3	2.02	0.41
1:C:210:THR:O	1:C:214:MET:HB2	2.21	0.41
1:B:27:VAL:HG12	1:B:27:VAL:O	2.21	0.41
1:D:23:TRP:NE1	1:D:55:MET:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:35:GLU:CA	1:Y:38:PRO:HD2	2.50	0.41
1:d:52:LEU:HD12	1:d:130:TYR:HD2	1.85	0.41
1:D:52:LEU:HD12	1:D:130:TYR:HD2	1.85	0.41
1:B:182:LYS:O	1:B:186:THR:HG22	2.21	0.41
1:D:130:TYR:CE2	1:D:134:ILE:HD11	2.56	0.41
1:G:101:GLY:HA2	1:G:104:ILE:HG22	2.03	0.41
1:Y:109:SER:OG	1:Y:110:THR:N	2.54	0.41
1:d:23:TRP:NE1	1:d:55:MET:O	2.53	0.41
1:d:149:SER:OG	1:d:150:ILE:N	2.54	0.41
1:A:131:LYS:HB2	1:A:131:LYS:HE3	1.69	0.41
1:C:5:ASN:OD1	1:C:9:GLN:N	2.54	0.41
1:C:5:ASN:HB3	1:D:6:ILE:HG21	2.02	0.41
1:D:109:SER:OG	1:D:110:THR:N	2.54	0.41
1:d:96:MET:HB3	1:d:117:TRP:HE1	1.85	0.41
1:G:20:LEU:HD23	1:G:20:LEU:HA	1.80	0.40
1:G:54:THR:O	1:G:58:THR:HG23	2.21	0.40
1:Y:104:ILE:CG1	1:Y:126:VAL:HG23	2.51	0.40
1:e:99:PRO:HG3	1:e:124:ILE:CG2	2.51	0.40
1:A:68:MET:SD	1:B:212:GLU:HB3	2.61	0.40
1:C:20:LEU:HD11	1:D:42:ALA:HB1	2.03	0.40
1:A:122:PRO:HA	1:A:123:PRO:HD3	1.95	0.40
1:D:35:GLU:O	1:D:38:PRO:CD	2.51	0.40
1:D:35:GLU:CA	1:D:38:PRO:HD2	2.50	0.40
1:d:109:SER:OG	1:d:110:THR:N	2.54	0.40
1:e:140:LYS:O	1:e:143:ARG:HG2	2.21	0.40
1:B:20:LEU:HD23	1:B:20:LEU:HA	1.87	0.40
1:H:96:MET:HB3	1:H:117:TRP:HE1	1.87	0.40
2:J:61:MET:SD	2:J:61:MET:C	3.04	0.40
1:k:215:MET:HE3	1:k:215:MET:HB2	1.81	0.40
1:A:101:GLY:HA2	1:A:104:ILE:HG22	2.03	0.40
1:B:64:ALA:O	1:B:68:MET:HG3	2.22	0.40
1:G:198:CYS:HA	1:G:201:ILE:HB	2.04	0.40
1:H:101:GLY:HA2	1:H:104:ILE:HG22	2.04	0.40
1:H:212:GLU:HG2	1:H:213:GLU:H	1.86	0.40
1:N:182:LYS:O	1:N:186:THR:HG22	2.21	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	144/220 (66%)	141 (98%)	3 (2%)	0	100	100
1	B	218/220 (99%)	216 (99%)	2 (1%)	0	100	100
1	C	216/220 (98%)	213 (99%)	3 (1%)	0	100	100
1	D	218/220 (99%)	215 (99%)	3 (1%)	0	100	100
1	G	218/220 (99%)	213 (98%)	5 (2%)	0	100	100
1	H	218/220 (99%)	214 (98%)	4 (2%)	0	100	100
1	N	72/220 (33%)	72 (100%)	0	0	100	100
1	Y	144/220 (66%)	142 (99%)	2 (1%)	0	100	100
1	d	218/220 (99%)	215 (99%)	3 (1%)	0	100	100
1	e	218/220 (99%)	213 (98%)	4 (2%)	1 (0%)	24	62
1	j	72/220 (33%)	71 (99%)	1 (1%)	0	100	100
1	k	218/220 (99%)	212 (97%)	6 (3%)	0	100	100
2	J	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
All	All	2336/2804 (83%)	2289 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	e	99	PRO

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	123/187 (66%)	123 (100%)	0	100	100
1	B	187/187 (100%)	187 (100%)	0	100	100
1	C	187/187 (100%)	187 (100%)	0	100	100
1	D	187/187 (100%)	187 (100%)	0	100	100
1	G	187/187 (100%)	187 (100%)	0	100	100
1	H	187/187 (100%)	187 (100%)	0	100	100
1	N	64/187 (34%)	64 (100%)	0	100	100
1	Y	123/187 (66%)	123 (100%)	0	100	100
1	d	187/187 (100%)	187 (100%)	0	100	100
1	e	187/187 (100%)	187 (100%)	0	100	100
1	j	64/187 (34%)	64 (100%)	0	100	100
1	k	187/187 (100%)	187 (100%)	0	100	100
2	J	132/132 (100%)	123 (93%)	9 (7%)	14	36
All	All	2002/2376 (84%)	1993 (100%)	9 (0%)	81	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	29	VAL
2	J	61	MET
2	J	84	GLU
2	J	91	LYS
2	J	120	GLU
2	J	134	GLU
2	J	144	ARG
2	J	151	LYS
2	J	165	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	95	GLN
1	B	5	ASN
1	B	9	GLN
1	B	53	ASN
1	B	63	GLN

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Mol	Chain	Res	Type
1	B	179	GLN
1	B	183	ASN
1	B	219	GLN
1	C	21	ASN
1	C	193	ASN
1	C	219	GLN
1	D	4	GLN
1	D	12	HIS
1	D	95	GLN
1	D	193	ASN
1	G	4	GLN
1	G	95	GLN
1	H	4	GLN
1	N	179	GLN
1	N	183	ASN
1	N	219	GLN
1	Y	4	GLN
1	Y	12	HIS
1	Y	95	GLN
1	d	4	GLN
1	d	12	HIS
1	d	95	GLN
1	d	193	ASN
1	e	5	ASN
1	e	7	GLN
1	e	9	GLN
1	e	21	ASN
1	e	53	ASN
1	e	63	GLN
1	e	219	GLN
1	j	219	GLN
1	k	21	ASN
1	k	63	GLN
1	k	84	HIS
1	k	95	GLN
1	k	193	ASN

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	147:PRO	C	148:THR	N	2.24

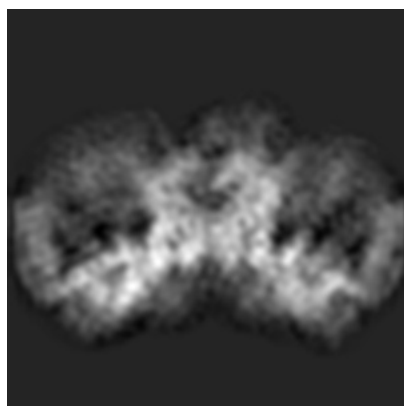
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10740. These allow visual inspection of the internal detail of the map and identification of artifacts.

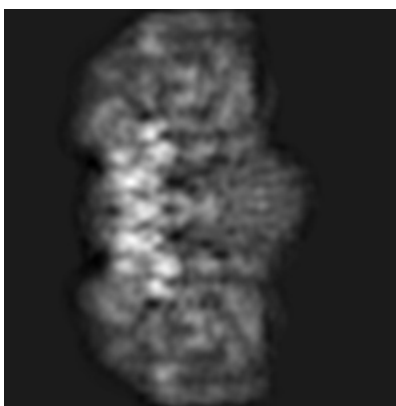
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

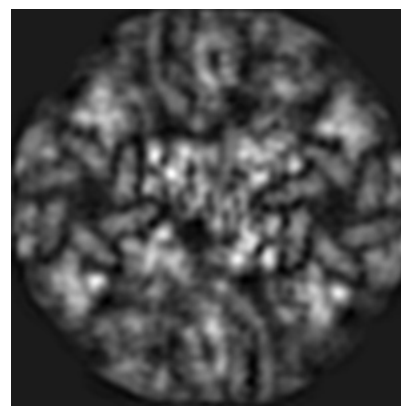
6.1.1 Primary map



X

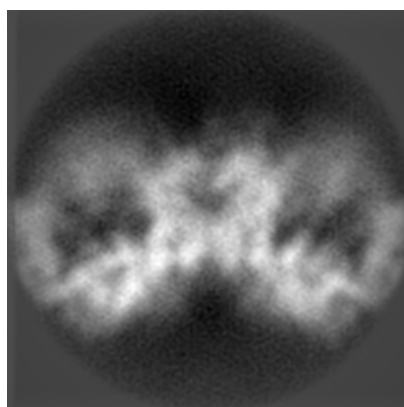


Y

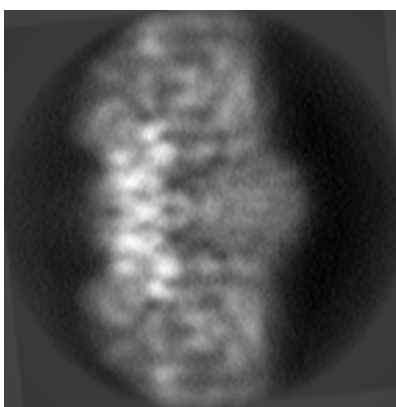


Z

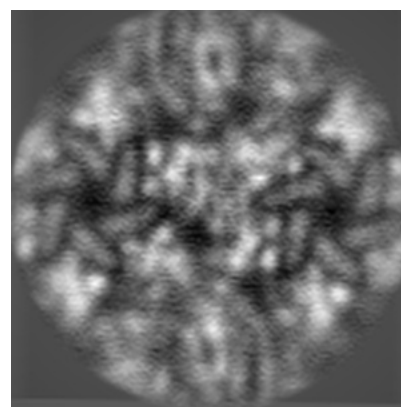
6.1.2 Raw map



X



Y

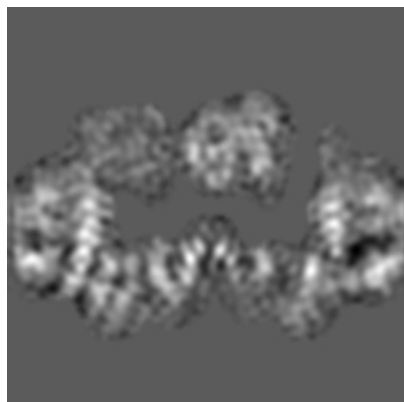


Z

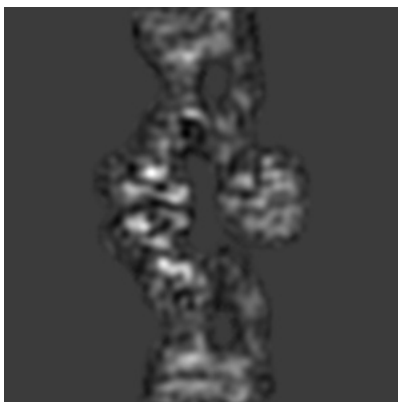
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

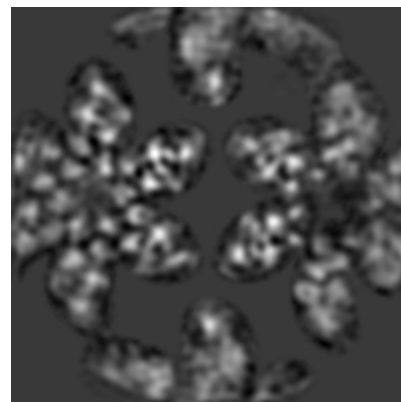
6.2.1 Primary map



X Index: 72

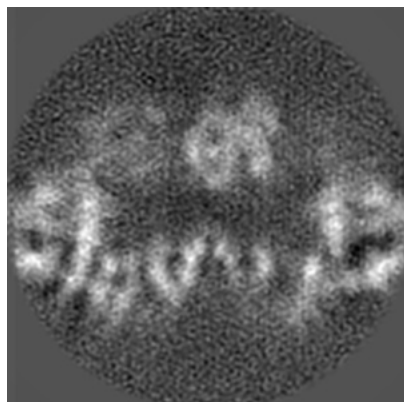


Y Index: 72

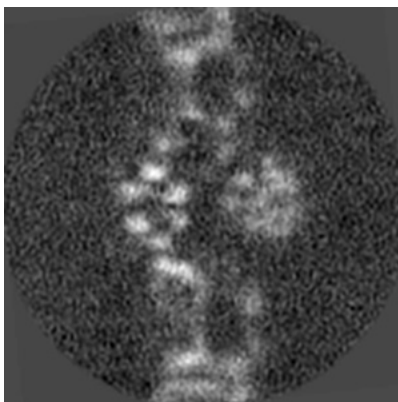


Z Index: 72

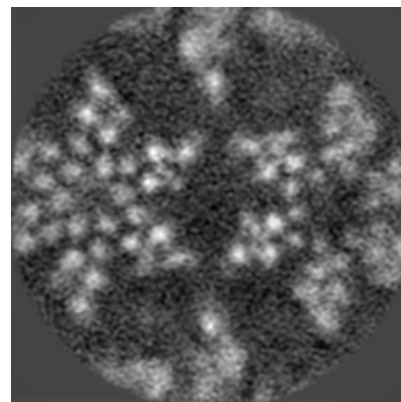
6.2.2 Raw map



X Index: 72



Y Index: 72

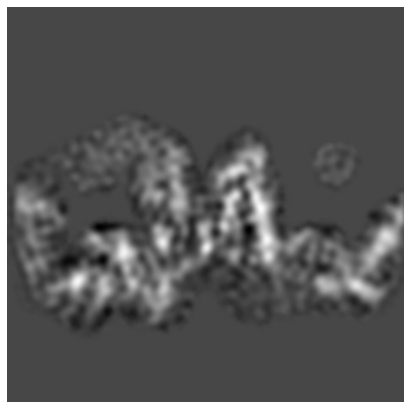


Z Index: 72

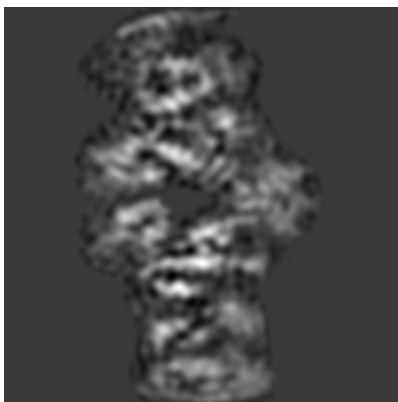
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

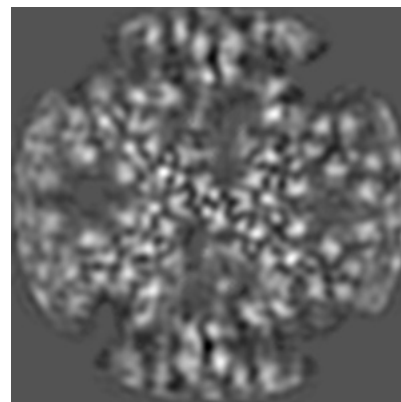
6.3.1 Primary map



X Index: 51

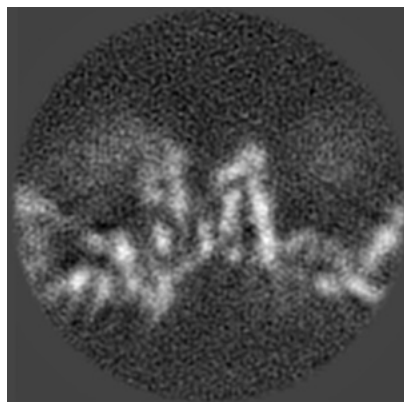


Y Index: 91

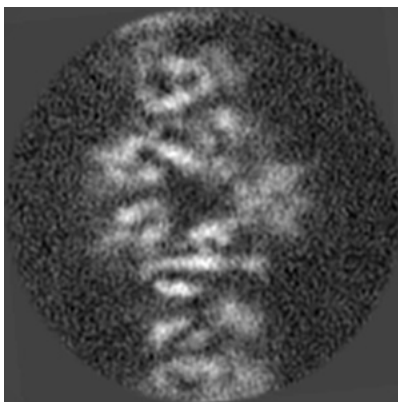


Z Index: 56

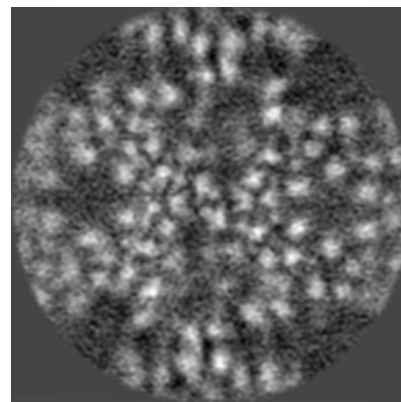
6.3.2 Raw map



X Index: 51



Y Index: 91

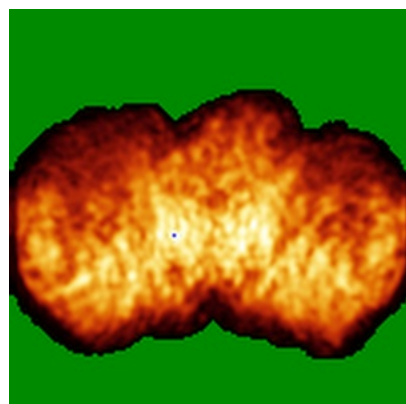


Z Index: 56

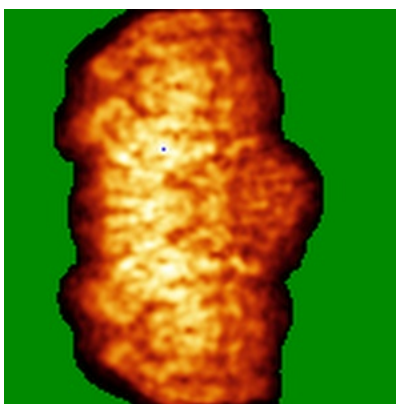
The images above show the largest variance slices of the map in three orthogonal directions.

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

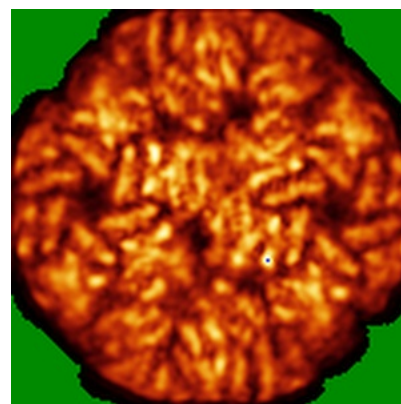
6.4.1 Primary map



X

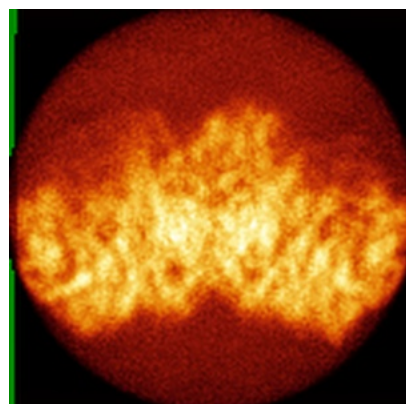


Y

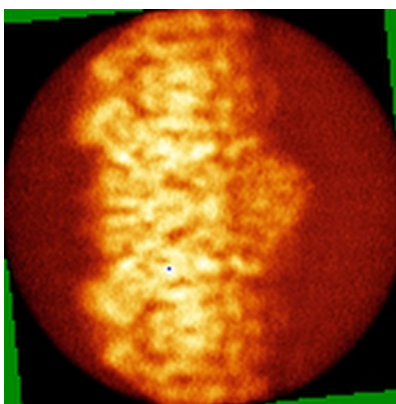


Z

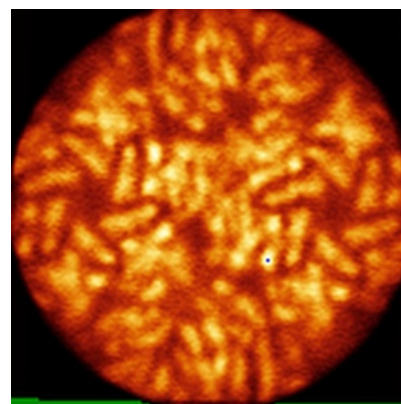
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

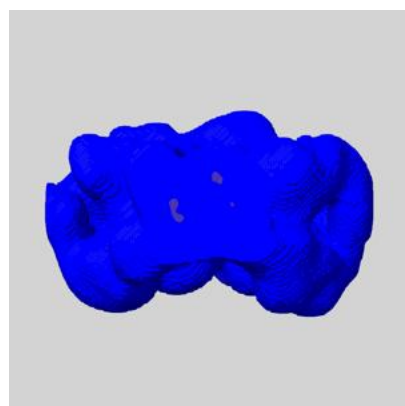
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

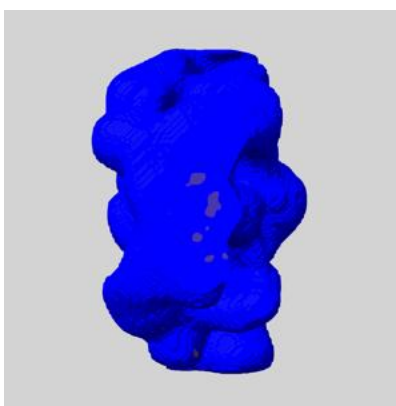
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

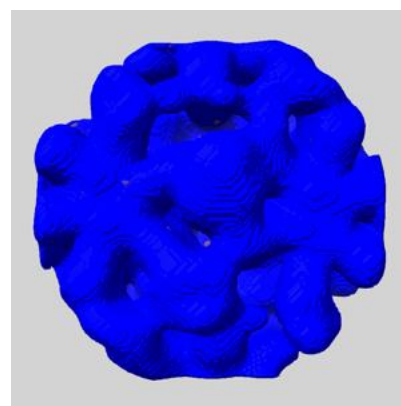
6.6.1 emd_10740_msk_1.map [i](#)



X



Y

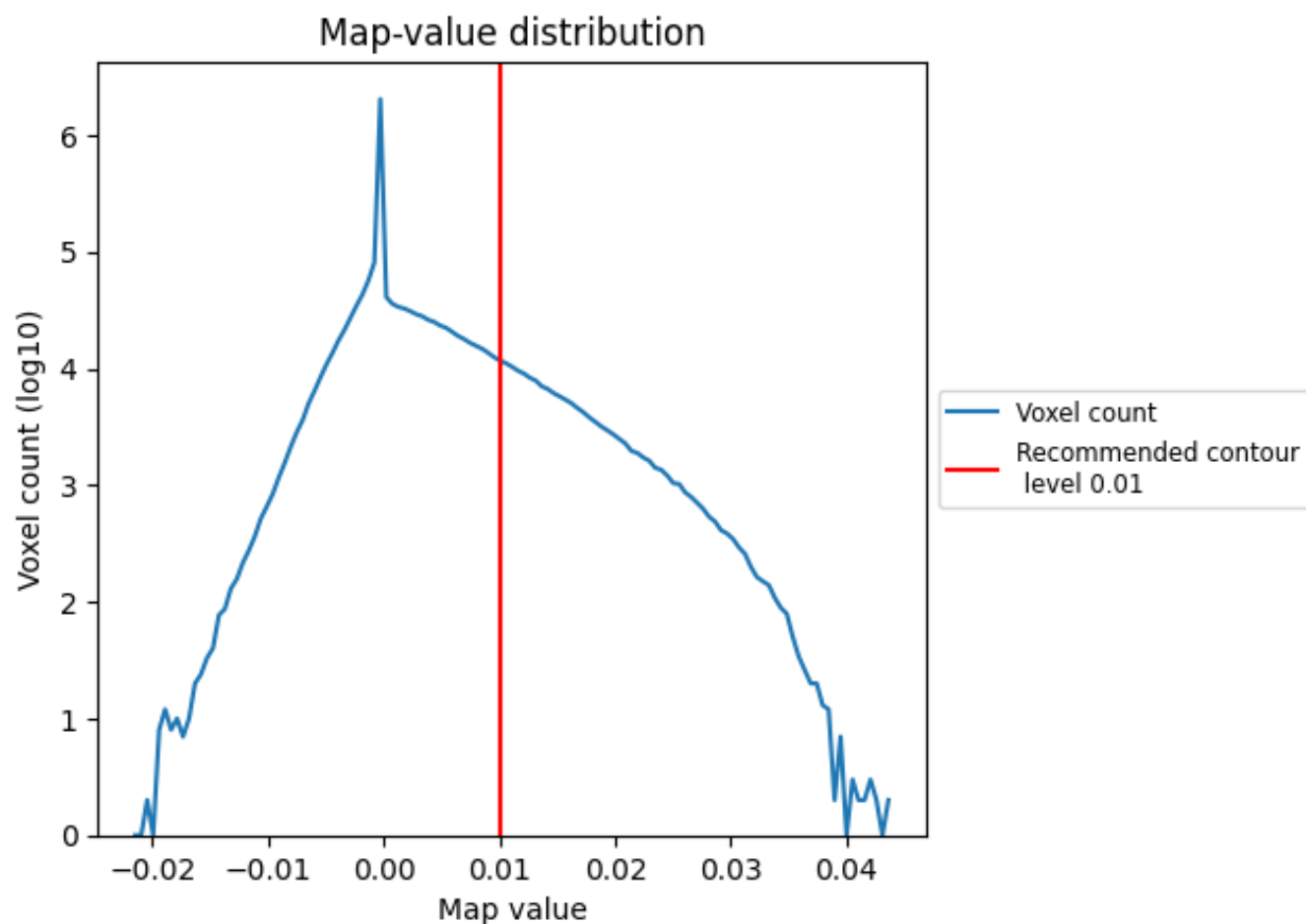


Z

7 Map analysis [i](#)

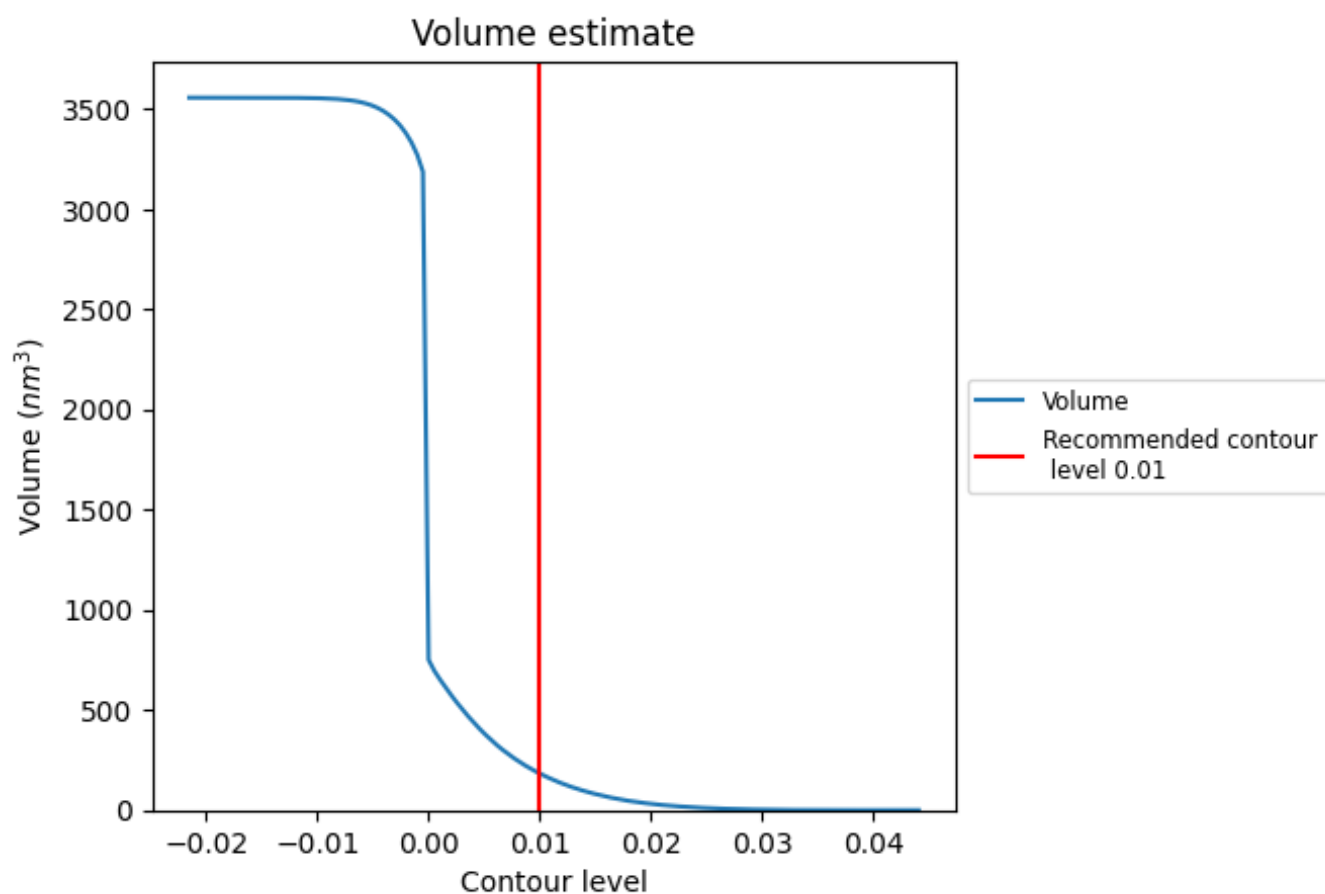
This section contains the results of statistical analysis of the map.

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.

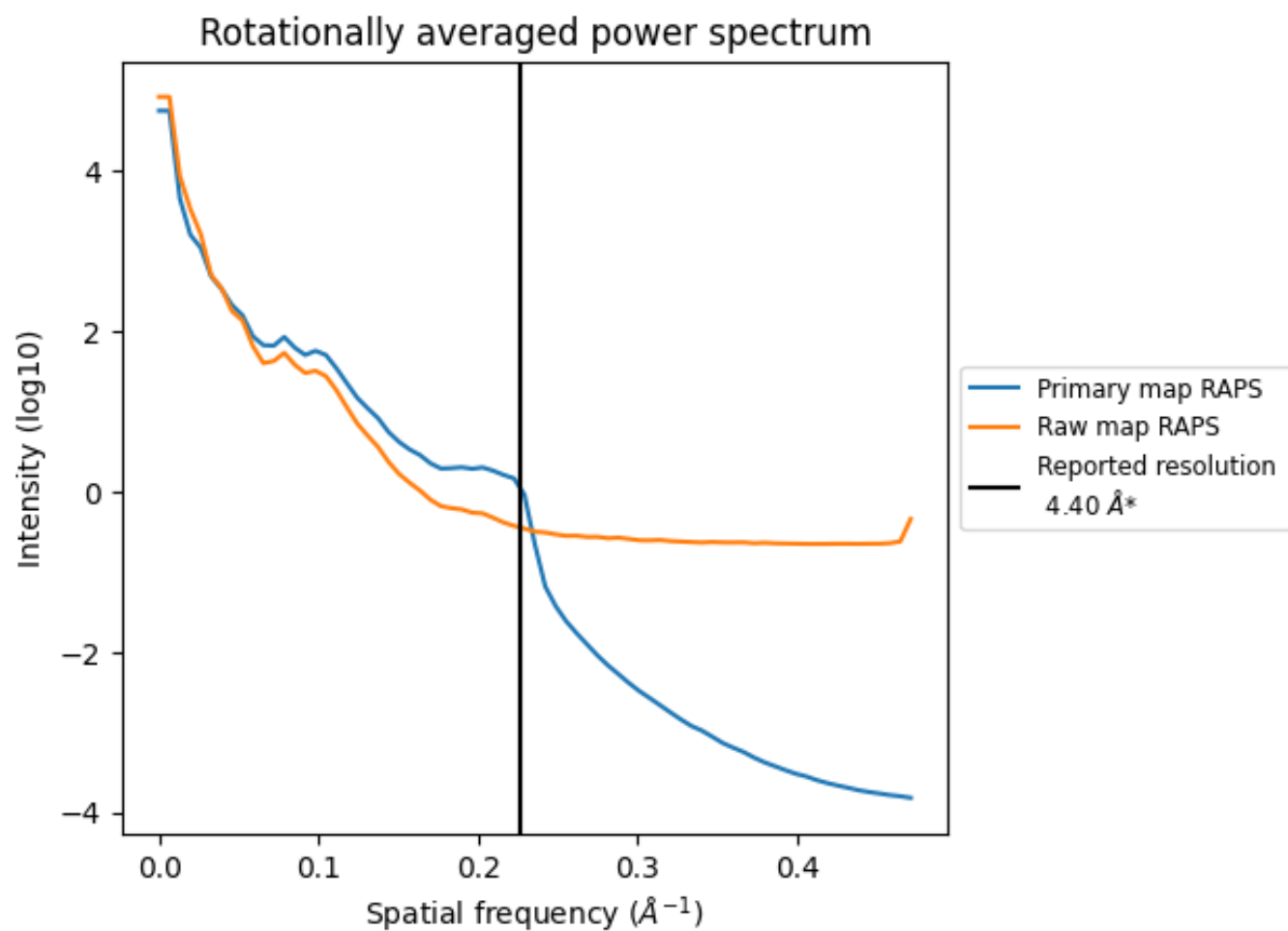
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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 ⓘ

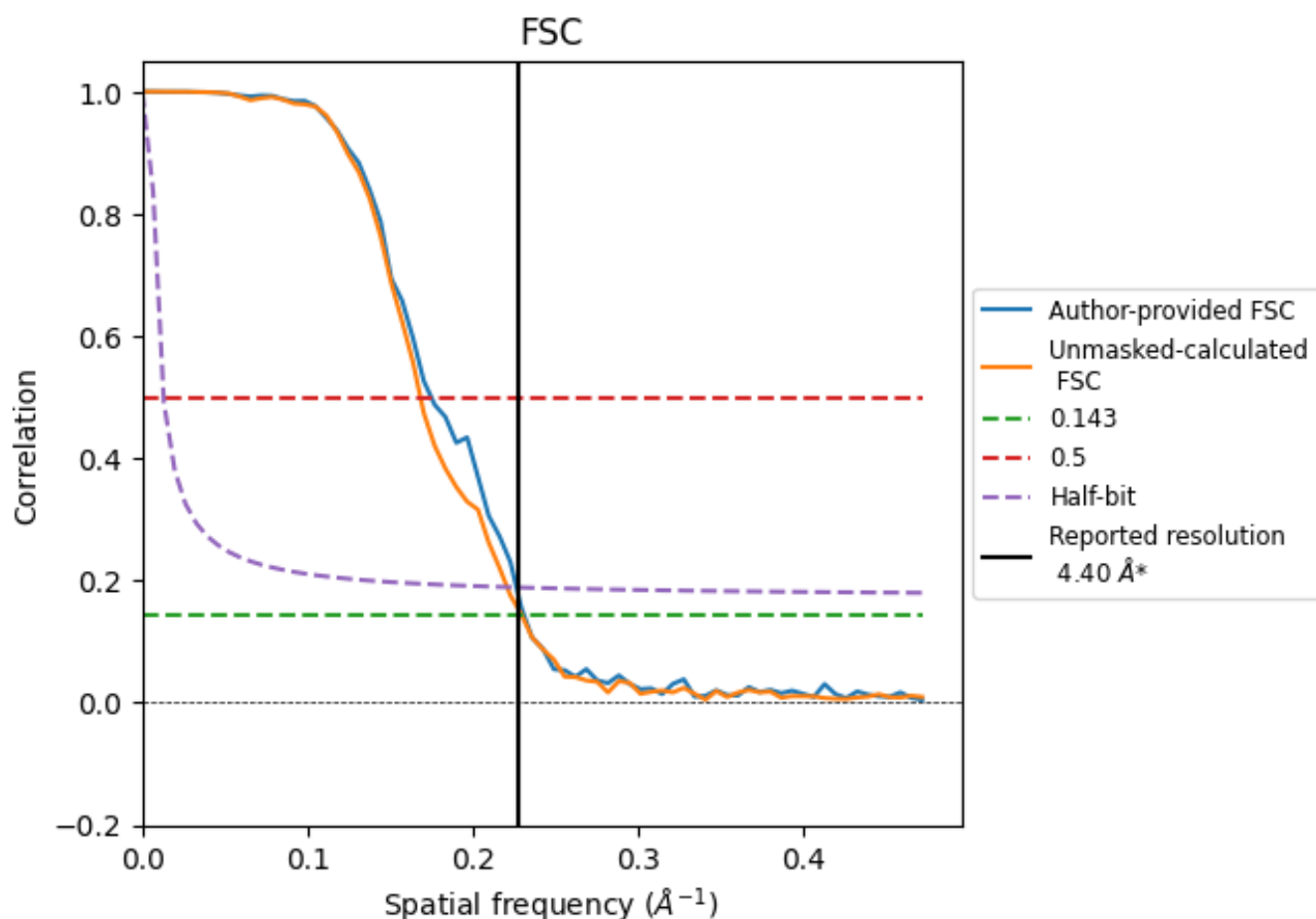


*Reported resolution corresponds to spatial frequency of $0.227 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

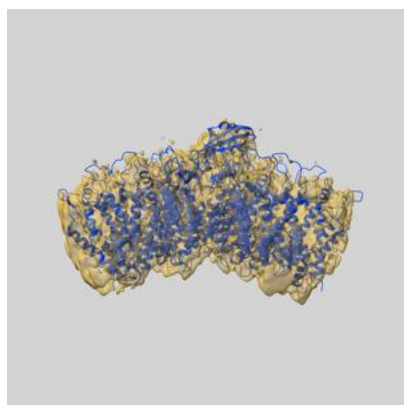
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.33	5.72	4.42
Unmasked-calculated*	4.36	5.94	4.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

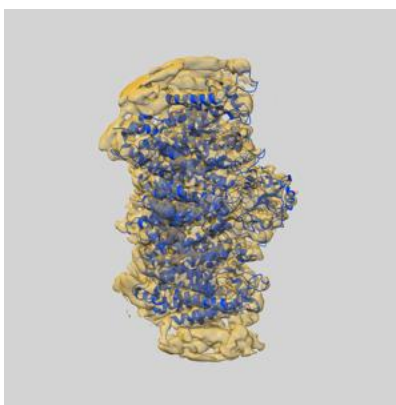
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10740 and PDB model 6Y9X. Per-residue inclusion information can be found in section [3](#) on page [5](#).

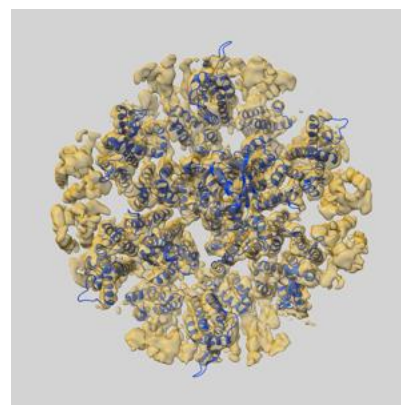
9.1 Map-model overlay [i](#)



X



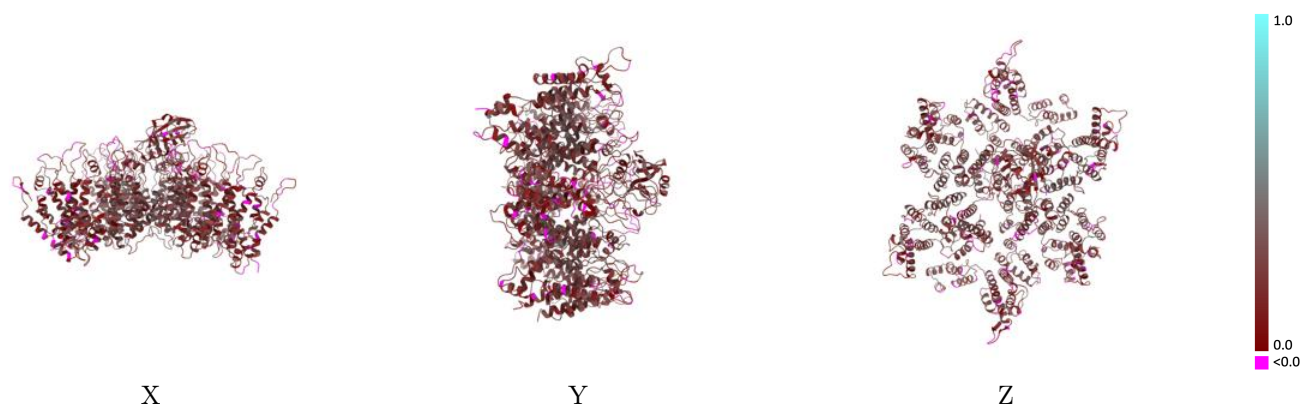
Y



Z

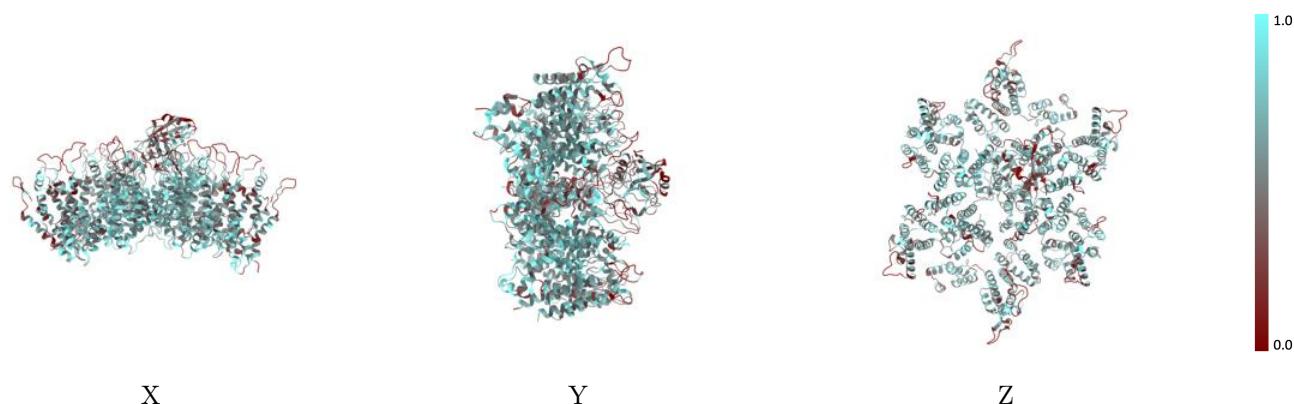
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



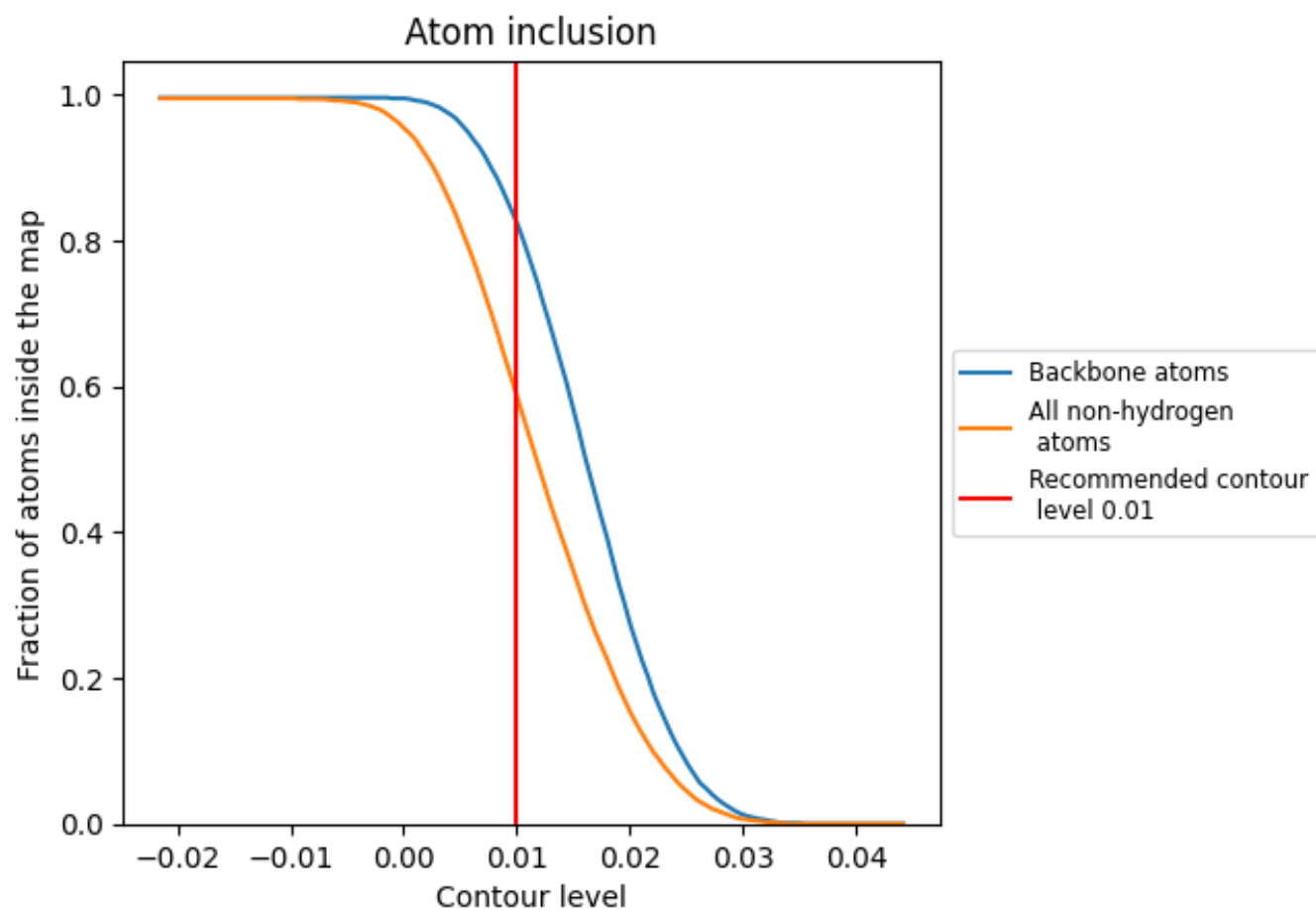
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 59% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5870	0.2190
A	0.5810	0.2290
B	0.6860	0.2570
C	0.6220	0.2420
D	0.5610	0.2000
G	0.5820	0.2230
H	0.5450	0.1800
J	0.4480	0.2230
N	0.5990	0.1880
Y	0.5490	0.2110
d	0.5330	0.1720
e	0.6380	0.2300
j	0.6230	0.2040
k	0.6470	0.2640

