Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 04:48 AM EST

PDB ID	:	7SEP
EMDB ID	:	EMD-25074
Title	:	Cryo-EM Structure of the RT component of the HIV-1 Pol Polyprotein
Authors	:	Lyumkis, D.; Passos, D.; Arnold, E.; Harrison, J.J.E.
Deposited on	:	2021-10-01
Resolution	:	3.80 Å(reported)
Based on initial models	:	1DLO, 3BGR

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:

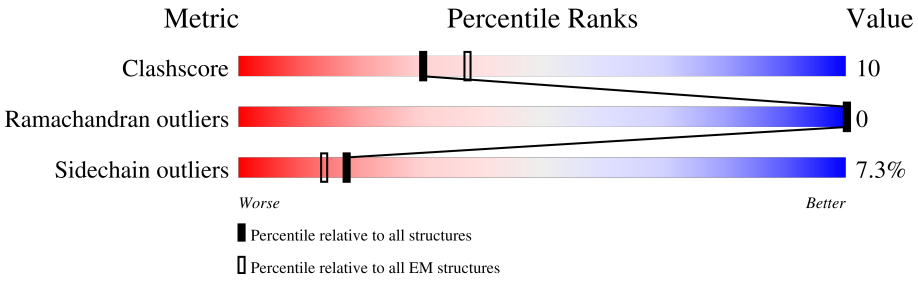
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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

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	1053	5% 36% 14% • 49%
1	B	1053	• 26% 10% • 62%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7641 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	532	Total	C	N	O	S	0	0
			4343	2817	719	799	8		
1	B	398	Total	C	N	O	S	0	0
			3298	2150	542	599	7		

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-204	MET	-	initiating methionine	UNP P03366
A	-203	GLY	-	expression tag	UNP P03366
A	-202	SER	-	expression tag	UNP P03366
A	-201	SER	-	expression tag	UNP P03366
A	-200	HIS	-	expression tag	UNP P03366
A	-199	HIS	-	expression tag	UNP P03366
A	-198	HIS	-	expression tag	UNP P03366
A	-197	HIS	-	expression tag	UNP P03366
A	-196	HIS	-	expression tag	UNP P03366
A	-195	HIS	-	expression tag	UNP P03366
A	-194	MET	-	expression tag	UNP P03366
A	-193	ALA	-	expression tag	UNP P03366
A	-192	THR	-	expression tag	UNP P03366
A	-191	VAL	-	expression tag	UNP P03366
A	-190	LYS	-	expression tag	UNP P03366
A	-189	PHE	-	expression tag	UNP P03366
A	-188	LYS	-	expression tag	UNP P03366
A	-187	TYR	-	expression tag	UNP P03366
A	-186	LYS	-	expression tag	UNP P03366
A	-185	GLY	-	expression tag	UNP P03366
A	-184	GLU	-	expression tag	UNP P03366
A	-183	GLU	-	expression tag	UNP P03366
A	-182	LYS	-	expression tag	UNP P03366
A	-181	GLU	-	expression tag	UNP P03366
A	-180	VAL	-	expression tag	UNP P03366
A	-179	ASP	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-178	ILE	-	expression tag	UNP P03366
A	-177	SER	-	expression tag	UNP P03366
A	-176	LYS	-	expression tag	UNP P03366
A	-175	ILE	-	expression tag	UNP P03366
A	-174	LYS	-	expression tag	UNP P03366
A	-173	LYS	-	expression tag	UNP P03366
A	-172	VAL	-	expression tag	UNP P03366
A	-171	TRP	-	expression tag	UNP P03366
A	-170	ARG	-	expression tag	UNP P03366
A	-169	VAL	-	expression tag	UNP P03366
A	-168	GLY	-	expression tag	UNP P03366
A	-167	LYS	-	expression tag	UNP P03366
A	-166	MET	-	expression tag	UNP P03366
A	-165	ILE	-	expression tag	UNP P03366
A	-164	SER	-	expression tag	UNP P03366
A	-163	PHE	-	expression tag	UNP P03366
A	-162	THR	-	expression tag	UNP P03366
A	-161	TYR	-	expression tag	UNP P03366
A	-160	ASP	-	expression tag	UNP P03366
A	-159	GLU	-	expression tag	UNP P03366
A	-158	GLY	-	expression tag	UNP P03366
A	-157	GLY	-	expression tag	UNP P03366
A	-156	GLY	-	expression tag	UNP P03366
A	-155	LYS	-	expression tag	UNP P03366
A	-154	THR	-	expression tag	UNP P03366
A	-153	GLY	-	expression tag	UNP P03366
A	-152	ARG	-	expression tag	UNP P03366
A	-151	GLY	-	expression tag	UNP P03366
A	-150	ALA	-	expression tag	UNP P03366
A	-149	VAL	-	expression tag	UNP P03366
A	-148	SER	-	expression tag	UNP P03366
A	-147	GLU	-	expression tag	UNP P03366
A	-146	LYS	-	expression tag	UNP P03366
A	-145	ASP	-	expression tag	UNP P03366
A	-144	ALA	-	expression tag	UNP P03366
A	-143	PRO	-	expression tag	UNP P03366
A	-142	LYS	-	expression tag	UNP P03366
A	-141	GLU	-	expression tag	UNP P03366
A	-140	LEU	-	expression tag	UNP P03366
A	-139	LEU	-	expression tag	UNP P03366
A	-138	GLN	-	expression tag	UNP P03366
A	-137	MET	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-136	LEU	-	expression tag	UNP P03366
A	-135	GLU	-	expression tag	UNP P03366
A	-134	LYS	-	expression tag	UNP P03366
A	-133	GLN	-	expression tag	UNP P03366
A	-132	LYS	-	expression tag	UNP P03366
A	-131	LYS	-	expression tag	UNP P03366
A	-130	ALA	-	expression tag	UNP P03366
A	-129	LEU	-	expression tag	UNP P03366
A	-128	GLU	-	expression tag	UNP P03366
A	-127	VAL	-	expression tag	UNP P03366
A	-126	LEU	-	expression tag	UNP P03366
A	-125	PHE	-	expression tag	UNP P03366
A	-124	GLN	-	expression tag	UNP P03366
A	-123	GLY	-	expression tag	UNP P03366
A	-122	PRO	-	expression tag	UNP P03366
A	-121	MET	-	expression tag	UNP P03366
A	-74	ALA	ASP	engineered mutation	UNP P03366
A	560	ASP	LEU	engineered mutation	UNP P03366
A	561	ASP	PHE	engineered mutation	UNP P03366
B	-204	MET	-	initiating methionine	UNP P03366
B	-203	GLY	-	expression tag	UNP P03366
B	-202	SER	-	expression tag	UNP P03366
B	-201	SER	-	expression tag	UNP P03366
B	-200	HIS	-	expression tag	UNP P03366
B	-199	HIS	-	expression tag	UNP P03366
B	-198	HIS	-	expression tag	UNP P03366
B	-197	HIS	-	expression tag	UNP P03366
B	-196	HIS	-	expression tag	UNP P03366
B	-195	HIS	-	expression tag	UNP P03366
B	-194	MET	-	expression tag	UNP P03366
B	-193	ALA	-	expression tag	UNP P03366
B	-192	THR	-	expression tag	UNP P03366
B	-191	VAL	-	expression tag	UNP P03366
B	-190	LYS	-	expression tag	UNP P03366
B	-189	PHE	-	expression tag	UNP P03366
B	-188	LYS	-	expression tag	UNP P03366
B	-187	TYR	-	expression tag	UNP P03366
B	-186	LYS	-	expression tag	UNP P03366
B	-185	GLY	-	expression tag	UNP P03366
B	-184	GLU	-	expression tag	UNP P03366
B	-183	GLU	-	expression tag	UNP P03366
B	-182	LYS	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-181	GLU	-	expression tag	UNP P03366
B	-180	VAL	-	expression tag	UNP P03366
B	-179	ASP	-	expression tag	UNP P03366
B	-178	ILE	-	expression tag	UNP P03366
B	-177	SER	-	expression tag	UNP P03366
B	-176	LYS	-	expression tag	UNP P03366
B	-175	ILE	-	expression tag	UNP P03366
B	-174	LYS	-	expression tag	UNP P03366
B	-173	LYS	-	expression tag	UNP P03366
B	-172	VAL	-	expression tag	UNP P03366
B	-171	TRP	-	expression tag	UNP P03366
B	-170	ARG	-	expression tag	UNP P03366
B	-169	VAL	-	expression tag	UNP P03366
B	-168	GLY	-	expression tag	UNP P03366
B	-167	LYS	-	expression tag	UNP P03366
B	-166	MET	-	expression tag	UNP P03366
B	-165	ILE	-	expression tag	UNP P03366
B	-164	SER	-	expression tag	UNP P03366
B	-163	PHE	-	expression tag	UNP P03366
B	-162	THR	-	expression tag	UNP P03366
B	-161	TYR	-	expression tag	UNP P03366
B	-160	ASP	-	expression tag	UNP P03366
B	-159	GLU	-	expression tag	UNP P03366
B	-158	GLY	-	expression tag	UNP P03366
B	-157	GLY	-	expression tag	UNP P03366
B	-156	GLY	-	expression tag	UNP P03366
B	-155	LYS	-	expression tag	UNP P03366
B	-154	THR	-	expression tag	UNP P03366
B	-153	GLY	-	expression tag	UNP P03366
B	-152	ARG	-	expression tag	UNP P03366
B	-151	GLY	-	expression tag	UNP P03366
B	-150	ALA	-	expression tag	UNP P03366
B	-149	VAL	-	expression tag	UNP P03366
B	-148	SER	-	expression tag	UNP P03366
B	-147	GLU	-	expression tag	UNP P03366
B	-146	LYS	-	expression tag	UNP P03366
B	-145	ASP	-	expression tag	UNP P03366
B	-144	ALA	-	expression tag	UNP P03366
B	-143	PRO	-	expression tag	UNP P03366
B	-142	LYS	-	expression tag	UNP P03366
B	-141	GLU	-	expression tag	UNP P03366
B	-140	LEU	-	expression tag	UNP P03366

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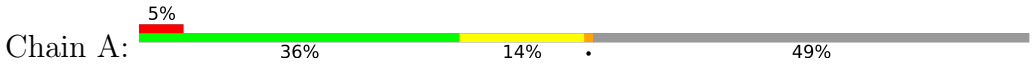
Chain	Residue	Modelled	Actual	Comment	Reference
B	-139	LEU	-	expression tag	UNP P03366
B	-138	GLN	-	expression tag	UNP P03366
B	-137	MET	-	expression tag	UNP P03366
B	-136	LEU	-	expression tag	UNP P03366
B	-135	GLU	-	expression tag	UNP P03366
B	-134	LYS	-	expression tag	UNP P03366
B	-133	GLN	-	expression tag	UNP P03366
B	-132	LYS	-	expression tag	UNP P03366
B	-131	LYS	-	expression tag	UNP P03366
B	-130	ALA	-	expression tag	UNP P03366
B	-129	LEU	-	expression tag	UNP P03366
B	-128	GLU	-	expression tag	UNP P03366
B	-127	VAL	-	expression tag	UNP P03366
B	-126	LEU	-	expression tag	UNP P03366
B	-125	PHE	-	expression tag	UNP P03366
B	-124	GLN	-	expression tag	UNP P03366
B	-123	GLY	-	expression tag	UNP P03366
B	-122	PRO	-	expression tag	UNP P03366
B	-121	MET	-	expression tag	UNP P03366
B	-74	ALA	ASP	engineered mutation	UNP P03366
B	560	ASP	LEU	engineered mutation	UNP P03366
B	561	ASP	PHE	engineered mutation	UNP P03366

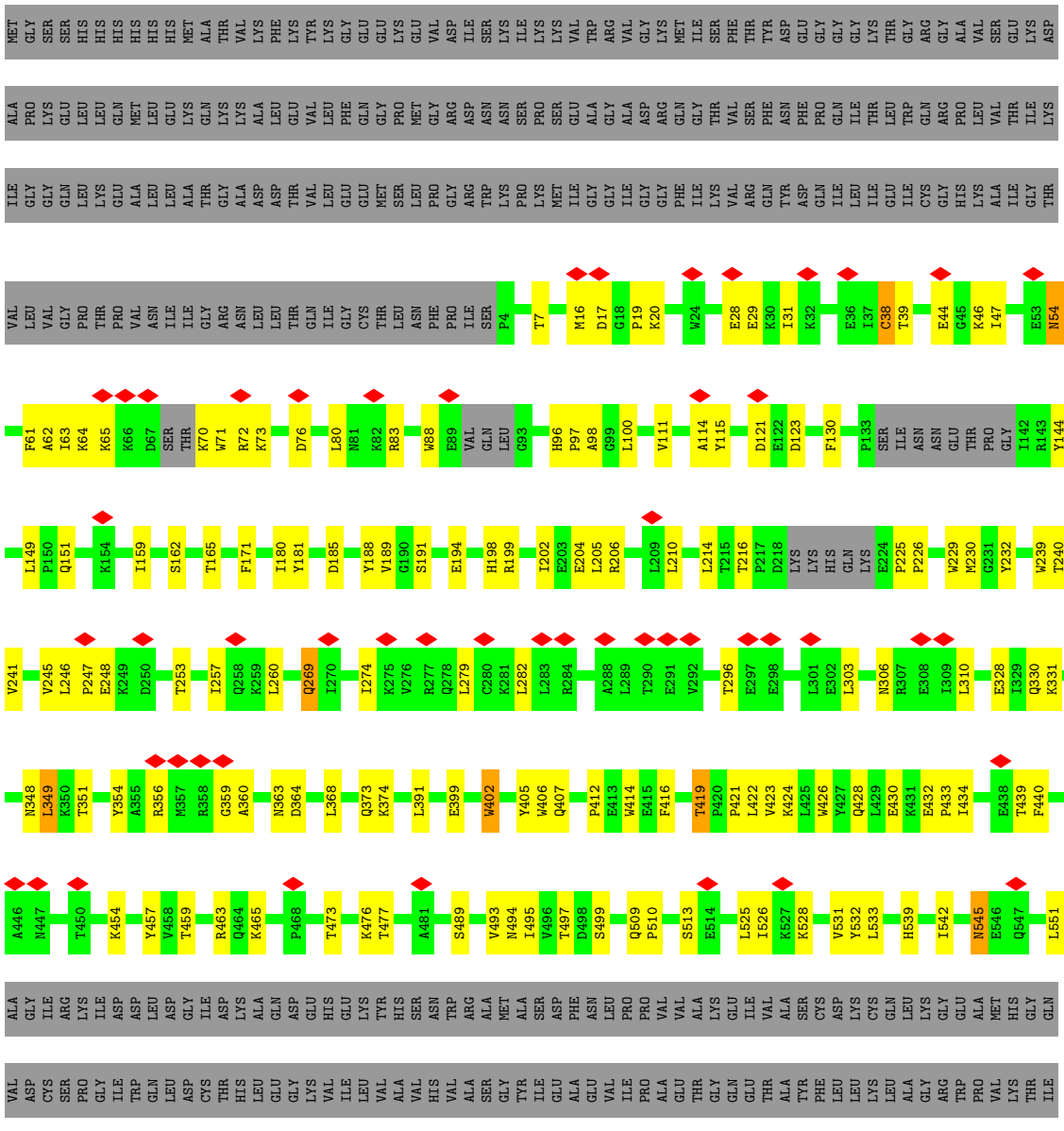
3 Residue-property plots (i)

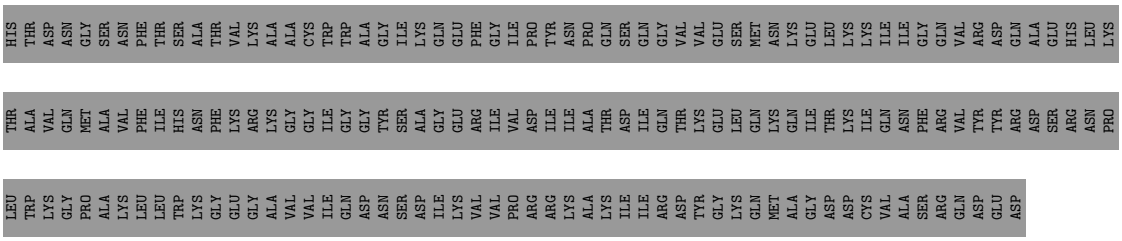
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

Chain A:

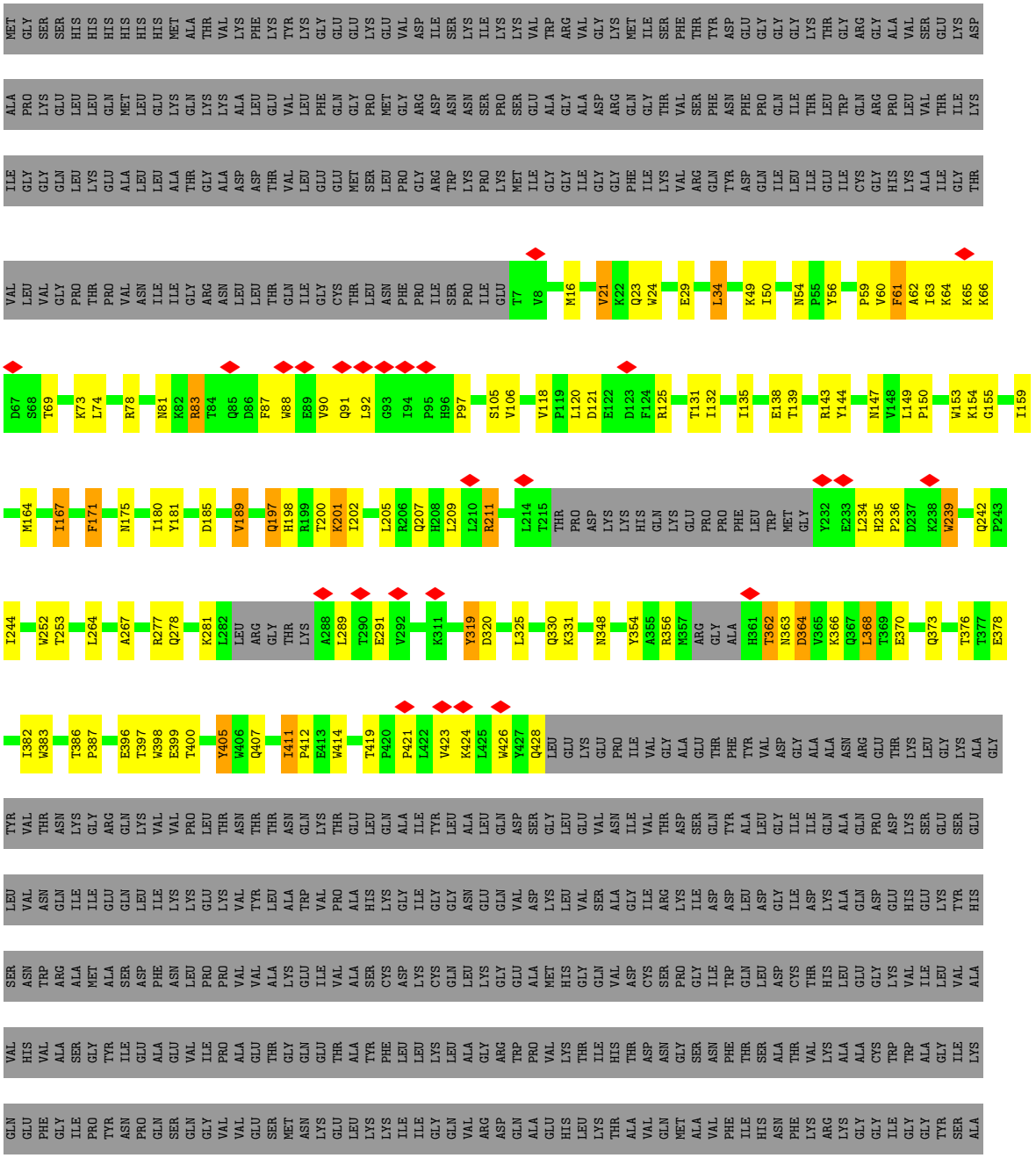






• Molecule 1: Gag-Pol polyprotein

Chain B:



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

ILE LYS VAL VAL PRO ARG ARG LYS ALA LYS ILE ILE ARG ASP TYR GLY LYS GLN MET ALA GLY ASP ASP CYS VAL ALA SER ARG GLN ASP GLU ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27555	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 ($e^-/Å^2$)	0.95	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	1.329	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	259.84, 259.84, 259.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.015, 1.015, 1.015	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	0.36	0/4454	0.48	0/6045
1	B	0.39	0/3391	0.48	0/4607
All	All	0.37	0/7845	0.48	0/10652

There are no bond length outliers.

There are no bond angle outliers.

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	4343	0	4391	84	0
1	B	3298	0	3321	70	0
All	All	7641	0	7712	152	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 10.

All (152) 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:181:TYR:HB2	1:A:188:TYR:HB3	1.69	0.74
1:B:125:ARG:HD3	1:B:147:ASN:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:TRP:HB3	1:A:526:ILE:HD11	1.69	0.73
1:A:328:GLU:OE2	1:A:330:GLN:NE2	2.26	0.69
1:B:23:GLN:NE2	1:B:131:THR:O	2.26	0.69
1:A:399:GLU:HA	1:A:402:TRP:HD1	1.57	0.69
1:B:330:GLN:HB2	1:B:424:LYS:HG2	1.76	0.68
1:A:545:ASN:OD1	1:A:545:ASN:N	2.16	0.67
1:B:90:VAL:HG23	1:B:91:GLN:HG2	1.75	0.66
1:A:19:PRO:HG3	1:A:80:LEU:HD23	1.77	0.66
1:A:73:LYS:O	1:A:151:GLN:NE2	2.30	0.65
1:B:289:LEU:HD23	1:B:289:LEU:H	1.62	0.63
1:A:489:SER:OG	1:A:528:LYS:NZ	2.30	0.63
1:B:24:TRP:HZ2	1:B:61:PHE:HE2	1.46	0.62
1:B:97:PRO:HG3	1:B:181:TYR:HB2	1.81	0.61
1:B:34:LEU:HG	1:B:62:ALA:HB2	1.83	0.61
1:A:364:ASP:N	1:A:364:ASP:OD1	2.29	0.60
1:B:138:GLU:HG3	1:B:139:THR:H	1.66	0.60
1:A:282:LEU:HD21	1:A:296:THR:HG23	1.84	0.58
1:A:130:PHE:HB3	1:A:144:TYR:HB2	1.85	0.58
1:B:362:THR:OG1	1:B:363:ASN:N	2.34	0.58
1:A:149:LEU:HD21	1:A:159:ILE:HG23	1.86	0.58
1:A:439:THR:HA	1:A:494:ASN:HB2	1.86	0.58
1:A:497:THR:HG22	1:A:499:SER:H	1.69	0.58
1:A:64:LYS:HA	1:A:70:LYS:HA	1.85	0.57
1:B:354:TYR:OH	1:B:370:GLU:OE1	2.23	0.57
1:A:65:LYS:HD2	1:A:72:ARG:HG3	1.87	0.57
1:A:210:LEU:HA	1:A:214:LEU:O	2.04	0.57
1:A:419:THR:OG1	1:A:421:PRO:O	2.23	0.57
1:B:81:ASN:OD1	1:B:154:LYS:N	2.37	0.56
1:A:111:VAL:HB	1:A:114:ALA:HB2	1.87	0.56
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.88	0.55
1:A:162:SER:O	1:A:165:THR:OG1	2.22	0.55
1:B:106:VAL:HG23	1:B:234:LEU:HB3	1.89	0.55
1:A:44:GLU:O	1:A:46:LYS:NZ	2.37	0.55
1:B:105:SER:HG	1:B:198:HIS:CE1	2.23	0.54
1:B:382:ILE:HG23	1:B:383:TRP:CD2	2.43	0.54
1:A:240:THR:HG22	1:A:241:VAL:N	2.23	0.54
1:B:378:GLU:O	1:B:382:ILE:HG22	2.08	0.54
1:B:368:LEU:HD12	1:B:398:TRP:HZ3	1.73	0.54
1:A:63:ILE:O	1:A:72:ARG:N	2.32	0.53
1:B:368:LEU:HD12	1:B:398:TRP:CZ3	2.43	0.53
1:A:63:ILE:HG13	1:A:65:LYS:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:HE1	1:A:204:GLU:HG3	1.73	0.53
1:B:180:ILE:HG12	1:B:189:VAL:HG12	1.90	0.53
1:A:199:ARG:O	1:A:202:ILE:HG22	2.09	0.53
1:A:206:ARG:NH2	1:A:216:THR:OG1	2.42	0.53
1:A:406:TRP:CD1	1:A:407:GLN:HG3	2.44	0.52
1:A:16:MET:HB3	1:A:83:ARG:HH11	1.74	0.52
1:B:88:TRP:HB2	1:B:154:LYS:HD3	1.92	0.52
1:B:24:TRP:CZ2	1:B:61:PHE:HE2	2.28	0.51
1:B:207:GLN:O	1:B:211:ARG:HB2	2.10	0.51
1:B:242:GLN:NE2	1:B:428:GLN:OE1	2.37	0.51
1:A:97:PRO:HG3	1:A:232:TYR:CG	2.45	0.51
1:A:232:TYR:OH	1:A:269:GLN:OE1	2.28	0.51
1:A:348:ASN:OD1	1:A:351:THR:OG1	2.29	0.51
1:B:24:TRP:HE1	1:B:61:PHE:HD2	1.58	0.51
1:A:54:ASN:OD1	1:A:54:ASN:N	2.41	0.51
1:A:191:SER:OG	1:A:198:HIS:ND1	2.36	0.50
1:B:62:ALA:HA	1:B:73:LYS:HA	1.93	0.50
1:B:319:TYR:HD1	1:B:320:ASP:N	2.09	0.50
1:A:246:LEU:HD22	1:A:260:LEU:HD22	1.93	0.49
1:B:198:HIS:O	1:B:202:ILE:HG12	2.12	0.49
1:A:489:SER:HB2	1:A:493:VAL:HG11	1.93	0.49
1:A:279:LEU:HG	1:A:303:LEU:HD11	1.95	0.48
1:B:65:LYS:HG3	1:B:66:LYS:HG3	1.95	0.48
1:B:149:LEU:HD22	1:B:153:TRP:HZ3	1.79	0.48
1:B:164:MET:O	1:B:167:ILE:N	2.46	0.48
1:B:21:VAL:HG13	1:B:59:PRO:HD3	1.96	0.48
1:B:421:PRO:HB2	1:B:423:VAL:HG23	1.96	0.48
1:A:98:ALA:HB1	1:A:349:LEU:HD12	1.95	0.48
1:B:253:THR:OG1	1:B:291:GLU:O	2.24	0.48
1:A:360:ALA:O	1:A:513:SER:HA	2.13	0.47
1:A:457:TYR:CE1	1:A:465:LYS:HG2	2.49	0.47
1:B:197:GLN:HA	1:B:200:THR:OG1	2.15	0.47
1:B:356:ARG:HD2	1:B:356:ARG:HA	1.76	0.47
1:A:363:ASN:ND2	1:A:509:GLN:O	2.47	0.47
1:A:368:LEU:HD11	1:A:391:LEU:HG	1.95	0.47
1:B:16:MET:HB3	1:B:83:ARG:HD2	1.96	0.47
1:B:106:VAL:HG22	1:B:236:PRO:HD3	1.96	0.47
1:A:180:ILE:HD13	1:A:189:VAL:HG22	1.95	0.47
1:A:525:LEU:HD21	1:A:531:VAL:HG11	1.96	0.47
1:B:120:LEU:HD12	1:B:121:ASP:H	1.80	0.46
1:B:396:GLU:O	1:B:399:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:O	1:A:477:THR:N	2.42	0.46
1:B:34:LEU:HD13	1:B:132:ILE:HG22	1.98	0.45
1:A:509:GLN:N	1:A:510:PRO:HD3	2.31	0.45
1:B:201:LYS:HD3	1:B:201:LYS:HA	1.69	0.45
1:B:167:ILE:HD13	1:B:167:ILE:HA	1.62	0.45
1:A:121:ASP:HB3	1:A:123:ASP:OD1	2.16	0.45
1:A:473:THR:HB	1:A:476:LYS:HB2	1.99	0.45
1:A:331:LYS:HD2	1:A:423:VAL:HG22	1.99	0.45
1:B:118:VAL:O	1:B:149:LEU:HG	2.17	0.45
1:B:366:LYS:HE2	1:B:405:TYR:CZ	2.53	0.44
1:A:247:PRO:HG2	1:A:260:LEU:HD11	2.00	0.44
1:B:23:GLN:HE22	1:B:60:VAL:HG12	1.82	0.44
1:B:63:ILE:HD13	1:B:74:LEU:HD11	2.00	0.44
1:B:264:LEU:O	1:B:267:ALA:N	2.49	0.44
1:A:412:PRO:O	1:A:414:TRP:HD1	2.00	0.44
1:A:62:ALA:HB1	1:A:71:TRP:HB3	1.98	0.44
1:A:100:LEU:HD11	1:A:229:TRP:CZ3	2.52	0.44
1:B:64:LYS:O	1:B:407:GLN:HG2	2.18	0.44
1:A:430:GLU:HG3	1:A:432:GLU:H	1.83	0.44
1:B:50:ILE:HD12	1:B:54:ASN:HB2	2.00	0.44
1:B:325:LEU:HD23	1:B:387:PRO:HB3	2.00	0.44
1:A:406:TRP:O	1:B:331:LYS:HE3	2.18	0.43
1:A:459:THR:OG1	1:A:463:ARG:N	2.51	0.43
1:B:135:ILE:O	1:B:138:GLU:HG2	2.19	0.43
1:B:78:ARG:HG3	1:B:411:ILE:HD13	2.01	0.43
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.33	0.43
1:A:188:TYR:HB2	1:A:229:TRP:NE1	2.33	0.43
1:A:194:GLU:O	1:A:198:HIS:N	2.46	0.43
1:A:225:PRO:HB2	1:A:226:PRO:HD3	2.00	0.43
1:B:83:ARG:HD3	1:B:83:ARG:HA	1.80	0.43
1:B:155:GLY:O	1:B:159:ILE:HG12	2.18	0.43
1:A:269:GLN:HE21	1:A:269:GLN:HB3	1.57	0.43
1:A:28:GLU:HA	1:A:31:ILE:HB	2.00	0.42
1:A:55:PRO:HD2	1:A:56:TYR:CE2	2.54	0.42
1:B:373:GLN:O	1:B:376:THR:HG22	2.19	0.42
1:A:38:CYS:SG	1:A:39:THR:N	2.92	0.42
1:A:16:MET:SD	1:A:83:ARG:NH1	2.93	0.42
1:A:253:THR:O	1:A:257:ILE:HG13	2.19	0.42
1:A:306:ASN:O	1:A:310:LEU:HG	2.18	0.42
1:B:264:LEU:HD12	1:B:264:LEU:HA	1.85	0.42
1:B:278:GLN:O	1:B:281:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASN:ND2	1:A:532:TYR:HB3	2.34	0.42
1:B:281:LYS:HB2	1:B:281:LYS:HE3	1.85	0.42
1:B:278:GLN:OE1	1:B:278:GLN:N	2.50	0.42
1:A:47:ILE:HG13	1:A:146:TYR:HA	2.02	0.41
1:A:402:TRP:CZ3	1:B:364:ASP:HB2	2.55	0.41
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.55	0.41
1:B:277:ARG:HA	1:B:277:ARG:HD2	1.89	0.41
1:A:240:THR:CG2	1:A:241:VAL:N	2.83	0.41
1:A:97:PRO:HD3	1:A:232:TYR:CZ	2.55	0.41
1:A:339:TYR:CZ	1:A:354:TYR:HB2	2.55	0.41
1:A:344:GLU:HB3	1:A:345:PRO:HD2	2.03	0.41
1:B:87:PHE:O	1:B:90:VAL:HG22	2.20	0.41
1:B:319:TYR:HE2	1:B:383:TRP:HB3	1.84	0.41
1:B:411:ILE:HA	1:B:412:PRO:HD3	1.91	0.41
1:A:356:ARG:HD2	1:A:359:GLY:HA2	2.02	0.41
1:B:150:PRO:HD2	1:B:153:TRP:HE3	1.86	0.41
1:B:235:HIS:O	1:B:239:TRP:HE3	2.04	0.41
1:A:274:ILE:HG23	1:A:306:ASN:HD21	1.86	0.41
1:A:97:PRO:HB2	1:A:239:TRP:CD2	2.56	0.41
1:A:111:VAL:HG22	1:A:185:ASP:O	2.21	0.40
1:A:405:TYR:HE2	1:A:407:GLN:HB2	1.87	0.40
1:A:61:PHE:HE2	1:A:76:ASP:HB2	1.87	0.40
1:A:171:PHE:CE2	1:A:205:LEU:HD13	2.57	0.40
1:B:132:ILE:HD11	1:B:144:TYR:HE2	1.86	0.40
1:B:244:ILE:HG13	1:B:426:TRP:CH2	2.56	0.40
1:A:440:PHE:CD1	1:A:459:THR:HG22	2.57	0.40
1:B:171:PHE:CE2	1:B:205:LEU:HD23	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/1053 (50%)	495 (95%)	27 (5%)	0	100	100
1	B	390/1053 (37%)	371 (95%)	19 (5%)	0	100	100
All	All	912/2106 (43%)	866 (95%)	46 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	475/909 (52%)	447 (94%)	28 (6%)	19	51
1	B	364/909 (40%)	331 (91%)	33 (9%)	9	36
All	All	839/1818 (46%)	778 (93%)	61 (7%)	18	45

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	17	ASP
1	A	20	LYS
1	A	29	GLU
1	A	38	CYS
1	A	54	ASN
1	A	88	TRP
1	A	115	TYR
1	A	145	GLN
1	A	230	MET
1	A	245	VAL
1	A	248	GLU
1	A	269	GLN
1	A	349	LEU
1	A	373	GLN
1	A	374	LYS
1	A	402	TRP
1	A	416	PHE

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Mol	Chain	Res	Type
1	A	419	THR
1	A	422	LEU
1	A	424	LYS
1	A	428	GLN
1	A	434	ILE
1	A	454	LYS
1	A	539	HIS
1	A	542	ILE
1	A	545	ASN
1	A	551	LEU
1	B	21	VAL
1	B	29	GLU
1	B	34	LEU
1	B	49	LYS
1	B	56	TYR
1	B	61	PHE
1	B	69	THR
1	B	83	ARG
1	B	92	LEU
1	B	143	ARG
1	B	167	ILE
1	B	171	PHE
1	B	175	ASN
1	B	185	ASP
1	B	189	VAL
1	B	197	GLN
1	B	201	LYS
1	B	209	LEU
1	B	211	ARG
1	B	239	TRP
1	B	252	TRP
1	B	319	TYR
1	B	348	ASN
1	B	362	THR
1	B	364	ASP
1	B	368	LEU
1	B	386	THR
1	B	397	THR
1	B	400	THR
1	B	405	TYR
1	B	411	ILE
1	B	414	TRP

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Mol	Chain	Res	Type
1	B	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	23	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no ligands in this entry.

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

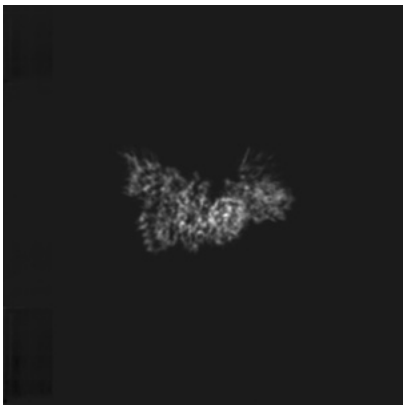
This section contains visualisations of the EMDB entry EMD-25074. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

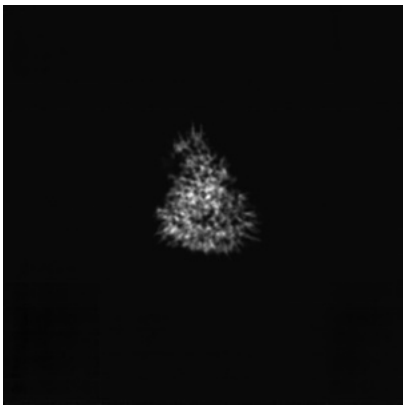
6.1 Orthogonal projections

6.1.1 Primary map

X

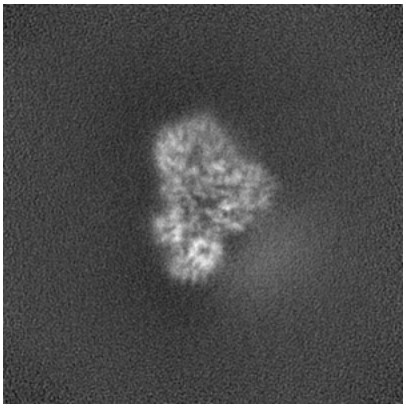


Y

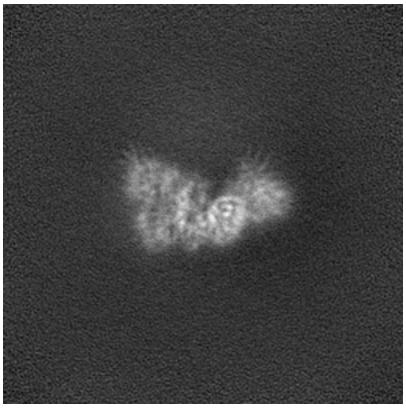


Z

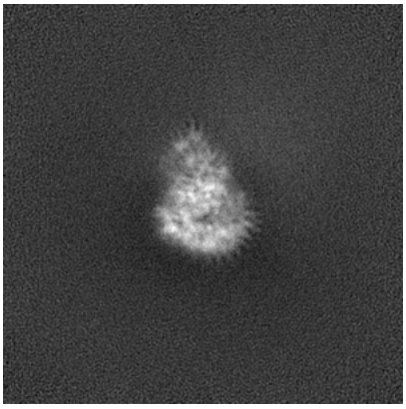
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

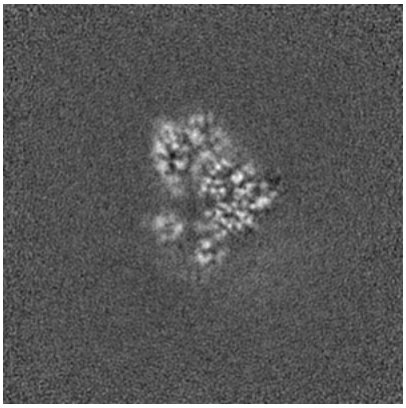
6.2.1 Primary map

X Index: 128

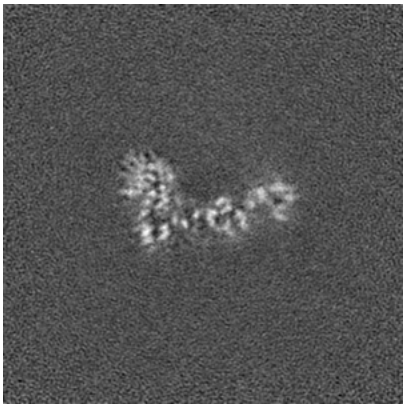
Y Index: 128

Z Index: 128

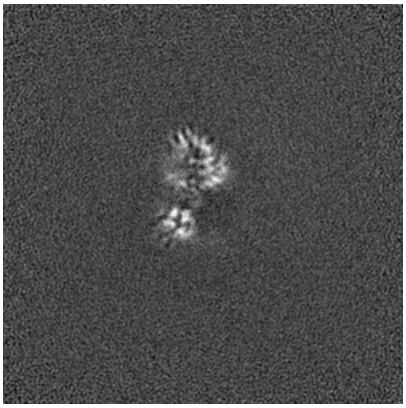
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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

6.3 Largest variance slices (i)

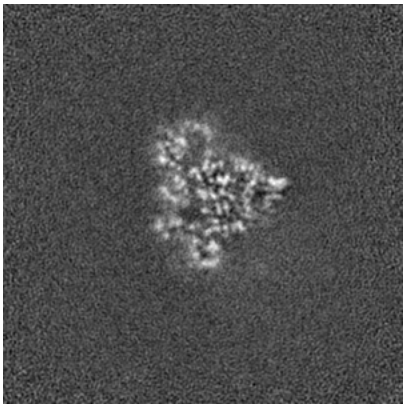
6.3.1 Primary map

X Index: 121

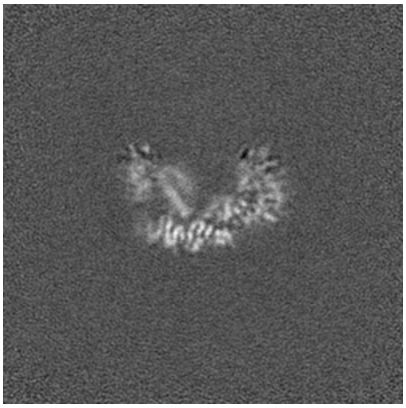
Y Index: 134

Z Index: 143

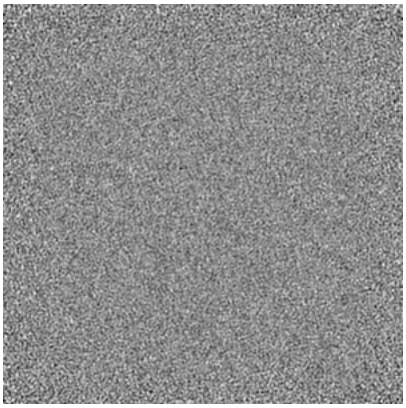
6.3.2 Raw map



X Index: 121



Y Index: 111



Z Index: 0

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

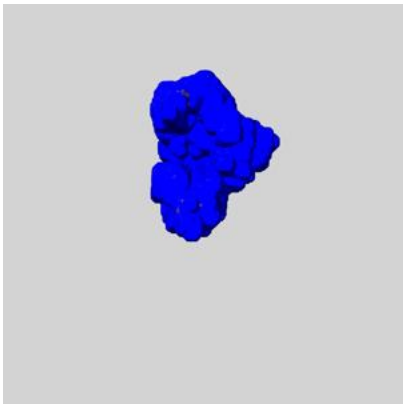
6.5 Mask visualisation (i)

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

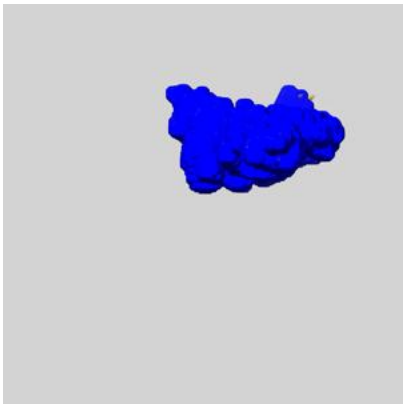
A mask typically either:

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

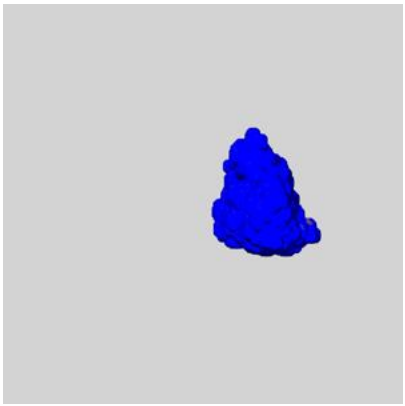
6.5.1 emd_25074_msk_1.map (i)



X



Y

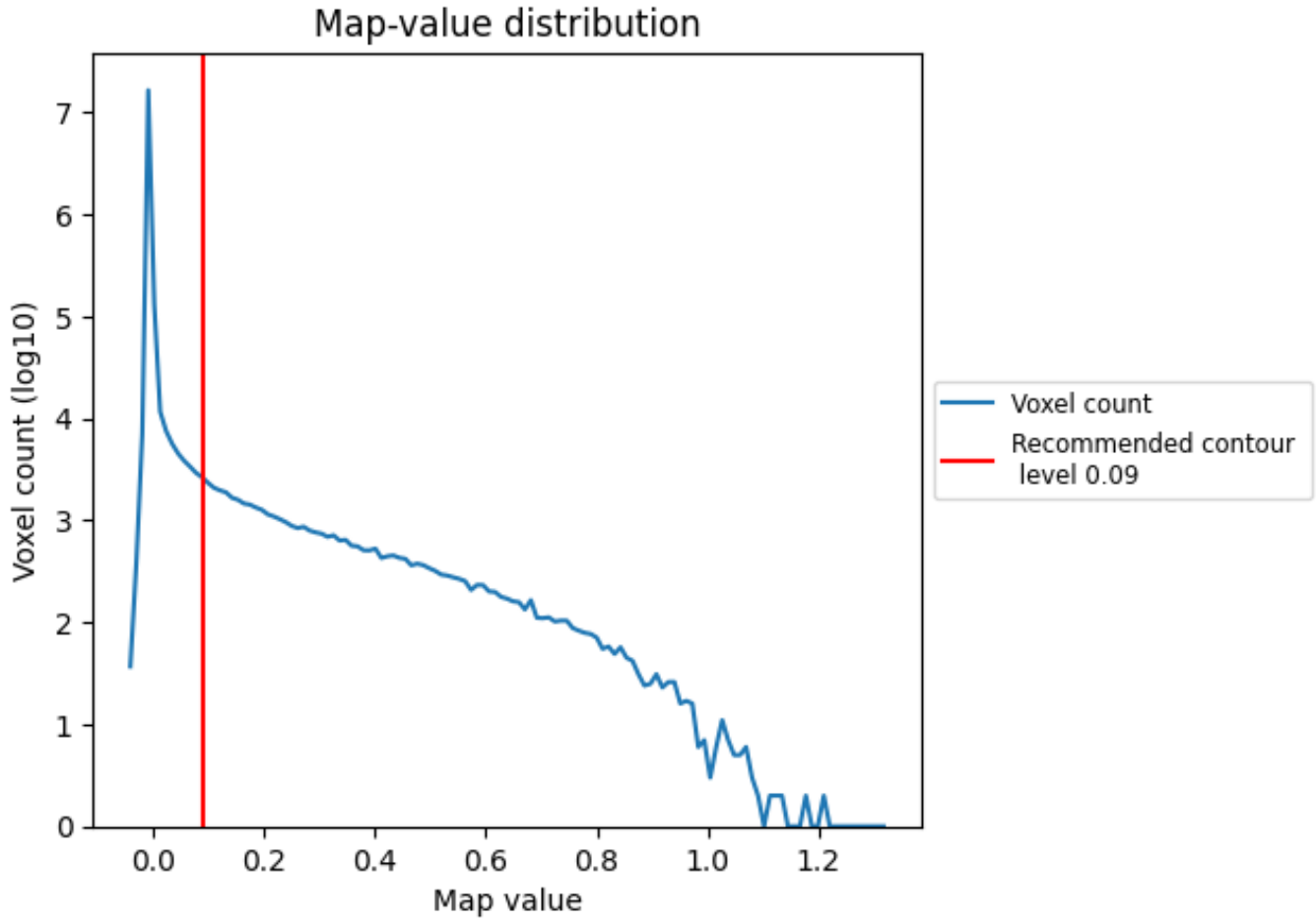


Z

7 Map analysis

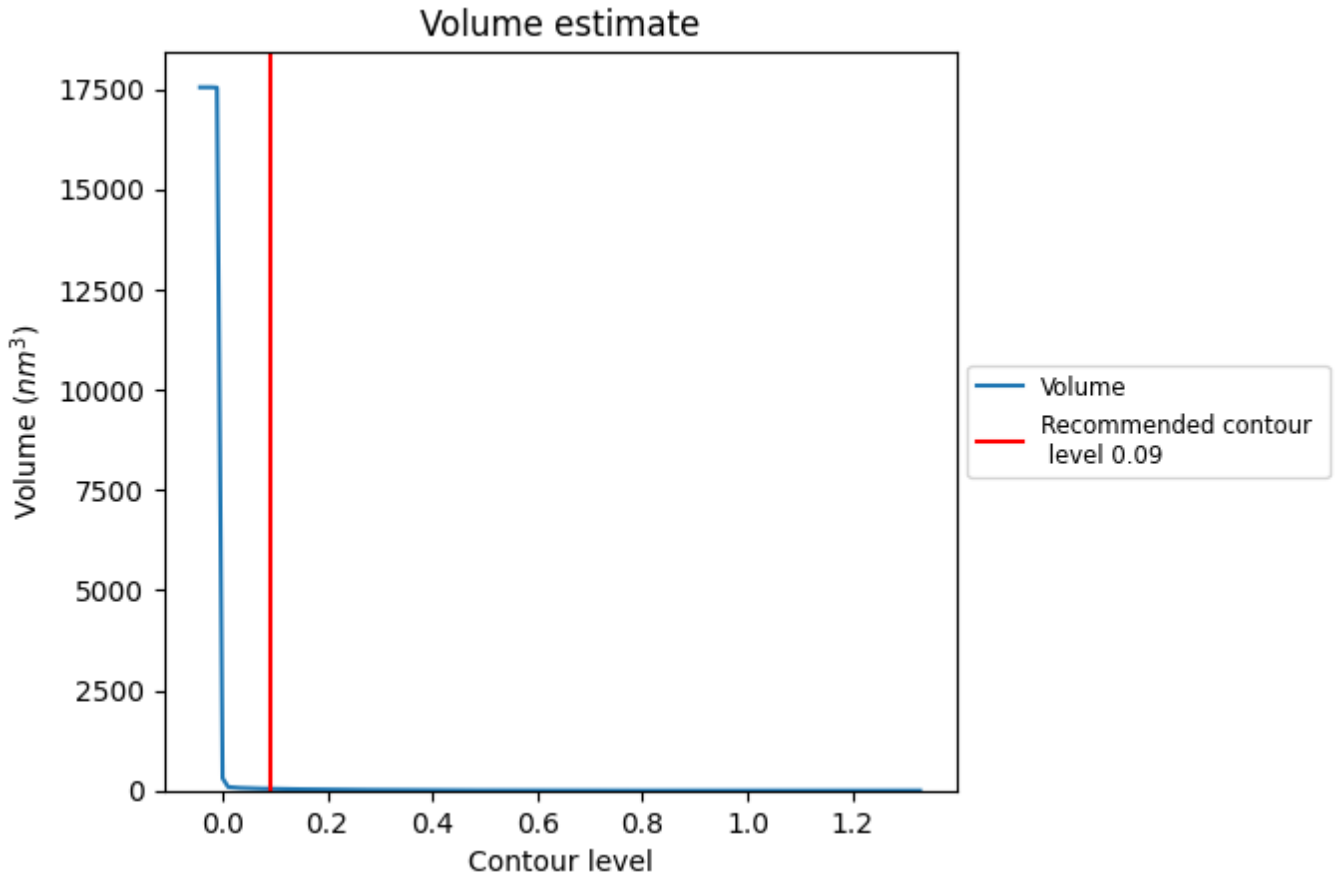
This section contains the results of statistical analysis of the map.

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.

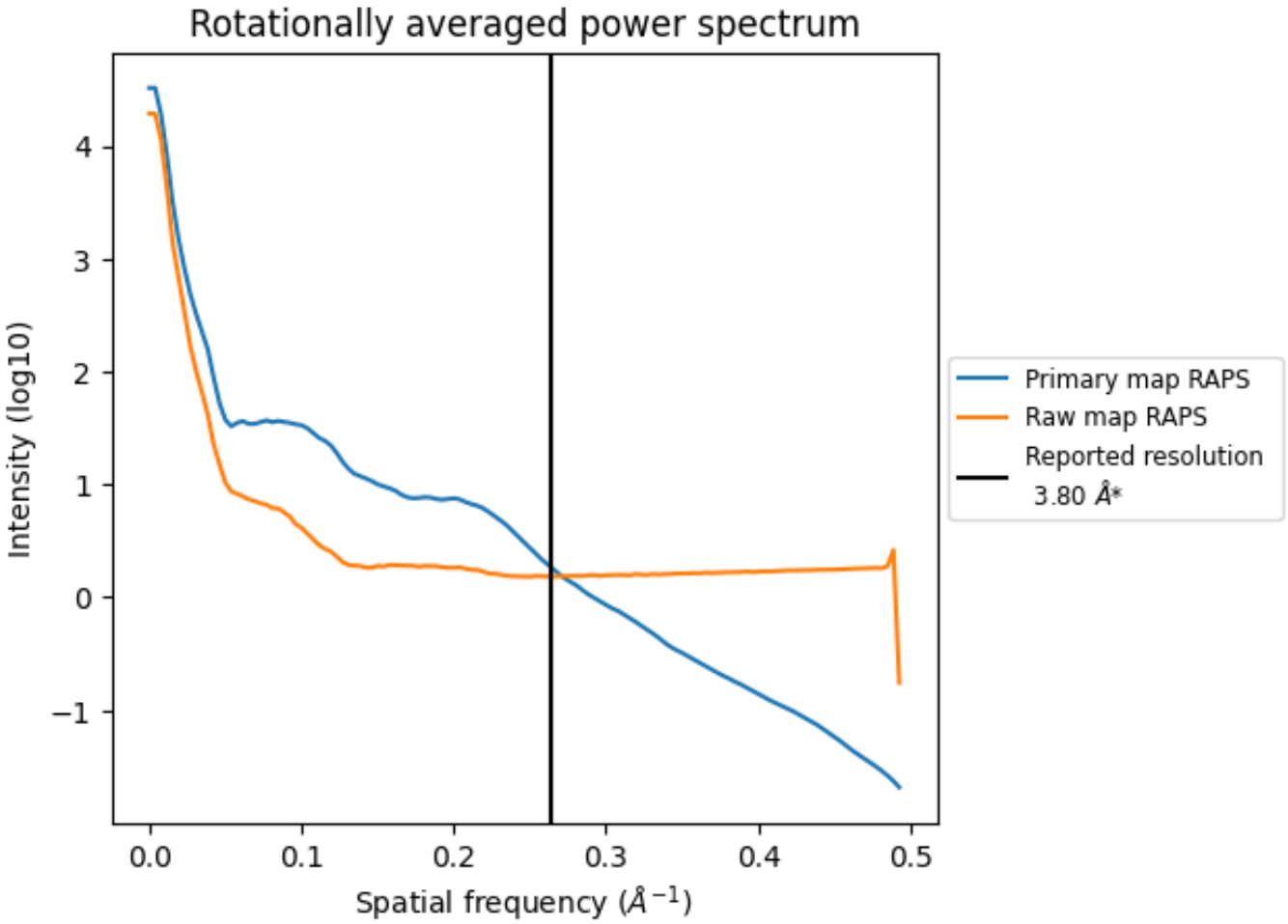
7.2 Volume estimate



The volume at the recommended contour level is 44 nm^3; this corresponds to an approximate mass of 40 kDa.

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

7.3 Rotationally averaged power spectrum (i)

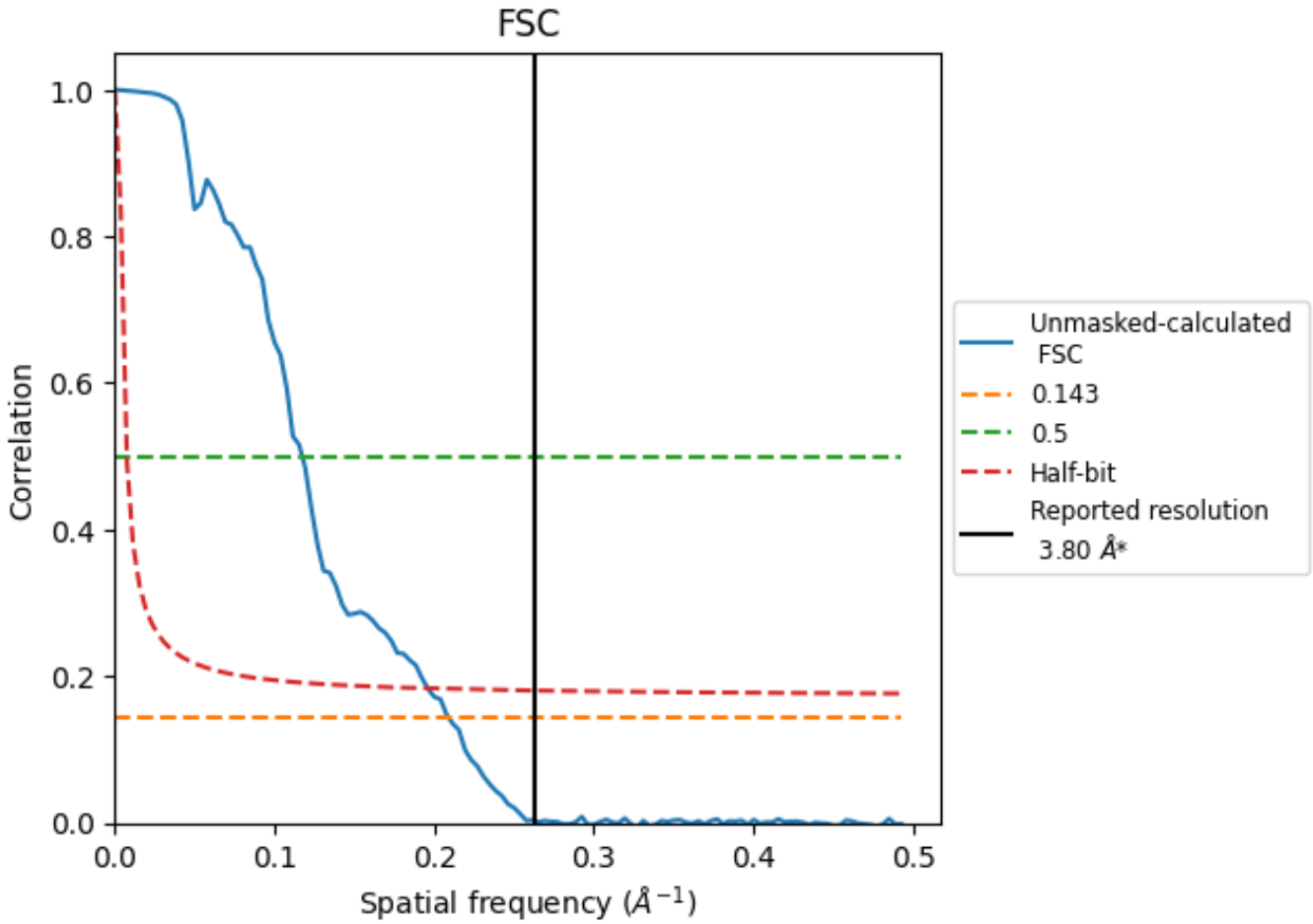


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

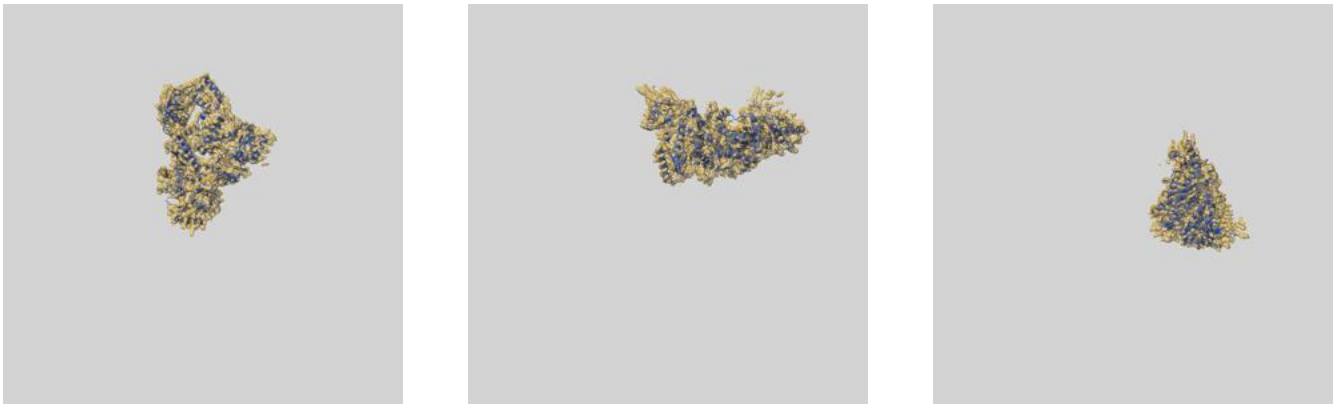
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.78	8.53	5.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.78 differs from the reported value 3.8 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25074 and PDB model 7SEP. Per-residue inclusion information can be found in section 3 on page 8.

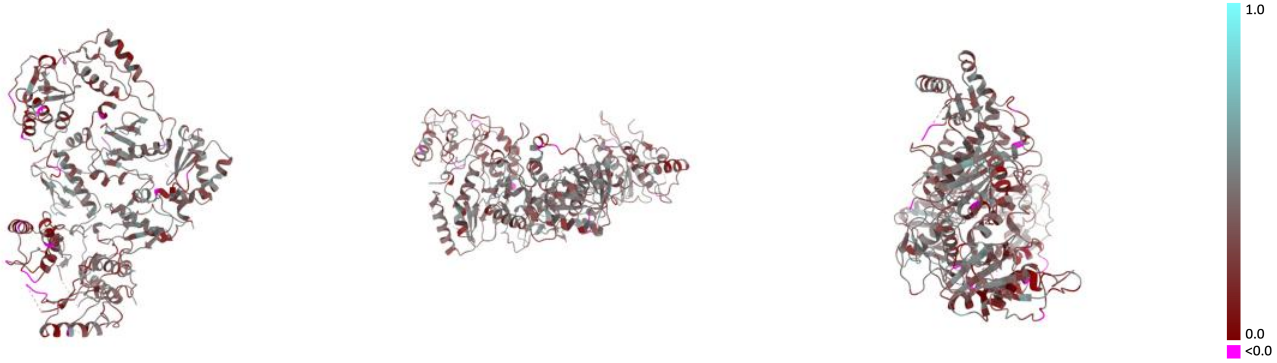
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

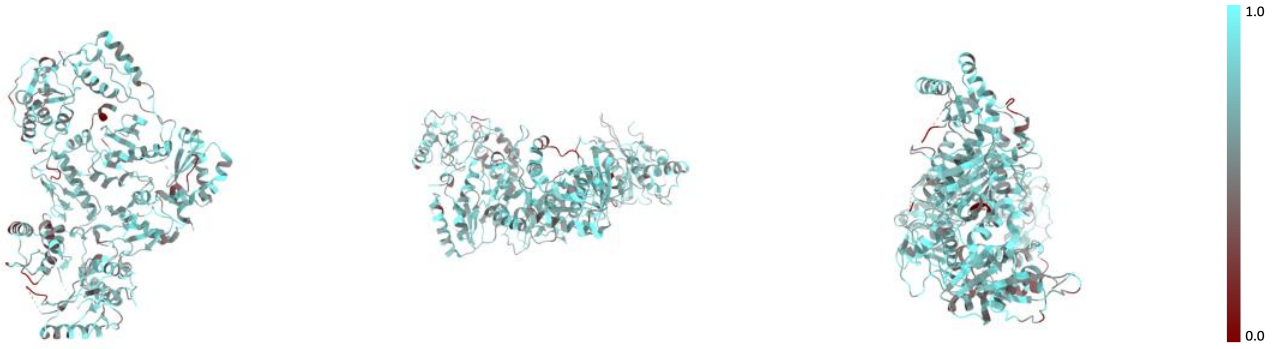
9.2 Q-score mapped to coordinate model



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.

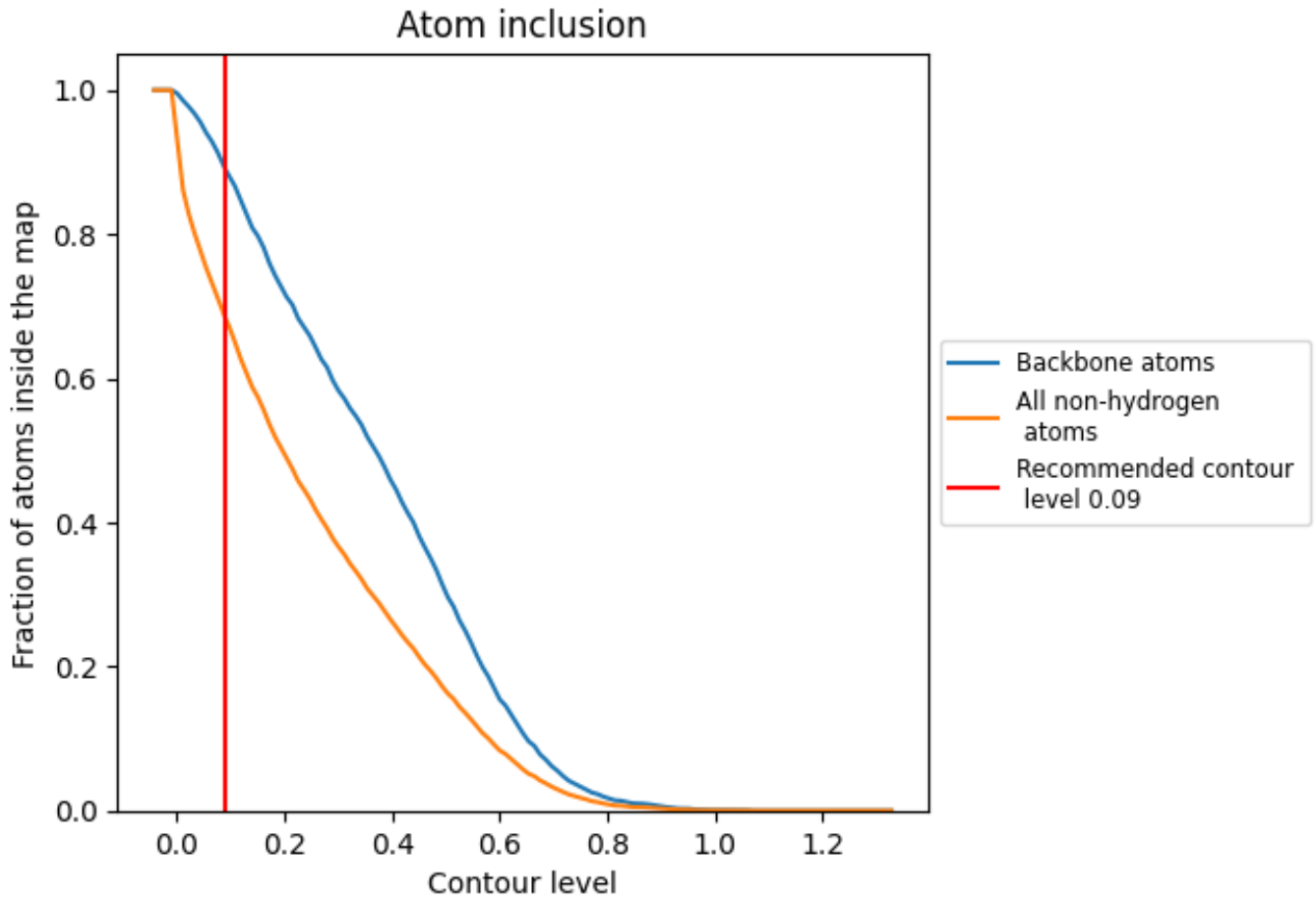
9.3 Atom inclusion mapped to coordinate model



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 68% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6837	0.3460
A	0.6732	0.3320
B	0.6974	0.3650