



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 02:57 AM UTC

PDB ID : 8U72 / pdb_00008u72
EMDB ID : EMD-41966
Title : Cryo-EM structure of the SPARTA oligomer with guide RNA and target DNA
Authors : Malik, R.; Kottur, J.; Aggarwal, A.K.
Deposited on : 2023-09-14
Resolution : 3.15 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

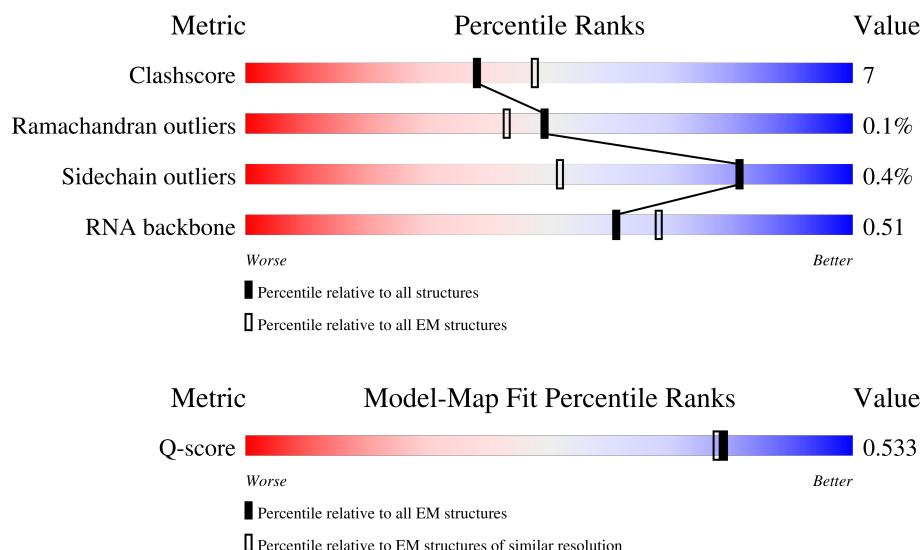
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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.



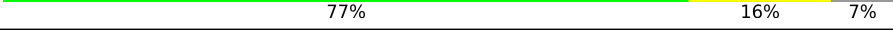
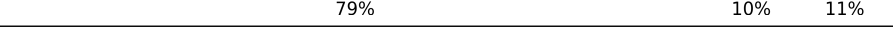
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14486 (2.65 - 3.65)

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	M	21	
1	S	21	
1	U	21	

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Mol	Chain	Length	Quality of chain
1	X	21	
2	N	45	
2	T	45	
2	V	45	
2	Y	45	
3	B	450	
3	D	450	
3	F	450	
3	H	450	
4	C	507	
4	E	507	
4	G	507	
4	I	507	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29712 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 RNA chain called RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*UP*GP*UP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	19	Total	C	N	O	P	0	0
			411	183	74	135	19		
1	M	19	Total	C	N	O	P	0	0
			411	183	74	135	19		
1	S	19	Total	C	N	O	P	0	0
			411	183	74	135	19		
1	X	19	Total	C	N	O	P	0	0
			411	183	74	135	19		

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	18	Total	C	N	O	P	0	0
			359	173	61	107	18		
2	N	18	Total	C	N	O	P	0	0
			359	173	61	107	18		
2	T	18	Total	C	N	O	P	0	0
			359	173	61	107	18		
2	Y	18	Total	C	N	O	P	0	0
			359	173	61	107	18		

- Molecule 3 is a protein called TIR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	417	Total	C	N	O	S	0	0
			3143	2068	545	523	7		
3	D	411	Total	C	N	O	S	0	0
			3142	2066	539	529	8		
3	B	417	Total	C	N	O	S	0	0
			3166	2093	538	527	8		
3	F	416	Total	C	N	O	S	0	0
			3170	2091	543	529	7		

- Molecule 4 is a protein called Piwi domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	454	Total	C	N	O	S	1	0
			3533	2312	591	619	11		
4	E	452	Total	C	N	O	S	0	0
			3452	2268	577	596	11		
4	C	452	Total	C	N	O	S	0	0
			3489	2282	580	616	11		
4	G	450	Total	C	N	O	S	1	0
			3476	2273	583	609	11		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	I	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	G	1	Total	Mg	0
			1	1	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	U	1	Total	O	0
			1	1	
6	H	8	Total	O	0
			8	8	
6	I	2	Total	O	0
			2	2	
6	E	1	Total	O	0
			1	1	
6	M	1	Total	O	0
			1	1	
6	N	1	Total	O	0
			1	1	
6	D	7	Total	O	0
			7	7	
6	B	17	Total	O	0
			17	17	

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Mol	Chain	Residues	Atoms		AltConf
6	C	4	Total 4	O 4	0
6	F	12	Total 12	O 12	0
6	G	3	Total 3	O 3	0

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.

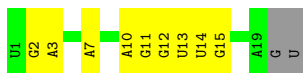
- Molecule 1: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*UP*GP*UP*AP*UP*A)-3')

Chain U: 



- Molecule 1: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*UP*GP*UP*AP*UP*A)-3')

Chain M: 

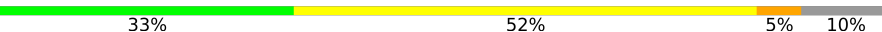


- Molecule 1: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*UP*GP*UP*AP*UP*A)-3')

Chain S: 



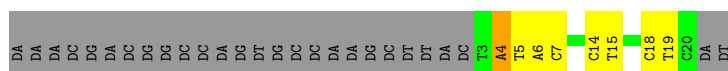
- Molecule 1: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*UP*GP*UP*AP*UP*A)-3')

Chain X: 

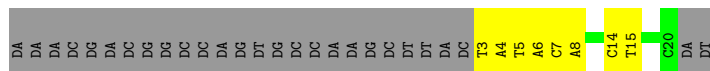


- Molecule 2: DNA (5'-D(P*TP*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*C P*TP*C)-3')

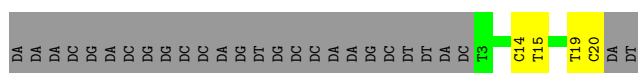
Chain V: 



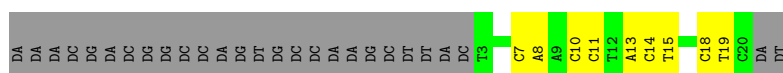
- Molecule 2: DNA (5'-D(P*TP*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*C P*TP*C)-3')



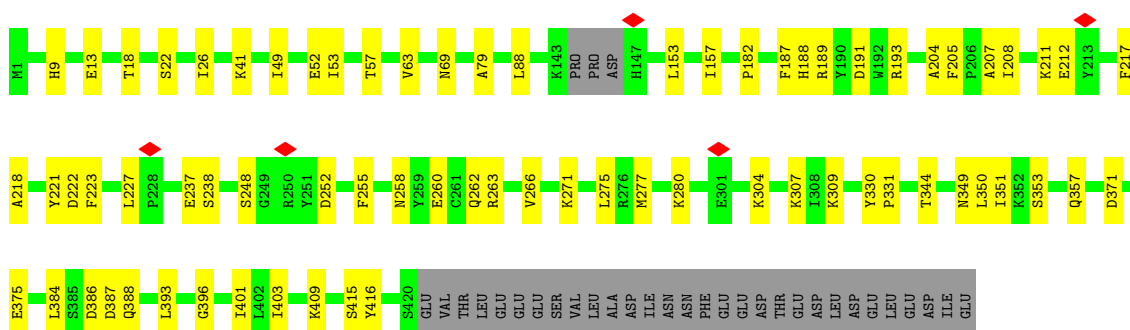
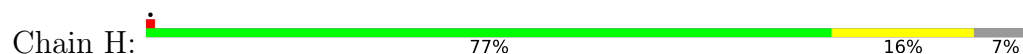
- Molecule 2: DNA (5'-D(P*TP*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*C P*TP*C)-3')



- Molecule 2: DNA (5'-D(P*TP*AP*TP*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*C P*TP*C)-3')

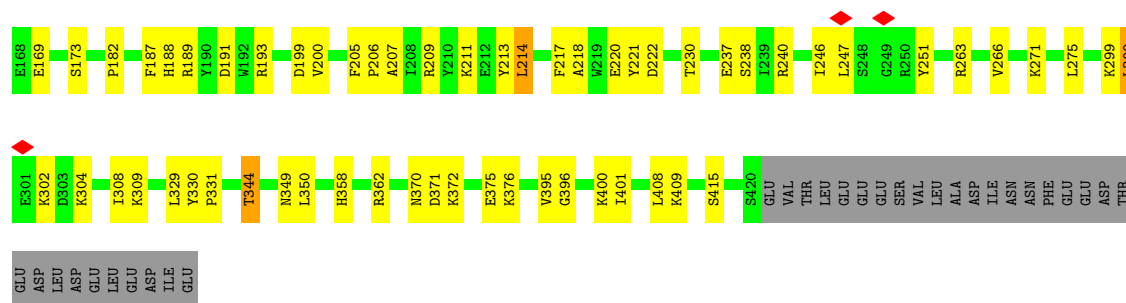


- Molecule 3: TIR domain-containing protein



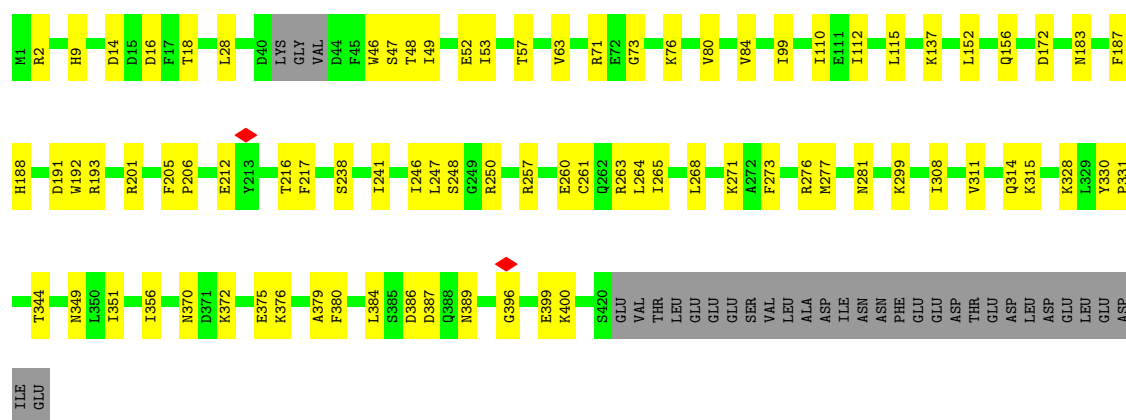
- Molecule 3: TIR domain-containing protein





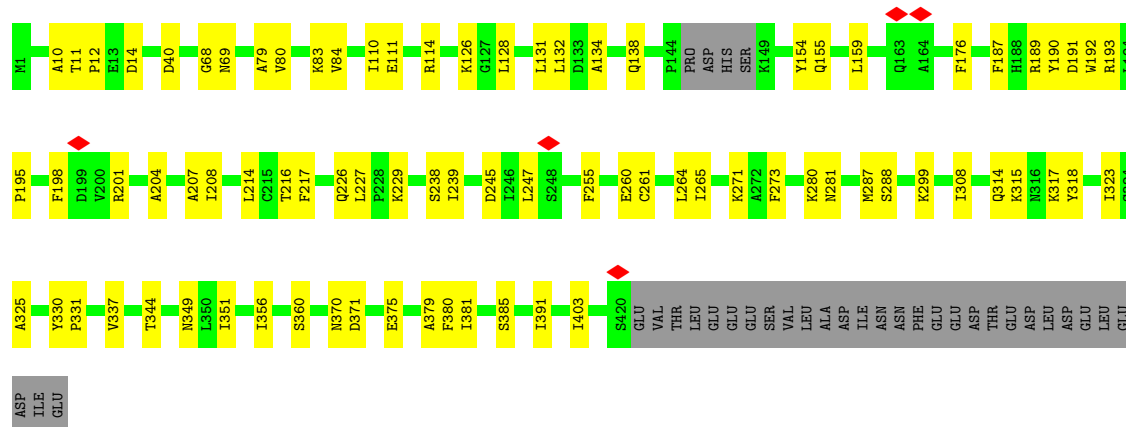
• Molecule 3: TIR domain-containing protein

Chain B: 74% 18% 7%



• Molecule 3: TIR domain-containing protein

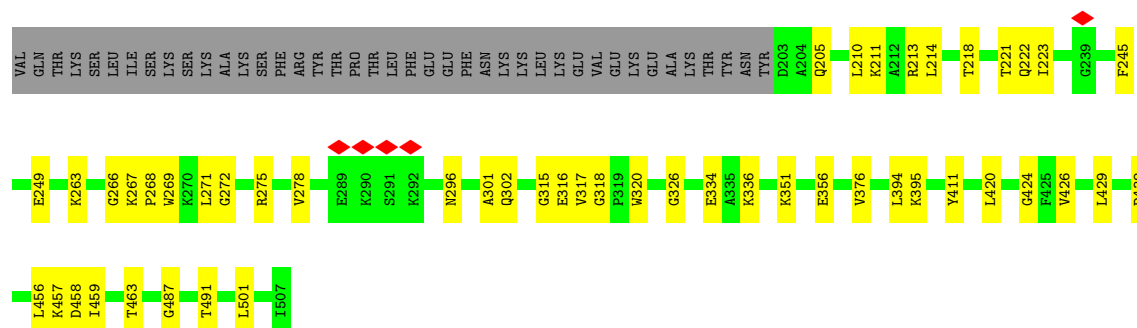
Chain F: 74% 18% 8%



• Molecule 4: Piwi domain-containing protein

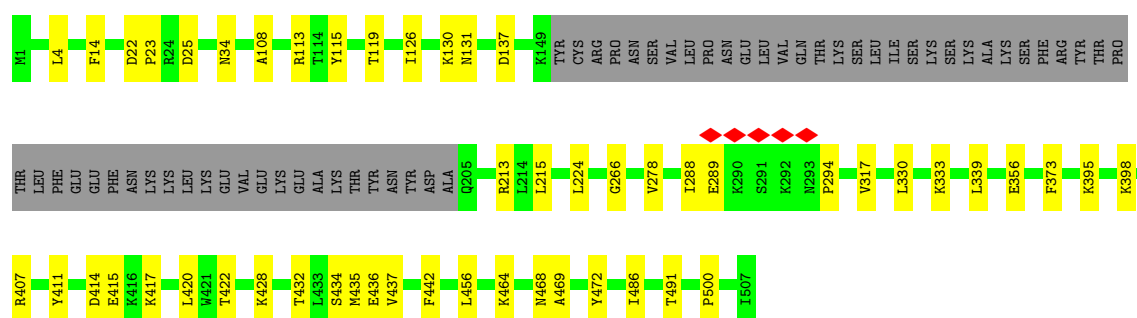
Chain I: 75% 15% 10%





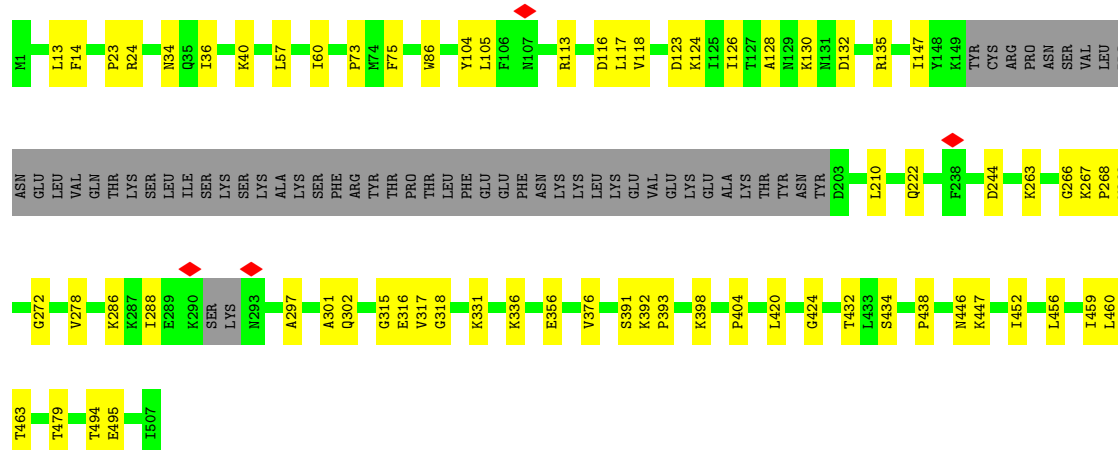
• Molecule 4: Piwi domain-containing protein

Chain E: 79% 10% 11%



• Molecule 4: Piwi domain-containing protein

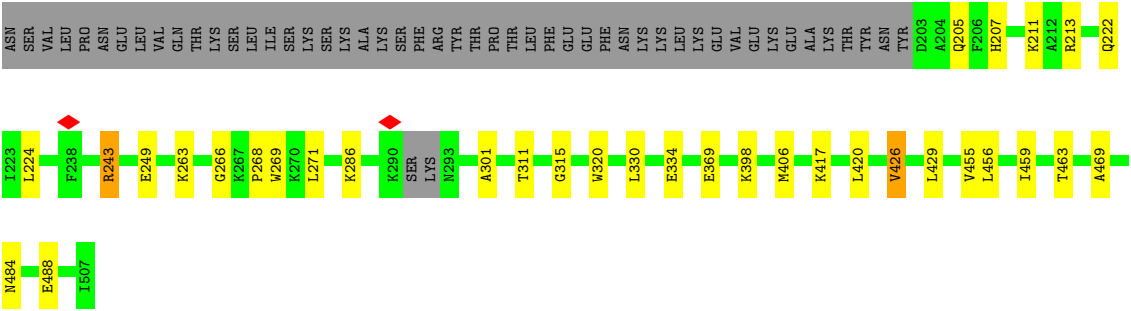
Chain C: 76% 14% 11%



• Molecule 4: Piwi domain-containing protein

Chain G: 77% 12% 11%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	238432	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 ($e^-/\text{\AA}^2$)	51.11	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.539	Depositor
Minimum map value	-0.412	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.564	Depositor
Map size (Å)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M	0.14	0/460	0.26	0/716
1	S	0.15	0/460	0.25	0/716
1	U	0.14	0/460	0.26	0/716
1	X	0.15	0/460	0.29	0/716
2	N	0.28	0/400	0.47	0/612
2	T	0.29	0/400	0.51	0/612
2	V	0.30	0/400	0.66	1/612 (0.2%)
2	Y	0.29	0/400	0.48	0/612
3	B	0.16	0/3247	0.40	0/4412
3	D	0.16	0/3221	0.40	1/4378 (0.0%)
3	F	0.23	0/3249	0.48	2/4410 (0.0%)
3	H	0.17	0/3220	0.39	0/4377
4	C	0.13	0/3578	0.29	0/4865
4	E	0.19	0/3541	0.33	0/4816
4	G	0.13	0/3566	0.29	0/4846
4	I	0.15	0/3630	0.33	1/4932 (0.0%)
All	All	0.17	0/30692	0.37	5/42348 (0.0%)

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
3	H	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	4	DA	O3'-P-O5'	10.63	119.95	104.00
4	I	36	ILE	N-CA-C	-8.16	96.32	108.97
3	F	14	ASP	N-CA-C	-7.39	100.74	111.30
3	D	214	LEU	N-CA-C	-7.35	101.54	111.54
3	F	190	TYR	CB-CA-C	5.95	120.17	111.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	189	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	411	0	203	8	0
1	S	411	0	203	8	0
1	U	411	0	203	7	0
1	X	411	0	203	9	0
2	N	359	0	204	6	0
2	T	359	0	204	2	0
2	V	359	0	204	6	0
2	Y	359	0	204	6	0
3	B	3166	0	2963	57	0
3	D	3142	0	2944	67	0
3	F	3170	0	2981	54	0
3	H	3143	0	2936	54	0
4	C	3489	0	3363	45	0
4	E	3452	0	3304	36	0
4	G	3476	0	3357	41	0
4	I	3533	0	3440	42	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	17	0	0	1	0
6	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	7	0	0	0	0
6	E	1	0	0	0	0
6	F	12	0	0	0	0
6	G	3	0	0	0	0
6	H	8	0	0	0	0
6	I	2	0	0	1	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	U	1	0	0	0	0
All	All	29712	0	26916	418	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 7.

All (418) 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)
3:D:344:THR:HG22	3:D:349:ASN:O	1.42	1.14
4:E:414:ASP:OD2	4:E:415:GLU:N	2.15	0.80
3:D:344:THR:HG23	3:D:350:LEU:HA	1.64	0.79
3:H:263:ARG:NH2	1:S:15:G:N2	2.33	0.77
3:D:344:THR:HG22	3:D:349:ASN:C	2.11	0.76
3:D:189:ARG:HD2	3:D:214:LEU:HG	1.68	0.75
3:D:189:ARG:CD	3:D:214:LEU:HG	2.18	0.74
3:F:370:ASN:HD21	4:G:398:LYS:H	1.34	0.74
3:F:204:ALA:H	3:F:226:GLN:HE22	1.36	0.73
3:H:263:ARG:NH2	1:S:15:G:H21	1.87	0.73
3:H:9:HIS:HD2	3:H:18:THR:HG21	1.55	0.71
3:H:13:GLU:N	3:H:13:GLU:OE2	2.24	0.70
3:D:344:THR:CG2	3:D:350:LEU:HA	2.22	0.69
4:G:420:LEU:HD12	4:G:456:LEU:HD22	1.74	0.69
3:D:188:HIS:HA	3:D:237:GLU:HG3	1.75	0.69
3:D:52:GLU:OE1	3:D:56:ASN:ND2	2.27	0.68
3:H:260:GLU:OE1	3:H:263:ARG:NH2	2.25	0.68
2:V:7:DC:O2	3:B:263:ARG:NH1	2.27	0.67
3:D:344:THR:CG2	3:D:349:ASN:O	2.34	0.67
4:I:278:VAL:HG12	4:I:356:GLU:HB3	1.77	0.67
4:C:135:ARG:NH1	4:G:137:ASP:OD2	2.28	0.67
4:C:278:VAL:HG12	4:C:356:GLU:HB3	1.76	0.67
3:H:188:HIS:HA	3:H:237:GLU:HG3	1.76	0.67
4:E:464:LYS:NZ	4:E:472:TYR:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:211:LYS:NZ	3:H:255:PHE:O	2.30	0.65
4:E:317:VAL:HG11	4:E:486:ILE:HG21	1.79	0.65
4:C:34:ASN:HD21	4:C:266:GLY:HA2	1.60	0.65
3:H:211:LYS:HG2	3:H:217:PHE:HZ	1.63	0.64
4:I:501:LEU:HB2	4:E:131:ASN:HB3	1.78	0.64
4:G:14:PHE:HZ	4:G:23:PRO:HA	1.62	0.64
4:E:119:THR:HG22	4:E:213:ARG:HH22	1.62	0.64
3:F:126:LYS:HE3	3:F:126:LYS:HA	1.79	0.64
3:F:195:PRO:HG2	3:F:198:PHE:HB2	1.79	0.64
3:B:276:ARG:NH2	3:B:386:ASP:OD1	2.31	0.64
1:U:14:U:H2'	1:U:15:G:H8	1.63	0.63
3:F:68:GLY:O	3:F:69:ASN:ND2	2.32	0.63
3:B:152:LEU:O	3:B:156:GLN:NE2	2.30	0.63
3:D:211:LYS:HG2	3:D:217:PHE:HZ	1.63	0.63
4:G:205:GLN:N	4:G:205:GLN:OE1	2.29	0.62
3:B:63:VAL:HG13	3:B:99:ILE:HD12	1.81	0.62
3:F:308:ILE:HD13	3:F:375:GLU:HB3	1.80	0.62
3:F:245:ASP:O	3:F:247:LEU:N	2.32	0.62
3:F:308:ILE:HD12	3:F:379:ALA:HB2	1.82	0.61
4:I:420:LEU:HD12	4:I:456:LEU:HD22	1.82	0.61
4:C:222:GLN:OE1	4:C:263:LYS:NZ	2.32	0.61
3:F:314:GLN:NE2	3:F:360:SER:OG	2.34	0.61
4:I:301:ALA:HA	4:I:315:GLY:HA2	1.82	0.61
4:G:100:GLU:O	4:G:104:TYR:HB2	2.01	0.61
3:B:308:ILE:HD13	3:B:375:GLU:HB3	1.81	0.60
2:N:3:DT:H2'	2:N:4:DA:H8	1.66	0.60
3:B:370:ASN:HD22	4:C:404:PRO:HA	1.65	0.60
3:H:371:ASP:O	3:H:375:GLU:HG2	2.01	0.60
4:G:330:LEU:N	4:G:369:GLU:OE2	2.27	0.60
4:E:108:ALA:HB3	4:E:113:ARG:HG3	1.83	0.60
3:B:370:ASN:HD21	4:C:398:LYS:H	1.50	0.60
3:H:263:ARG:CZ	1:S:15:G:N2	2.64	0.59
3:D:49:ILE:O	3:D:53:ILE:HG13	2.02	0.59
4:I:426:VAL:HG11	4:I:429:LEU:HD12	1.83	0.59
3:B:71:ARG:O	3:B:73:GLY:N	2.35	0.59
3:F:191:ASP:C	3:F:193:ARG:H	2.11	0.59
1:U:14:U:H2'	1:U:15:G:C8	2.38	0.59
3:H:304:LYS:HE3	3:H:307:LYS:HA	1.85	0.58
2:V:5:DT:H2''	2:V:6:DA:OP2	2.03	0.58
3:B:188:HIS:HB2	3:B:216:THR:HB	1.84	0.58
3:F:391:ILE:HB	3:F:403:ILE:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:424:GLY:HA2	4:I:438:PRO:HG3	1.86	0.58
3:B:281:ASN:HB3	3:B:299:LYS:HE2	1.86	0.58
3:B:330:TYR:HB3	3:B:331:PRO:HD3	1.86	0.58
4:G:54:LYS:HG2	4:G:88:SER:HB2	1.84	0.58
4:G:61:GLN:NE2	4:G:86:TRP:O	2.37	0.58
3:H:344:THR:OG1	3:H:349:ASN:O	2.20	0.57
3:H:415:SER:OG	3:H:416:TYR:N	2.38	0.57
3:F:344:THR:OG1	3:F:349:ASN:O	2.22	0.57
3:H:271:LYS:O	3:H:275:LEU:HD12	2.04	0.57
4:I:46:THR:HG23	4:I:49:GLY:H	1.69	0.57
3:B:187:PHE:HE1	3:B:217:PHE:CE1	2.23	0.57
3:B:344:THR:OG1	3:B:349:ASN:O	2.23	0.57
3:D:187:PHE:HB2	3:D:238:SER:HB3	1.86	0.57
4:C:446:ASN:ND2	4:C:446:ASN:O	2.38	0.57
4:E:34:ASN:HD21	4:E:266:GLY:HA2	1.70	0.57
3:B:308:ILE:HD12	3:B:379:ALA:HB2	1.85	0.57
3:F:281:ASN:O	3:F:299:LYS:NZ	2.35	0.57
4:I:114:THR:HG21	4:I:205:GLN:HB3	1.87	0.57
3:B:46:TRP:CD1	3:B:47:SER:H	2.23	0.57
3:B:261:CYS:HA	3:B:264:LEU:HD12	1.86	0.57
4:C:288:ILE:HD11	4:C:297:ALA:HB2	1.87	0.57
3:D:167:LYS:HB3	3:D:415:SER:HB2	1.87	0.56
4:C:117:LEU:HD13	4:C:147:ILE:HG23	1.86	0.56
3:B:399:GLU:O	3:B:400:LYS:NZ	2.31	0.56
2:N:8:DA:H1'	3:D:263:ARG:HD3	1.87	0.56
4:E:398:LYS:H	3:D:370:ASN:HD21	1.51	0.56
4:E:435:MET:HG2	4:E:436:GLU:HG3	1.87	0.56
2:Y:18:DC:H2'	2:Y:19:DT:C6	2.41	0.56
4:G:271:LEU:H	4:G:311:THR:HG21	1.69	0.56
3:H:280:LYS:NZ	3:H:384:LEU:O	2.34	0.56
3:D:218:ALA:HB1	3:D:220:GLU:O	2.06	0.56
3:D:344:THR:CG2	3:D:349:ASN:C	2.78	0.56
3:H:280:LYS:NZ	3:H:386:ASP:OD1	2.37	0.56
4:I:222:GLN:OE1	4:I:263:LYS:NZ	2.38	0.56
3:H:211:LYS:HA	1:S:17:A:H4'	1.87	0.56
1:X:14:U:H2'	1:X:15:G:H8	1.70	0.55
4:C:301:ALA:HA	4:C:315:GLY:HA2	1.88	0.55
3:F:273:PHE:CE1	3:F:325:ALA:HB3	2.42	0.55
3:D:371:ASP:O	3:D:375:GLU:HG2	2.07	0.55
3:F:187:PHE:HA	3:F:216:THR:O	2.06	0.55
3:B:396:GLY:O	3:B:400:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:17:A:H4'	3:B:212:GLU:H	1.71	0.55
4:G:301:ALA:HA	4:G:315:GLY:HA2	1.89	0.54
3:D:207:ALA:HA	3:D:217:PHE:O	2.07	0.54
3:D:237:GLU:N	3:D:237:GLU:OE1	2.40	0.54
4:I:214:LEU:O	4:I:218:THR:N	2.41	0.54
4:C:432:THR:OG1	4:C:434:SER:O	2.25	0.54
4:C:446:ASN:C	4:C:446:ASN:HD22	2.14	0.54
4:G:104:TYR:CE1	4:G:116:ASP:HB3	2.43	0.54
3:H:182:PRO:HD3	3:H:401:ILE:HG12	1.89	0.54
4:I:135:ARG:NH1	4:E:137:ASP:OD2	2.40	0.54
4:I:459:ILE:O	4:I:463:THR:HG23	2.07	0.54
4:C:36:ILE:HG13	4:C:36:ILE:O	2.07	0.54
3:D:182:PRO:HD3	3:D:401:ILE:HG12	1.90	0.54
3:F:330:TYR:HB3	3:F:331:PRO:HD3	1.91	0.54
4:E:417:LYS:HD3	4:E:442:PHE:HZ	1.72	0.53
4:E:22:ASP:HB2	4:E:428:LYS:HE2	1.89	0.53
1:X:14:U:H2'	1:X:15:G:C8	2.43	0.53
4:G:320:TRP:HB3	4:G:334:GLU:HB3	1.90	0.53
1:S:13:U:H2'	1:S:14:U:C6	2.43	0.53
2:N:7:DC:H2'	2:N:8:DA:C8	2.43	0.53
3:F:371:ASP:OD1	3:F:371:ASP:N	2.42	0.53
3:D:309:LYS:O	3:D:376:LYS:NZ	2.41	0.53
3:B:246:ILE:HG22	3:B:247:LEU:H	1.73	0.53
3:H:205:PHE:CD2	3:H:396:GLY:HA2	2.45	0.52
3:D:200:VAL:HG21	3:D:209:ARG:HG3	1.92	0.52
3:B:206:PRO:HB3	3:B:271:LYS:HG2	1.91	0.52
4:G:455:VAL:O	4:G:459:ILE:HG12	2.10	0.52
1:S:14:U:H2'	1:S:15:G:H8	1.74	0.52
1:X:2:G:H5'	4:G:224:LEU:HD23	1.92	0.52
2:Y:14:DC:H2'	2:Y:15:DT:C6	2.44	0.52
3:B:9:HIS:CD2	3:B:18:THR:HG21	2.45	0.52
3:H:237:GLU:N	3:H:237:GLU:OE1	2.43	0.52
3:D:15:ASP:O	3:D:18:THR:OG1	2.23	0.52
3:F:11:THR:O	3:F:12:PRO:C	2.53	0.52
4:E:278:VAL:HG12	4:E:356:GLU:HB3	1.92	0.51
4:E:432:THR:HG22	4:E:434:SER:H	1.75	0.51
4:G:89:GLN:OE1	4:G:89:GLN:N	2.42	0.51
1:U:13:U:H2'	1:U:14:U:H6	1.74	0.51
3:D:266:VAL:HG12	3:D:329:LEU:HD13	1.92	0.51
4:G:426:VAL:HG13	4:G:429:LEU:HB2	1.91	0.51
1:M:13:U:H2'	1:M:14:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:9:HIS:CG	3:D:18:THR:HG21	2.45	0.51
3:D:187:PHE:HE2	3:D:217:PHE:CZ	2.29	0.51
4:I:320:TRP:HB3	4:I:334:GLU:HB3	1.91	0.51
3:D:372:LYS:O	3:D:376:LYS:HG3	2.11	0.51
4:C:420:LEU:HD13	4:C:456:LEU:HD22	1.92	0.51
1:S:13:U:H2'	1:S:14:U:H6	1.74	0.50
3:D:344:THR:HG23	3:D:350:LEU:HD23	1.92	0.50
3:B:217:PHE:CZ	3:B:264:LEU:HD13	2.46	0.50
3:B:183:ASN:OD1	3:B:183:ASN:N	2.44	0.50
4:C:105:LEU:HD12	4:C:113:ARG:HD3	1.93	0.50
4:C:302:GLN:HB2	4:C:316:GLU:HG2	1.93	0.50
4:G:484:ASN:O	4:G:488:GLU:HG3	2.11	0.50
3:F:155:GLN:HG2	3:F:159:LEU:HD23	1.93	0.50
3:D:240:ARG:NH1	3:D:251:TYR:O	2.45	0.50
4:C:123:ASP:OD1	4:C:124:LYS:N	2.45	0.50
3:F:134:ALA:O	3:F:138:GLN:HG3	2.11	0.50
3:H:271:LYS:HG3	3:H:275:LEU:HD11	1.94	0.50
3:B:257:ARG:NE	6:B:503:HOH:O	2.44	0.50
3:H:187:PHE:HE1	3:H:217:PHE:CE2	2.30	0.50
1:X:13:U:H2'	1:X:14:U:H6	1.77	0.50
3:F:201:ARG:HG3	3:F:271:LYS:HZ1	1.77	0.50
2:N:3:DT:H2'	2:N:4:DA:C8	2.45	0.50
1:U:12:G:H2'	1:U:13:U:C6	2.47	0.49
3:D:71:ARG:HB3	3:D:74:VAL:HG12	1.93	0.49
3:D:308:ILE:HG12	3:D:375:GLU:HB3	1.93	0.49
4:C:268:PRO:HB2	4:C:269:TRP:CE3	2.47	0.49
4:E:395:LYS:HE3	4:E:437:VAL:HB	1.93	0.49
1:M:14:U:H2'	1:M:15:G:H8	1.77	0.49
4:C:446:ASN:O	4:C:447:LYS:HG2	2.12	0.49
4:E:398:LYS:N	3:D:370:ASN:HD21	2.10	0.49
4:G:123:ASP:OD1	4:G:124:LYS:N	2.45	0.49
3:H:218:ALA:HB3	3:H:223:PHE:HZ	1.77	0.49
3:F:80:VAL:O	3:F:84:VAL:HG23	2.12	0.49
3:B:380:PHE:HE1	3:B:384:LEU:HD11	1.78	0.49
1:M:14:U:H2'	1:M:15:G:C8	2.47	0.49
4:C:459:ILE:O	4:C:463:THR:HG23	2.13	0.49
3:H:351:ILE:HB	3:H:357:GLN:HE21	1.77	0.49
1:M:13:U:H2'	1:M:14:U:H6	1.78	0.48
3:F:208:ILE:HD11	3:F:264:LEU:HG	1.95	0.48
3:H:153:LEU:O	3:H:157:ILE:HG13	2.12	0.48
4:E:126:ILE:O	4:E:130:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:330:TYR:HB3	3:D:331:PRO:HD3	1.95	0.48
3:F:187:PHE:CD1	3:F:238:SER:HB2	2.48	0.48
2:V:6:DA:O3'	3:B:201:ARG:NH1	2.46	0.48
3:D:112:ILE:HA	3:D:115:LEU:HD12	1.95	0.48
3:B:387:ASP:OD1	3:B:389:ASN:N	2.44	0.48
4:G:50:LEU:HD11	4:G:91:ILE:HG21	1.96	0.48
3:D:149:LYS:O	3:D:153:LEU:HG	2.14	0.48
3:D:221:TYR:CG	3:D:222:ASP:N	2.82	0.48
4:C:494:THR:OG1	4:C:495:GLU:N	2.47	0.48
3:F:201:ARG:HG3	3:F:271:LYS:NZ	2.29	0.48
4:I:72:ARG:NH1	6:I:701:HOH:O	2.46	0.48
3:B:351:ILE:HG21	3:B:356:ILE:HD11	1.95	0.48
3:H:191:ASP:C	3:H:193:ARG:H	2.22	0.48
4:E:420:LEU:HD22	4:E:456:LEU:HD22	1.96	0.48
4:I:24:ARG:HD2	4:I:73:PRO:HD2	1.95	0.48
2:N:5:DT:H2'	2:N:6:DA:H8	1.77	0.48
3:F:330:TYR:HE2	4:G:417:LYS:HD2	1.78	0.48
1:U:13:U:H2'	1:U:14:U:C6	2.49	0.48
3:H:221:TYR:CG	3:H:222:ASP:N	2.82	0.48
1:S:14:U:H2'	1:S:15:G:C8	2.49	0.47
3:D:395:VAL:HG22	3:D:400:LYS:HA	1.96	0.47
4:C:391:SER:O	4:C:391:SER:OG	2.28	0.47
3:H:409:LYS:HB3	3:H:409:LYS:HE3	1.61	0.47
3:H:227:LEU:HD12	3:H:227:LEU:O	2.14	0.47
2:V:4:DA:H2''	2:V:5:DT:OP1	2.14	0.47
4:E:14:PHE:HZ	4:E:23:PRO:HA	1.80	0.47
3:H:41:LYS:HD2	3:D:118:ILE:HG12	1.95	0.47
2:V:18:DC:H2'	2:V:19:DT:C6	2.50	0.47
3:H:205:PHE:HB2	3:H:223:PHE:HE1	1.79	0.47
2:T:14:DC:H2'	2:T:15:DT:C6	2.50	0.47
3:D:189:ARG:HD2	3:D:214:LEU:CG	2.42	0.47
3:B:380:PHE:CE1	3:B:384:LEU:HD11	2.50	0.47
3:B:389:ASN:O	3:B:389:ASN:ND2	2.46	0.47
4:C:118:VAL:HG13	4:C:210:LEU:HD13	1.96	0.47
3:H:387:ASP:OD1	3:H:388:GLN:N	2.45	0.47
4:G:117:LEU:HD13	4:G:147:ILE:HG23	1.96	0.47
3:D:16:ASP:HA	3:D:19:ARG:HG3	1.97	0.47
4:I:296:ASN:ND2	4:I:326:GLY:O	2.48	0.47
3:F:260:GLU:HG3	3:F:264:LEU:HD13	1.97	0.47
4:I:336:LYS:HA	4:I:376:VAL:HG21	1.97	0.46
1:X:13:U:H2'	1:X:14:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:191:ASP:O	3:D:193:ARG:HG3	2.16	0.46
4:C:104:TYR:CD2	4:C:116:ASP:HB3	2.49	0.46
4:C:126:ILE:O	4:C:130:LYS:HG2	2.15	0.46
3:D:80:VAL:O	3:D:84:VAL:HG23	2.15	0.46
3:F:330:TYR:CD1	3:F:330:TYR:C	2.93	0.46
4:E:25:ASP:OD2	3:D:154:TYR:OH	2.34	0.46
2:N:14:DC:H2'	2:N:15:DT:C6	2.51	0.46
3:H:262:GLN:O	3:H:266:VAL:HG23	2.15	0.46
4:I:210:LEU:HD22	4:I:223:ILE:HD11	1.97	0.46
2:T:19:DT:H4'	2:T:20:DC:C2	2.51	0.46
1:X:12:G:H2'	1:X:13:U:C6	2.51	0.46
4:G:56:TYR:O	4:G:60:ILE:HG23	2.16	0.46
2:V:14:DC:H2'	2:V:15:DT:C6	2.50	0.46
3:F:191:ASP:O	3:F:193:ARG:N	2.49	0.46
3:F:239:ILE:H	3:F:239:ILE:HG13	1.54	0.46
3:D:18:THR:O	3:D:22:SER:OG	2.25	0.46
3:F:273:PHE:HE1	3:F:325:ALA:HB3	1.80	0.46
4:G:268:PRO:HB2	4:G:269:TRP:CE3	2.51	0.46
4:I:128:ALA:O	4:I:132:ASP:HB2	2.16	0.46
4:I:268:PRO:HB2	4:I:269:TRP:CE3	2.51	0.46
3:B:205:PHE:HE2	3:B:396:GLY:C	2.24	0.46
3:B:261:CYS:O	3:B:265:ILE:HG13	2.15	0.46
4:E:215:LEU:HD21	4:E:500:PRO:HD2	1.98	0.45
4:E:469:ALA:HB2	1:M:3:A:H4'	1.98	0.45
3:B:273:PHE:CZ	3:B:277:MET:HE3	2.51	0.45
3:F:351:ILE:HG21	3:F:356:ILE:HD11	1.98	0.45
4:G:105:LEU:HD13	4:G:117:LEU:HD11	1.97	0.45
3:H:204:ALA:C	3:H:205:PHE:HD1	2.24	0.45
1:U:12:G:H2'	1:U:13:U:H6	1.81	0.45
3:B:112:ILE:HA	3:B:115:LEU:HD12	1.99	0.45
3:F:187:PHE:CE1	3:F:238:SER:HB2	2.52	0.45
3:B:46:TRP:C	3:B:48:THR:H	2.24	0.45
3:F:128:LEU:O	3:F:132:LEU:HD23	2.16	0.45
3:D:358:HIS:O	3:D:362:ARG:HG2	2.16	0.45
4:C:244:ASP:OD1	4:C:244:ASP:N	2.48	0.45
4:G:14:PHE:CZ	4:G:23:PRO:HA	2.49	0.45
4:I:14:PHE:HZ	4:I:23:PRO:HA	1.81	0.45
4:E:224:LEU:HD23	1:M:2:G:H5'	1.99	0.45
3:D:33:TRP:NE1	3:D:52:GLU:OE2	2.49	0.45
3:D:213:TYR:O	3:D:214:LEU:C	2.58	0.45
3:H:9:HIS:HA	3:H:63:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:394:LEU:HD12	4:I:395:LYS:H	1.82	0.45
3:D:191:ASP:C	3:D:193:ARG:H	2.24	0.45
3:B:49:ILE:O	3:B:53:ILE:HG13	2.17	0.45
3:B:52:GLU:O	3:B:57:THR:HG23	2.16	0.45
3:B:328:LYS:HZ3	3:B:331:PRO:HD2	1.82	0.45
3:F:79:ALA:O	3:F:83:LYS:HG2	2.17	0.45
4:G:57:LEU:O	4:G:61:GLN:HG2	2.17	0.45
4:G:249:GLU:H	4:G:249:GLU:CD	2.23	0.45
4:G:286:LYS:HB3	4:G:286:LYS:HE3	1.65	0.45
4:I:126:ILE:O	4:I:130:LYS:HG2	2.17	0.44
4:I:275:ARG:NH2	4:I:458:ASP:OD2	2.47	0.44
4:C:460:LEU:O	4:C:463:THR:OG1	2.29	0.44
4:I:501:LEU:HB2	4:E:131:ASN:CB	2.45	0.44
4:I:211:LYS:HE2	4:I:221:THR:HG23	1.99	0.44
4:I:487:GLY:O	4:I:491:THR:HG23	2.16	0.44
3:B:191:ASP:C	3:B:193:ARG:H	2.25	0.44
3:H:353:SER:O	3:H:357:GLN:HG3	2.18	0.44
4:E:4:LEU:HD22	4:E:411:TYR:HB2	1.99	0.44
3:B:28:LEU:HD12	3:B:28:LEU:HA	1.75	0.44
3:F:385:SER:HA	3:F:391:ILE:HD13	1.99	0.44
3:F:110:ILE:O	3:F:111:GLU:HG2	2.18	0.44
4:E:288:ILE:HD13	4:E:491:THR:HG23	2.00	0.44
4:I:94:LYS:HE2	4:I:128:ALA:HB2	1.99	0.44
4:I:302:GLN:HB2	4:I:316:GLU:HG2	2.00	0.44
4:E:289:GLU:HA	4:E:294:PRO:HA	1.99	0.43
4:E:339:LEU:HD22	4:E:373:PHE:CD1	2.53	0.43
3:F:227:LEU:O	3:F:229:LYS:N	2.51	0.43
4:I:15:ALA:HB2	4:I:32:PRO:O	2.18	0.43
4:G:34:ASN:HD21	4:G:266:GLY:HA2	1.82	0.43
3:H:52:GLU:O	3:H:57:THR:HG23	2.17	0.43
1:M:12:G:H2'	1:M:13:U:C6	2.53	0.43
3:B:137:LYS:HE2	3:F:40:ASP:OD1	2.17	0.43
3:F:318:TYR:HB2	3:F:344:THR:HG22	2.00	0.43
3:H:212:GLU:H	3:H:212:GLU:CD	2.26	0.43
3:D:187:PHE:N	3:D:238:SER:O	2.46	0.43
3:D:246:ILE:HG22	3:D:247:LEU:H	1.83	0.43
3:B:372:LYS:O	3:B:376:LYS:HG3	2.18	0.43
4:G:222:GLN:OE1	4:G:263:LYS:NZ	2.45	0.43
4:C:13:LEU:HD13	4:C:272:GLY:HA3	2.01	0.43
4:C:424:GLY:HA2	4:C:438:PRO:HG3	1.99	0.43
3:H:252:ASP:HB3	3:H:258:ASN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:304:LYS:HG2	3:H:309:LYS:HG3	2.00	0.43
3:D:173:SER:OG	3:D:408:LEU:O	2.28	0.43
3:B:260:GLU:HG3	3:B:264:LEU:HD11	2.01	0.43
3:H:211:LYS:HG2	3:H:217:PHE:CZ	2.47	0.43
3:D:199:ASP:OD1	3:D:199:ASP:N	2.49	0.43
3:B:328:LYS:NZ	3:B:331:PRO:HD2	2.34	0.43
4:C:267:LYS:H	4:C:267:LYS:HG3	1.68	0.43
4:I:351:LYS:HA	4:I:351:LYS:HD3	1.87	0.43
3:B:80:VAL:O	3:B:84:VAL:HG23	2.18	0.43
4:C:452:ILE:HD12	4:C:452:ILE:HA	1.91	0.43
3:F:176:PHE:CE2	3:F:381:ILE:HG12	2.54	0.43
4:C:331:LYS:HA	4:C:331:LYS:HD3	1.85	0.43
4:G:57:LEU:HD23	4:G:57:LEU:HA	1.85	0.43
4:G:207:HIS:CE1	4:G:211:LYS:HG3	2.54	0.43
4:I:457:LYS:HB3	4:I:457:LYS:HE2	1.91	0.42
4:C:24:ARG:HD2	4:C:73:PRO:HD2	2.00	0.42
4:I:122:ASN:ND2	4:I:213:ARG:HB2	2.34	0.42
3:D:189:ARG:HD3	3:D:214:LEU:CD2	2.49	0.42
4:C:57:LEU:HA	4:C:57:LEU:HD12	1.79	0.42
3:D:206:PRO:HG3	3:D:275:LEU:HD21	2.01	0.42
3:B:187:PHE:HD2	3:B:238:SER:HG	1.67	0.42
3:B:217:PHE:HD2	3:B:268:LEU:HD11	1.84	0.42
4:C:14:PHE:HZ	4:C:23:PRO:HA	1.84	0.42
3:F:10:ALA:O	3:F:11:THR:C	2.61	0.42
4:C:57:LEU:HD11	4:C:86:TRP:CE2	2.54	0.42
3:H:69:ASN:OD1	3:H:69:ASN:C	2.63	0.42
2:Y:7:DC:H2'	2:Y:8:DA:C8	2.54	0.42
3:D:263:ARG:HD2	3:D:263:ARG:O	2.19	0.42
3:H:207:ALA:C	3:H:208:ILE:HD13	2.45	0.42
4:I:315:GLY:O	4:I:501:LEU:HG	2.19	0.42
4:C:392:LYS:HA	4:C:393:PRO:HD3	1.86	0.42
3:H:277:MET:SD	3:H:384:LEU:HD13	2.60	0.42
1:X:5:G:H2'	1:X:6:U:C6	2.54	0.42
3:B:14:ASP:C	3:B:16:ASP:H	2.27	0.42
3:F:280:LYS:HD2	3:F:280:LYS:HA	1.92	0.42
4:G:406:MET:HE2	4:G:406:MET:HB3	1.89	0.42
4:I:13:LEU:HD13	4:I:272:GLY:HA3	2.02	0.42
3:B:201:ARG:HE	3:B:201:ARG:HB2	1.67	0.42
3:F:132:LEU:HD12	3:F:154:TYR:HE1	1.85	0.42
3:H:49:ILE:O	3:H:53:ILE:HG13	2.19	0.41
3:B:183:ASN:O	3:B:241:ILE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:131:LEU:HD23	3:F:131:LEU:HA	1.82	0.41
3:H:9:HIS:CD2	3:H:18:THR:HG21	2.45	0.41
3:H:350:LEU:HD23	3:H:350:LEU:HA	1.89	0.41
1:X:9:U:OP2	3:F:288:SER:OG	2.34	0.41
3:F:261:CYS:O	3:F:265:ILE:HG13	2.20	0.41
4:G:119:THR:OG1	4:G:213:ARG:NH2	2.54	0.41
4:I:317:VAL:HG22	4:I:318:GLY:H	1.85	0.41
3:D:22:SER:O	3:D:26:ILE:HG13	2.21	0.41
3:F:187:PHE:HD2	3:F:217:PHE:CE1	2.39	0.41
4:G:15:ALA:HB2	4:G:32:PRO:O	2.20	0.41
4:G:243[A]:ARG:HA	4:G:243[A]:ARG:HD2	1.80	0.41
4:I:18:GLN:HG3	4:I:30:PHE:CE1	2.55	0.41
4:I:245:PHE:O	4:I:249:GLU:HG3	2.20	0.41
4:I:271:LEU:HD23	4:I:271:LEU:HA	1.91	0.41
2:Y:13:DA:H2''	2:Y:14:DC:H6	1.84	0.41
3:D:302:LYS:O	3:D:304:LYS:HG3	2.20	0.41
3:B:314:GLN:CG	3:B:315:LYS:H	2.33	0.41
3:F:207:ALA:HA	3:F:217:PHE:O	2.21	0.41
3:F:214:LEU:HD13	3:F:255:PHE:CE1	2.56	0.41
4:E:22:ASP:HB3	4:E:25:ASP:HB2	2.02	0.41
3:D:271:LYS:O	3:D:275:LEU:HG	2.20	0.41
3:F:325:ALA:HB2	3:F:337:VAL:HA	2.02	0.41
3:H:205:PHE:CD1	3:H:205:PHE:N	2.87	0.41
1:X:3:A:H4'	4:G:469:ALA:HB2	2.02	0.41
3:D:110:ILE:HG22	3:D:111:GLU:H	1.85	0.41
3:D:299:LYS:O	3:D:300:LEU:HB2	2.21	0.41
4:C:420:LEU:HD21	4:C:460:LEU:HD13	2.02	0.41
4:I:4:LEU:HD22	4:I:411:TYR:HB2	2.02	0.41
4:E:14:PHE:CZ	4:E:23:PRO:HA	2.55	0.41
4:E:468:ASN:ND2	1:M:3:A:H5'	2.36	0.41
3:D:409:LYS:HE3	3:D:409:LYS:HB3	1.65	0.41
4:C:128:ALA:O	4:C:132:ASP:HB2	2.21	0.41
4:C:317:VAL:HG22	4:C:318:GLY:H	1.85	0.41
3:F:315:LYS:O	3:F:317:LYS:HG3	2.21	0.41
4:G:459:ILE:O	4:G:463:THR:HG23	2.21	0.41
3:H:79:ALA:HB2	3:F:114:ARG:NH1	2.36	0.41
3:H:330:TYR:HB3	3:H:331:PRO:HD3	2.01	0.41
3:B:248:SER:O	3:B:250:ARG:N	2.47	0.41
4:C:40:LYS:HE3	4:C:40:LYS:HB3	1.85	0.41
4:C:301:ALA:HB3	4:C:479:THR:HG23	2.03	0.41
4:G:113:ARG:O	4:G:117:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:187:PHE:HB2	3:H:238:SER:HB3	2.03	0.40
3:H:393:LEU:HD11	3:H:403:ILE:HD11	2.04	0.40
4:E:330:LEU:HD12	4:E:330:LEU:HA	1.94	0.40
3:D:152:LEU:O	3:D:156:GLN:HG3	2.21	0.40
3:B:2:ARG:HA	3:B:2:ARG:NE	2.36	0.40
3:F:323:ILE:HG12	3:F:380:PHE:CE1	2.56	0.40
4:I:134:GLU:H	4:I:134:GLU:HG3	1.68	0.40
4:I:34:ASN:HD21	4:I:266:GLY:HA2	1.85	0.40
4:E:115:TYR:O	4:E:119:THR:HG23	2.22	0.40
4:E:407:ARG:NH1	4:E:422:THR:O	2.48	0.40
2:Y:10:DC:H2'	2:Y:11:DC:H6	1.86	0.40
3:D:205:PHE:CE2	3:D:396:GLY:HA2	2.56	0.40
4:C:336:LYS:HG2	4:C:376:VAL:HG23	2.03	0.40
4:G:128:ALA:O	4:G:132:ASP:HB2	2.21	0.40
2:Y:10:DC:H2'	2:Y:11:DC:C6	2.57	0.40
3:B:76:LYS:O	3:B:80:VAL:HG23	2.20	0.40
3:B:172:ASP:N	3:B:172:ASP:OD1	2.54	0.40
4:C:286:LYS:HE3	4:C:286:LYS:HB3	1.77	0.40
3:H:22:SER:O	3:H:26:ILE:HG13	2.21	0.40
3:H:88:LEU:HD12	3:H:88:LEU:HA	1.93	0.40
4:E:333:LYS:HB3	4:E:333:LYS:HE2	1.92	0.40
4:E:398:LYS:HZ3	3:D:169:GLU:CD	2.29	0.40
3:D:46:TRP:HE1	3:B:110:ILE:HB	1.86	0.40
3:D:152:LEU:HD12	3:D:152:LEU:HA	1.90	0.40
4:C:60:ILE:HG23	4:C:75:PHE:HE2	1.86	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	
3	B	413/450 (92%)	353 (86%)	60 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	407/450 (90%)	368 (90%)	38 (9%)	1 (0%)	43	71
3	F	412/450 (92%)	354 (86%)	56 (14%)	2 (0%)	24	55
3	H	413/450 (92%)	370 (90%)	42 (10%)	1 (0%)	43	71
4	C	446/507 (88%)	416 (93%)	30 (7%)	0	100	100
4	E	448/507 (88%)	419 (94%)	29 (6%)	0	100	100
4	G	443/507 (87%)	417 (94%)	26 (6%)	0	100	100
4	I	451/507 (89%)	427 (95%)	24 (5%)	0	100	100
All	All	3433/3828 (90%)	3124 (91%)	305 (9%)	4 (0%)	49	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	248	SER
3	F	192	TRP
3	D	300	LEU
3	F	189	ARG

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	
3	B	279/415 (67%)	277 (99%)	2 (1%)	76	80
3	D	284/415 (68%)	282 (99%)	2 (1%)	76	80
3	F	284/415 (68%)	283 (100%)	1 (0%)	84	84
3	H	279/415 (67%)	279 (100%)	0	100	100
4	C	335/446 (75%)	335 (100%)	0	100	100
4	E	319/446 (72%)	319 (100%)	0	100	100
4	G	333/446 (75%)	330 (99%)	3 (1%)	70	77
4	I	344/446 (77%)	340 (99%)	4 (1%)	63	74
All	All	2457/3444 (71%)	2445 (100%)	12 (0%)	81	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	36	ILE
4	I	97	THR
4	I	267[A]	LYS
4	I	267[B]	LYS
3	D	230	THR
3	D	344	THR
3	B	192	TRP
3	B	311	VAL
3	F	287	MET
4	G	243[A]	ARG
4	G	243[B]	ARG
4	G	426	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	262	GLN
3	H	357	GLN
3	H	364	GLN
4	I	217	HIS
4	I	329	HIS
4	I	409	ASN
4	I	468	ASN
4	E	217	HIS
3	D	267	GLN
3	D	320	HIS
3	D	367	ASN
3	D	370	ASN
3	D	389	ASN
3	B	370	ASN
4	C	68	ASN
4	C	205	GLN
4	C	295	GLN
4	C	409	ASN
3	F	9	HIS
3	F	314	GLN
3	F	340	HIS
3	F	364	GLN
3	F	370	ASN
4	G	207	HIS
4	G	209	GLN

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Mol	Chain	Res	Type
4	G	217	HIS
4	G	329	HIS
4	G	360	HIS
4	G	446	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	18/21 (85%)	3 (16%)	0
1	S	18/21 (85%)	3 (16%)	0
1	U	18/21 (85%)	3 (16%)	0
1	X	18/21 (85%)	4 (22%)	0
All	All	72/84 (85%)	13 (18%)	0

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	2	G
1	U	7	A
1	U	10	A
1	M	7	A
1	M	10	A
1	M	11	G
1	S	2	G
1	S	7	A
1	S	11	G
1	X	2	G
1	X	7	A
1	X	10	A
1	X	11	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

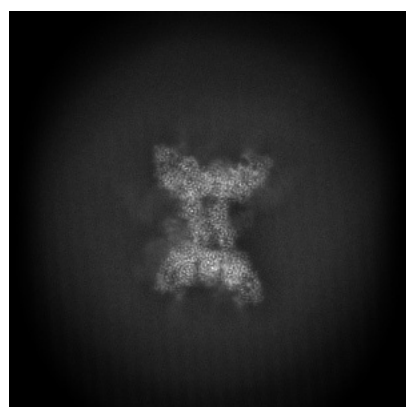
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41966. These allow visual inspection of the internal detail of the map and identification of artifacts.

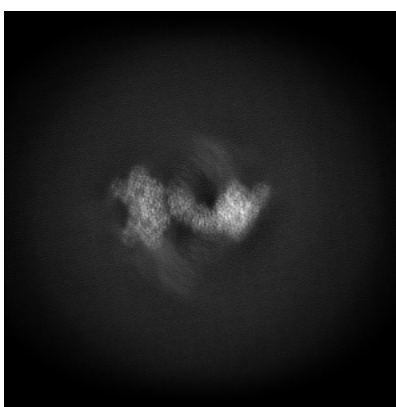
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

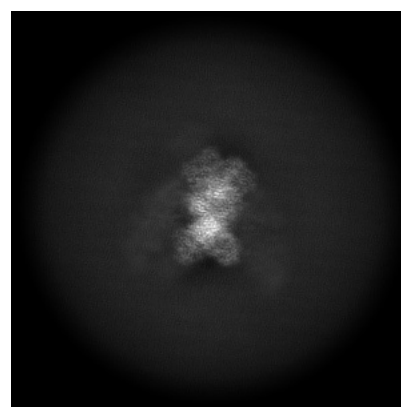
6.1.1 Primary map



X



Y

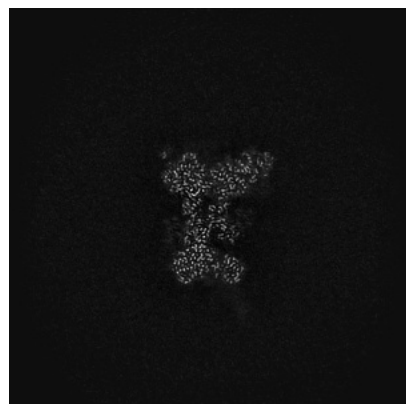


Z

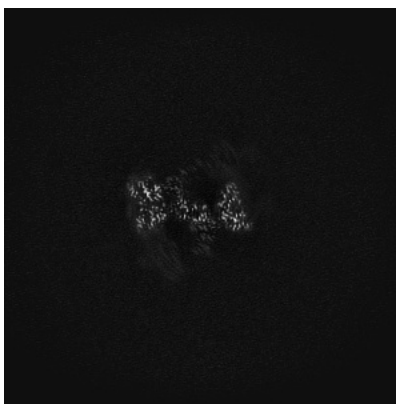
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

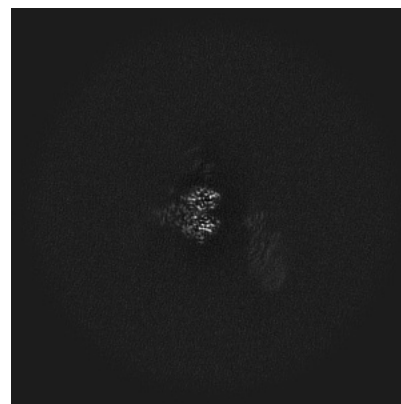
6.2.1 Primary map



X Index: 240



Y Index: 240

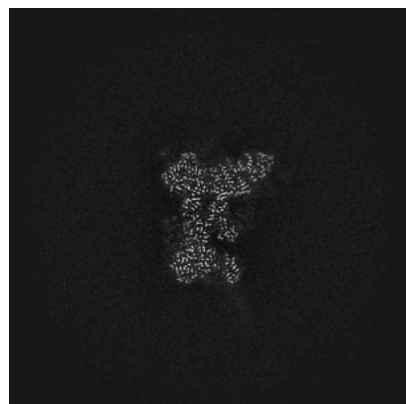


Z Index: 240

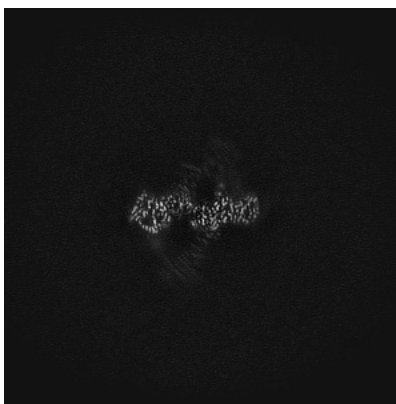
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

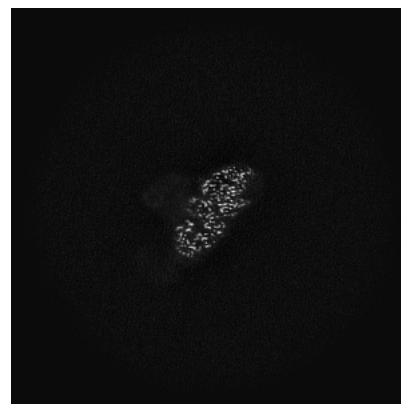
6.3.1 Primary map



X Index: 238



Y Index: 220



Z Index: 171

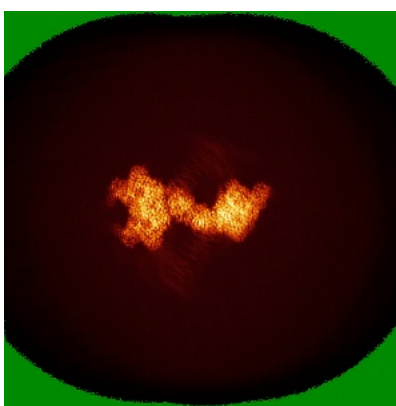
The images above show the largest variance slices of the map in three orthogonal directions.

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

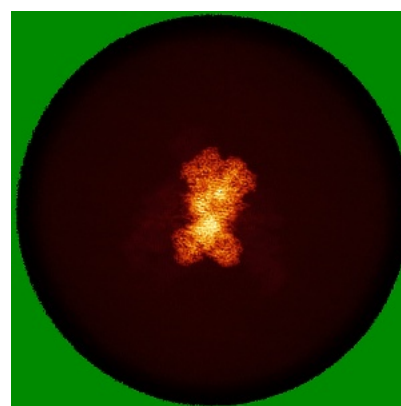
6.4.1 Primary map



X



Y



Z

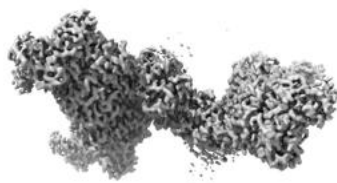
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

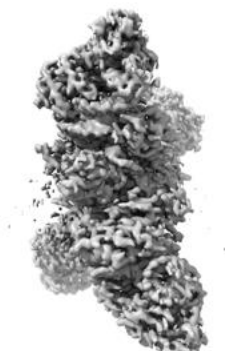
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.564. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

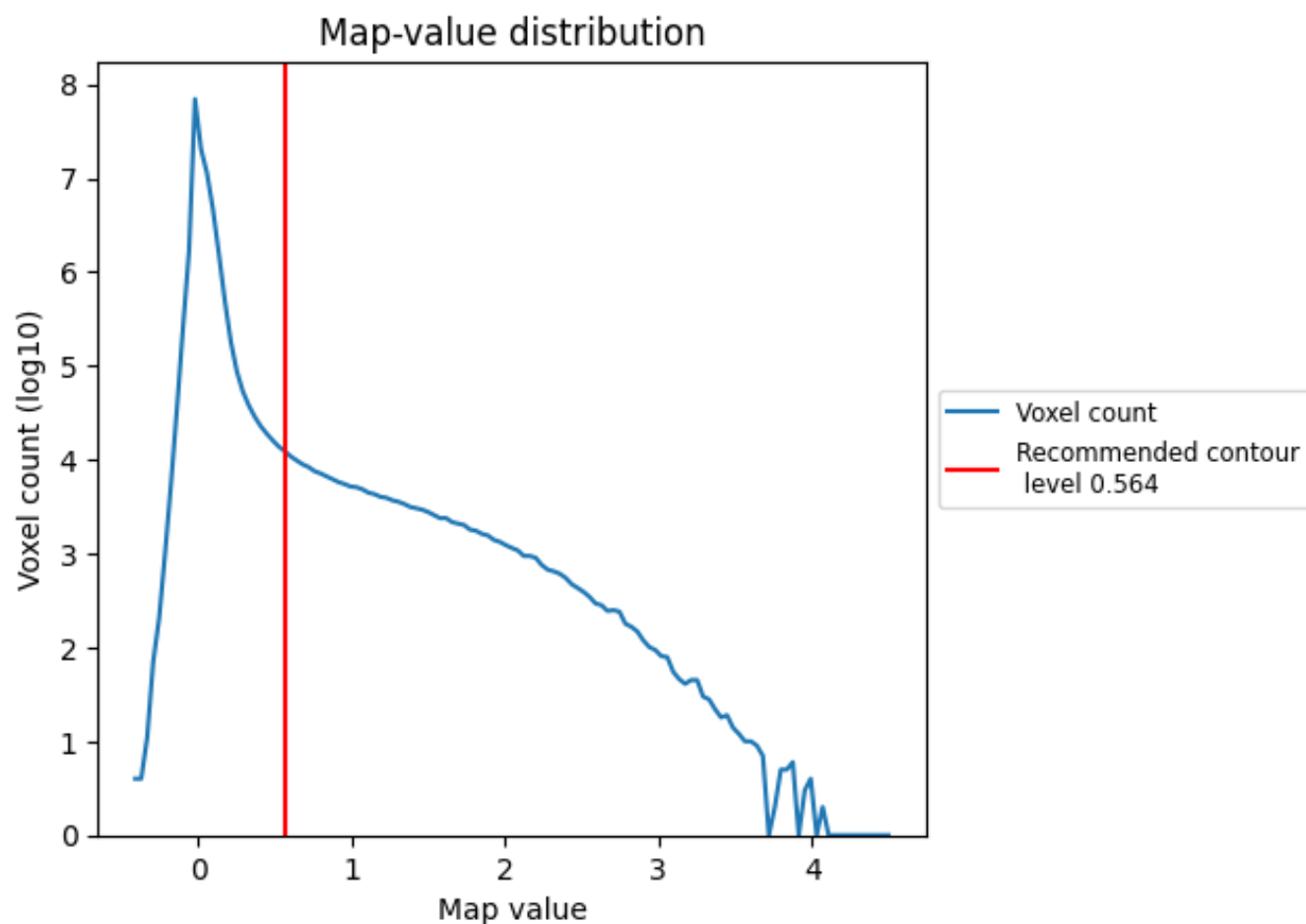
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

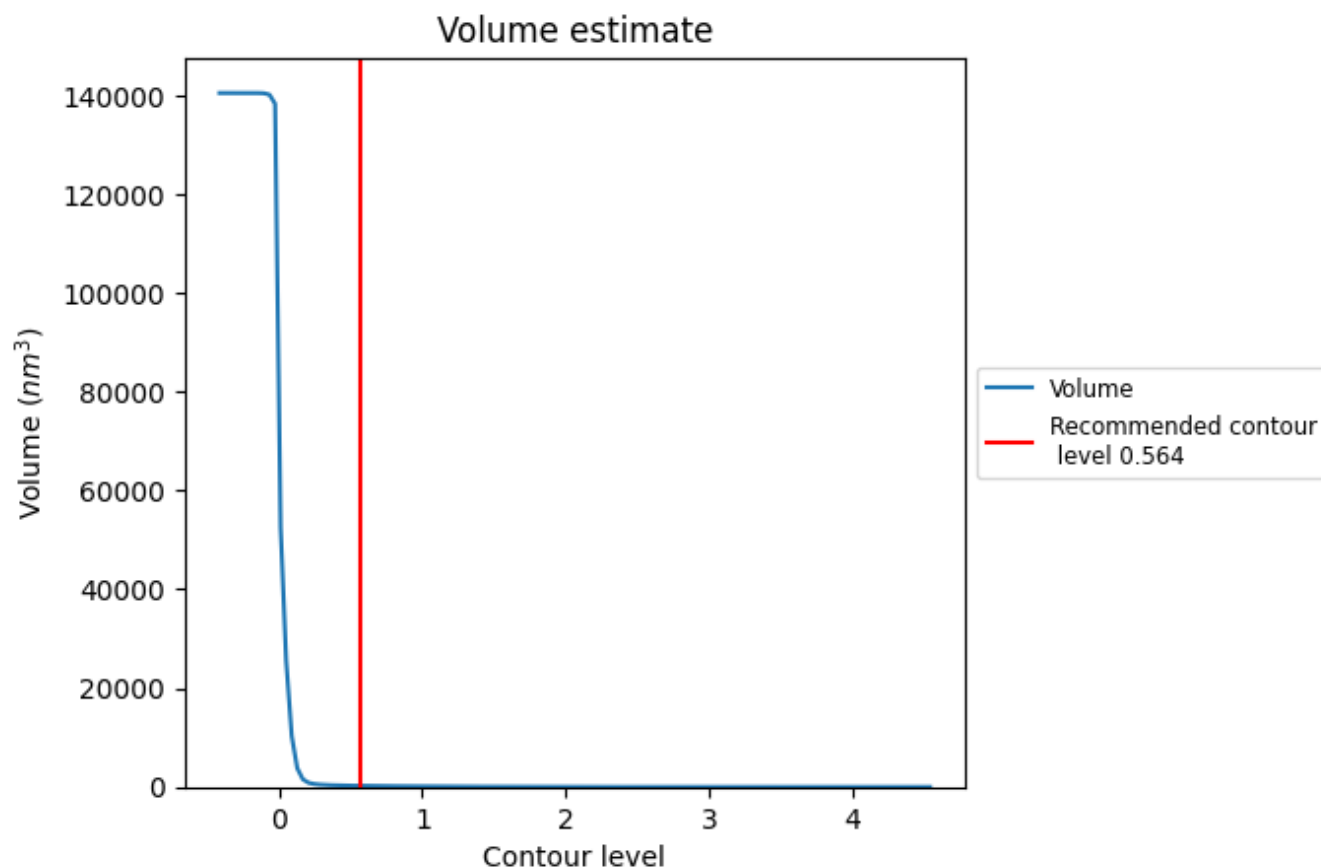
This section contains the results of statistical analysis of the map.

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.

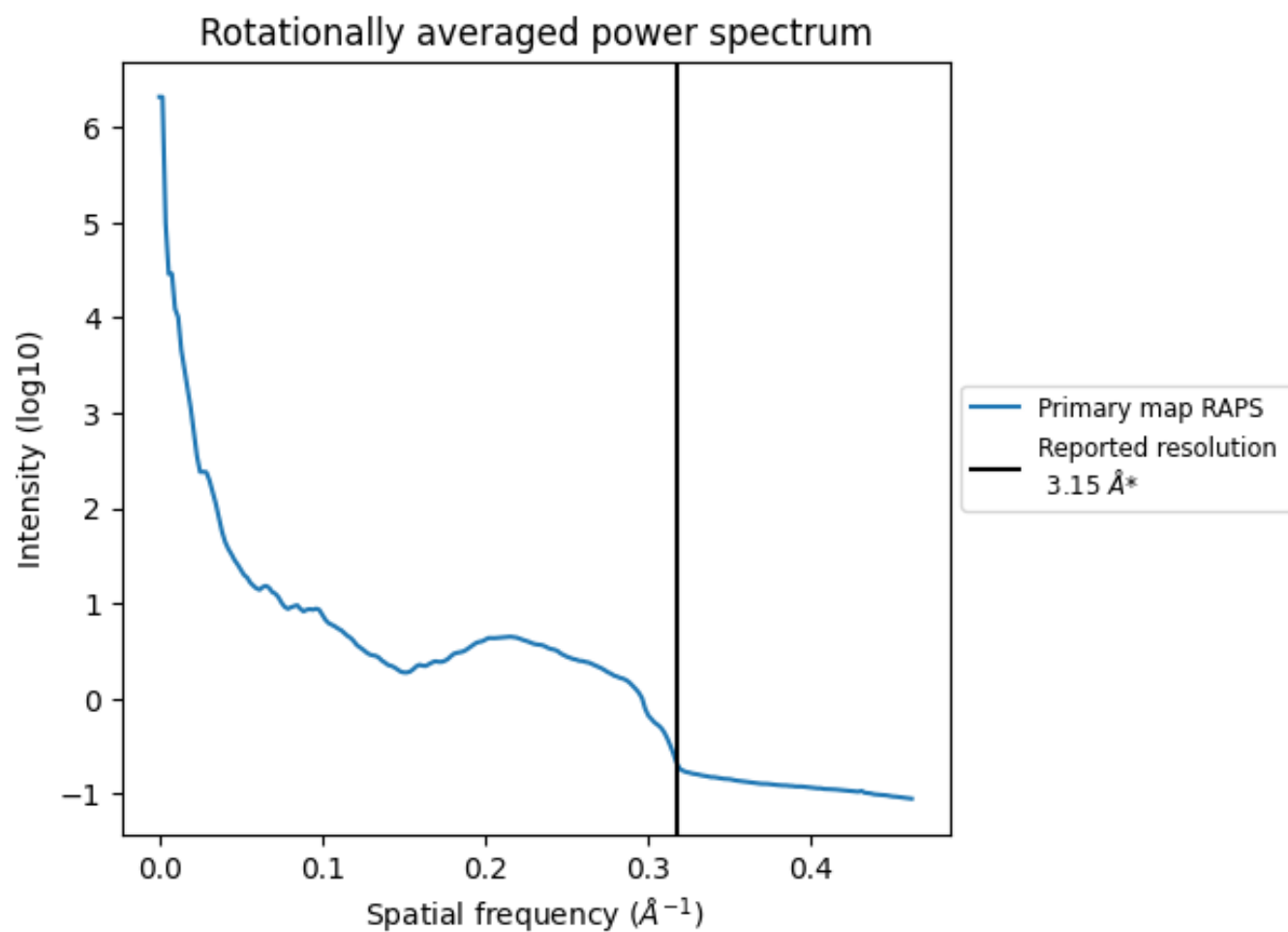
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm^3 ; this corresponds to an approximate mass of 207 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 0.317 Å⁻¹

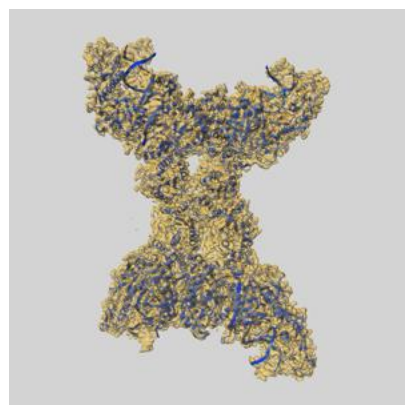
8 Fourier-Shell correlation ⓘ

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

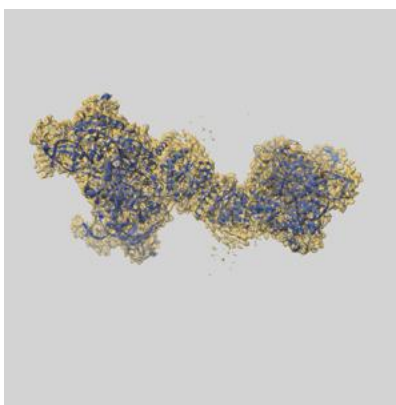
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41966 and PDB model 8U72. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

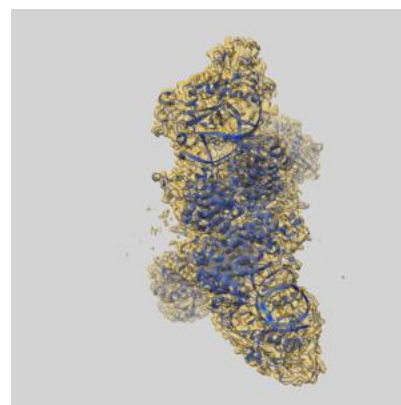
9.1 Map-model overlay [i](#)



X



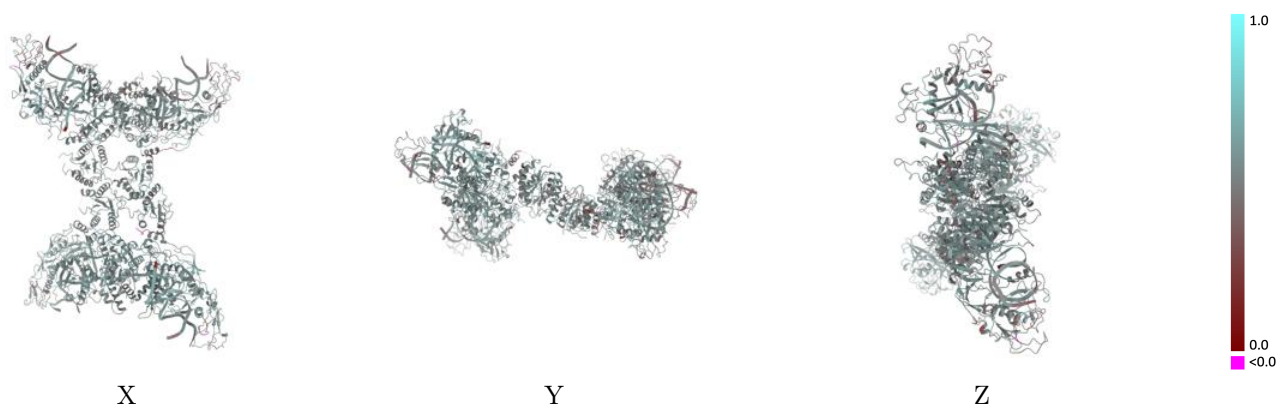
Y



Z

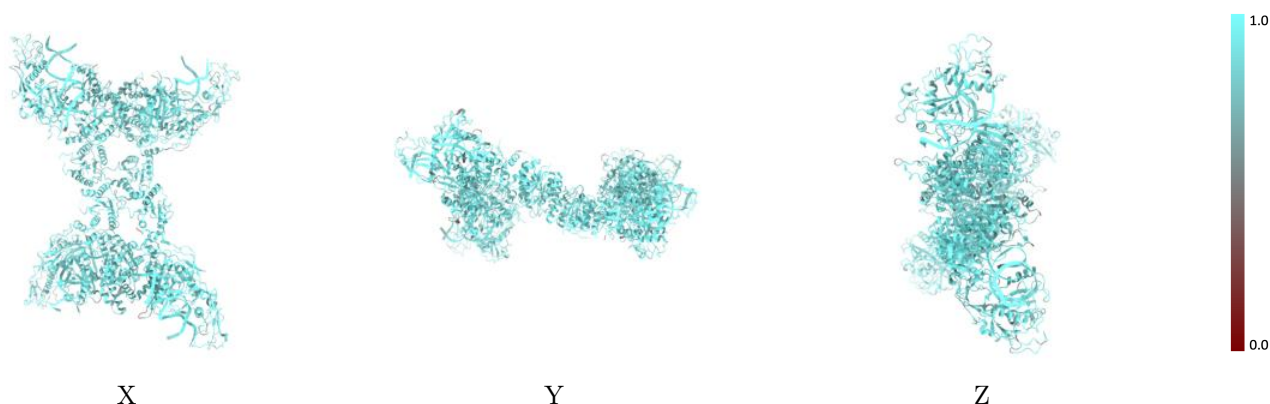
The images above show the 3D surface view of the map at the recommended contour level 0.564 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



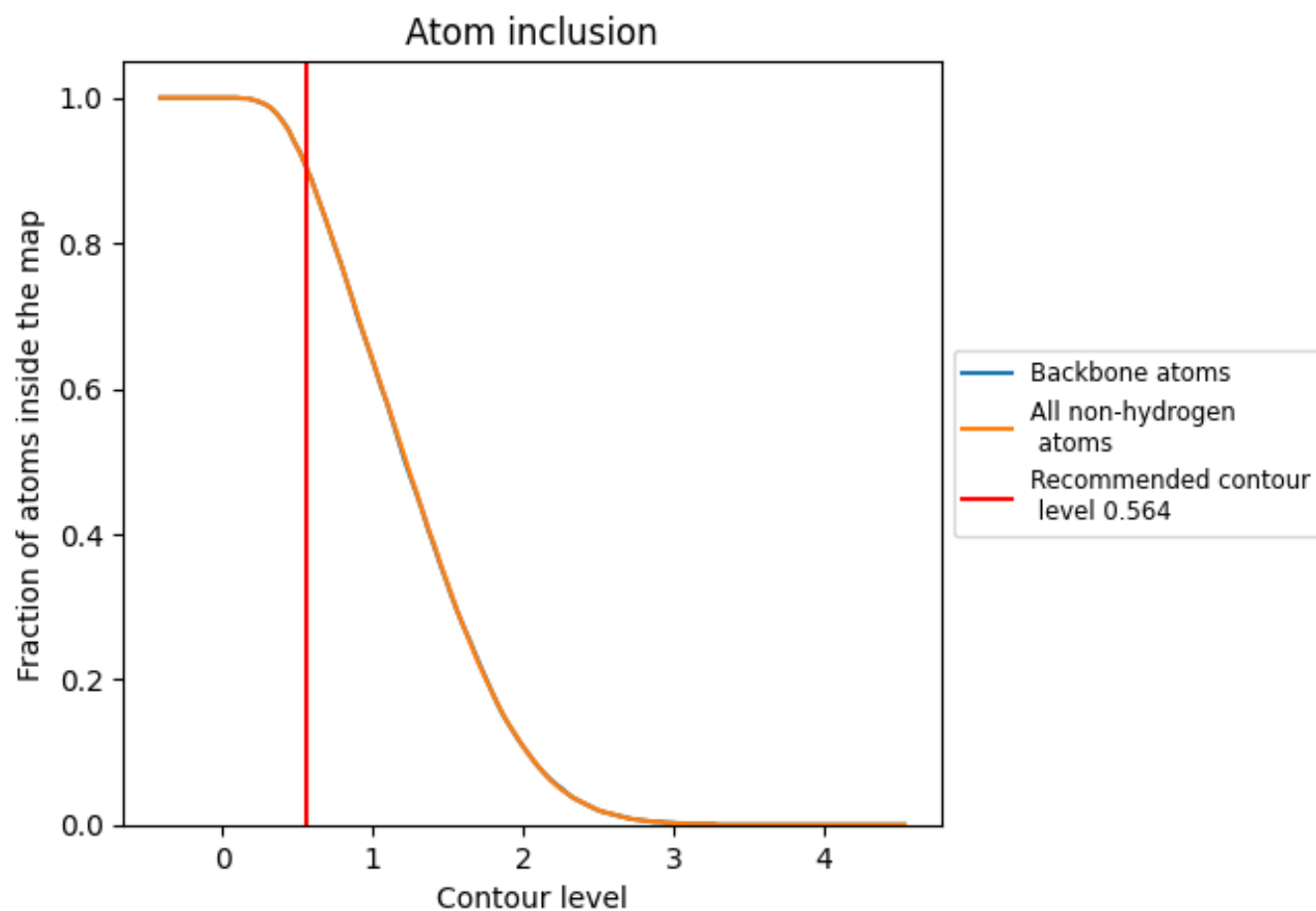
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.564).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.564) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.5330
B	 0.8820	 0.5110
C	 0.8950	 0.5410
D	 0.9040	 0.5310
E	 0.9240	 0.5580
F	 0.8820	 0.5090
G	 0.9020	 0.5370
H	 0.9070	 0.5270
I	 0.9030	 0.5520
M	 0.9710	 0.5540
N	 0.9390	 0.5310
S	 0.9680	 0.5540
T	 0.9330	 0.5250
U	 0.9470	 0.5280
V	 0.8910	 0.5110
X	 0.9660	 0.5350
Y	 0.8660	 0.4750

