



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:59 AM UTC

PDB ID : 6X67 / pdb_00006x67
EMDB ID : EMD-22072
Title : Cryo-EM structure of piggyBac transposase strand transfer complex (STC)
Authors : Chen, Q.; Hickman, A.B.; Dyda, F.
Deposited on : 2020-05-27
Resolution : 3.47 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:

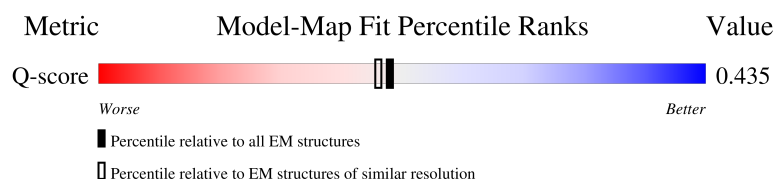
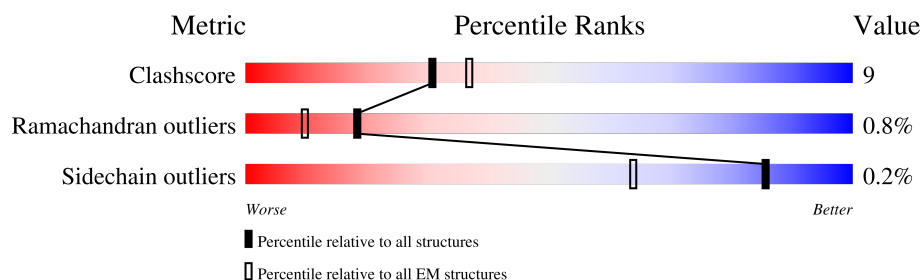
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.47 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.



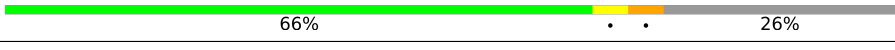
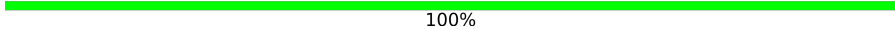
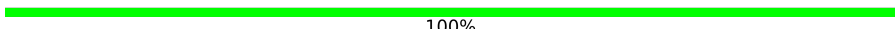
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 (2.97 - 3.97)

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	C	594	
1	D	594	
2	E	37	
2	J	37	

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Mol	Chain	Length	Quality of chain
3	F	47	 89% 11%
3	K	47	 66% 26%
4	G	8	 100%
4	L	8	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10984 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 Transposase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	478	Total	C	N	O	S	0	0
			3848	2424	676	704	44		
1	D	478	Total	C	N	O	S	0	0
			3848	2424	676	704	44		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	500	LYS	GLU	variant	UNP Q283G1
D	500	LYS	GLU	variant	UNP Q283G1

- Molecule 2 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	37	Total	C	N	O	P	0	0
			762	363	147	216	36		
2	J	25	Total	C	N	O	P	0	0
			514	245	100	145	24		

- Molecule 3 is a DNA chain called DNA (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	47	Total	C	N	O	P	0	0
			961	460	167	287	47		
3	K	35	Total	C	N	O	P	0	0
			717	343	125	214	35		

- Molecule 4 is a DNA chain called DNA (tDNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	8	Total	C	N	O	P	0	0
			163	77	31	47	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	8	Total	C	N	O	P	0	0
			163	77	31	47	8		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Zn	0
			2	2	
5	D	2	Total	Zn	0
			2	2	

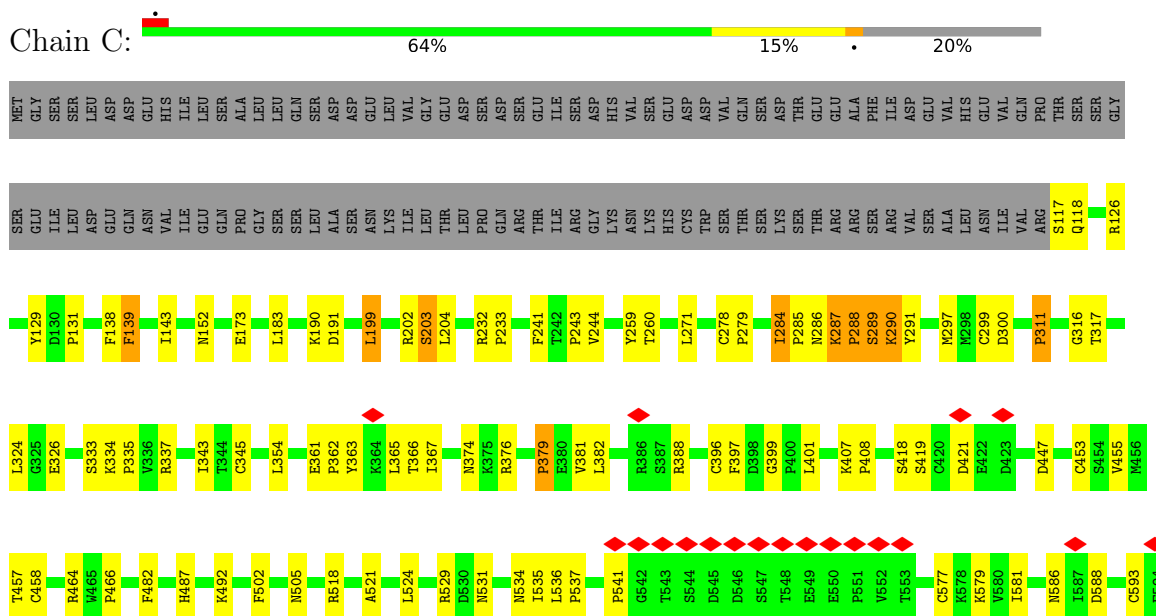
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	C	2	Total	Ca	0
			2	2	
6	D	2	Total	Ca	0
			2	2	

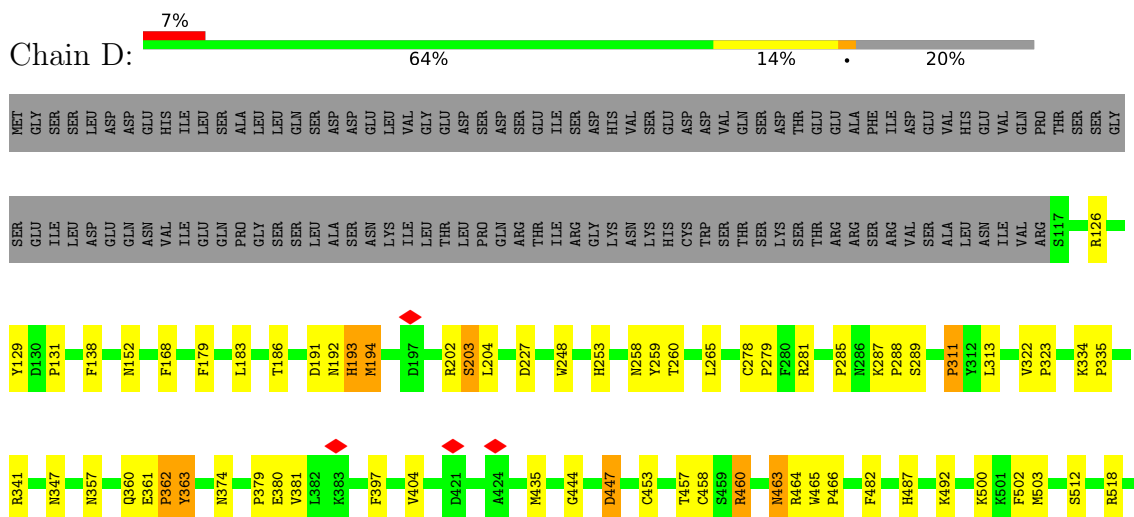
3 Residue-property plots [i](#)

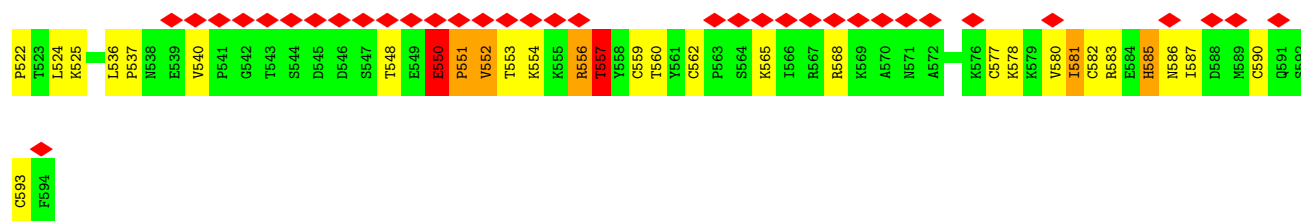
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

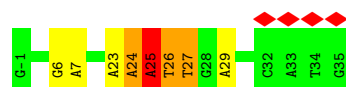
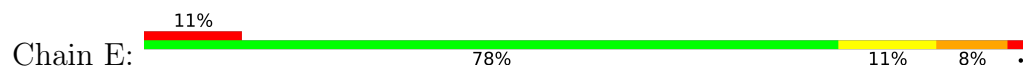


- Molecule 1: Transposase

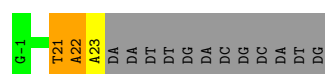




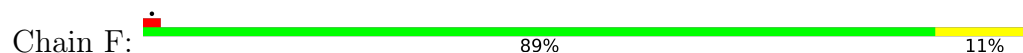
- Molecule 2: DNA (37-MER)



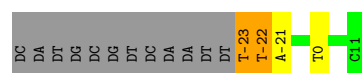
- Molecule 2: DNA (37-MER)



- Molecule 3: DNA (47-MER)



- Molecule 3: DNA (47-MER)



- Molecule 4: DNA (tDNA)



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (tDNA)



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43512	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 ($e^-/\text{\AA}^2$)	46.6	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	0.056	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	201.4, 201.4, 201.4	wwPDB
Map dimensions	190, 190, 190	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	C	1.00	2/3926 (0.1%)	1.31	45/5286 (0.9%)
1	D	0.99	4/3926 (0.1%)	1.33	43/5286 (0.8%)
2	E	0.72	0/857	1.15	4/1322 (0.3%)
2	J	0.71	1/578 (0.2%)	1.18	4/891 (0.4%)
3	F	0.62	0/1075	1.00	1/1657 (0.1%)
3	K	0.76	2/802 (0.2%)	1.29	7/1236 (0.6%)
4	G	0.50	0/182	0.85	0/278
4	L	0.53	0/182	0.82	0/278
All	All	0.91	9/11528 (0.1%)	1.26	104/16234 (0.6%)

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
2	E	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	288	PRO	C-N	-6.71	1.24	1.33
2	J	21	DT	O3'-P	-6.16	1.51	1.61
3	K	-23	DT	O3'-P	5.62	1.69	1.61
1	D	289	SER	N-CA	-5.52	1.39	1.46
1	D	248	TRP	N-CA	-5.46	1.39	1.46
3	K	-23	DT	C4'-C3'	5.40	1.63	1.52
1	D	179	PHE	N-CA	-5.24	1.40	1.46
1	C	537	PRO	CA-C	-5.20	1.43	1.52
1	D	253	HIS	N-CA	-5.09	1.40	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	-23	DT	P-O3'-C3'	16.40	144.80	120.20
2	J	21	DT	P-O3'-C3'	-12.23	101.85	120.20
3	K	-23	DT	O3'-P-O5'	9.89	118.83	104.00
1	D	193	HIS	CA-CB-CG	-9.69	104.11	113.80
1	D	556	ARG	N-CA-C	-9.17	91.26	110.80
1	C	138	PHE	CA-CB-CG	-8.94	104.86	113.80
1	D	192	ASN	CA-CB-CG	-8.48	104.12	112.60
1	D	362	PRO	CB-CA-C	-8.41	99.93	110.95
1	D	522	PRO	CB-CA-C	-8.35	100.00	111.85
3	K	-23	DT	C2'-C3'-O3'	8.18	123.76	111.50
1	D	487	HIS	CA-CB-CG	-7.85	105.95	113.80
1	D	279	PRO	CB-CA-C	-7.80	100.78	111.85
2	E	26	DT	P-O3'-C3'	7.77	131.86	120.20
2	E	25	DA	P-O5'-C5'	-7.75	108.38	120.00
1	C	541	PRO	CB-CA-C	-7.52	99.15	111.56
1	D	285	PRO	CB-CA-C	-7.50	99.90	111.22
1	C	291	TYR	N-CA-C	7.41	121.63	112.59
1	D	536	LEU	CA-C-N	7.35	127.05	119.56
1	D	536	LEU	C-N-CA	7.35	127.05	119.56
1	D	540	VAL	CA-C-N	7.35	127.30	120.03
1	D	540	VAL	C-N-CA	7.35	127.30	120.03
1	C	204	LEU	N-CA-C	-7.32	102.95	112.68
1	D	131	PRO	CB-CA-C	-7.14	101.07	112.21
1	D	204	LEU	N-CA-C	-7.11	103.22	112.68
1	D	168	PHE	CA-CB-CG	-7.00	106.80	113.80
3	K	-23	DT	C6-N1-C1'	6.74	129.46	119.35
1	C	535	ILE	N-CA-C	-6.72	106.46	111.90
1	C	139	PHE	CA-CB-CG	-6.71	107.09	113.80
1	D	557	THR	N-CA-C	-6.68	96.56	110.80
1	C	536	LEU	CA-C-N	6.51	126.44	119.28
1	C	536	LEU	C-N-CA	6.51	126.44	119.28
1	C	284	ILE	CA-C-N	6.43	126.35	119.28
1	C	284	ILE	C-N-CA	6.43	126.35	119.28
1	D	323	PRO	CB-CA-C	-6.37	102.90	111.12
1	C	260	THR	CA-C-N	6.35	126.31	120.03
1	C	260	THR	C-N-CA	6.35	126.31	120.03
1	C	279	PRO	CB-CA-C	-6.31	102.36	112.21
1	C	287	LYS	CA-C-N	6.29	126.20	119.28
1	C	287	LYS	C-N-CA	6.29	126.20	119.28
1	D	322	VAL	CA-C-N	6.29	126.65	119.92
1	D	322	VAL	C-N-CA	6.29	126.65	119.92
1	C	311	PRO	CB-CA-C	-6.21	103.11	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	LYS	CA-C-N	6.11	126.00	119.28
1	D	287	LYS	C-N-CA	6.11	126.00	119.28
1	D	550	GLU	CA-C-N	6.10	125.78	119.56
1	D	550	GLU	C-N-CA	6.10	125.78	119.56
1	D	138	PHE	CA-CB-CG	-6.08	107.72	113.80
1	C	367	ILE	N-CA-C	6.03	117.37	108.45
1	D	311	PRO	CB-CA-C	-6.01	103.54	111.23
1	C	447	ASP	CA-CB-CG	-6.01	106.59	112.60
3	K	-23	DT	C5'-C4'-C3'	5.96	123.84	114.90
1	D	447	ASP	CA-CB-CG	-5.95	106.66	112.60
1	D	581	ILE	N-CA-C	5.91	118.71	108.90
1	C	290	LYS	N-CA-C	5.88	120.73	113.50
1	C	482	PHE	CA-CB-CG	-5.88	107.92	113.80
1	C	408	PRO	CB-CA-C	-5.82	103.19	111.68
1	C	299	CYS	CA-C-N	-5.76	114.07	122.19
1	C	299	CYS	C-N-CA	-5.76	114.07	122.19
1	D	512	SER	N-CA-C	5.75	117.23	111.07
1	D	482	PHE	CA-CB-CG	-5.74	108.06	113.80
1	C	374	ASN	CA-CB-CG	-5.73	106.87	112.60
3	K	-22	DT	O5'-C5'-C4'	5.65	119.28	110.80
1	D	227	ASP	N-CA-C	5.64	116.52	108.74
1	C	259	TYR	N-CA-C	5.55	117.53	108.76
1	C	126	ARG	N-CA-C	5.54	117.12	111.14
1	C	278	CYS	CA-C-N	5.48	125.31	119.28
1	C	278	CYS	C-N-CA	5.48	125.31	119.28
1	D	374	ASN	CA-CB-CG	-5.48	107.12	112.60
1	D	585	HIS	CA-CB-CG	-5.48	108.32	113.80
1	C	285	PRO	N-CA-C	5.47	121.03	113.65
1	C	397	PHE	CA-CB-CG	-5.44	108.36	113.80
2	J	21	DT	C4'-C3'-C2'	5.44	110.56	102.40
3	F	2	DA	N9-C1'-C2'	5.41	121.62	113.50
1	D	260	THR	CA-C-N	5.40	125.70	119.92
1	D	260	THR	C-N-CA	5.40	125.70	119.92
2	E	24	DA	P-O3'-C3'	-5.40	112.10	120.20
3	K	0	DT	P-O3'-C3'	5.40	128.30	120.20
1	C	531	ASN	CA-CB-CG	-5.39	107.20	112.60
1	C	152	ASN	CA-CB-CG	-5.39	107.21	112.60
1	C	199	LEU	CB-CA-C	-5.37	100.69	110.63
1	C	505	ASN	CA-CB-CG	-5.36	107.24	112.60
1	D	152	ASN	CA-CB-CG	-5.36	107.24	112.60
1	C	289	SER	N-CA-C	-5.34	99.73	108.76
1	C	285	PRO	CB-CA-C	-5.32	103.91	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	557	THR	N-CA-CB	5.32	119.48	110.49
2	J	22	DA	P-O3'-C3'	5.29	128.13	120.20
1	C	521	ALA	CA-C-N	5.25	124.87	119.56
1	C	521	ALA	C-N-CA	5.25	124.87	119.56
1	D	548	THR	N-CA-C	5.21	116.64	111.07
2	J	22	DA	C3'-C2'-C1'	-5.21	93.79	101.60
1	C	399	GLY	CA-C-N	5.20	124.71	119.19
1	C	399	GLY	C-N-CA	5.20	124.71	119.19
1	D	126	ARG	N-CA-C	5.20	117.86	111.82
1	C	487	HIS	CA-CB-CG	-5.20	108.60	113.80
1	D	397	PHE	CA-CB-CG	-5.15	108.65	113.80
1	D	362	PRO	N-CA-C	-5.14	103.70	111.41
1	C	379	PRO	CB-CA-C	-5.13	104.23	110.95
1	D	551	PRO	CB-CA-C	-5.10	104.61	111.85
1	D	357	ASN	CA-CB-CG	-5.08	107.52	112.60
1	C	297	MET	N-CA-C	5.07	116.78	109.07
2	E	27	DT	C3'-C2'-C1'	-5.05	94.02	101.60
1	D	537	PRO	CB-CA-C	-5.05	104.68	111.85
1	C	534	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	324	LEU	N-CA-C	5.02	117.48	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	25	DA	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	C	3848	0	3888	46	0
1	D	3848	0	3889	90	0
2	E	762	0	417	37	0
2	J	514	0	282	3	0
3	F	961	0	534	12	0
3	K	717	0	398	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	163	0	90	0	0
4	L	163	0	90	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	10984	0	9588	181	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 9.

All (181) 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:K:-23:DT:H3'	3:K:-22:DT:C7	1.59	1.32
3:K:-23:DT:C3'	3:K:-22:DT:H71	1.67	1.24
3:K:-23:DT:C3'	3:K:-22:DT:C7	2.23	1.12
1:D:554:LYS:HE3	1:D:557:THR:HG21	1.13	1.12
1:D:554:LYS:CE	1:D:557:THR:HG21	1.82	1.09
1:C:129:TYR:CE2	1:C:492:LYS:HD2	1.89	1.07
3:K:-23:DT:H3'	3:K:-22:DT:H73	1.37	1.07
3:K:-22:DT:H6	3:K:-22:DT:O5'	1.44	1.00
2:E:24:DA:C2	2:E:25:DA:C4	2.61	0.88
1:D:500:LYS:NZ	2:E:6:DG:H3'	1.87	0.87
1:D:556:ARG:HB2	1:D:580:VAL:HG11	1.55	0.87
3:K:-23:DT:C2'	3:K:-22:DT:H71	2.04	0.87
2:E:25:DA:H61	3:F:-26:DA:N6	1.73	0.87
2:E:23:DA:C2	2:E:24:DA:C4	2.63	0.86
3:K:-23:DT:O3'	3:K:-22:DT:H71	1.75	0.86
1:D:554:LYS:HE3	1:D:557:THR:CG2	2.03	0.85
3:K:-22:DT:O5'	3:K:-22:DT:C6	2.29	0.85
1:D:586:ASN:HB3	1:D:590:CYS:HA	1.62	0.82
1:D:550:GLU:HG2	1:D:578:LYS:HE3	1.61	0.82
2:E:25:DA:N6	3:F:-26:DA:H61	1.80	0.79
1:D:562:CYS:SG	1:D:585:HIS:HE1	2.06	0.78
2:E:25:DA:N6	3:F:-26:DA:N6	2.33	0.77
1:D:554:LYS:HG3	1:D:557:THR:CG2	2.15	0.76
1:D:503:MET:HA	1:D:503:MET:HE2	1.67	0.76
2:E:26:DT:H2''	2:E:27:DT:C6	2.20	0.75
1:D:554:LYS:CE	1:D:557:THR:CG2	2.65	0.74
1:D:554:LYS:HG3	1:D:557:THR:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:GLU:HA	1:D:578:LYS:CE	2.18	0.73
2:J:21:DT:C2'	2:J:22:DA:O5'	2.34	0.71
1:D:550:GLU:HA	1:D:578:LYS:HE3	1.73	0.71
1:D:554:LYS:CG	1:D:557:THR:CG2	2.68	0.70
1:C:376:ARG:NE	3:F:9:DT:OP2	2.24	0.69
2:E:26:DT:C2'	2:E:27:DT:C6	2.75	0.69
1:D:550:GLU:O	1:D:578:LYS:HD2	1.92	0.69
3:K:-23:DT:O3'	3:K:-22:DT:C7	2.38	0.69
1:C:382:LEU:HD11	1:C:396:CYS:SG	2.33	0.68
1:D:129:TYR:CE2	1:D:492:LYS:HD2	2.28	0.68
1:D:183:LEU:HB3	1:D:458:CYS:SG	2.32	0.68
1:D:565:LYS:CE	3:F:-35:DC:OP2	2.42	0.68
3:K:-23:DT:C2'	3:K:-22:DT:C7	2.70	0.67
1:D:460:ARG:HG2	1:D:460:ARG:HH11	1.61	0.66
1:D:500:LYS:NZ	2:E:6:DG:C3'	2.57	0.65
1:D:129:TYR:CZ	1:D:492:LYS:HD2	2.31	0.65
1:D:500:LYS:HZ1	2:E:6:DG:H3'	1.60	0.64
1:D:556:ARG:HB2	1:D:580:VAL:CG1	2.27	0.63
1:D:556:ARG:H	1:D:580:VAL:HG21	1.63	0.63
2:E:25:DA:C2'	2:E:26:DT:O5'	2.44	0.63
1:C:129:TYR:CZ	1:C:492:LYS:HD2	2.32	0.63
1:C:326:GLU:HG3	1:C:354:LEU:HB2	1.80	0.62
1:D:500:LYS:CE	2:E:6:DG:H3'	2.29	0.62
1:D:550:GLU:HA	1:D:578:LYS:HD2	1.81	0.62
1:C:453:CYS:O	1:C:457:THR:HB	2.01	0.60
3:K:-23:DT:H2'	3:K:-22:DT:C7	2.31	0.60
1:D:559:CYS:HB2	1:D:582:CYS:HB3	1.84	0.60
1:D:556:ARG:O	1:D:557:THR:HG23	2.02	0.60
1:C:577:CYS:HB3	1:C:593:CYS:SG	2.41	0.59
1:D:193:HIS:O	1:D:194:MET:O	2.20	0.59
1:D:202:ARG:O	1:D:203:SER:CB	2.51	0.59
2:E:25:DA:H61	3:F:-26:DA:H62	1.49	0.58
1:D:334:LYS:HB3	1:D:335:PRO:HD3	1.86	0.57
1:D:460:ARG:HH11	1:D:460:ARG:CG	2.15	0.57
2:E:25:DA:H2'	2:E:26:DT:O5'	2.04	0.57
1:D:311:PRO:HB2	1:D:313:LEU:HG	1.86	0.57
3:K:-23:DT:H2'	3:K:-22:DT:H71	1.84	0.57
1:C:202:ARG:O	1:C:203:SER:CB	2.53	0.57
1:D:577:CYS:HB3	1:D:593:CYS:SG	2.45	0.57
2:E:23:DA:H2''	2:E:24:DA:H8	1.69	0.57
1:D:193:HIS:O	1:D:194:MET:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:CYS:SG	1:C:579:LYS:HG2	2.46	0.56
1:D:447:ASP:N	1:D:447:ASP:OD1	2.31	0.56
1:C:232:ARG:N	1:C:233:PRO:CD	2.68	0.56
1:D:500:LYS:HE2	2:E:7:DA:OP2	2.05	0.55
1:D:552:VAL:HG12	1:D:553:THR:N	2.21	0.55
3:K:-22:DT:H2''	3:K:-21:DA:O5'	2.04	0.55
2:J:21:DT:H2'	2:J:22:DA:O5'	2.05	0.55
2:E:24:DA:C2	2:E:25:DA:C5	2.95	0.54
1:D:565:LYS:HE3	3:F:-35:DC:OP2	2.05	0.54
1:D:550:GLU:HA	1:D:578:LYS:CD	2.36	0.54
3:K:-22:DT:H71	3:K:-22:DT:P	2.47	0.54
1:D:460:ARG:CG	1:D:460:ARG:NH1	2.70	0.54
1:D:581:ILE:HD12	1:D:586:ASN:HB2	1.88	0.54
1:C:129:TYR:HE2	1:C:492:LYS:HB2	1.72	0.53
1:D:463:ASN:HD22	1:D:463:ASN:H	1.56	0.53
1:D:500:LYS:NZ	2:E:6:DG:C2'	2.72	0.53
1:D:186:THR:HG23	1:D:191:ASP:O	2.09	0.53
1:D:463:ASN:HD22	1:D:463:ASN:N	2.07	0.53
1:D:379:PRO:HB2	1:D:381:VAL:HG22	1.91	0.52
1:D:129:TYR:CE2	1:D:492:LYS:HB2	2.45	0.52
1:D:463:ASN:H	1:D:463:ASN:ND2	2.07	0.52
1:D:500:LYS:HZ3	2:E:6:DG:C3'	2.22	0.52
1:C:588:ASP:OD1	1:C:588:ASP:N	2.42	0.52
1:D:554:LYS:CG	1:D:557:THR:HG23	2.39	0.52
1:C:316:GLY:O	1:C:317:THR:C	2.52	0.51
1:D:362:PRO:HB2	1:D:363:TYR:CD1	2.45	0.51
2:E:26:DT:H2'	2:E:27:DT:C6	2.44	0.51
1:D:278:CYS:HB3	1:D:281:ARG:HB2	1.92	0.51
1:D:565:LYS:HE3	3:F:-35:DC:P	2.50	0.51
1:C:284:ILE:O	1:C:290:LYS:HG2	2.09	0.51
2:E:23:DA:C2'	2:E:24:DA:H8	2.23	0.51
1:C:202:ARG:O	1:C:203:SER:OG	2.25	0.51
1:C:241:PHE:CZ	1:C:311:PRO:HG3	2.45	0.51
1:C:337:ARG:HB2	1:C:363:TYR:CD2	2.46	0.51
1:C:244:VAL:HG13	1:C:466:PRO:HB3	1.93	0.51
1:D:568:ARG:NH2	2:E:29:DA:OP2	2.44	0.50
1:C:232:ARG:N	1:C:233:PRO:HD2	2.27	0.50
1:C:343:ILE:HG22	1:C:345:CYS:SG	2.51	0.50
1:C:190:LYS:NZ	1:C:455:VAL:O	2.45	0.50
1:D:347:ASN:C	1:D:347:ASN:OD1	2.54	0.50
1:C:581:ILE:HD12	1:C:586:ASN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:GLU:HB2	1:D:551:PRO:HD3	1.94	0.50
1:C:529:ARG:HH11	1:C:529:ARG:HG3	1.76	0.50
1:D:550:GLU:CG	1:D:578:LYS:HE3	2.39	0.50
1:D:565:LYS:HE2	3:F:-35:DC:OP2	2.12	0.50
1:D:554:LYS:HG2	1:D:557:THR:HG23	1.95	0.49
1:C:232:ARG:NH2	1:C:243:PRO:HB3	2.28	0.49
1:D:556:ARG:HG3	1:D:560:THR:CG2	2.42	0.49
1:C:129:TYR:CE2	1:C:492:LYS:CD	2.81	0.49
1:C:388:ARG:HG2	1:C:407:LYS:HD3	1.95	0.48
3:K:-22:DT:C2'	3:K:-21:DA:O5'	2.61	0.48
2:E:23:DA:C2	2:E:24:DA:C5	3.02	0.48
2:E:23:DA:H2''	2:E:24:DA:C8	2.47	0.48
2:E:24:DA:C2	2:E:25:DA:N3	2.80	0.48
2:E:23:DA:C2'	2:E:24:DA:C8	2.97	0.48
1:D:583:ARG:O	1:D:587:ILE:HD13	2.14	0.47
1:C:183:LEU:HD22	1:C:458:CYS:SG	2.54	0.47
1:D:202:ARG:O	1:D:203:SER:HB3	2.15	0.46
2:E:23:DA:C4	2:E:24:DA:C8	3.03	0.46
1:D:552:VAL:HG12	1:D:553:THR:H	1.79	0.46
1:C:376:ARG:NH2	3:F:9:DT:OP2	2.48	0.46
1:C:334:LYS:HB3	1:C:335:PRO:HD3	1.97	0.46
1:D:556:ARG:N	1:D:580:VAL:HG21	2.28	0.46
3:K:-23:DT:C3'	3:K:-22:DT:H73	2.18	0.46
2:E:23:DA:C6	2:E:24:DA:C6	3.04	0.45
2:E:26:DT:H2'	2:E:27:DT:C5	2.51	0.45
1:D:502:PHE:CD2	1:D:503:MET:HE3	2.52	0.45
2:E:24:DA:C6	2:E:25:DA:C6	3.05	0.45
1:D:129:TYR:HE2	1:D:492:LYS:HB2	1.82	0.45
2:E:25:DA:C6	3:F:-26:DA:N6	2.81	0.45
2:E:23:DA:N3	2:E:24:DA:C8	2.85	0.45
1:D:258:ASN:O	1:D:259:TYR:HB3	2.16	0.44
1:D:463:ASN:N	1:D:463:ASN:ND2	2.65	0.44
1:C:333:SER:HB3	1:C:365:LEU:CD1	2.48	0.43
1:C:191:ASP:HB3	1:C:199:LEU:HD21	2.00	0.43
3:K:-22:DT:C7	3:K:-22:DT:P	3.06	0.43
1:D:500:LYS:HZ1	2:E:6:DG:C3'	2.25	0.43
1:C:379:PRO:HB2	1:C:381:VAL:HG12	2.00	0.43
1:C:464:ARG:C	1:C:466:PRO:HD2	2.44	0.43
1:D:464:ARG:C	1:D:466:PRO:HD2	2.44	0.43
1:C:173:GLU:H	1:C:173:GLU:CD	2.27	0.43
1:C:361:GLU:HB3	1:C:362:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:ARG:HG2	1:D:524:LEU:CD2	2.49	0.42
1:C:131:PRO:HB3	1:C:502:PHE:CE1	2.55	0.42
1:C:139:PHE:O	1:C:143:ILE:HB	2.19	0.42
2:J:23:DA:H61	3:K:-23:DT:H3	1.68	0.42
1:D:463:ASN:HD22	1:D:463:ASN:C	2.27	0.42
1:D:554:LYS:HE2	1:D:557:THR:HG21	1.88	0.42
1:C:518:ARG:HG2	1:C:524:LEU:CD2	2.49	0.42
1:D:453:CYS:O	1:D:457:THR:HB	2.19	0.42
1:D:465:TRP:N	1:D:466:PRO:CD	2.83	0.42
1:C:286:ASN:OD1	1:C:286:ASN:N	2.50	0.42
1:D:500:LYS:HZ3	2:E:6:DG:C2'	2.31	0.42
1:D:265:LEU:HD11	1:D:341:ARG:HD2	2.02	0.42
2:E:24:DA:N1	2:E:25:DA:C6	2.88	0.42
1:D:404:VAL:HG12	1:D:435:MET:CE	2.50	0.41
1:C:287:LYS:HB3	1:C:288:PRO:HD2	2.01	0.41
1:D:360:GLN:O	1:D:361:GLU:C	2.64	0.41
1:C:117:SER:O	1:C:118:GLN:HB2	2.21	0.41
1:C:300:ASP:OD1	1:C:300:ASP:N	2.54	0.41
1:D:444:GLY:HA2	1:D:447:ASP:OD1	2.21	0.41
1:C:366:THR:OG1	1:C:419:SER:OG	2.33	0.41
1:C:271:LEU:HD23	1:C:289:SER:O	2.19	0.41
1:C:418:SER:OG	1:C:421:ASP:HB2	2.21	0.41
1:D:500:LYS:HE2	2:E:7:DA:P	2.61	0.41
1:D:502:PHE:HD2	1:D:503:MET:HE3	1.85	0.41
1:D:559:CYS:CB	1:D:582:CYS:HB3	2.50	0.41
1:D:500:LYS:HZ1	2:E:6:DG:C2'	2.34	0.41
1:D:380:GLU:H	1:D:380:GLU:CD	2.27	0.40
1:D:553:THR:OG1	1:D:554:LYS:N	2.50	0.40
1:D:311:PRO:HB2	1:D:313:LEU:CD2	2.52	0.40
1:D:288:PRO:HG3	3:F:-2:DG:H5'	2.03	0.40
1:C:401:LEU:HD22	1:C:419:SER:HB3	2.03	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	C	476/594 (80%)	453 (95%)	22 (5%)	1 (0%)	43	74
1	D	476/594 (80%)	447 (94%)	22 (5%)	7 (2%)	8	37
All	All	952/1188 (80%)	900 (94%)	44 (5%)	8 (1%)	18	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	194	MET
1	D	525	LYS
1	D	557	THR
1	D	203	SER
1	D	550	GLU
1	D	552	VAL
1	C	203	SER
1	D	363	TYR

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	C	442/549 (80%)	442 (100%)	0	100	100
1	D	442/549 (80%)	440 (100%)	2 (0%)	81	80
All	All	884/1098 (80%)	882 (100%)	2 (0%)	85	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	460	ARG
1	D	463	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	253	HIS
1	C	264	HIS
1	C	270	GLN
1	C	487	HIS
1	C	531	ASN
1	D	253	HIS
1	D	254	GLN
1	D	463	ASN
1	D	487	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

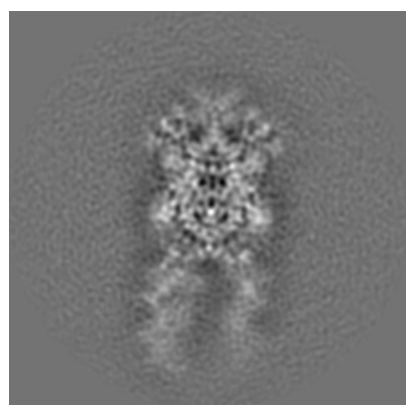
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22072. These allow visual inspection of the internal detail of the map and identification of artifacts.

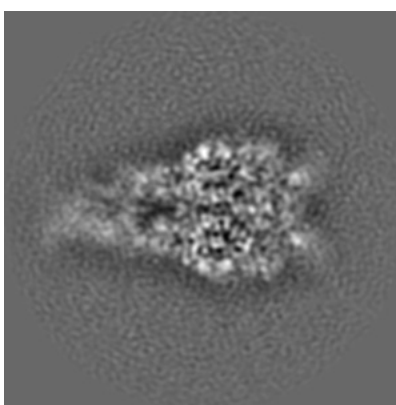
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

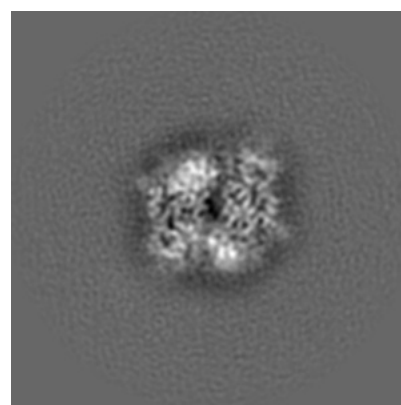
6.1.1 Primary map



X



Y

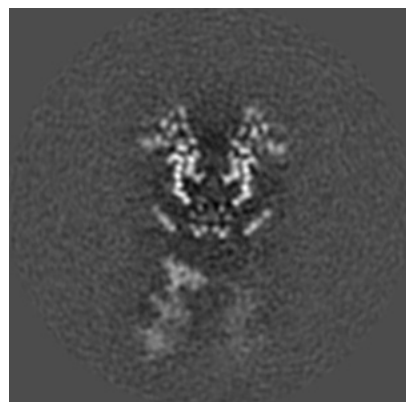


Z

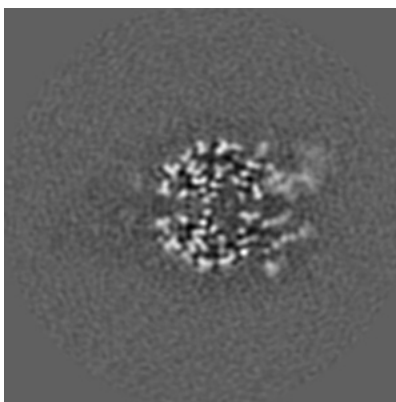
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

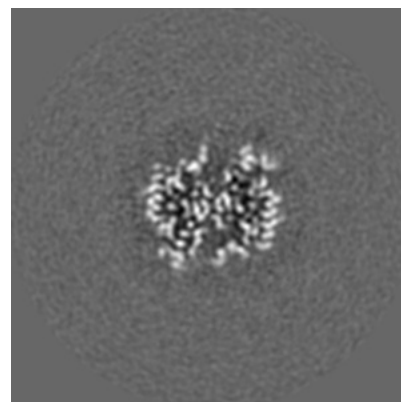
6.2.1 Primary map



X Index: 95



Y Index: 95

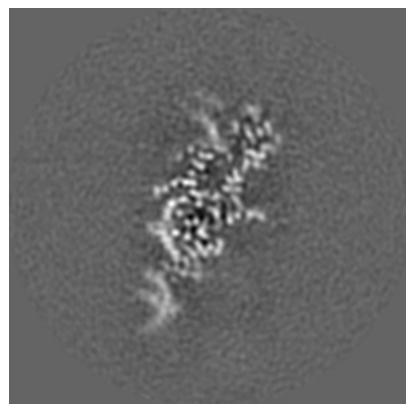


Z Index: 95

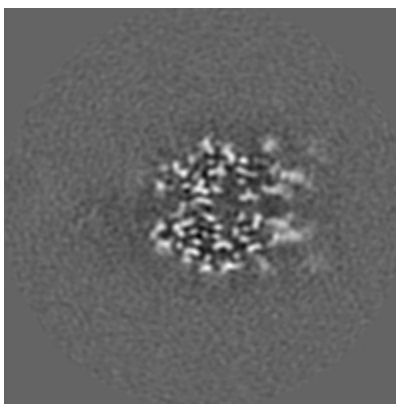
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

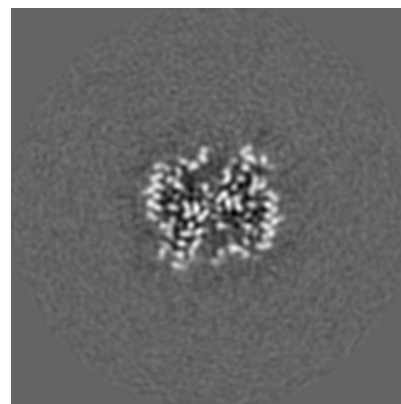
6.3.1 Primary map



X Index: 104



Y Index: 98

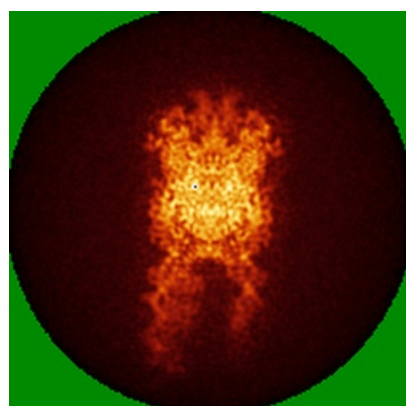


Z Index: 94

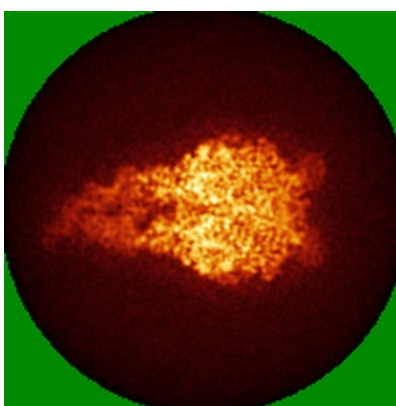
The images above show the largest variance slices of the map in three orthogonal directions.

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

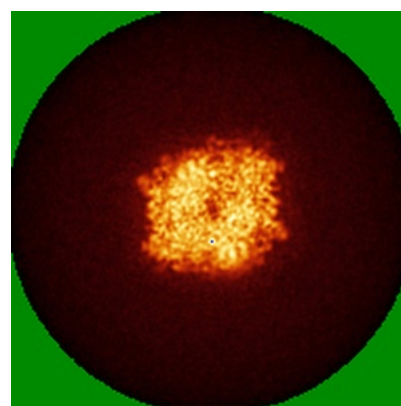
6.4.1 Primary map



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

This section was not generated.

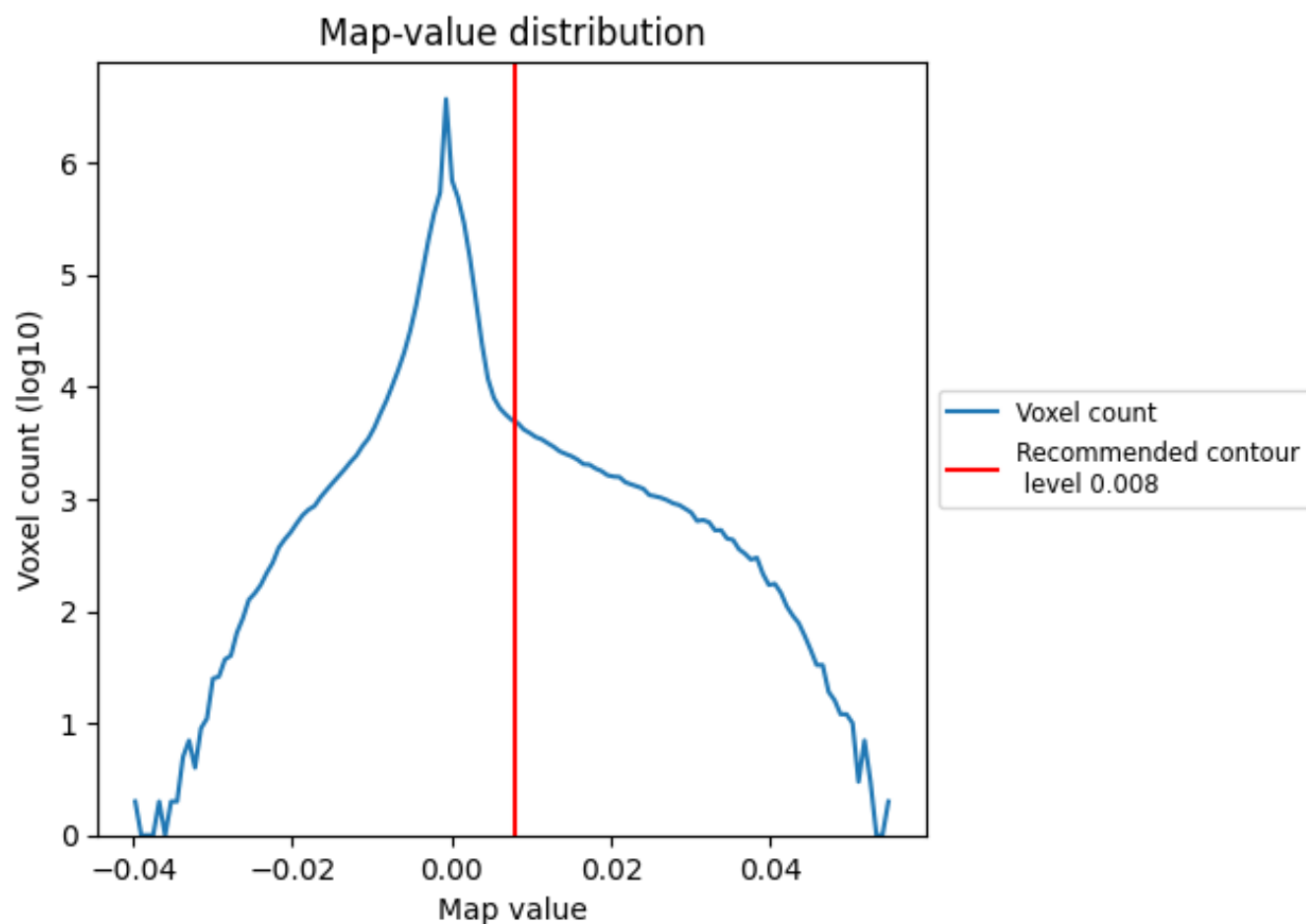
6.6 Mask visualisation

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

7 Map analysis [i](#)

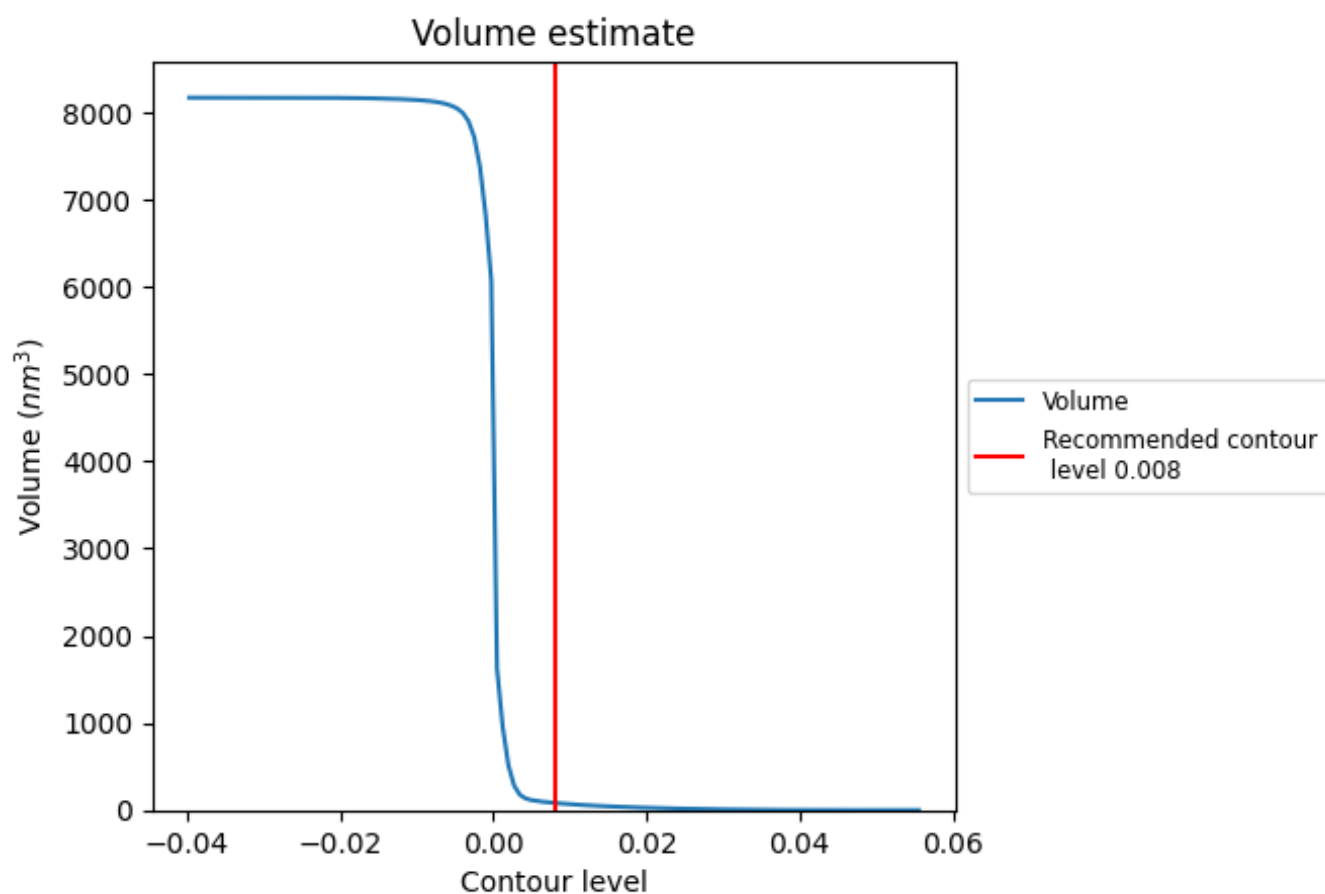
This section contains the results of statistical analysis of the map.

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.

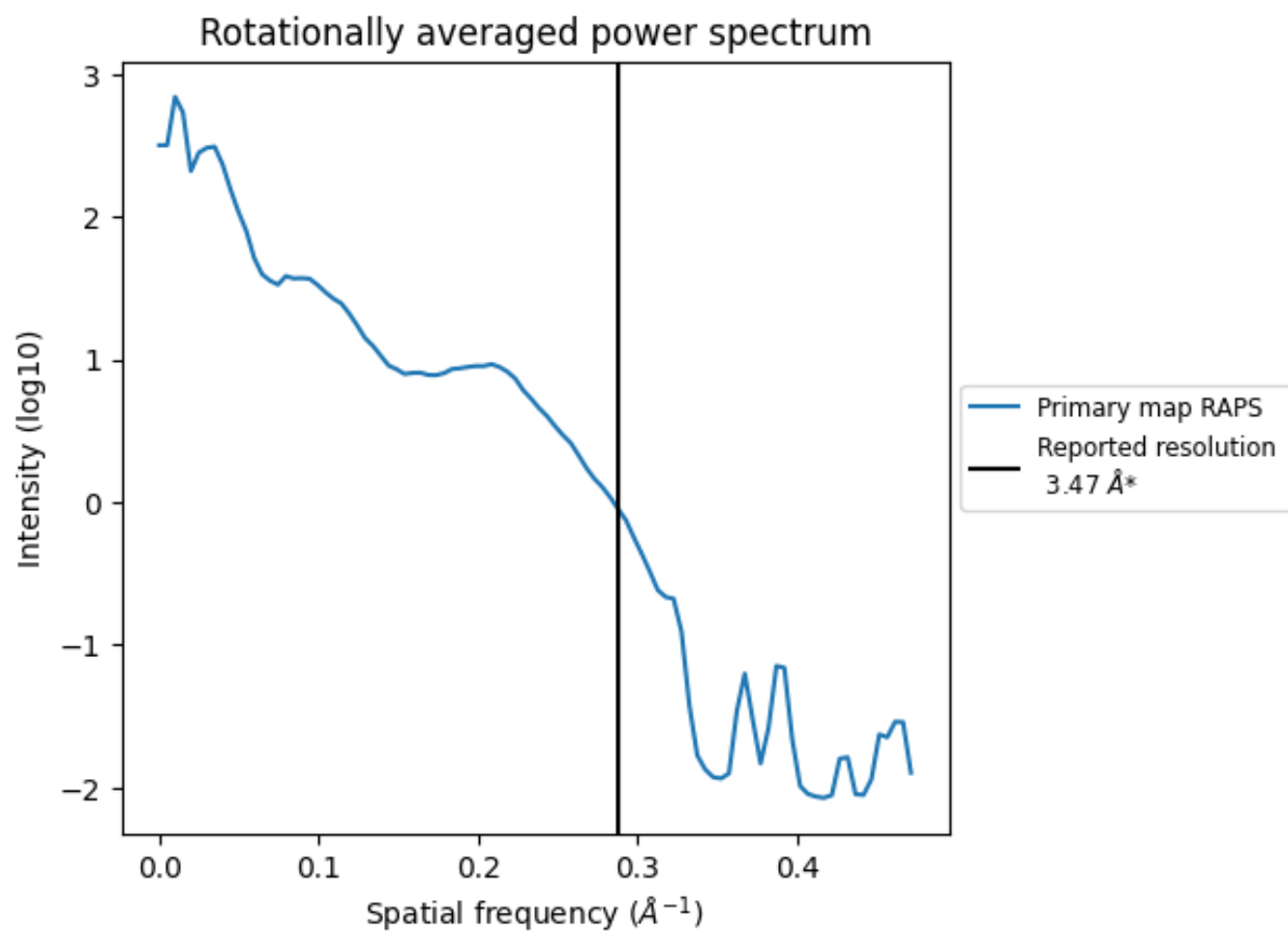
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm³; this corresponds to an approximate mass of 74 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 0.288 Å⁻¹

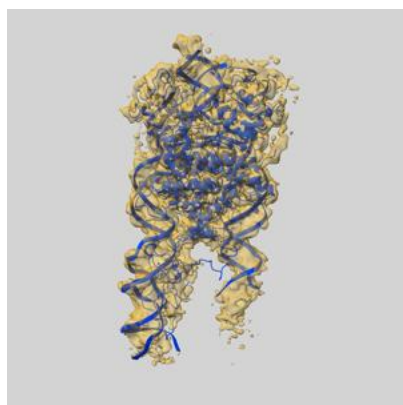
8 Fourier-Shell correlation ⓘ

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

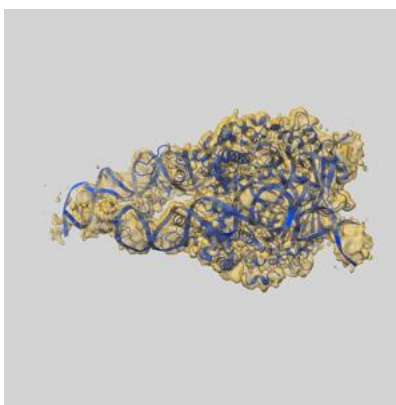
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22072 and PDB model 6X67. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

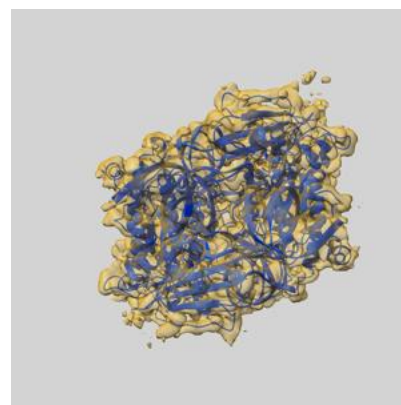
9.1 Map-model overlay [i](#)



X



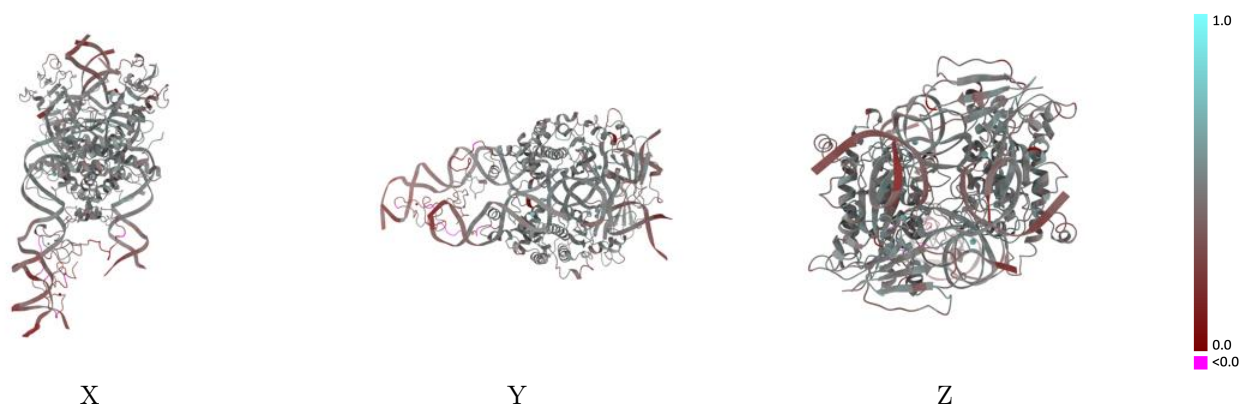
Y



Z

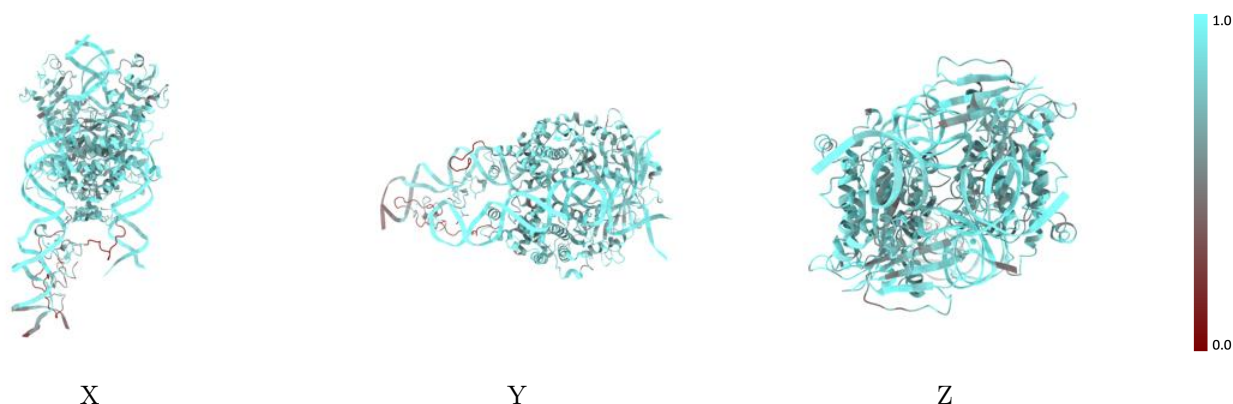
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



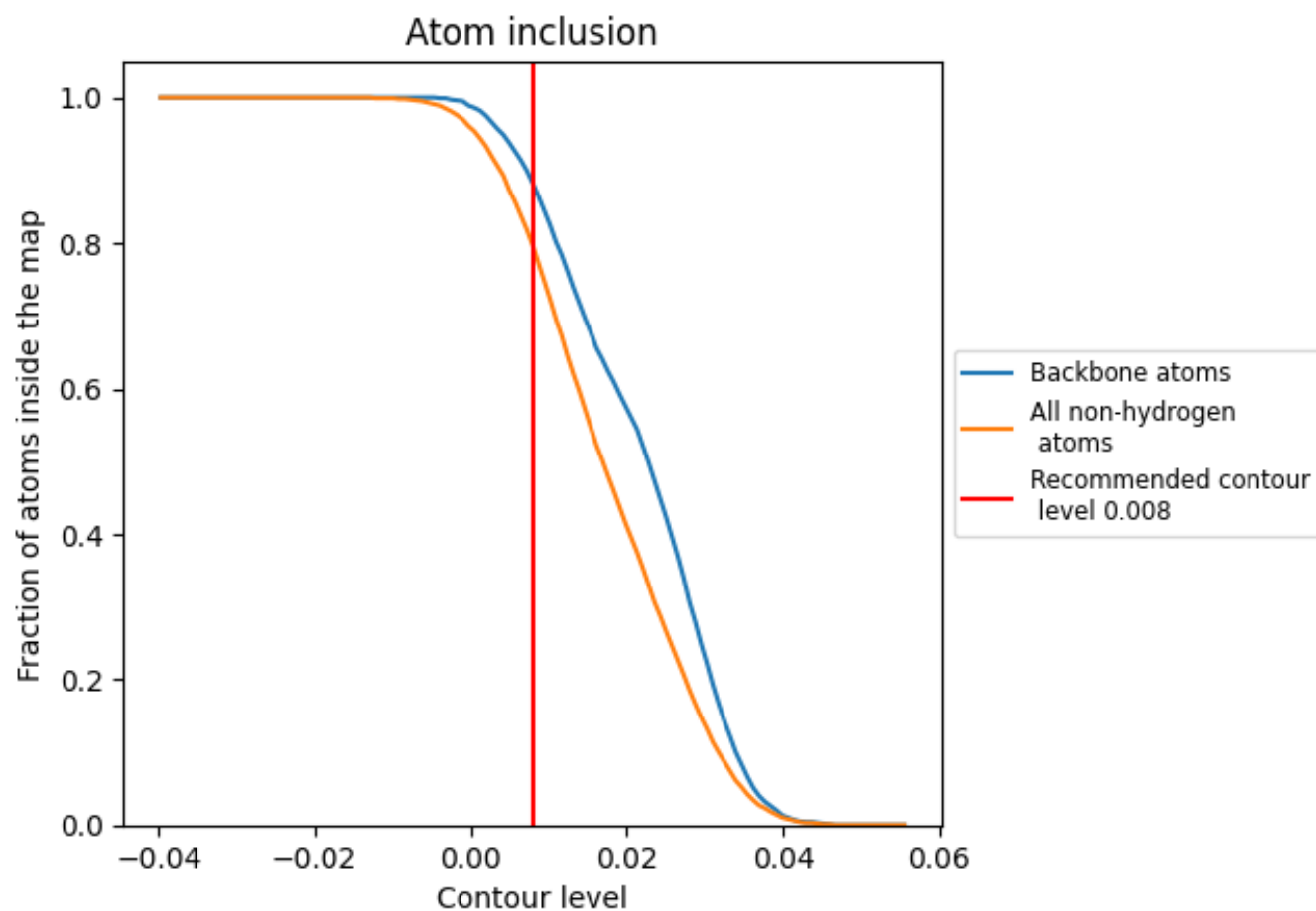
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.4350
C	0.7710	0.4550
D	0.7450	0.4330
E	0.8150	0.4030
F	0.8640	0.4190
G	0.8770	0.3610
J	0.9490	0.4490
K	0.9180	0.4290
L	0.8530	0.3420

