



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:17 AM UTC

PDB ID : 8T7S / pdb_00008t7s
EMDB ID : EMD-41093
Title : SpRYmer bound to NAC PAM DNA
Authors : Hibshman, G.N.; Bravo, J.P.K.; Taylor, D.W.
Deposited on : 2023-06-21
Resolution : 3.01 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:

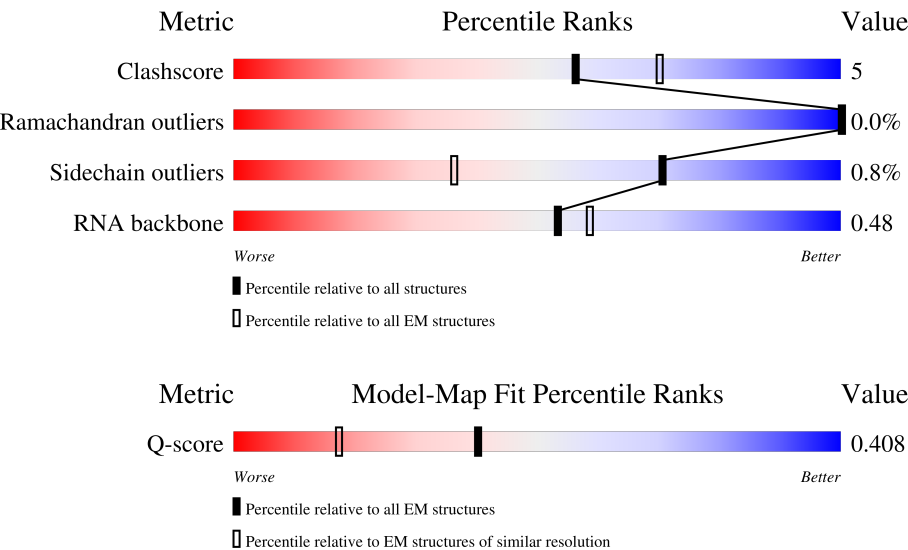
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.01 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.



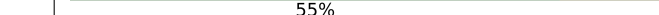
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13882 (2.51 - 3.51)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1369	
1	G	1369	
2	B	98	

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Mol	Chain	Length	Quality of chain
2	H	98	
3	C	55	
3	c	55	
4	D	55	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24994 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 CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1312	Total	C	N	O	S	0	0
			10774	6864	1885	2003	22		
1	G	1157	Total	C	N	O	S	0	0
			9139	5843	1570	1709	17		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP Q99ZW2
A	61	ARG	ALA	engineered mutation	UNP Q99ZW2
A	1111	ARG	LEU	engineered mutation	UNP Q99ZW2
A	1135	LEU	ASP	engineered mutation	UNP Q99ZW2
A	1136	TRP	SER	engineered mutation	UNP Q99ZW2
A	1218	LYS	GLY	engineered mutation	UNP Q99ZW2
A	1219	GLN	GLU	engineered mutation	UNP Q99ZW2
A	1317	ARG	ASN	engineered mutation	UNP Q99ZW2
A	1322	ARG	ALA	engineered mutation	UNP Q99ZW2
A	1333	PRO	ARG	engineered mutation	UNP Q99ZW2
A	1335	GLN	ARG	engineered mutation	UNP Q99ZW2
A	1337	ARG	THR	engineered mutation	UNP Q99ZW2
A	1369	GLY	-	expression tag	UNP Q99ZW2
G	1	GLU	-	expression tag	UNP Q99ZW2
G	61	ARG	ALA	engineered mutation	UNP Q99ZW2
G	1111	ARG	LEU	engineered mutation	UNP Q99ZW2
G	1135	LEU	ASP	engineered mutation	UNP Q99ZW2
G	1136	TRP	SER	engineered mutation	UNP Q99ZW2
G	1218	LYS	GLY	engineered mutation	UNP Q99ZW2
G	1219	GLN	GLU	engineered mutation	UNP Q99ZW2
G	1317	ARG	ASN	engineered mutation	UNP Q99ZW2
G	1322	ARG	ALA	engineered mutation	UNP Q99ZW2
G	1333	PRO	ARG	engineered mutation	UNP Q99ZW2
G	1335	GLN	ARG	engineered mutation	UNP Q99ZW2
G	1337	ARG	THR	engineered mutation	UNP Q99ZW2
G	1369	GLY	-	expression tag	UNP Q99ZW2

- Molecule 2 is a RNA chain called gRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	P	0	0
			2103	941	389	675	98		
2	H	88	Total	C	N	O	P	0	0
			1887	844	346	609	88		

- Molecule 3 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	21	Total	C	N	O	P	0	0
			433	206	76	130	21		
3	c	15	Total	C	N	O	P	0	0
			302	146	46	95	15		

- Molecule 4 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	17	Total	C	N	O	P	0	0
			349	166	68	98	17		

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

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total	Mg	0
			4	4	
5	c	1	Total	Mg	0
			1	1	

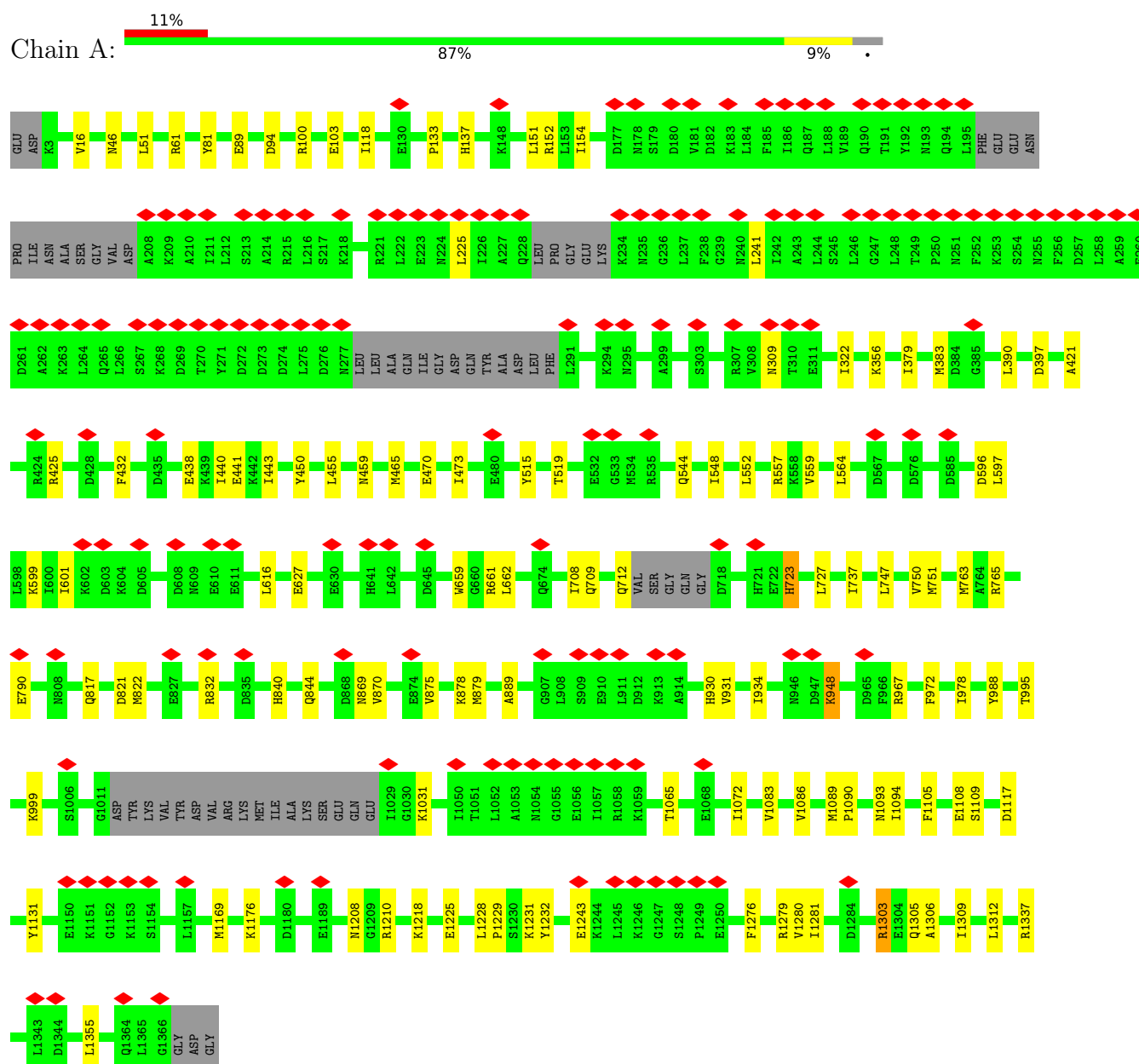
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	O	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: CRISPR-associated endonuclease Cas9/Csn1



Chain G:





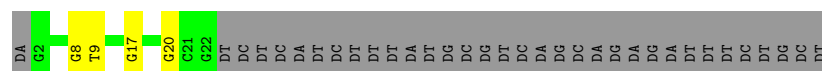
• Molecule 2: gRNA



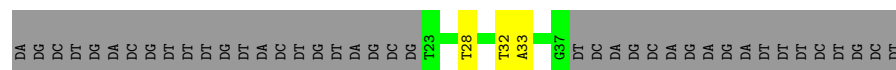
• Molecule 2: gRNA



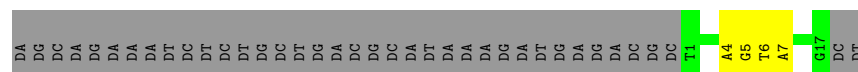
• Molecule 3: TS



• Molecule 3: TS



• Molecule 4: NTS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62283	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.578	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0797	Depositor
Map size ($\text{\AA}$)	311.04, 311.04, 311.04	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.81, 0.81, 0.81	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: 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	A	0.31	1/10963 (0.0%)	0.68	8/14719 (0.1%)
1	G	0.67	8/9308 (0.1%)	1.48	186/12582 (1.5%)
2	B	0.52	5/2355 (0.2%)	0.83	11/3665 (0.3%)
2	H	0.27	0/2114	0.56	0/3294
3	C	0.35	0/484	0.63	0/746
3	c	0.35	0/335	0.57	0/514
4	D	0.28	0/392	0.57	0/602
All	All	0.49	14/25951 (0.1%)	1.04	205/36122 (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
1	A	0	2
1	G	2	27
2	B	0	1
All	All	2	30

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	G	C3'-O3'	14.49	1.63	1.42
2	B	4	G	C1'-N9	9.44	1.62	1.48
1	G	643	PHE	CE2-CZ	-8.81	1.12	1.38
2	B	4	G	C3'-C2'	8.49	1.65	1.52
1	G	212	LEU	CG-CD2	8.33	1.80	1.52
1	A	1090	PRO	CG-CD	-8.16	1.23	1.50
1	G	246	LEU	CG-CD1	-8.09	1.25	1.52
1	G	623	LEU	CG-CD1	-6.85	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	G	C2'-C1'	6.51	1.63	1.53
2	B	4	G	N9-C4	5.51	1.49	1.38
1	G	301	LEU	CG-CD1	-5.45	1.34	1.52
1	G	300	ILE	CG1-CD1	-5.28	1.31	1.51
1	G	1169	MET	CB-CG	5.23	1.68	1.52
1	G	621	LEU	CG-CD1	-5.13	1.35	1.52

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	G	C3'-C2'-C1'	18.36	119.66	101.30
1	G	616	LEU	CB-CG-CD1	17.92	164.45	110.70
1	G	246	LEU	CD1-CG-CD2	-17.84	71.56	110.80
1	A	133	PRO	N-CD-CG	-17.46	77.01	103.20
1	G	383	MET	CG-SD-CE	15.65	135.33	100.90
2	B	4	G	O4'-C1'-C2'	-15.12	92.48	107.60
2	B	4	G	C4'-C3'-O3'	15.02	135.53	113.00
2	B	4	G	C4'-C3'-C2'	-14.99	87.61	102.60
1	G	616	LEU	CD1-CG-CD2	-13.84	80.36	110.80
1	G	513	LEU	CD1-CG-CD2	-13.78	80.48	110.80
1	G	1043	MET	CG-SD-CE	13.21	129.97	100.90
2	B	4	G	N9-C1'-C2'	13.08	131.62	112.00
1	G	338	LEU	CB-CG-CD2	12.60	148.51	110.70
1	G	301	LEU	CD1-CG-CD2	-12.48	83.33	110.80
1	G	513	LEU	CB-CG-CD1	12.41	147.92	110.70
1	G	237	LEU	CD1-CG-CD2	-12.23	83.90	110.80
1	G	1169	MET	CG-SD-CE	-11.95	74.62	100.90
1	G	623	LEU	CD1-CG-CD2	-11.76	84.94	110.80
1	G	1288	ASP	CB-CG-OD2	11.09	143.91	118.40
1	G	1139	VAL	CG1-CB-CG2	-11.06	86.47	110.80
1	G	513	LEU	CB-CG-CD2	-11.05	77.55	110.70
2	B	4	G	C2'-C3'-O3'	10.86	129.99	113.70
1	G	1097	LYS	CD-CE-NZ	-10.82	77.27	111.90
1	G	763	MET	CA-CB-CG	-10.72	92.65	114.10
1	G	648	MET	CA-CB-CG	10.45	134.99	114.10
1	G	621	LEU	CD1-CG-CD2	-10.26	88.22	110.80
1	A	1090	PRO	CA-N-CD	-10.24	97.66	112.00
1	G	302	LEU	CD1-CG-CD2	-10.22	88.33	110.80
1	G	76	LYS	CD-CE-NZ	10.09	144.18	111.90
1	G	1261	GLN	CG-CD-NE2	-10.01	101.39	116.40
1	G	751	MET	CG-SD-CE	-9.73	79.50	100.90
1	G	921	LEU	CB-CG-CD2	-9.69	81.65	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1288	ASP	CB-CG-OD1	-9.62	96.27	118.40
1	G	90	MET	CB-CA-C	-9.56	94.92	110.79
1	A	133	PRO	CA-CB-CG	-9.50	86.45	104.50
1	G	1007	GLU	CA-CB-CG	9.42	132.94	114.10
1	G	321	MET	CG-SD-CE	9.41	121.61	100.90
1	G	338	LEU	CB-CG-CD1	-9.24	82.98	110.70
1	G	1043	MET	CA-CB-CG	8.65	131.41	114.10
1	A	1090	PRO	N-CD-CG	-8.62	90.27	103.20
1	G	763	MET	N-CA-CB	8.58	123.86	109.87
1	G	623	LEU	N-CA-CB	-8.26	96.28	110.32
1	G	470	GLU	N-CA-CB	8.26	120.60	110.53
1	G	1261	GLN	CB-CA-C	8.24	126.58	109.68
1	G	212	LEU	CD1-CG-CD2	-8.12	92.94	110.80
1	A	133	PRO	CA-N-CD	-7.95	100.87	112.00
1	G	616	LEU	CB-CG-CD2	-7.78	87.37	110.70
1	G	419	LEU	CB-CG-CD2	7.72	133.86	110.70
1	G	403	ARG	CD-NE-CZ	7.69	135.17	124.40
1	G	1332	ASP	OD1-CG-OD2	-7.66	104.52	122.90
1	G	90	MET	CG-SD-CE	7.62	117.66	100.90
1	G	1331	ILE	CG1-CB-CG2	-7.60	87.89	110.70
1	G	1043	MET	N-CA-CB	-7.56	98.08	110.40
1	G	1261	GLN	CG-CD-OE1	7.56	135.92	120.80
1	G	212	LEU	CA-C-N	7.55	134.91	123.05
1	G	212	LEU	C-N-CA	7.55	134.91	123.05
1	G	222	LEU	CB-CG-CD1	7.43	132.98	110.70
1	G	223	GLU	CA-CB-CG	7.39	128.88	114.10
1	G	1331	ILE	CA-C-N	7.22	141.49	120.97
1	G	1331	ILE	C-N-CA	7.22	141.49	120.97
1	G	513	LEU	CA-CB-CG	7.11	141.19	116.30
1	G	337	ALA	CA-C-N	7.10	130.02	120.65
1	G	337	ALA	C-N-CA	7.10	130.02	120.65
1	G	750	VAL	CG1-CB-CG2	-7.09	95.19	110.80
1	G	470	GLU	CG-CD-OE1	-7.05	102.18	118.40
1	G	1123	LYS	CD-CE-NZ	7.05	134.46	111.90
1	G	620	VAL	N-CA-C	-7.04	102.71	112.50
1	A	1303	ARG	CB-CG-CD	7.02	127.45	111.30
1	G	621	LEU	CB-CG-CD2	-7.02	89.64	110.70
1	G	339	VAL	CG1-CB-CG2	-7.00	95.39	110.80
1	G	90	MET	N-CA-CB	7.00	120.41	110.12
1	G	296	LEU	CD1-CG-CD2	-7.00	95.41	110.80
1	G	724	ILE	CB-CA-C	6.96	121.54	112.14
1	G	1196	ILE	CG1-CB-CG2	-6.90	90.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	648	MET	CB-CG-SD	-6.88	92.05	112.70
1	G	1316	THR	CA-CB-CG2	6.87	122.17	110.50
1	G	1332	ASP	CB-CG-OD1	6.81	134.06	118.40
1	G	631	MET	CG-SD-CE	6.81	115.87	100.90
1	G	938	ARG	CA-CB-CG	6.78	127.67	114.10
1	G	544	GLN	CA-CB-CG	6.78	127.66	114.10
1	G	302	LEU	CB-CA-C	6.77	122.36	110.85
1	G	419	LEU	CB-CA-C	-6.73	100.60	110.96
1	G	1043	MET	CB-CA-C	6.72	124.04	109.99
1	G	623	LEU	CB-CA-C	6.71	124.48	110.32
1	G	617	GLU	CA-CB-CG	-6.70	100.70	114.10
1	G	746	GLU	OE1-CD-OE2	-6.69	106.84	122.90
1	G	1316	THR	OG1-CB-CG2	6.65	122.60	109.30
1	G	921	LEU	CD1-CG-CD2	-6.62	96.24	110.80
1	G	296	LEU	CB-CG-CD2	-6.59	90.93	110.70
1	G	1261	GLN	CB-CG-CD	6.58	123.79	112.60
1	G	1358	THR	OG1-CB-CG2	6.58	122.46	109.30
1	G	460	SER	CA-C-N	6.58	129.75	120.28
1	G	460	SER	C-N-CA	6.58	129.75	120.28
1	G	1068	GLU	CA-C-N	6.57	132.94	121.52
1	G	1068	GLU	C-N-CA	6.57	132.94	121.52
2	B	4	G	C4-N9-C1'	6.46	145.86	126.50
1	G	470	GLU	CG-CD-OE2	6.45	133.24	118.40
1	G	76	LYS	CB-CG-CD	6.43	126.09	111.30
1	G	339	VAL	CA-CB-CG1	6.41	121.30	110.40
1	G	338	LEU	CA-C-N	6.41	128.64	120.56
1	G	338	LEU	C-N-CA	6.41	128.64	120.56
1	G	330	GLN	CG-CD-NE2	-6.40	106.80	116.40
1	G	1358	THR	CA-CB-CG2	6.40	121.39	110.50
1	G	90	MET	CA-CB-CG	-6.39	101.32	114.10
1	G	297	SER	CA-CB-OG	6.39	123.88	111.10
1	G	622	THR	CA-CB-CG2	-6.36	99.68	110.50
1	G	383	MET	CB-CA-C	6.36	123.49	109.94
1	G	922	VAL	CG1-CB-CG2	-6.35	96.83	110.80
1	G	643	PHE	CE1-CZ-CE2	-6.35	108.57	120.00
1	G	1261	GLN	CA-CB-CG	6.34	126.78	114.10
1	G	1195	ILE	CA-C-N	-6.33	114.69	123.10
1	G	1195	ILE	C-N-CA	-6.33	114.69	123.10
1	G	301	LEU	CB-CA-C	6.32	121.28	110.79
1	G	403	ARG	CA-CB-CG	-6.27	101.56	114.10
1	G	939	MET	CG-SD-CE	6.26	114.66	100.90
1	G	1079	ASP	N-CA-C	-6.24	104.02	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	330	GLN	N-CA-CB	6.14	119.25	110.16
1	G	45	LYS	CD-CE-NZ	6.14	131.53	111.90
1	G	594	TYR	OH-CZ-CE2	-6.11	101.56	119.90
1	G	482	VAL	CG1-CB-CG2	-6.11	97.36	110.80
1	G	763	MET	CB-CA-C	-6.10	100.28	110.29
1	G	1069	THR	CA-CB-OG1	6.09	118.73	109.60
1	G	751	MET	CA-CB-CG	6.08	126.25	114.10
1	G	212	LEU	CB-CG-CD2	-6.07	92.50	110.70
1	G	594	TYR	CE1-CZ-OH	6.07	138.10	119.90
1	G	514	LEU	CD1-CG-CD2	-6.06	97.47	110.80
1	G	1139	VAL	CA-CB-CG2	-6.05	100.12	110.40
1	G	302	LEU	CB-CG-CD1	-6.03	92.61	110.70
1	G	419	LEU	CA-C-N	6.01	128.33	120.28
1	G	419	LEU	C-N-CA	6.01	128.33	120.28
1	G	1069	THR	OG1-CB-CG2	5.97	121.25	109.30
1	G	76	LYS	CG-CD-CE	-5.93	97.67	111.30
1	G	212	LEU	CB-CA-C	5.93	120.45	109.54
1	G	921	LEU	CB-CG-CD1	5.91	128.42	110.70
1	G	469	SER	CA-C-N	-5.90	113.32	122.05
1	G	469	SER	C-N-CA	-5.90	113.32	122.05
1	G	942	LYS	CD-CE-NZ	5.88	130.72	111.90
1	G	237	LEU	CB-CG-CD2	-5.85	93.14	110.70
1	G	622	THR	CA-C-N	5.81	129.90	120.60
1	G	622	THR	C-N-CA	5.81	129.90	120.60
1	A	948	LYS	CB-CG-CD	5.81	124.66	111.30
1	G	613	GLU	CA-C-N	-5.81	110.83	121.52
1	G	613	GLU	C-N-CA	-5.81	110.83	121.52
1	G	1069	THR	CA-C-N	-5.78	110.33	121.78
1	G	1069	THR	C-N-CA	-5.78	110.33	121.78
1	G	1073	VAL	CA-CB-CG2	5.76	120.19	110.40
1	G	1237	TYR	OH-CZ-CE2	-5.72	102.74	119.90
1	G	184	LEU	CB-CG-CD2	-5.70	93.61	110.70
1	G	222	LEU	CA-C-N	-5.70	111.65	120.31
1	G	222	LEU	C-N-CA	-5.70	111.65	120.31
2	B	4	G	O4'-C4'-C3'	5.61	109.61	104.00
1	G	1237	TYR	CE1-CZ-OH	5.59	136.67	119.90
1	A	470	GLU	CA-CB-CG	5.58	125.26	114.10
1	G	291	LEU	CB-CG-CD2	-5.58	93.96	110.70
1	G	648	MET	CG-SD-CE	5.56	113.13	100.90
2	B	4	G	C8-N9-C4	-5.53	89.80	106.40
1	G	341	GLN	CB-CG-CD	5.50	121.95	112.60
1	G	394	ASN	CA-C-N	-5.48	113.72	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	394	ASN	C-N-CA	-5.48	113.72	122.66
1	G	616	LEU	CA-C-N	-5.47	112.94	120.28
1	G	616	LEU	C-N-CA	-5.47	112.94	120.28
1	G	607	LEU	CA-CB-CG	5.46	135.39	116.30
1	G	433	LEU	CB-CG-CD2	-5.45	94.34	110.70
1	G	321	MET	CA-C-N	5.43	127.40	120.56
1	G	321	MET	C-N-CA	5.43	127.40	120.56
1	G	1261	GLN	N-CA-CB	-5.42	102.61	110.36
1	G	1169	MET	CA-CB-CG	5.40	124.91	114.10
2	B	4	G	O4'-C1'-N9	5.40	116.60	108.50
1	G	212	LEU	N-CA-CB	-5.39	102.41	110.17
1	G	636	LEU	CD1-CG-CD2	-5.38	98.97	110.80
1	G	920	GLN	CG-CD-NE2	-5.38	108.34	116.40
1	G	222	LEU	CD1-CG-CD2	-5.37	98.99	110.80
1	G	622	THR	OG1-CB-CG2	-5.33	98.64	109.30
1	G	922	VAL	CA-CB-CG2	-5.33	101.33	110.40
1	G	183	LYS	CA-C-N	-5.32	111.63	120.68
1	G	183	LYS	C-N-CA	-5.32	111.63	120.68
1	G	1069	THR	CA-CB-CG2	5.32	119.54	110.50
1	G	338	LEU	CB-CA-C	-5.31	102.78	110.96
1	G	750	VAL	CA-C-N	5.27	129.66	122.34
1	G	750	VAL	C-N-CA	5.27	129.66	122.34
1	G	433	LEU	CB-CG-CD1	5.26	126.49	110.70
1	G	724	ILE	CG1-CB-CG2	-5.25	94.95	110.70
1	G	330	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	G	246	LEU	CB-CG-CD1	-5.22	95.04	110.70
1	G	303	SER	CA-CB-OG	5.22	121.54	111.10
1	G	220	ARG	CA-C-N	5.21	127.26	120.28
1	G	220	ARG	C-N-CA	5.21	127.26	120.28
1	G	725	ALA	CA-C-N	-5.20	113.27	122.26
1	G	725	ALA	C-N-CA	-5.20	113.27	122.26
2	B	4	G	C1'-O4'-C4'	5.19	115.09	109.90
1	G	964	SER	CA-CB-OG	-5.17	100.75	111.10
1	G	1090	PRO	CB-CA-C	-5.17	102.98	111.31
1	G	291	LEU	CB-CG-CD1	5.17	126.21	110.70
1	G	701	SER	CA-CB-OG	-5.15	100.80	111.10
1	G	1236	LEU	CD1-CG-CD2	-5.14	99.49	110.80
1	G	384	ASP	N-CA-C	5.14	118.38	110.42
1	G	161	MET	CG-SD-CE	5.13	112.19	100.90
1	G	1148	LYS	CD-CE-NZ	5.13	128.31	111.90
1	G	469	SER	CA-CB-OG	5.13	121.36	111.10
1	G	630	GLU	N-CA-CB	5.12	117.74	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	345	GLU	CA-C-N	5.06	131.21	121.54
1	G	345	GLU	C-N-CA	5.06	131.21	121.54
1	G	713	VAL	CG1-CB-CG2	-5.06	99.67	110.80
1	G	922	VAL	N-CA-C	5.04	115.17	108.11
1	G	1257	LEU	CB-CG-CD2	-5.03	95.60	110.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	1069	THR	CB
1	G	1358	THR	CB

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	ASN	Peptide
1	A	832	ARG	Sidechain
2	B	4	G	Sidechain
1	G	1104	GLY	Mainchain
1	G	1140	ALA	Mainchain
1	G	1171	ARG	Sidechain
1	G	1288	ASP	Sidechain
1	G	1307	GLU	Sidechain
1	G	1332	ASP	Sidechain
1	G	1337	ARG	Sidechain
1	G	144	ASP	Peptide
1	G	220	ARG	Sidechain
1	G	324	ARG	Sidechain
1	G	330	GLN	Sidechain
1	G	342	GLN	Sidechain
1	G	382	LYS	Mainchain
1	G	384	ASP	Mainchain
1	G	424	ARG	Sidechain
1	G	500	LYS	Mainchain
1	G	586	ARG	Sidechain
1	G	629	ARG	Sidechain
1	G	641	HIS	Sidechain
1	G	643	PHE	Sidechain
1	G	725	ALA	Mainchain
1	G	746	GLU	Sidechain
1	G	752	GLY	Mainchain
1	G	76	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	G	919	ARG	Sidechain
1	G	920	GLN	Sidechain
1	G	938	ARG	Sidechain

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	10774	0	10978	88	0
1	G	9139	0	8954	111	0
2	B	2103	0	1058	35	0
2	H	1887	0	947	11	0
3	C	433	0	238	3	0
3	c	302	0	173	3	0
4	D	349	0	191	3	0
5	A	4	0	0	0	0
5	c	1	0	0	0	0
6	A	2	0	0	0	0
All	All	24994	0	22539	233	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 5.

All (233) 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:G:212:LEU:CG	1:G:212:LEU:CD2	1.80	1.58
2:B:4:G:C3'	2:B:4:G:O3'	1.63	1.42
2:B:4:G:H2'	2:B:5:C:P	1.72	1.29
1:A:661:ARG:HB2	2:B:4:G:O3'	1.45	1.15
2:B:4:G:O3'	2:B:4:G:H3'	1.33	1.10
2:B:4:G:C2'	2:B:5:C:P	2.38	1.09
1:G:212:LEU:CD2	1:G:212:LEU:CD1	2.33	1.05
1:G:212:LEU:CD2	1:G:212:LEU:CB	2.41	0.97
1:A:661:ARG:CB	2:B:4:G:O3'	2.17	0.93
2:B:4:G:C3'	2:B:5:C:P	2.61	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ARG:HB2	2:B:4:G:H3'	1.59	0.85
1:A:661:ARG:HB2	2:B:4:G:C3'	2.08	0.84
1:A:723:HIS:CE1	1:A:727:LEU:HD21	2.16	0.81
1:A:661:ARG:CG	2:B:4:G:H3'	2.12	0.80
1:G:212:LEU:HD23	1:G:212:LEU:HA	1.63	0.79
1:A:661:ARG:CB	2:B:4:G:H3'	2.16	0.76
1:G:212:LEU:CD2	1:G:212:LEU:HD13	2.16	0.73
1:A:597:LEU:HD13	1:A:616:LEU:HD11	1.71	0.71
1:A:1309:ILE:HA	1:A:1312:LEU:HD13	1.73	0.71
1:A:878:LYS:HG3	1:A:879:MET:HG3	1.73	0.69
1:G:619:ILE:O	1:G:623:LEU:HB2	1.93	0.68
1:G:134:THR:HG23	2:H:45:U:H4'	1.76	0.67
1:G:184:LEU:HD21	1:G:296:LEU:HB2	1.77	0.67
1:G:24:GLU:OE2	1:G:1079:ASP:OD1	2.13	0.67
1:A:875:VAL:HA	1:A:878:LYS:HG2	1.77	0.66
1:G:212:LEU:CD2	1:G:212:LEU:HA	2.25	0.66
1:A:661:ARG:HG3	2:B:4:G:H3'	1.78	0.66
1:G:32:PHE:CE2	1:G:1355:LEU:HD12	2.30	0.66
1:G:455:LEU:HD13	1:G:473:ILE:HG21	1.78	0.65
1:G:1147:ALA:HB2	1:G:1190:VAL:HG12	1.77	0.65
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.27	0.65
1:G:921:LEU:HD23	1:G:922:VAL:HG23	1.78	0.64
1:A:763:MET:HE2	1:A:765:ARG:HH11	1.63	0.64
1:G:237:LEU:HD21	1:G:255:ASN:HB3	1.78	0.64
1:A:548:ILE:HD13	1:A:564:LEU:HD11	1.80	0.63
1:A:515:TYR:OH	2:B:4:G:O3'	2.13	0.63
1:A:817:GLN:HG2	1:A:822:MET:HE2	1.80	0.62
1:G:596:ASP:OD2	1:G:656:TYR:OH	2.16	0.62
1:A:723:HIS:HE1	1:A:727:LEU:HD21	1.66	0.61
1:G:746:GLU:OE1	1:G:1351:SER:HB2	2.00	0.60
1:G:745:ASP:OD2	1:G:938:ARG:NH1	2.34	0.60
2:B:37:U:H2'	2:B:38:A:C8	2.37	0.60
1:G:919:ARG:HG2	1:G:919:ARG:HH11	1.67	0.59
1:G:1243:GLU:N	1:G:1243:GLU:OE2	2.35	0.59
2:H:73:G:N2	2:H:76:A:OP2	2.35	0.59
1:A:438:GLU:HA	1:A:441:GLU:HB2	1.85	0.59
1:G:212:LEU:CD2	1:G:212:LEU:CA	2.80	0.59
1:G:419:LEU:HD13	1:G:444:LEU:HD13	1.85	0.58
1:A:627:GLU:N	1:A:627:GLU:OE1	2.36	0.58
1:G:586:ARG:HG2	1:G:587:PHE:N	2.18	0.58
2:B:83:C:H2'	2:B:84:A:H8	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:ARG:HG3	1:A:1280:VAL:HA	1.85	0.57
3:C:17:DG:C2	4:D:4:DA:C2	2.92	0.57
1:A:869:ASN:OD1	1:A:870:VAL:N	2.38	0.56
2:B:4:G:C3'	2:B:4:G:HO3'	2.07	0.56
2:H:27:G:N2	2:H:44:U:OP2	2.39	0.56
1:A:1243:GLU:OE1	1:A:1303:ARG:NH1	2.39	0.56
1:G:952:GLU:H	1:G:952:GLU:CD	2.14	0.56
1:A:151:LEU:HA	1:A:154:ILE:HD12	1.88	0.55
1:G:212:LEU:HD21	1:G:246:LEU:HD21	1.87	0.55
1:A:750:VAL:HG21	1:A:1355:LEU:HD12	1.87	0.55
1:A:1105:PHE:CG	1:A:1169:MET:HG3	2.41	0.55
1:G:421:ALA:O	1:G:425:ARG:CB	2.54	0.55
1:A:661:ARG:CG	2:B:4:G:O3'	2.54	0.55
1:G:343:LEU:HB2	1:G:383:MET:HE3	1.88	0.55
1:G:297:SER:O	1:G:301:LEU:HB2	2.06	0.54
2:B:8:A:H2'	2:B:9:A:C8	2.42	0.54
1:A:1228:LEU:HD11	1:A:1232:TYR:HB2	1.90	0.54
1:G:237:LEU:CD2	1:G:255:ASN:HB3	2.37	0.54
2:B:83:C:H2'	2:B:84:A:C8	2.43	0.54
3:c:32:DT:H2'	3:c:33:DA:C8	2.43	0.53
1:G:621:LEU:O	1:G:625:LEU:HB2	2.08	0.53
1:A:225:LEU:HD11	1:A:241:LEU:HD22	1.90	0.53
2:B:46:A:H2'	2:B:47:A:C8	2.44	0.53
1:A:1306:ALA:HA	1:A:1309:ILE:HD12	1.90	0.53
2:B:4:G:H2'	2:B:5:C:OP2	2.06	0.53
1:G:14:ASN:OD1	1:G:55:SER:OG	2.18	0.52
1:G:615:ILE:HG23	1:G:639:TYR:CE1	2.44	0.52
1:A:597:LEU:O	1:A:601:ILE:N	2.43	0.52
1:G:467:ARG:HD2	1:G:470:GLU:OE2	2.09	0.52
1:A:450:TYR:OH	1:A:627:GLU:OE2	2.23	0.51
1:A:995:THR:HG22	1:A:999:LYS:HE2	1.92	0.51
2:B:37:U:H2'	2:B:38:A:H8	1.74	0.51
1:G:1086:VAL:HA	1:G:1089:MET:HE2	1.91	0.51
1:A:875:VAL:HG22	1:A:879:MET:HE2	1.93	0.51
2:B:4:G:O3'	2:B:5:C:P	2.69	0.51
1:G:184:LEU:C	1:G:184:LEU:HD23	2.37	0.50
1:A:1228:LEU:HD12	1:A:1229:PRO:HD2	1.94	0.50
1:A:459:ASN:O	1:A:459:ASN:ND2	2.45	0.50
2:B:38:A:H2'	2:B:39:G:C8	2.46	0.50
1:A:46:ASN:O	1:A:1093:ASN:ND2	2.38	0.49
1:A:596:ASP:O	1:A:599:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:LEU:HD11	1:G:153:LEU:HB3	1.94	0.49
2:H:46:A:H2'	2:H:47:A:C8	2.48	0.49
1:A:1208:ASN:OD1	1:A:1279:ARG:HG3	2.13	0.49
1:G:1203:LEU:HD13	1:G:1213:MET:HE3	1.95	0.49
1:G:1111:ARG:HG3	1:G:1135:LEU:HD12	1.94	0.49
1:G:492:ILE:HG12	1:G:625:LEU:HD11	1.94	0.49
1:G:677:LYS:HB3	1:G:681:ASP:HB2	1.95	0.49
1:A:519:THR:HG23	2:B:5:C:H4'	1.94	0.48
3:c:32:DT:H2'	3:c:33:DA:H8	1.78	0.48
1:G:18:TRP:CH2	1:G:1355:LEU:HD21	2.48	0.48
1:G:212:LEU:CD2	1:G:212:LEU:HB3	2.36	0.48
1:G:249:THR:HG23	1:G:265:GLN:HB2	1.95	0.48
1:G:26:LYS:HE3	1:G:26:LYS:HB3	1.51	0.48
1:A:356:LYS:HB3	1:A:356:LYS:HE3	1.68	0.48
1:G:643:PHE:HB2	1:G:648:MET:SD	2.53	0.48
2:B:54:G:H2'	2:B:55:C:C6	2.49	0.48
1:A:94:ASP:OD2	1:A:152:ARG:NH1	2.47	0.47
1:A:544:GLN:O	1:A:548:ILE:HG13	2.15	0.47
1:G:424:ARG:HG2	1:G:427:GLU:CD	2.39	0.47
1:A:737:ILE:HG23	1:A:931:VAL:HG22	1.97	0.47
1:G:511:HIS:ND1	1:G:656:TYR:HB3	2.29	0.47
1:A:661:ARG:HB3	2:B:4:G:H5''	1.97	0.47
1:A:662:LEU:HD21	2:B:4:G:C5'	2.45	0.47
1:G:225:LEU:HD13	1:G:242:ILE:HG21	1.97	0.47
1:G:921:LEU:HB2	1:G:1042:ILE:HD13	1.96	0.47
1:G:24:GLU:HB3	1:G:26:LYS:HG2	1.97	0.47
1:G:145:SER:O	1:G:145:SER:OG	2.27	0.47
1:A:137:HIS:HA	1:A:322:ILE:HD11	1.97	0.47
1:G:217:SER:N	1:G:220:ARG:HH11	2.12	0.47
1:G:603:ASP:OD1	1:G:603:ASP:N	2.39	0.47
1:G:980:ASN:H	1:G:1225:GLU:CD	2.22	0.47
1:A:118:ILE:O	1:A:152:ARG:HD2	2.15	0.46
1:A:552:LEU:HD13	1:A:559:VAL:HG21	1.96	0.46
1:G:302:LEU:HA	1:G:302:LEU:HD22	1.68	0.46
1:G:321:MET:HE1	1:G:324:ARG:NH1	2.30	0.46
1:A:455:LEU:HD13	1:A:473:ILE:HG21	1.98	0.46
1:A:930:HIS:O	1:A:934:ILE:HG13	2.14	0.46
1:G:244:LEU:HD21	1:G:271:TYR:OH	2.16	0.46
1:G:718:ASP:OD1	1:G:718:ASP:N	2.47	0.46
1:G:991:ALA:O	1:G:995:THR:OG1	2.31	0.46
1:G:184:LEU:HD11	1:G:295:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:469:SER:HB3	1:G:481:VAL:HG13	1.97	0.45
1:G:171:GLU:CD	1:G:629:ARG:HD2	2.41	0.45
1:A:1131:TYR:HA	2:B:24:U:H4'	1.97	0.45
3:C:8:DG:H2'	3:C:9:DT:C6	2.50	0.45
1:G:1194:LEU:HD21	1:G:1365:LEU:HB3	1.97	0.45
1:G:720:LEU:O	1:G:724:ILE:HG12	2.17	0.45
1:A:790:GLU:HG2	1:A:889:ALA:HA	1.98	0.45
1:A:821:ASP:OD1	1:A:822:MET:N	2.50	0.45
2:B:89:G:H4'	2:B:90:U:H5'	1.99	0.45
1:A:81:TYR:HB2	1:A:443:ILE:HD12	1.98	0.45
1:G:24:GLU:C	1:G:26:LYS:H	2.24	0.45
1:G:217:SER:H	1:G:220:ARG:HD2	1.82	0.45
1:G:909:SER:H	1:G:912:ASP:HB2	1.82	0.45
1:G:1169:MET:HE3	1:G:1169:MET:HB2	1.15	0.45
1:G:663:SER:O	1:G:667:ILE:HG13	2.18	0.44
1:G:692:ASN:OD1	1:G:694:MET:HG2	2.17	0.44
1:G:622:THR:HG23	1:G:635:ARG:HD3	1.98	0.44
1:A:723:HIS:CE1	1:A:727:LEU:CD2	2.94	0.44
1:A:840:HIS:CE1	1:A:844:GLN:HE21	2.35	0.44
1:A:1305:GLN:O	1:A:1309:ILE:HG13	2.18	0.44
1:G:143:VAL:HG13	1:G:421:ALA:HB1	1.99	0.44
1:A:16:VAL:HG22	1:A:51:LEU:HB3	1.99	0.44
1:A:1280:VAL:HG23	1:A:1281:ILE:HG12	1.99	0.44
1:A:948:LYS:HE3	1:A:948:LYS:HA	2.00	0.44
1:A:978:ILE:HG21	1:A:1228:LEU:HD23	2.00	0.44
1:G:967:ARG:HA	1:G:972:PHE:HB3	1.99	0.44
1:A:421:ALA:O	1:A:425:ARG:HG2	2.18	0.44
1:A:661:ARG:CB	2:B:4:G:H5'	2.48	0.43
1:A:390:LEU:HD12	1:A:390:LEU:HA	1.86	0.43
2:H:25:U:H2'	2:H:26:A:C8	2.54	0.43
2:H:84:A:H2'	2:H:85:C:C6	2.54	0.43
1:A:100:ARG:HA	1:A:103:GLU:HG2	2.01	0.43
1:A:1231:LYS:HE3	1:A:1232:TYR:CZ	2.53	0.43
2:B:85:C:H2'	2:B:86:C:C6	2.53	0.43
1:G:18:TRP:CE3	1:G:747:LEU:HD11	2.53	0.43
1:G:212:LEU:HD23	1:G:212:LEU:CA	2.41	0.43
1:G:1360:ILE:HD13	1:G:1360:ILE:HG21	1.82	0.43
1:G:763:MET:HE2	1:G:763:MET:HB2	1.47	0.43
1:A:61:ARG:NH1	1:A:1108:GLU:OE2	2.47	0.43
1:A:1176:LYS:HE3	1:A:1176:LYS:HB3	1.80	0.42
1:G:90:MET:HE3	1:G:151:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:451:TYR:HA	1:G:491:PHE:CD1	2.54	0.42
1:G:977:GLU:OE1	1:G:1317:ARG:NH2	2.52	0.42
1:A:708:ILE:O	1:A:712:GLN:HG2	2.18	0.42
1:G:11:ILE:HD13	1:G:11:ILE:HG21	1.79	0.42
1:G:184:LEU:HD21	1:G:296:LEU:CB	2.47	0.42
1:G:670:ILE:HD13	1:G:670:ILE:HG21	1.73	0.42
1:G:671:ARG:HG2	1:G:678:THR:HG22	2.01	0.42
1:A:659:TRP:NE1	3:c:28:DT:OP1	2.48	0.42
2:B:8:A:H2'	2:B:9:A:H8	1.81	0.42
1:A:597:LEU:HD23	1:A:597:LEU:HA	1.78	0.42
1:G:25:TYR:HB3	1:G:992:VAL:HG12	2.02	0.42
2:B:23:U:H2'	2:B:24:U:C6	2.55	0.41
1:G:419:LEU:HD21	1:G:440:ILE:HG22	2.00	0.41
1:G:1302:ILE:HG21	1:G:1302:ILE:HD13	1.85	0.41
1:A:723:HIS:ND1	1:A:723:HIS:C	2.78	0.41
1:G:335:LEU:O	1:G:338:LEU:HB3	2.21	0.41
1:G:1358:THR:HG23	2:H:68:A:H2	1.86	0.41
1:A:879:MET:HE3	1:A:879:MET:HB2	1.49	0.41
1:G:560:THR:HG23	1:G:563:GLN:H	1.86	0.41
1:G:615:ILE:HD13	1:G:615:ILE:HG21	1.89	0.41
1:G:94:ASP:OD2	1:G:152:ARG:NH1	2.49	0.41
1:G:289:LEU:HA	1:G:289:LEU:HD23	1.85	0.41
1:G:419:LEU:HD23	1:G:423:LEU:CD1	2.51	0.41
1:G:548:ILE:HD13	1:G:548:ILE:HA	1.78	0.41
1:G:724:ILE:HG21	1:G:724:ILE:HD13	1.72	0.41
2:H:38:A:H2'	2:H:39:G:C8	2.55	0.41
1:A:379:ILE:HG22	1:A:383:MET:HE3	2.03	0.41
1:A:1065:THR:HG22	1:A:1072:ILE:HA	2.02	0.41
1:G:966:PHE:CD1	1:G:966:PHE:C	2.98	0.41
2:H:84:A:H2'	2:H:85:C:H6	1.85	0.41
1:G:116:HIS:HA	1:G:117:PRO:HD3	1.85	0.41
1:G:474:THR:O	1:G:478:PHE:HB2	2.21	0.41
1:A:1109:SER:N	3:C:20:DG:OP1	2.40	0.41
1:G:760:VAL:C	1:G:761:ILE:HD13	2.45	0.41
1:A:440:ILE:O	1:A:443:ILE:HG22	2.20	0.41
1:A:459:ASN:OD1	2:B:56:U:N3	2.52	0.41
1:A:747:LEU:O	1:A:751:MET:HG2	2.21	0.41
1:A:1086:VAL:O	1:A:1089:MET:HG3	2.21	0.41
1:G:256:PHE:CZ	1:G:282:ILE:HD12	2.55	0.41
4:D:5:DG:H1'	4:D:6:DT:H5'	2.02	0.41
1:A:988:TYR:HE2	1:A:1083:VAL:HG13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:LYS:HE3	1:A:1337:ARG:HH22	1.86	0.41
1:G:918:LYS:HD2	1:G:918:LYS:C	2.46	0.40
1:G:1195:ILE:HD13	1:G:1195:ILE:HG21	1.63	0.40
1:G:24:GLU:O	1:G:26:LYS:N	2.54	0.40
4:D:6:DT:H1'	4:D:7:DA:C8	2.57	0.40
1:A:972:PHE:HD1	1:A:972:PHE:HA	1.70	0.40
1:A:1276:PHE:O	1:A:1280:VAL:HG22	2.22	0.40
1:G:611:GLU:OE1	1:G:611:GLU:N	2.51	0.40
1:A:967:ARG:NH1	1:A:972:PHE:O	2.52	0.40
1:A:1094:ILE:HG21	1:A:1225:GLU:OE2	2.22	0.40
1:G:512:SER:HA	1:G:620:VAL:HG21	2.03	0.40
1:G:1105:PHE:CD1	1:G:1168:ILE:HG22	2.56	0.40
1:G:1270:ILE:HA	1:G:1273:ILE:HG22	2.04	0.40
2:H:94:U:H2'	2:H:95:G:C8	2.56	0.40
1:A:89:GLU:HG3	1:A:432:PHE:CD1	2.56	0.40
1:G:450:TYR:HE1	2:H:15:A:C5	2.39	0.40
1:G:727:LEU:HD22	1:G:930:HIS:HB3	2.03	0.40
1:G:1105:PHE:HD1	1:G:1168:ILE:HG22	1.86	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	1300/1369 (95%)	1269 (98%)	31 (2%)	0	100	100
1	G	1145/1369 (84%)	1099 (96%)	45 (4%)	1 (0%)	48	79
All	All	2445/2738 (89%)	2368 (97%)	76 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	25	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	A	1184/1230 (96%)	1178 (100%)	6 (0%)	81	88
1	G	955/1230 (78%)	943 (99%)	12 (1%)	61	80
All	All	2139/2460 (87%)	2121 (99%)	18 (1%)	70	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	ASP
1	A	465	MET
1	A	709	GLN
1	A	723	HIS
1	A	1031	LYS
1	A	1117	ASP
1	G	23	ASP
1	G	26	LYS
1	G	82	LEU
1	G	279	LEU
1	G	302	LEU
1	G	383	MET
1	G	623	LEU
1	G	702	LEU
1	G	751	MET
1	G	1069	THR
1	G	1261	GLN
1	G	1297	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	178	ASN
1	A	415	HIS
1	A	641	HIS
1	A	650	GLN
1	A	668	ASN
1	A	695	GLN
1	A	844	GLN
1	A	971	GLN
1	A	979	ASN
1	A	1256	GLN
1	G	342	GLN
1	G	412	HIS
1	G	501	ASN
1	G	556	ASN
1	G	609	ASN
1	G	612	ASN
1	G	930	HIS
1	G	933	GLN
1	G	985	HIS
1	G	990	ASN
1	G	1262	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	97/98 (98%)	21 (21%)	3 (3%)
2	H	87/98 (88%)	20 (22%)	2 (2%)
All	All	184/196 (93%)	41 (22%)	5 (2%)

All (41) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	3	C
2	B	4	G
2	B	5	C
2	B	9	A
2	B	17	A
2	B	20	C
2	B	28	A
2	B	29	G
2	B	33	G

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Mol	Chain	Res	Type
2	B	35	A
2	B	36	A
2	B	37	U
2	B	39	G
2	B	51	A
2	B	56	U
2	B	57	A
2	B	58	G
2	B	59	U
2	B	68	A
2	B	89	G
2	B	91	C
2	H	20	C
2	H	28	A
2	H	30	C
2	H	32	A
2	H	33	G
2	H	34	A
2	H	35	A
2	H	36	A
2	H	37	U
2	H	38	A
2	H	39	G
2	H	51	A
2	H	56	U
2	H	57	A
2	H	59	U
2	H	68	A
2	H	89	G
2	H	90	U
2	H	91	C
2	H	96	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	2	A
2	B	8	A
2	B	38	A
2	H	36	A
2	H	38	A

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 5 ligands modelled in this entry, 5 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1:G	O3'	2:A	P	4.01
1	B	4:G	O3'	5:C	P	2.69

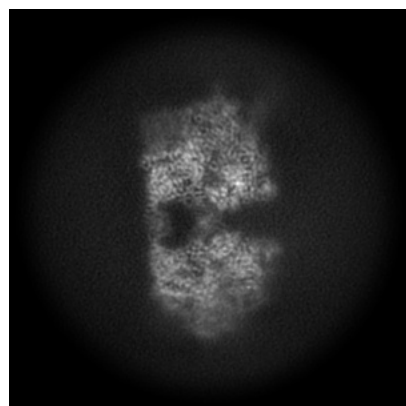
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41093. These allow visual inspection of the internal detail of the map and identification of artifacts.

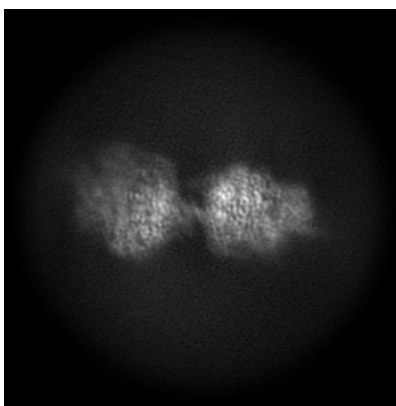
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

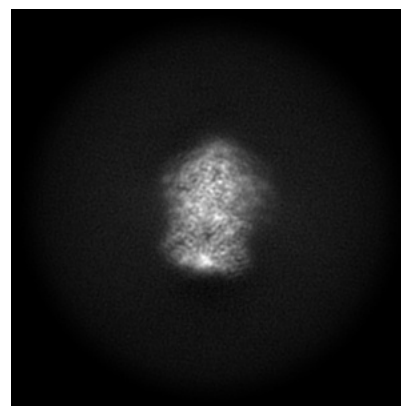
6.1.1 Primary map



X

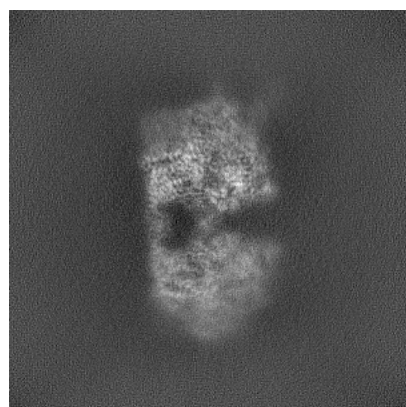


Y

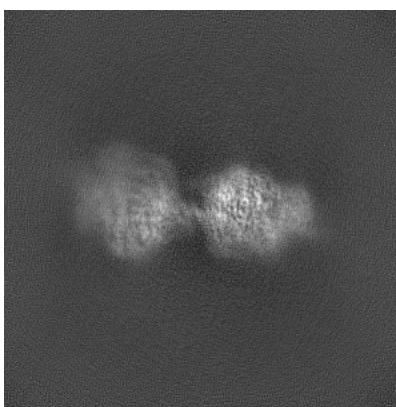


Z

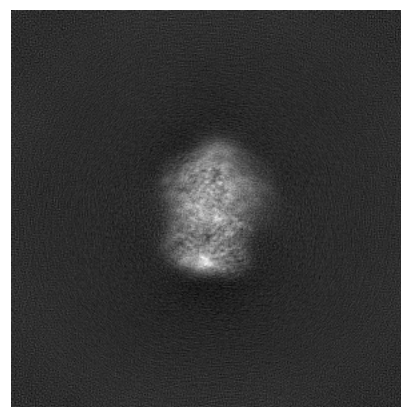
6.1.2 Raw map



X



Y

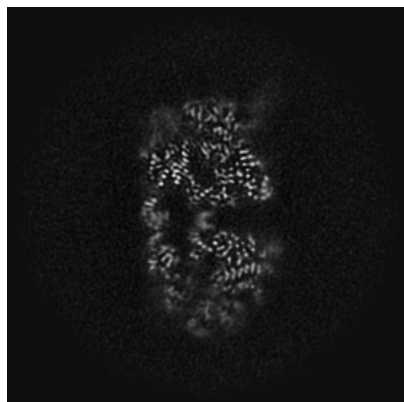


Z

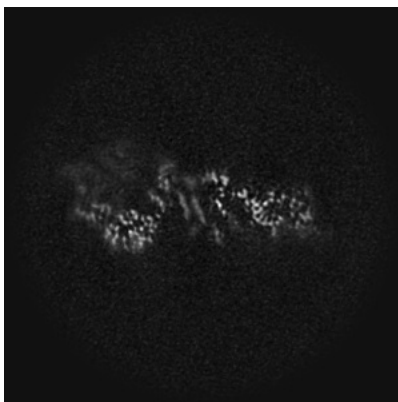
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

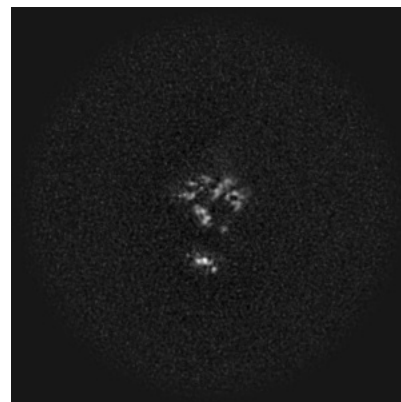
6.2.1 Primary map



X Index: 192



Y Index: 192

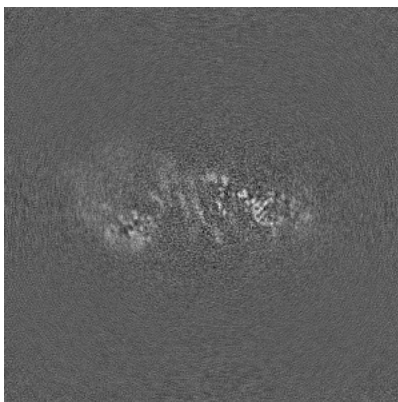


Z Index: 192

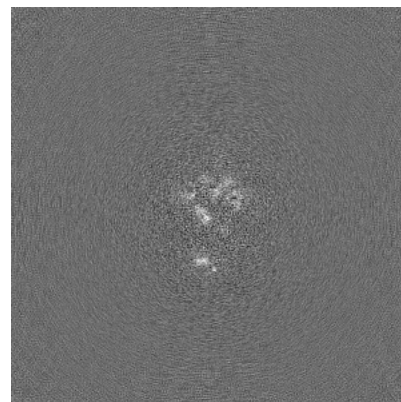
6.2.2 Raw map



X Index: 192



Y Index: 192

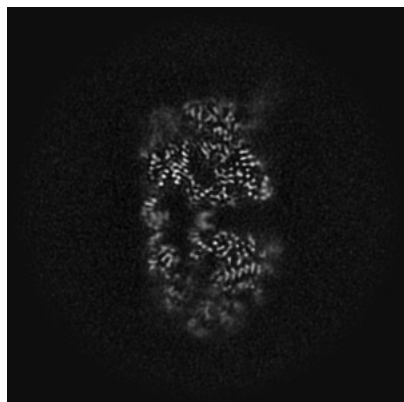


Z Index: 192

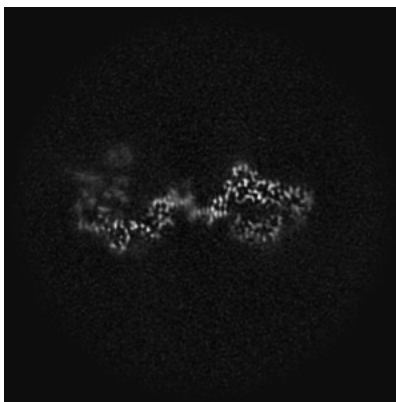
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

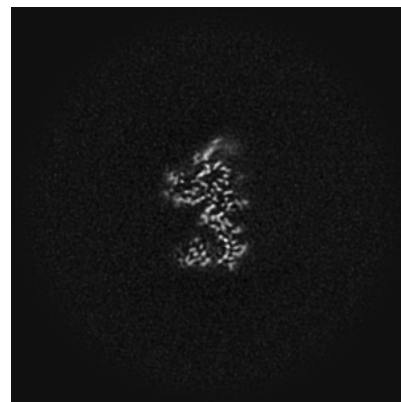
6.3.1 Primary map



X Index: 192

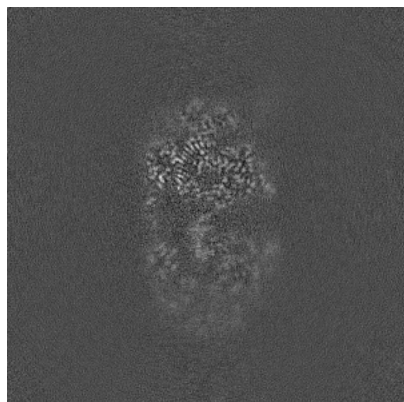


Y Index: 183

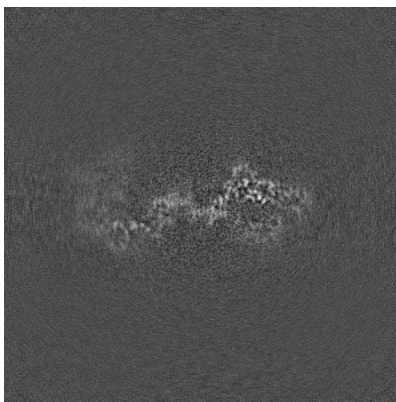


Z Index: 207

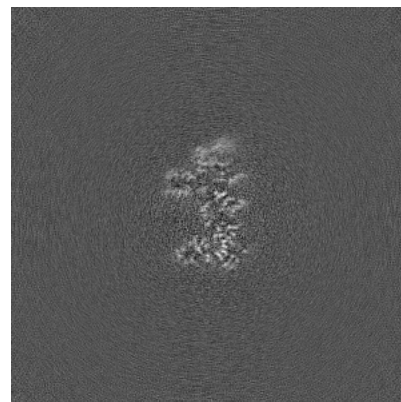
6.3.2 Raw map



X Index: 197



Y Index: 183

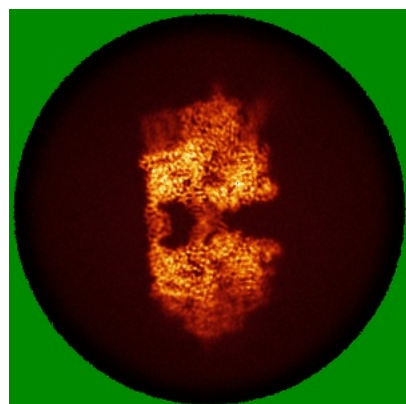


Z Index: 211

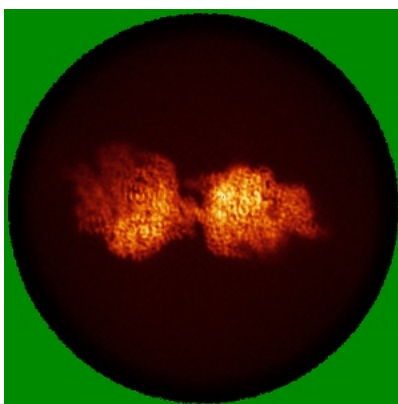
The images above show the largest variance slices of the map in three orthogonal directions.

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

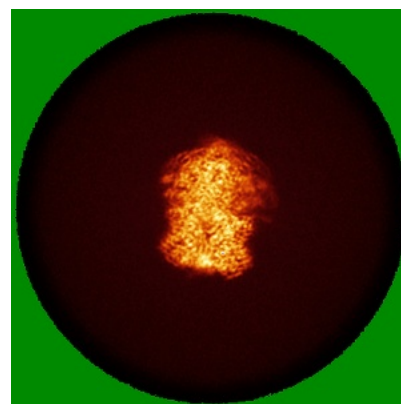
6.4.1 Primary map



X

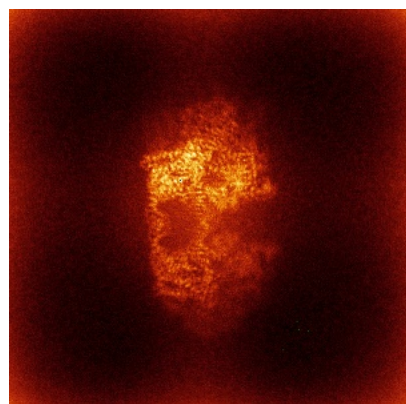


Y

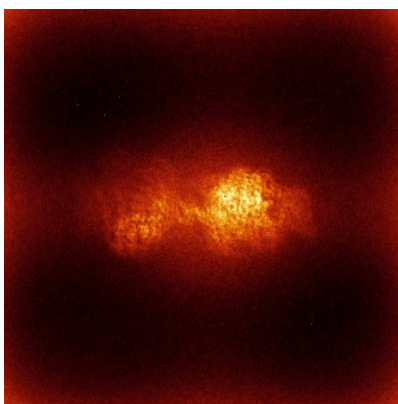


Z

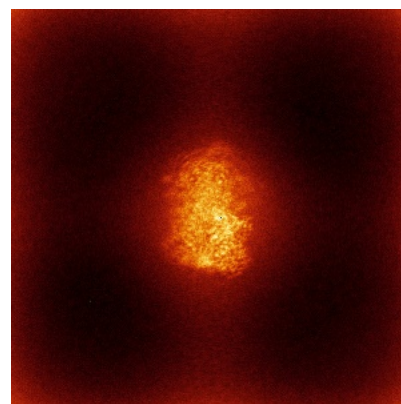
6.4.2 Raw map



X



Y

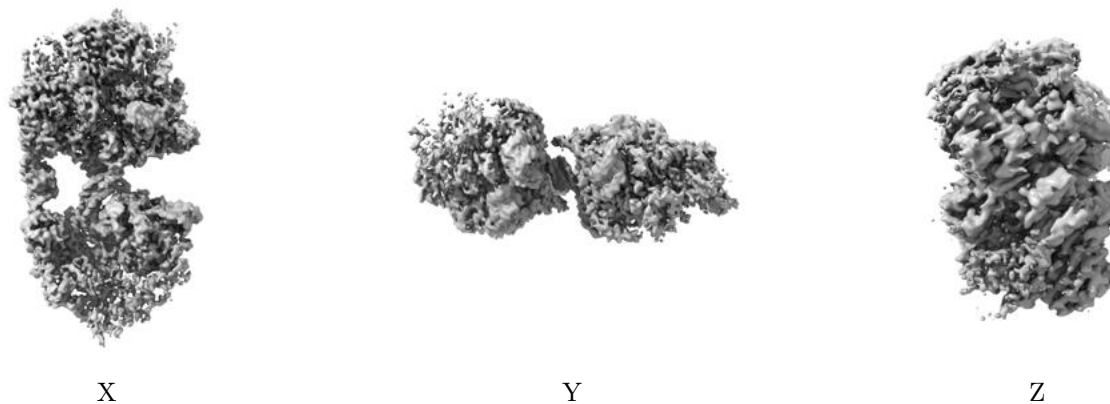


Z

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

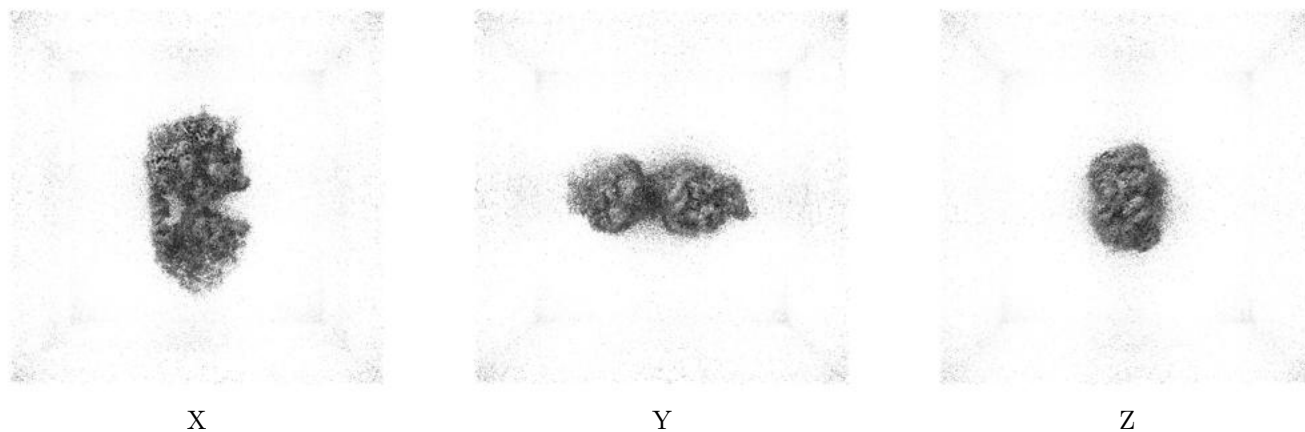
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0797. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

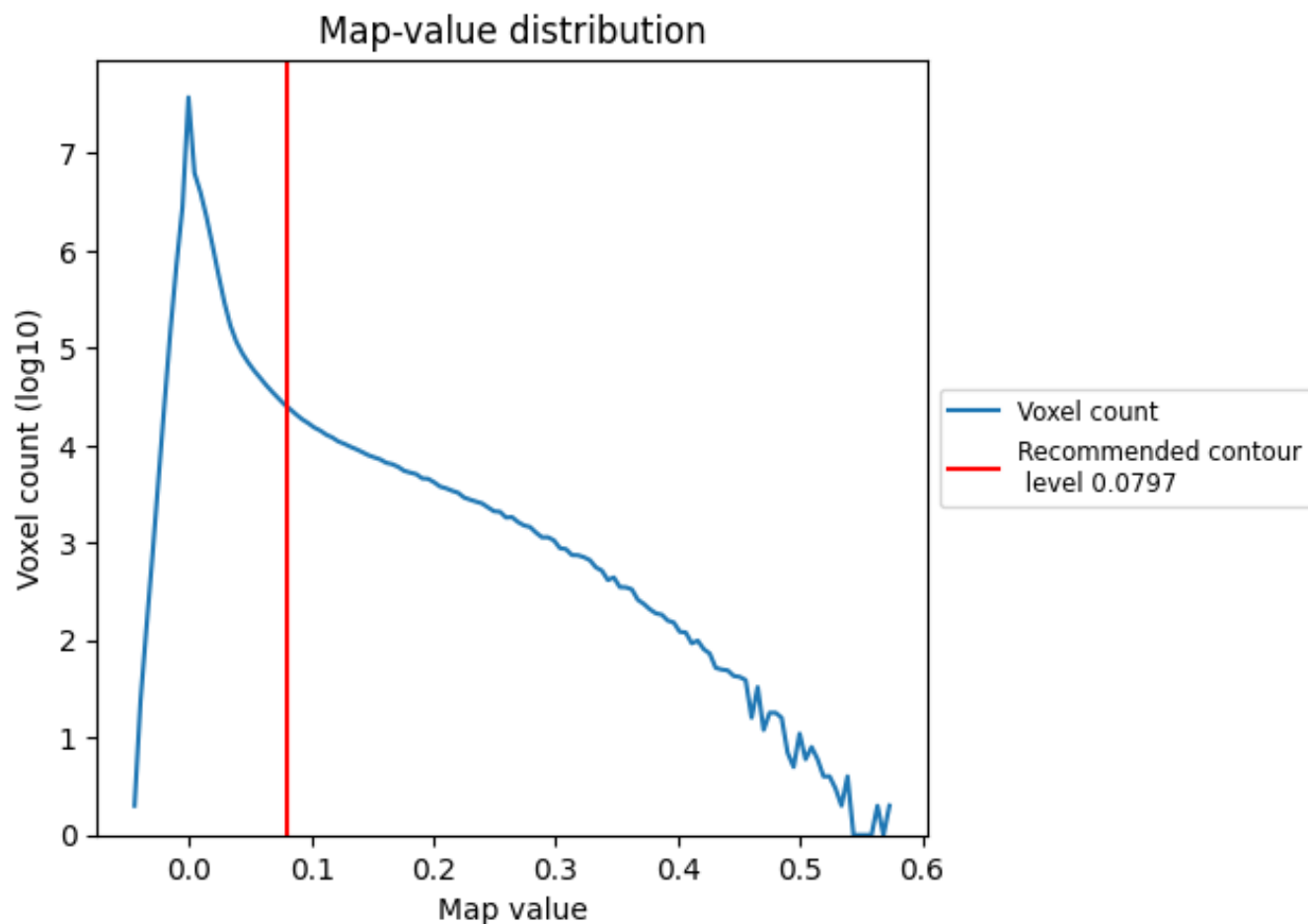
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

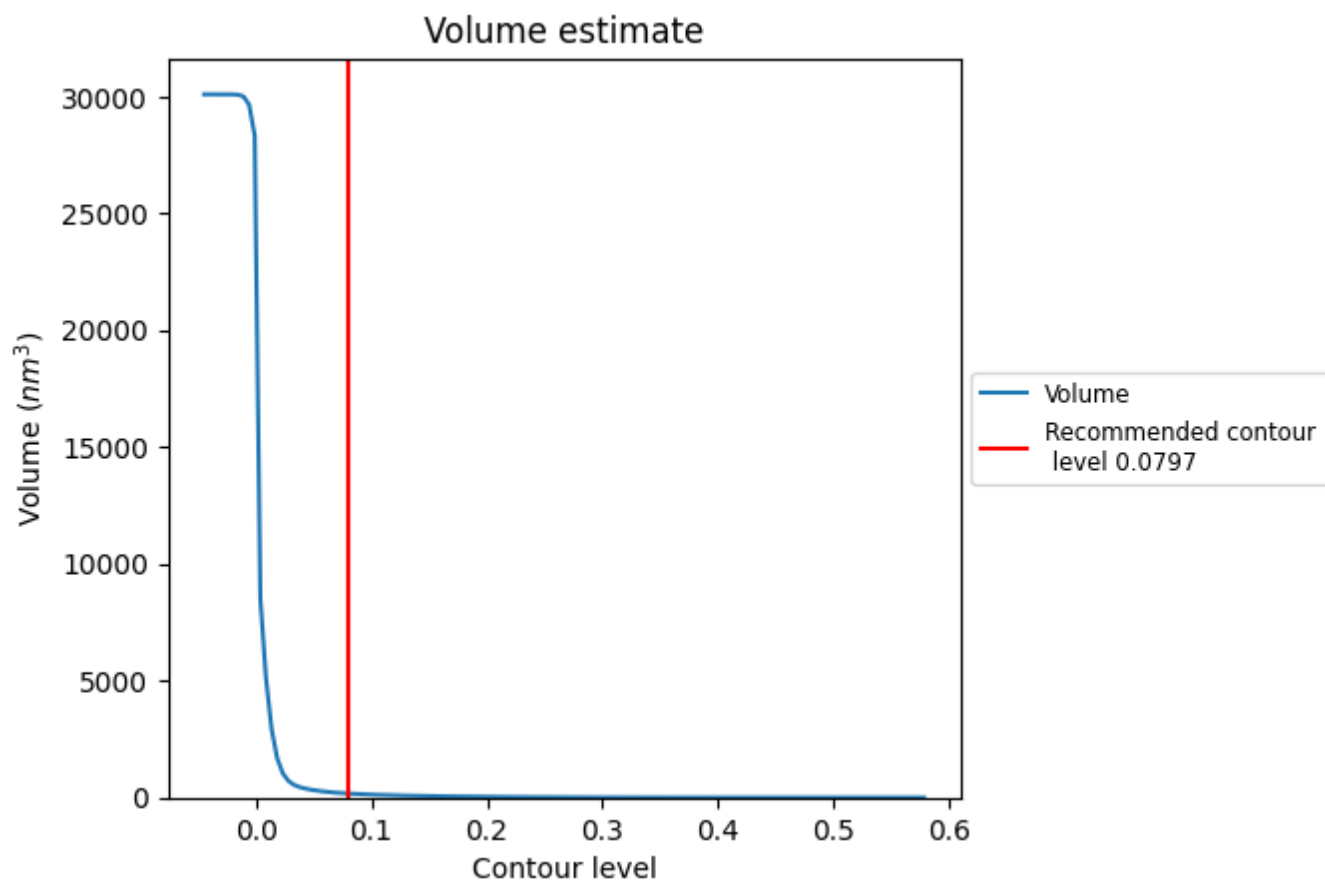
This section contains the results of statistical analysis of the map.

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.

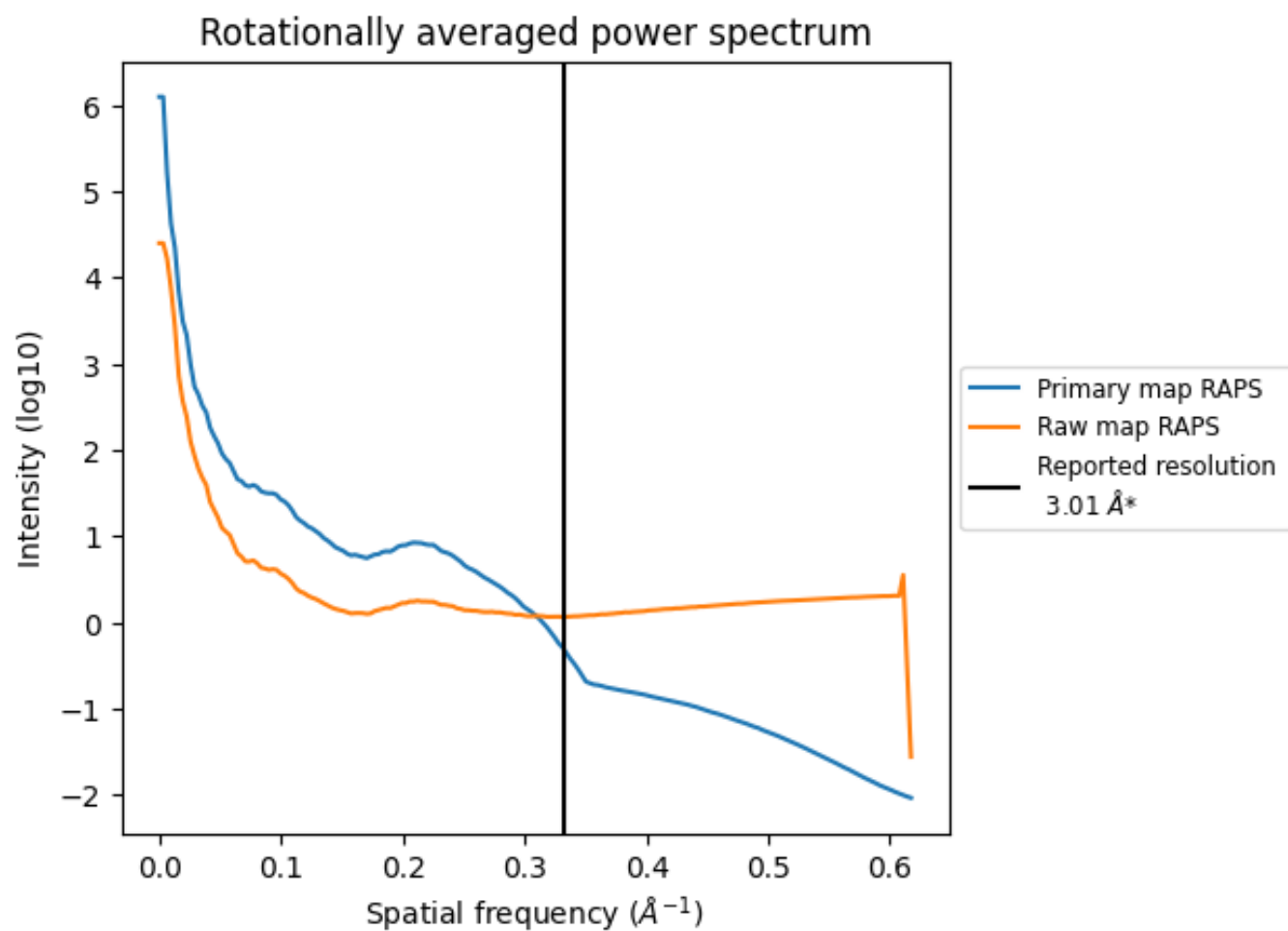
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 156 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 ⓘ

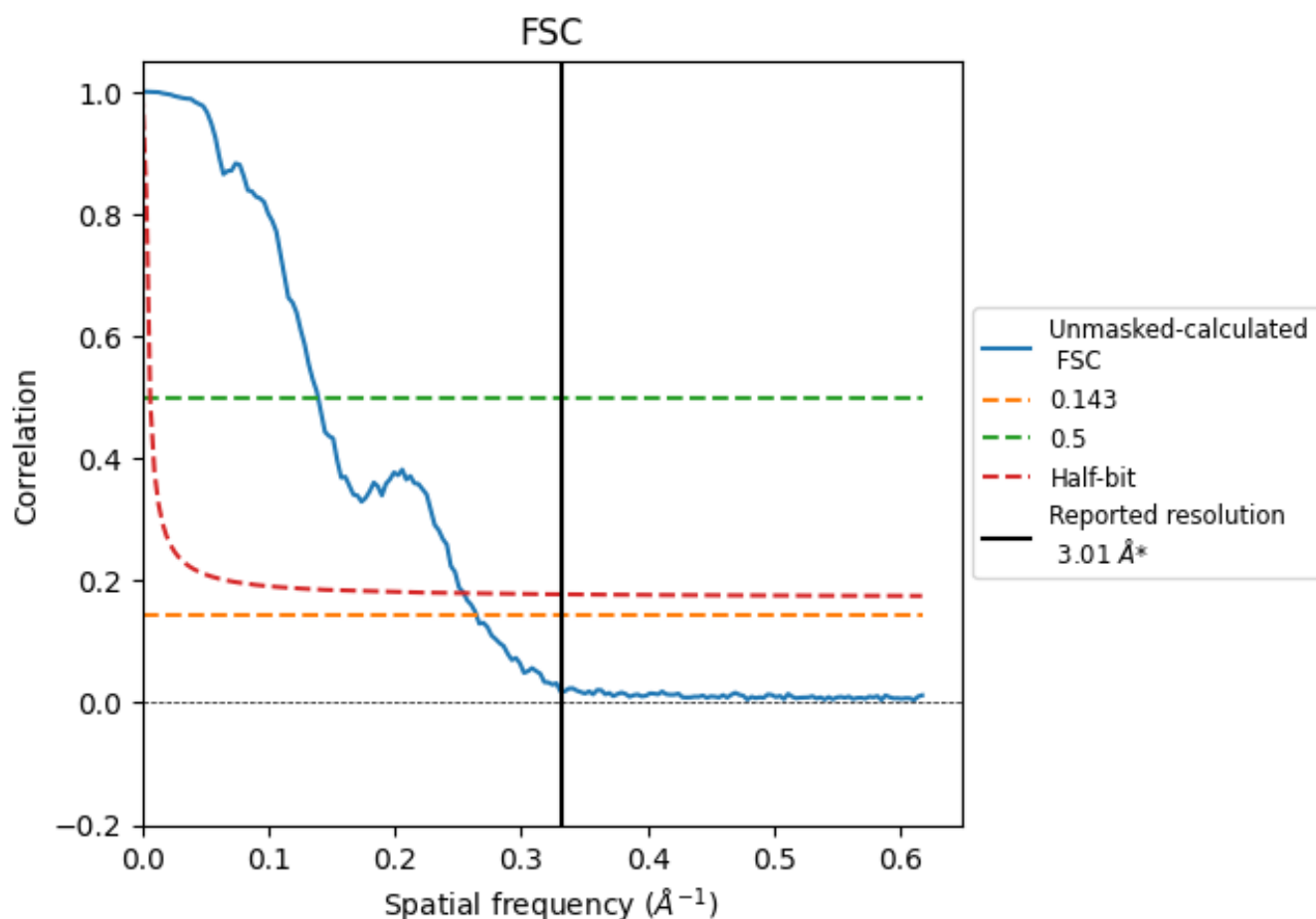


*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.332 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

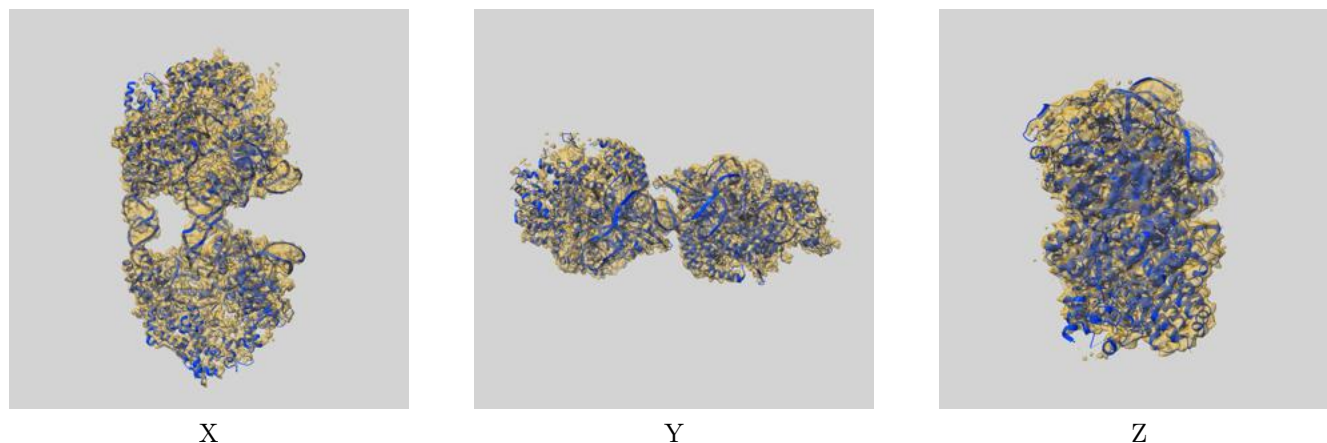
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	7.19	3.93

*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 3.78 differs from the reported value 3.01 by more than 10 %

9 Map-model fit [i](#)

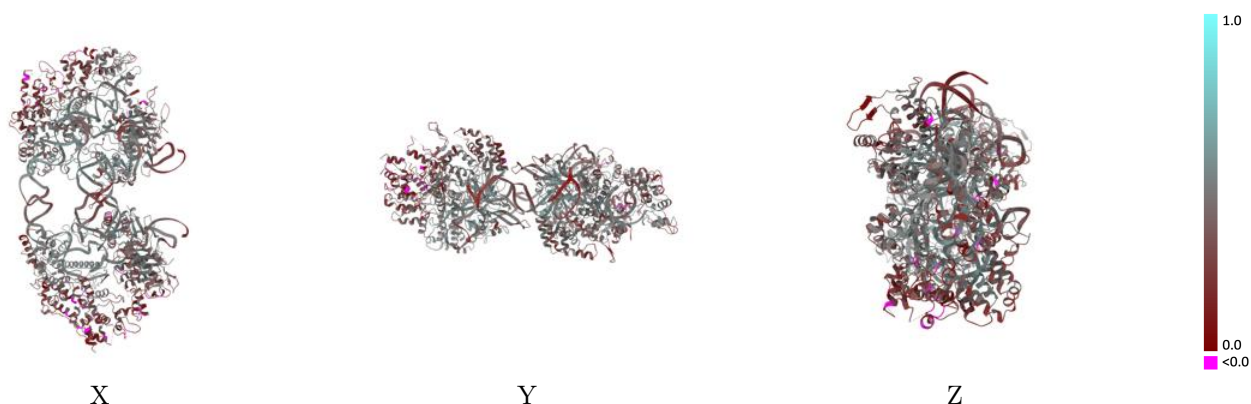
This section contains information regarding the fit between EMDB map EMD-41093 and PDB model 8T7S. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



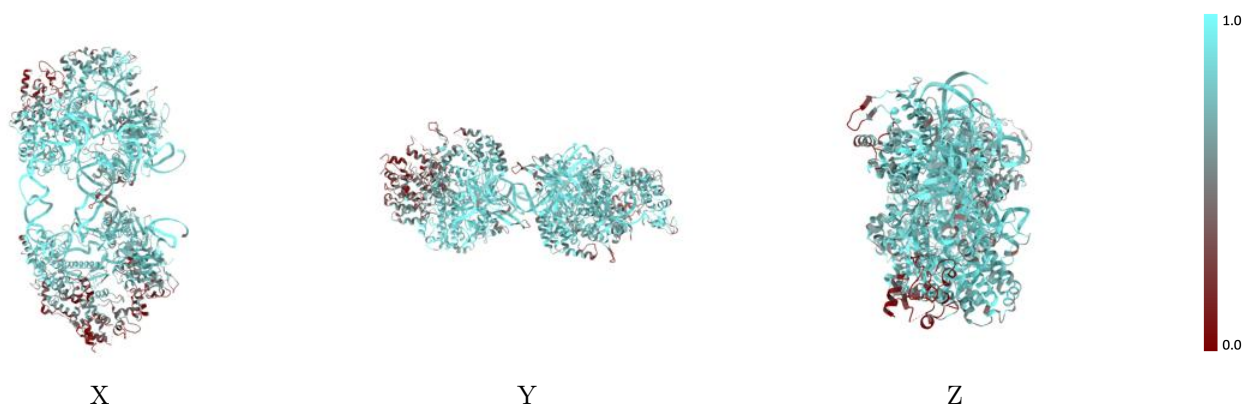
The images above show the 3D surface view of the map at the recommended contour level 0.0797 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



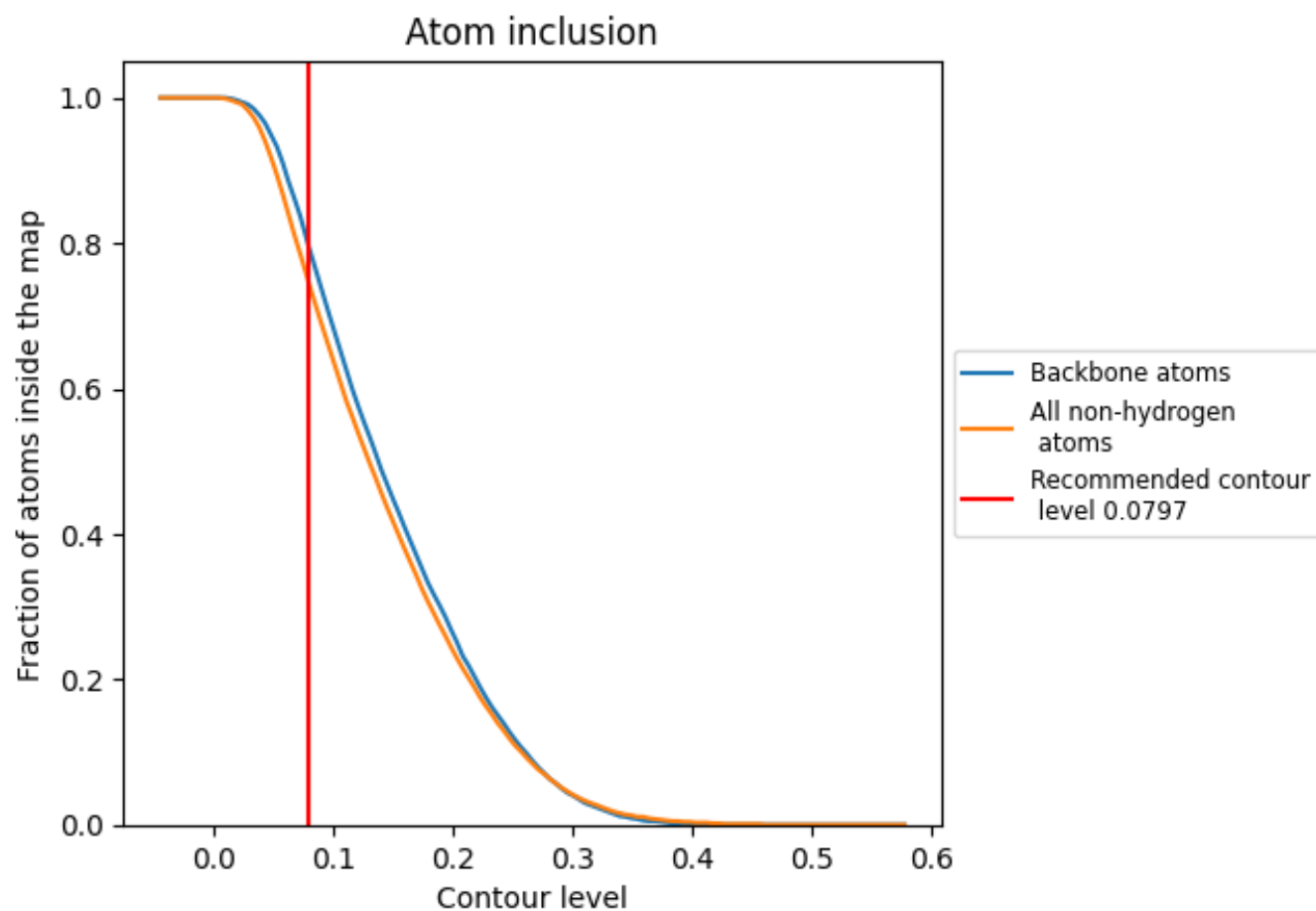
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0797).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 74% 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 (0.0797) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.4080
A	0.7300	0.4020
B	0.9210	0.4320
C	0.9100	0.4550
D	0.9400	0.4530
G	0.6690	0.3960
H	0.9010	0.4320
c	0.9600	0.5430

1.0

0.0

<0.0