WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

May 4, 2024 – 02:44 PM EDT

PDB ID	:	8T7S
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:

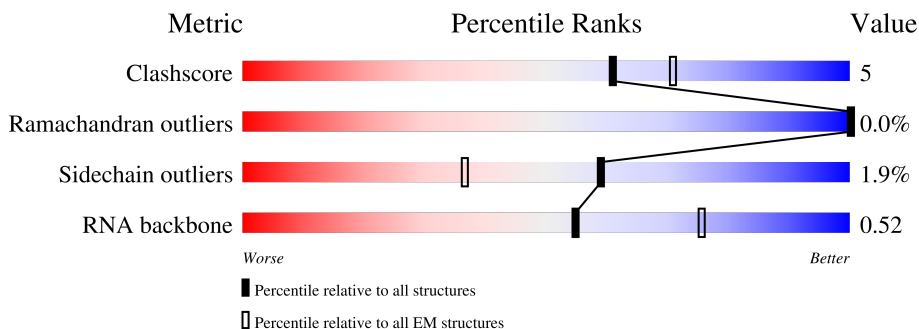|		
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.01 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.0%
Sidechain outliers		1.9%
RNA backbone		0.52

Worse *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1369	11% 85% 10% · ·
1	G	1369	17% 66% 15% · · 15%
2	B	98	64% 24% 9% ·
2	H	98	· 55% 31% · 10%
3	C	55	29% 7% · 62%
3	c	55	25% · 73%
4	D	55	24% 7% 69%

2 Entity 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 10774	C 6864	N 1885	O 2003	S 22	0	0
1	G	1157	Total 9139	C 5843	N 1570	O 1709	S 17	0	0

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 2103	C 941	N 389	O 675	P 98	0	0
2	H	88	Total 1887	C 844	N 346	O 609	P 88	0	0

- Molecule 3 is a DNA chain called TS.

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

- Molecule 4 is a DNA chain called NTS.

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

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

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

- Molecule 6 is water.

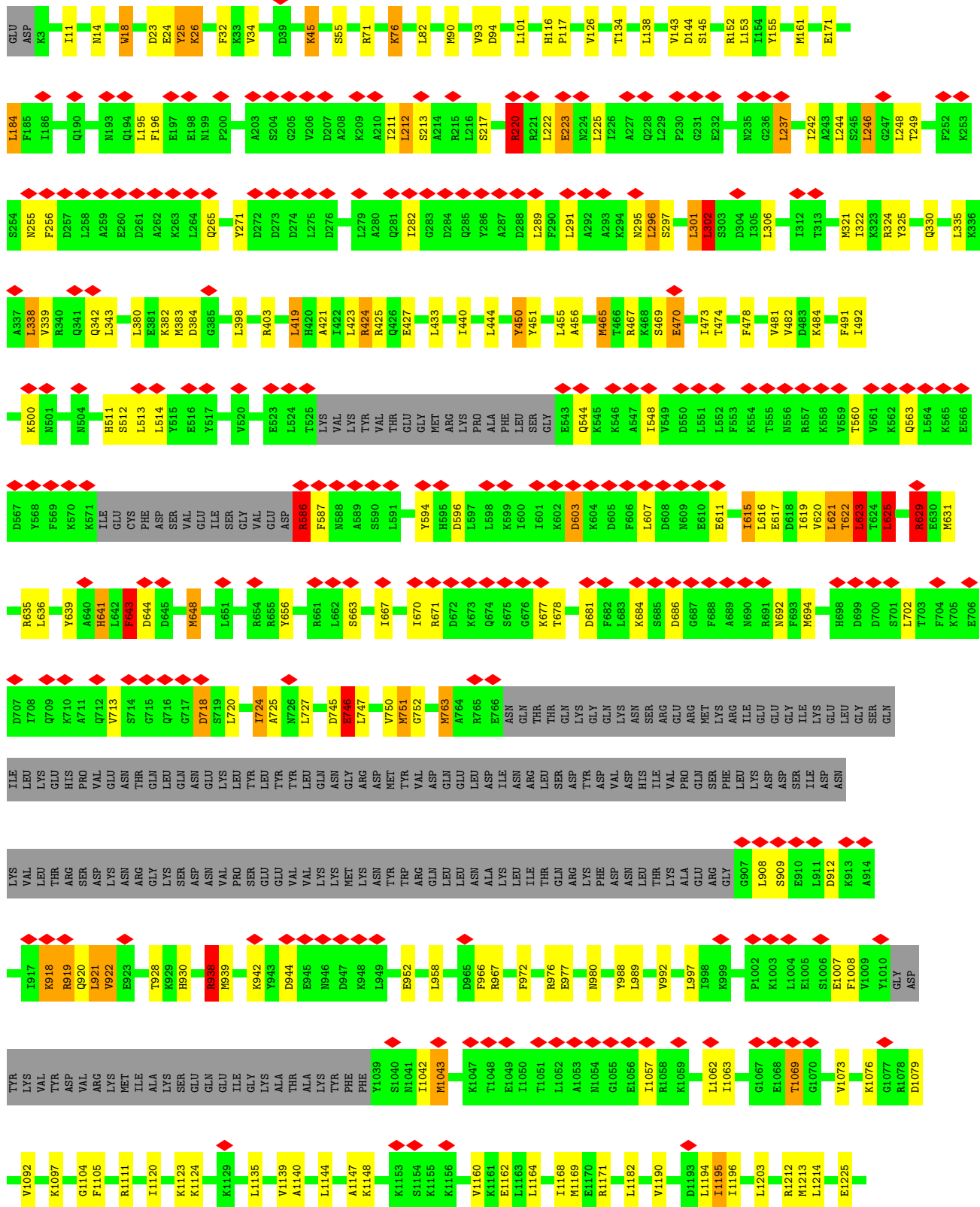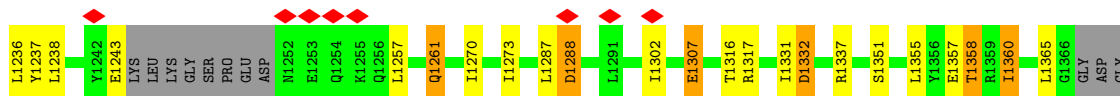| Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total 2	O 2	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

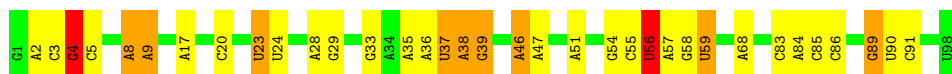• Molecule 1: CRISPR-associated endonuclease Cas9/Csn1
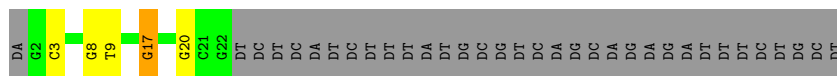
• Molecule 1: CRISPR-associated endonuclease Cas9/Csn1

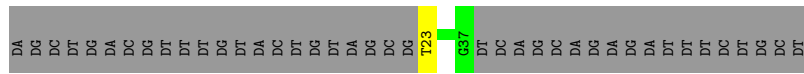L1236 Y1237 L1238 Y1242 E1243 LYS LEU LYS GLY SER PRO GLU ASP N1252 E1253 Q1254 K1255 Q1256 L1257 Q1261 I1270 I1273 L1287 D1288 L1291 I1302 E1307 T1316 R1317 I1331 D1332 R1337 S1351 L1355 Y1356 E1357 T1358 R1359 I1360 L1365 G1366 GLY ASP GLY

• Molecule 2: gRNA

Chain B:

64% 24% 9% ·

G1 A2 C3 G4 C5 A8 A9 A17 C20 U23 U24 A28 G29 G33 A34 A35 A36 U37 A38 G39 A46 A47 A51 G54 C55 U56 A57 G58 U59 A68 C83 A84 C85 C86 G89 U90 C91 U98

• Molecule 2: gRNA

Chain H:

·

55% 31% · 10%

G A C G C A U A A A G11 A15 C20 U25 A26 G27 A28 G29 C30 U31 A32 G33 A34 A35 A36 U37 A38 G39 U44 U45 A46 A47 A51 U56 A57 G58 U59 A68 G73 A76 A84 C85 G89 U90 C91 U94 G95 C96

U97 U98

• Molecule 3: TS

Chain C:

29% 7% · 62%

DA G2 C3 G8 T9 G17 G20 C21 G22 DT DC DT DC DA DT DC DT DT DA DT DG DC DG DC DT DC DG DC DA DG DC DA DG DA DG DA DT DT DT DC DT DG DC DT

• Molecule 3: TS

Chain c:

25% · 73%

DA DG DC DT DG DA DC DG DT DT DG DA DC DT DG DT DA DC DG DC DG T23 G37 DT DC DA DG DC DA DG DC DA DG DA DT DT DC DT DG DC DT

• Molecule 4: NTS

Chain D:

24% 7% 69%

DA DG DC DA DG DA DA DA DT DC DT DC DT DG DC DT DG DA DC DG DC DA DT DA DA DA DG DA DT DG DA DG DA DC DG DC T1 A4 G5 T6 A7 G17 DC DT

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 $(e^-/\text{Å}^2)$	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 (Å)	311.04, 311.04, 311.04	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	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	A	0.36	1/10963 (0.0%)	0.74	20/14719 (0.1%)
1	G	0.70	16/9308 (0.2%)	1.57	200/12582 (1.6%)
2	B	0.77	10/2355 (0.4%)	1.60	27/3665 (0.7%)
2	H	0.45	0/2114	1.14	3/3294 (0.1%)
3	C	0.73	1/484 (0.2%)	1.10	1/746 (0.1%)
3	c	0.67	0/335	1.22	1/514 (0.2%)
4	D	0.69	0/392	1.01	0/602
All	All	0.57	28/25951 (0.1%)	1.24	252/36122 (0.7%)

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 (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	G	C3'-O3'	15.53	1.63	1.42
2	B	4	G	N9-C4	13.79	1.49	1.38
1	G	643	PHE	CE2-CZ	-13.22	1.12	1.37
2	B	4	G	C3'-C2'	11.39	1.65	1.52
2	B	4	G	C1'-N9	8.90	1.62	1.48
2	B	4	G	C2'-C1'	8.88	1.63	1.53
1	G	746	GLU	CD-OE1	-8.75	1.16	1.25
1	A	1090	PRO	CG-CD	-8.38	1.23	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	G	C5-C4	8.09	1.44	1.38
1	G	470	GLU	CD-OE1	-8.05	1.16	1.25
2	B	4	G	C2-N3	7.88	1.39	1.32
1	G	212	LEU	CG-CD2	7.62	1.80	1.51
1	G	746	GLU	CG-CD	-7.56	1.40	1.51
1	G	1139	VAL	CB-CG1	-7.38	1.37	1.52
1	G	750	VAL	CB-CG1	-7.07	1.38	1.52
1	G	246	LEU	CG-CD1	-7.03	1.25	1.51
1	G	1092	VAL	CB-CG1	-6.75	1.38	1.52
2	B	4	G	C6-O6	6.51	1.30	1.24
1	G	1160	VAL	CB-CG2	-6.18	1.39	1.52
2	B	4	G	N3-C4	5.92	1.39	1.35
1	G	623	LEU	CG-CD1	-5.92	1.29	1.51
1	G	220	ARG	CG-CD	5.46	1.65	1.51
2	B	4	G	N7-C5	-5.34	1.36	1.39
3	C	17	DG	C1'-N9	-5.27	1.39	1.47
1	G	1169	MET	CB-CG	5.25	1.68	1.51
1	G	1162	GLU	CB-CG	5.10	1.61	1.52
1	G	470	GLU	CD-OE2	5.03	1.31	1.25
1	G	18	TRP	CE3-CZ3	-5.02	1.29	1.38

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	G	C8-N9-C4	-41.50	89.80	106.40
1	G	616	LEU	CB-CG-CD1	31.44	164.45	111.00
1	G	1288	ASP	CB-CG-OD2	28.45	143.91	118.30
1	G	1288	ASP	CB-CG-OD1	-24.48	96.27	118.30
2	B	4	G	C3'-C2'-C1'	22.70	119.66	101.50
1	G	338	LEU	CB-CG-CD2	22.07	148.51	111.00
1	G	383	MET	CG-SD-CE	21.96	135.33	100.20
1	G	513	LEU	CB-CG-CD1	21.72	147.92	111.00
2	B	4	G	N3-C4-C5	-20.58	118.31	128.60
1	G	513	LEU	CB-CG-CD2	-19.68	77.55	111.00
2	B	4	G	N7-C8-N9	19.49	122.84	113.10
1	G	1043	MET	CG-SD-CE	18.61	129.97	100.20
1	G	1332	ASP	CB-CG-OD1	17.52	134.06	118.30
1	A	133	PRO	N-CD-CG	-17.46	77.01	103.20
1	G	921	LEU	CB-CG-CD2	-17.27	81.65	111.00
1	G	338	LEU	CB-CG-CD1	-16.48	82.98	111.00
1	G	1169	MET	CG-SD-CE	-15.99	74.62	100.20
1	G	1139	VAL	CG1-CB-CG2	-15.27	86.47	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4	G	C4'-C3'-C2'	-14.99	87.61	102.60
1	G	1097	LYS	CD-CE-NZ	-14.97	77.27	111.70
2	B	4	G	C4-N9-C1'	14.89	145.86	126.50
2	B	4	G	C4-C5-C6	14.77	127.66	118.80
2	B	4	G	C5-N7-C8	-14.19	97.20	104.30
1	G	76	LYS	CD-CE-NZ	14.12	144.18	111.70
1	G	616	LEU	CB-CG-CD2	-13.90	87.37	111.00
1	G	746	GLU	OE1-CD-OE2	-13.72	106.84	123.30
2	B	4	G	N9-C1'-C2'	13.55	131.62	114.00
1	G	419	LEU	CB-CG-CD2	13.45	133.86	111.00
1	G	321	MET	CG-SD-CE	13.38	121.61	100.20
2	B	4	G	O4'-C1'-C2'	-13.32	92.48	105.80
1	G	246	LEU	CD1-CG-CD2	-12.98	71.56	110.50
1	G	751	MET	CG-SD-CE	-12.94	79.50	100.20
1	G	222	LEU	CB-CG-CD1	12.93	132.98	111.00
1	G	648	MET	CA-CB-CG	12.76	134.99	113.30
1	G	621	LEU	CB-CG-CD2	-12.57	89.64	111.00
1	G	763	MET	CA-CB-CG	-12.15	92.65	113.30
2	B	4	G	N3-C4-N9	12.14	133.29	126.00
1	G	296	LEU	CB-CG-CD2	-11.81	90.93	111.00
2	B	4	G	C6-C5-N7	-11.32	123.61	130.40
2	B	4	G	C4'-C3'-O3'	11.26	135.53	113.00
1	G	513	LEU	CA-CB-CG	11.26	141.19	115.30
1	G	90	MET	CG-SD-CE	10.91	117.66	100.20
1	G	212	LEU	CB-CG-CD2	-10.88	92.50	111.00
1	G	302	LEU	CB-CG-CD1	-10.82	92.61	111.00
1	G	1331	ILE	CG1-CB-CG2	-10.69	87.89	111.40
1	G	1043	MET	CA-CB-CG	10.65	131.41	113.30
1	G	237	LEU	CB-CG-CD2	-10.51	93.14	111.00
2	B	4	G	O4'-C1'-N9	10.51	116.60	108.20
1	G	921	LEU	CB-CG-CD1	10.25	128.42	111.00
1	G	184	LEU	CB-CG-CD2	-10.23	93.61	111.00
1	G	616	LEU	CD1-CG-CD2	-10.05	80.36	110.50
1	G	291	LEU	CB-CG-CD2	-10.02	93.96	111.00
1	G	513	LEU	CD1-CG-CD2	-10.01	80.48	110.50
1	G	1123	LYS	CD-CE-NZ	9.90	134.46	111.70
1	A	1090	PRO	CA-N-CD	-9.88	97.66	111.50
1	G	1332	ASP	OD1-CG-OD2	-9.88	104.52	123.30
1	G	750	VAL	CG1-CB-CG2	-9.82	95.19	110.90
1	G	433	LEU	CB-CG-CD2	-9.80	94.34	111.00
1	G	631	MET	CG-SD-CE	9.80	115.87	100.20
1	G	1196	ILE	CG1-CB-CG2	-9.72	90.01	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	339	VAL	CG1-CB-CG2	-9.69	95.39	110.90
1	G	246	LEU	CB-CG-CD1	-9.39	95.04	111.00
2	B	4	G	C2'-C3'-O3'	9.31	129.99	109.50
1	A	133	PRO	CA-CB-CG	-9.24	86.45	104.00
1	G	643	PHE	CB-CG-CD2	-9.18	114.37	120.80
1	G	643	PHE	CB-CG-CD1	9.12	127.18	120.80
1	G	433	LEU	CB-CG-CD1	9.11	126.49	111.00
1	G	622	THR	CA-CB-CG2	-9.08	99.68	112.40
1	G	301	LEU	CD1-CG-CD2	-9.05	83.33	110.50
1	G	1257	LEU	CB-CG-CD2	-9.06	95.60	111.00
1	G	939	MET	CG-SD-CE	9.04	114.66	100.20
1	G	291	LEU	CB-CG-CD1	8.95	126.21	111.00
1	G	1007	GLU	CA-CB-CG	8.88	132.94	113.40
1	G	237	LEU	CD1-CG-CD2	-8.87	83.90	110.50
1	G	644	ASP	CB-CG-OD1	8.82	126.23	118.30
1	G	922	VAL	CG1-CB-CG2	-8.80	96.83	110.90
1	G	607	LEU	CA-CB-CG	8.74	135.39	115.30
1	G	1236	LEU	CB-CG-CD2	-8.72	96.17	111.00
1	G	629	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	G	45	LYS	CD-CE-NZ	8.62	131.53	111.70
1	A	1090	PRO	N-CD-CG	-8.62	90.27	103.20
1	G	623	LEU	CD1-CG-CD2	-8.52	84.94	110.50
1	G	482	VAL	CG1-CB-CG2	-8.46	97.36	110.90
1	A	829	ASP	CB-CG-OD1	8.42	125.88	118.30
1	G	942	LYS	CD-CE-NZ	8.27	130.72	111.70
1	G	403	ARG	CD-NE-CZ	8.27	135.17	123.60
1	G	222	LEU	CB-CG-CD2	-8.25	96.97	111.00
1	G	1261	GLN	CB-CA-C	8.09	126.58	110.40
1	G	648	MET	CG-SD-CE	8.08	113.13	100.20
2	B	4	G	C2-N3-C4	8.07	115.94	111.90
1	G	470	GLU	CG-CD-OE1	-8.06	102.18	118.30
1	G	1332	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	G	212	LEU	CB-CG-CD1	7.93	124.48	111.00
1	G	1331	ILE	C-N-CA	7.92	141.49	121.70
1	A	1004	LEU	CA-CB-CG	7.82	133.29	115.30
2	B	4	G	N3-C2-N2	7.78	125.34	119.90
1	G	90	MET	CB-CA-C	-7.74	94.92	110.40
1	G	306	LEU	CB-CG-CD2	-7.72	97.88	111.00
1	G	751	MET	CA-CB-CG	7.62	126.25	113.30
1	A	133	PRO	CA-N-CD	-7.59	100.87	111.50
1	G	623	LEU	CB-CA-C	7.52	124.48	110.20
2	B	4	G	N9-C4-C5	7.50	108.40	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	161	MET	CG-SD-CE	7.49	112.19	100.20
1	G	724	ILE	CG1-CB-CG2	-7.48	94.95	111.40
1	G	470	GLU	CG-CD-OE2	7.47	133.24	118.30
1	G	514	LEU	CB-CG-CD2	-7.46	98.33	111.00
1	G	621	LEU	CD1-CG-CD2	-7.43	88.22	110.50
1	G	237	LEU	CA-CB-CG	7.42	132.37	115.30
1	G	302	LEU	CD1-CG-CD2	-7.39	88.33	110.50
1	G	616	LEU	CA-CB-CG	7.38	132.28	115.30
1	G	1307	GLU	OE1-CD-OE2	-7.38	114.44	123.30
2	B	4	G	C5-C6-N1	-7.38	107.81	111.50
1	G	763	MET	N-CA-CB	7.37	123.86	110.60
1	G	1062	LEU	CB-CG-CD1	7.31	123.42	111.00
1	G	403	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	G	1148	LYS	CD-CE-NZ	7.22	128.31	111.70
1	G	403	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	G	1139	VAL	CA-CB-CG2	-7.19	100.12	110.90
1	G	997	LEU	CB-CG-CD2	-7.16	98.83	111.00
1	G	1261	GLN	CG-CD-OE1	7.16	135.92	121.60
1	G	398	LEU	CB-CG-CD2	-7.13	98.88	111.00
1	G	1287	LEU	CB-CG-CD2	7.07	123.02	111.00
1	G	623	LEU	N-CA-CB	-7.06	96.28	110.40
1	G	90	MET	CA-CB-CG	-7.05	101.32	113.30
1	G	223	GLU	CA-CB-CG	7.04	128.88	113.40
1	G	702	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	G	713	VAL	CG1-CB-CG2	-7.02	99.67	110.90
1	G	212	LEU	CA-CB-CG	-7.01	99.19	115.30
1	G	1316	THR	CA-CB-CG2	6.98	122.17	112.40
1	G	1043	MET	N-CA-CB	-6.96	98.08	110.60
1	G	339	VAL	CA-CB-CG1	6.93	121.30	110.90
1	G	594	TYR	OH-CZ-CE2	-6.87	101.56	120.10
1	G	636	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	G	1169	MET	CA-CB-CG	6.83	124.91	113.30
1	G	1043	MET	CB-CA-C	6.82	124.04	110.40
1	G	684	LYS	CD-CE-NZ	6.79	127.32	111.70
1	G	648	MET	CB-CG-SD	-6.78	92.05	112.40
3	c	23	DT	OP1-P-OP2	-6.76	109.46	119.60
1	A	379	ILE	CG1-CB-CG2	-6.68	96.71	111.40
1	G	615	ILE	CG1-CB-CG2	-6.68	96.71	111.40
1	G	594	TYR	CE1-CZ-OH	6.67	138.10	120.10
1	G	989	LEU	CA-CB-CG	-6.66	99.98	115.30
1	G	93	VAL	CG1-CB-CG2	-6.61	100.33	110.90
1	A	416	LEU	CB-CG-CD1	-6.61	99.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ASP	CB-CG-OD1	6.58	124.22	118.30
1	G	1124	LYS	CD-CE-NZ	6.58	126.83	111.70
1	G	383	MET	CB-CA-C	6.54	123.49	110.40
1	G	586	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	B	4	G	C1'-O4'-C4'	6.49	115.09	109.90
1	G	938	ARG	CA-CB-CG	6.49	127.67	113.40
1	G	544	GLN	CA-CB-CG	6.48	127.66	113.40
1	G	1073	VAL	CG1-CB-CG2	6.47	121.25	110.90
1	G	1237	TYR	OH-CZ-CE2	-6.43	102.74	120.10
1	G	1076	LYS	CD-CE-NZ	6.42	126.48	111.70
1	G	1358	THR	CA-CB-CG2	6.42	121.39	112.40
1	G	302	LEU	CB-CA-C	6.40	122.36	110.20
1	G	1261	GLN	CG-CD-NE2	-6.38	101.39	116.70
1	G	922	VAL	CA-CB-CG2	-6.38	101.33	110.90
2	B	59	U	C2-N1-C1'	6.37	125.34	117.70
1	A	644	ASP	CB-CG-OD1	6.36	124.03	118.30
1	G	643	PHE	CE1-CZ-CE2	-6.35	108.57	120.00
1	G	908	LEU	CA-CB-CG	6.27	129.72	115.30
1	G	1214	LEU	CA-CB-CG	6.27	129.72	115.30
1	G	484	LYS	CD-CE-NZ	6.23	126.03	111.70
1	G	603	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	G	1073	VAL	CA-CB-CG2	6.19	120.19	110.90
1	G	1214	LEU	CB-CG-CD2	-6.18	100.50	111.00
1	G	918	LYS	CD-CE-NZ	6.17	125.89	111.70
1	G	1237	TYR	CE1-CZ-OH	6.14	136.67	120.10
1	G	1057	ILE	CG1-CB-CG2	6.12	124.87	111.40
1	A	1303	ARG	CB-CG-CD	6.10	127.45	111.60
1	G	625	LEU	CB-CG-CD1	-6.09	100.64	111.00
1	G	1261	GLN	CA-CB-CG	6.08	126.78	113.40
1	A	147	ASP	CB-CG-OD1	6.07	123.76	118.30
1	G	1288	ASP	OD1-CG-OD2	-6.04	111.83	123.30
1	A	791	LEU	CA-CB-CG	6.00	129.10	115.30
1	G	702	LEU	CB-CG-CD1	5.94	121.09	111.00
1	G	686	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	G	322	ILE	CG1-CB-CG2	-5.93	98.35	111.40
1	G	629	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	G	958	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	A	1214	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	138	LEU	CA-CB-CG	5.86	128.78	115.30
1	G	212	LEU	CD1-CG-CD2	-5.86	92.94	110.50
1	G	1092	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	G	1144	LEU	CA-CB-CG	5.85	128.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	921	LEU	CA-CB-CG	5.85	128.75	115.30
1	G	301	LEU	CB-CA-C	5.83	121.28	110.20
1	A	597	LEU	CA-CB-CG	-5.82	101.91	115.30
1	G	617	GLU	CA-CB-CG	-5.77	100.70	113.40
1	G	1195	ILE	CG1-CB-CG2	-5.77	98.71	111.40
1	G	213	SER	N-CA-CB	5.74	119.11	110.50
1	G	718	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	G	1069	THR	C-N-CA	-5.70	110.33	122.30
2	B	4	G	N1-C2-N2	-5.69	111.08	116.20
1	G	306	LEU	CB-CG-CD1	5.64	120.58	111.00
1	G	1144	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	G	623	LEU	CB-CG-CD1	-5.62	101.45	111.00
2	B	23	U	C6-N1-C2	-5.60	117.64	121.00
1	G	343	LEU	CA-CB-CG	5.60	128.17	115.30
1	G	1182	LEU	CB-CG-CD2	-5.60	101.49	111.00
1	G	248	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	A	1312	LEU	CA-CB-CG	5.58	128.12	115.30
1	G	76	LYS	CB-CG-CD	5.57	126.09	111.60
1	G	470	GLU	N-CA-CB	5.56	120.60	110.60
1	G	93	VAL	CA-CB-CG2	-5.55	102.57	110.90
1	G	195	LEU	CB-CG-CD2	5.55	120.44	111.00
1	G	155	TYR	CE1-CZ-OH	-5.51	105.21	120.10
1	G	325	TYR	OH-CZ-CE2	-5.51	105.23	120.10
1	G	1236	LEU	CB-CG-CD1	5.49	120.33	111.00
1	G	1316	THR	OG1-CB-CG2	5.48	122.60	110.00
1	G	1360	ILE	CG1-CB-CG2	-5.47	99.36	111.40
2	H	20	C	N3-C2-O2	-5.45	118.08	121.90
1	G	90	MET	N-CA-CB	5.45	120.41	110.60
1	G	380	LEU	CB-CG-CD2	-5.43	101.76	111.00
2	B	56	U	N3-C2-O2	-5.43	118.40	122.20
1	G	1358	THR	OG1-CB-CG2	5.42	122.46	110.00
2	H	20	C	N1-C2-O2	5.40	122.14	118.90
1	G	212	LEU	CB-CA-C	5.39	120.45	110.20
1	A	470	GLU	CA-CB-CG	5.39	125.26	113.40
1	G	403	ARG	CA-CB-CG	-5.38	101.56	113.40
2	B	4	G	C4-C5-N7	-5.37	108.65	110.80
2	B	56	U	N1-C2-O2	5.35	126.55	122.80
1	G	1257	LEU	CB-CG-CD1	5.35	120.10	111.00
1	G	101	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	G	1063	ILE	CG1-CB-CG2	-5.34	99.65	111.40
1	G	944	ASP	CB-CG-OD1	5.31	123.08	118.30
1	G	1238	LEU	CB-CG-CD2	-5.29	102.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	325	TYR	CE1-CZ-OH	5.29	134.37	120.10
1	G	212	LEU	C-N-CA	5.28	134.91	121.70
1	G	398	LEU	CB-CG-CD1	5.26	119.94	111.00
1	G	1164	LEU	CB-CG-CD1	-5.20	102.15	111.00
2	B	46	A	O5'-P-OP1	-5.17	101.04	105.70
2	H	20	C	C6-N1-C2	-5.17	118.23	120.30
1	G	211	ILE	CG1-CB-CG2	5.12	122.67	111.40
1	G	1062	LEU	CA-CB-CG	-5.12	103.52	115.30
1	G	1069	THR	CA-CB-CG2	5.10	119.54	112.40
1	G	966	PHE	CB-CG-CD1	5.09	124.36	120.80
1	G	465	MET	CB-CG-SD	5.09	127.66	112.40
1	G	34	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	G	196	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	G	126	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	G	1120	ILE	CG1-CB-CG2	-5.07	100.25	111.40
3	C	3	DC	O4'-C1'-N1	5.06	111.54	108.00
1	G	988	TYR	OH-CZ-CE2	5.06	133.76	120.10
1	G	763	MET	CB-CA-C	-5.06	100.28	110.40
1	G	419	LEU	CB-CA-C	-5.05	100.60	110.20
1	G	586	ARG	CD-NE-CZ	5.05	130.67	123.60
1	G	988	TYR	CE1-CZ-OH	-5.04	106.50	120.10
1	G	296	LEU	CD1-CG-CD2	-5.03	95.41	110.50
1	A	948	LYS	CB-CG-CD	5.02	124.66	111.60
1	G	586	ARG	NE-CZ-NH1	5.00	122.80	120.30

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

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Mol	Chain	Res	Type	Group
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
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	82	0
1	G	9139	0	8954	103	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	0	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	217	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 (217) 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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:763:MET:HE2	1:G:928:THR:HG23	1.85	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
1:A:1210:ARG:HG3	1:A:1280:VAL:HA	1.85	0.57
2:B:4:G:C3'	2:B:4:G:HO3'	2.07	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: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: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: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
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
1:G:145:SER:OG	1:G:145:SER:O	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:952:GLU:H	1:G:952:GLU:CD	2.14	0.51
2:B:4:G:O3'	2:B:5:C:P	2.69	0.51
1:A:763:MET:HE2	1:A:765:ARG:HH11	1.77	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
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: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
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: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:45:LYS:NZ	1:G:1357:GLU:OE2	2.41	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: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: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:1203:LEU:HD13	1:G:1213:MET:HE3	1.98	0.46
1:G:302:LEU:HA	1:G:302:LEU:HD22	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:184:LEU:C	1:G:184:LEU:HD23	2.37	0.45
1:G:184:LEU:HD11	1:G:295:ASN:HB3	1.98	0.45
1:G:469:SER:HB3	1:G:481:VAL:HG13	1.97	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: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: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
1:G:456:ALA:O	1:G:465:MET:HE1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424:ARG:HG2	1:G:427:GLU:CD	2.39	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: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
2:B:8:A:H2'	2:B:9:A:H8	1.81	0.42
1:G:980:ASN:H	1:G:1225:GLU:CD	2.22	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: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: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:1065:THR:HG22	1:A:1072:ILE:HA	2.02	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: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
1:A:1218:LYS:HE3	1:A:1337:ARG:HH22	1.86	0.41
1:G:171:GLU:CD	1:G:629:ARG:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1300/1369 (95%)	1269 (98%)	31 (2%)	0	100	100
1	G	1145/1369 (84%)	1099 (96%)	45 (4%)	1 (0%)	51	85
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%)	1162 (98%)	22 (2%)	57	83
1	G	955/1230 (78%)	937 (98%)	18 (2%)	57	83
All	All	2139/2460 (87%)	2099 (98%)	40 (2%)	59	83

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	144	ASP
1	A	215	ARG
1	A	263	LYS
1	A	397	ASP
1	A	420	HIS
1	A	429	PHE
1	A	432	PHE
1	A	543	GLU
1	A	630	GLU
1	A	645	ASP
1	A	723	HIS
1	A	776	ASN
1	A	832	ARG
1	A	970	PHE
1	A	972	PHE
1	A	1031	LYS
1	A	1039	TYR
1	A	1080	PHE
1	A	1116	SER
1	A	1117	ASP
1	A	1356	TYR
1	G	23	ASP
1	G	26	LYS
1	G	71	ARG
1	G	82	LEU
1	G	223	GLU

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Mol	Chain	Res	Type
1	G	302	LEU
1	G	450	TYR
1	G	623	LEU
1	G	625	LEU
1	G	641	HIS
1	G	751	MET
1	G	918	LYS
1	G	976	ARG
1	G	1008	PHE
1	G	1043	MET
1	G	1069	THR
1	G	1212	ARG
1	G	1261	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	990	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/98 (97%)	19 (19%)	3 (3%)
2	H	87/98 (88%)	20 (22%)	2 (2%)
All	All	183/196 (93%)	39 (21%)	5 (2%)

All (39) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	3	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
2	B	35	A
2	B	36	A
2	B	37	U
2	B	39	G

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Mol	Chain	Res	Type
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 ⓘ

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 ⓘ

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 ⓘ
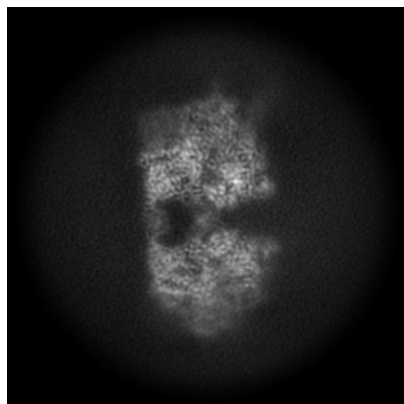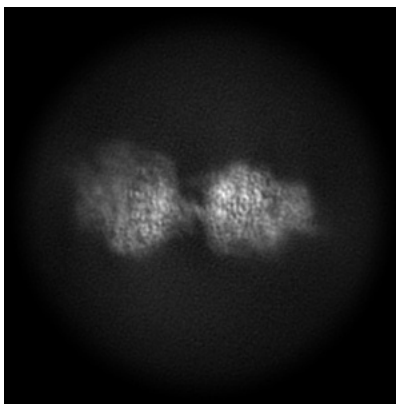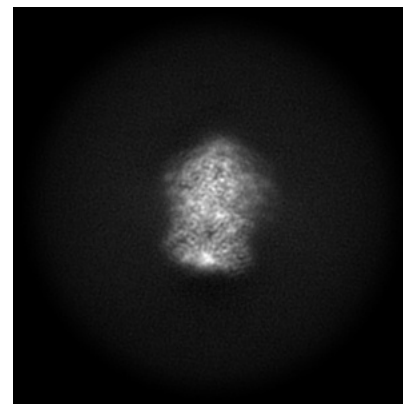
6.1.1 Primary map

X Y Z

6.1.2 Raw map

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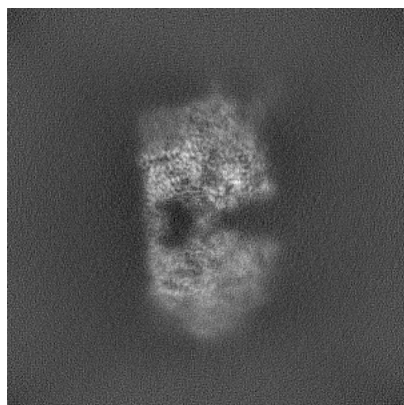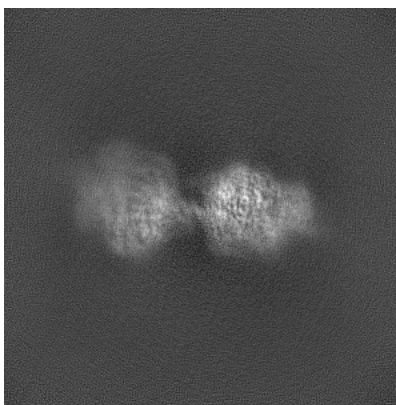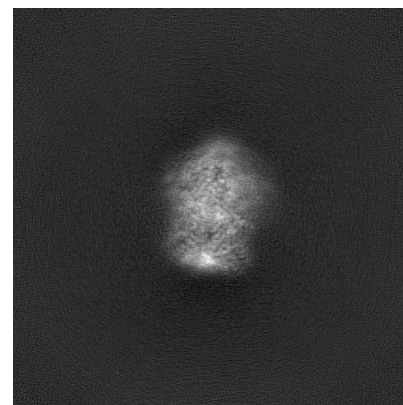
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
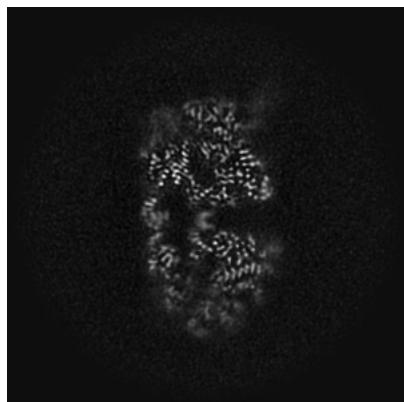
6.2.1 Primary map
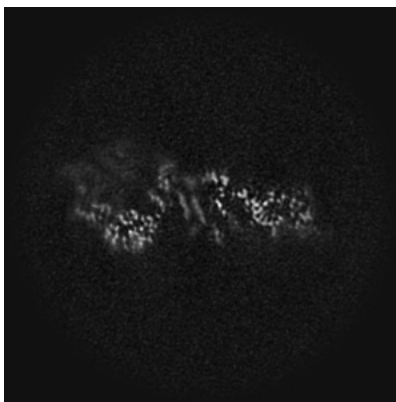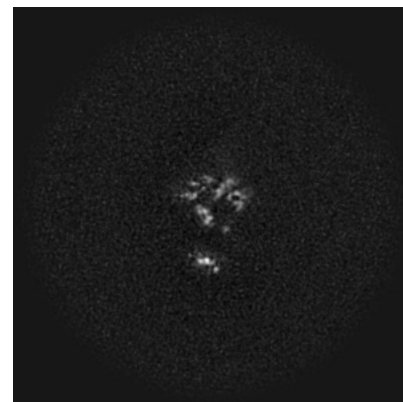
X Index: 192   Y Index: 192   Z Index: 192

6.2.2 Raw map
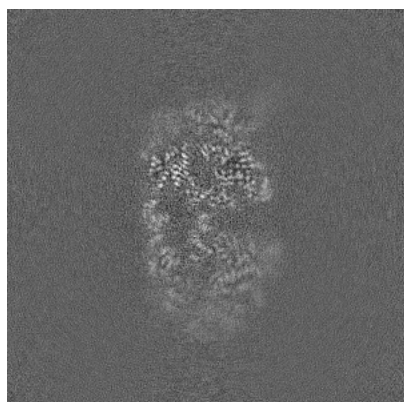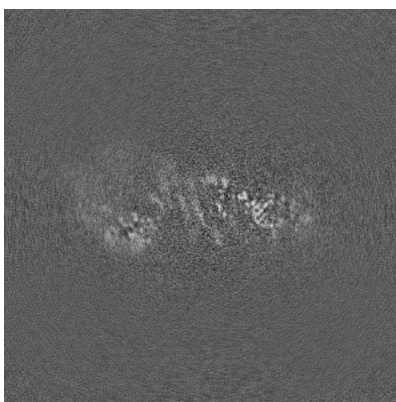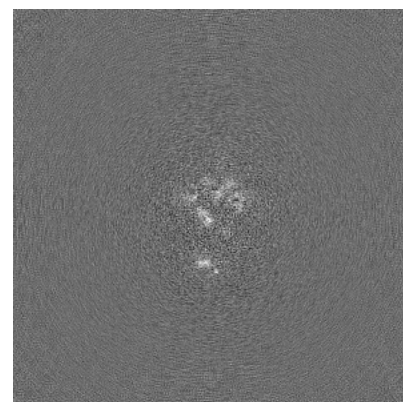
X Index: 192   Y Index: 192   Z Index: 192

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

6.3　Largest variance slices ⓘ

6.3.1　Primary map
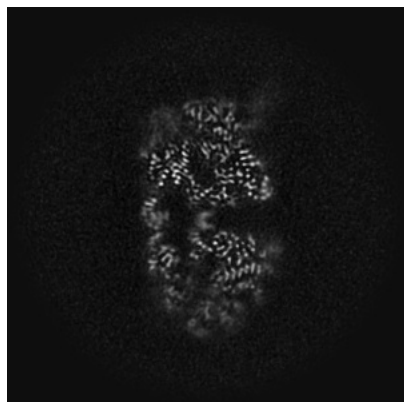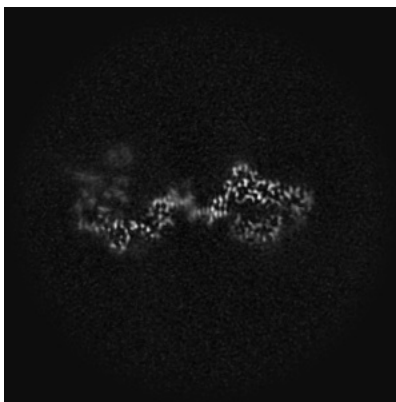
| X Index: 192 | Y Index: 183 | Z Index: 207 |
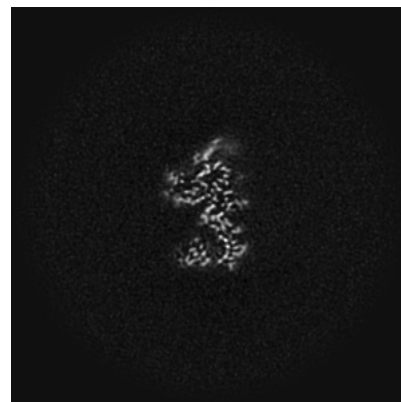
6.3.2　Raw map
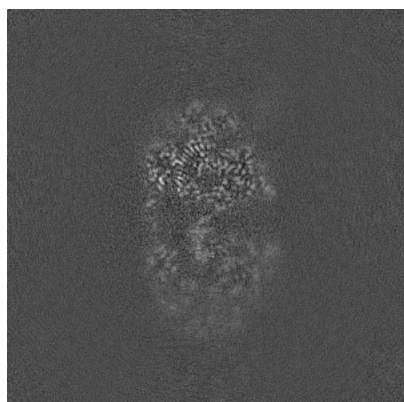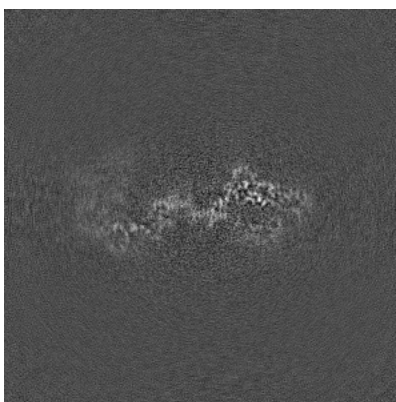
| X Index: 197 | Y Index: 183 | Z Index: 211 |
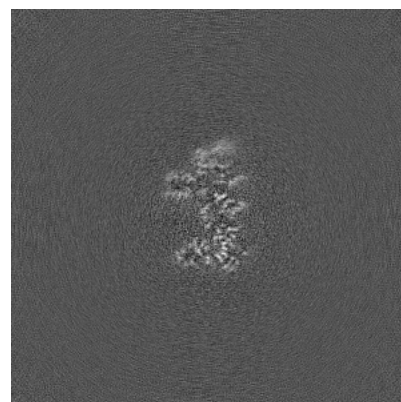
The images above show the largest variance slices of the map in three orthogonal directions.

6.4　Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1　Primary map
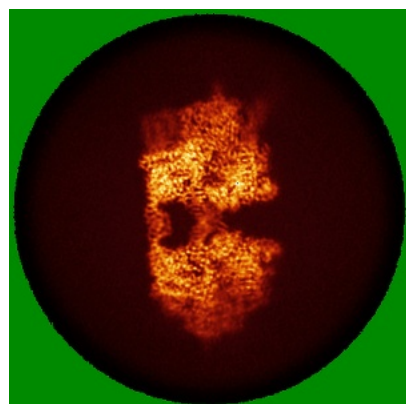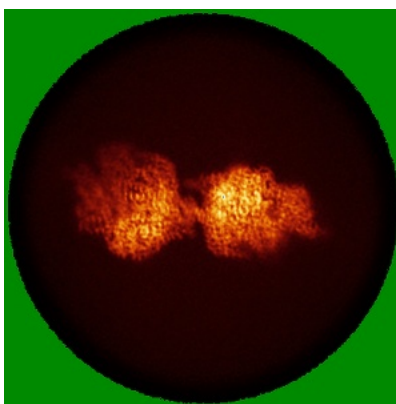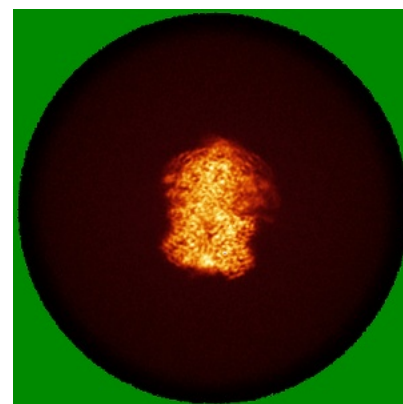
| X | Y | Z |

6.4.2　Raw map

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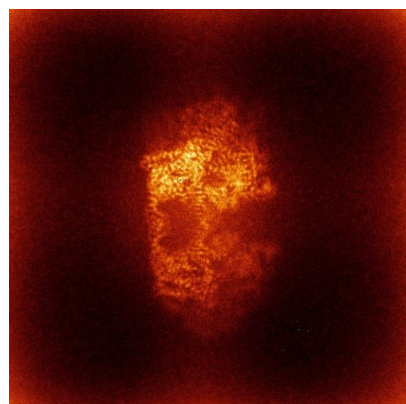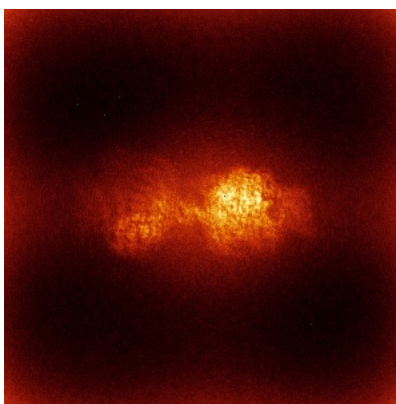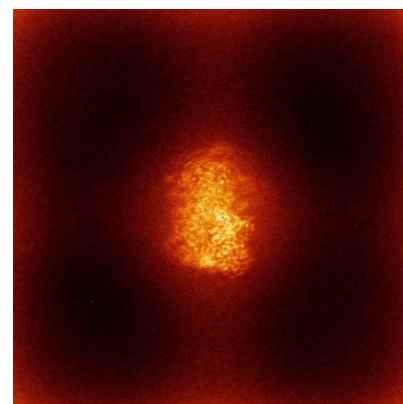
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

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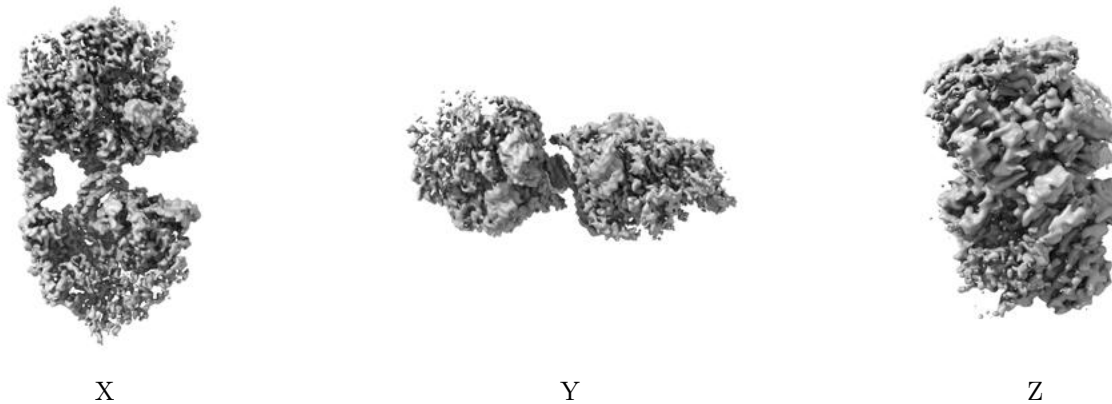
The images above show the 3D surface view of the map at the recommended contour level 0.0797. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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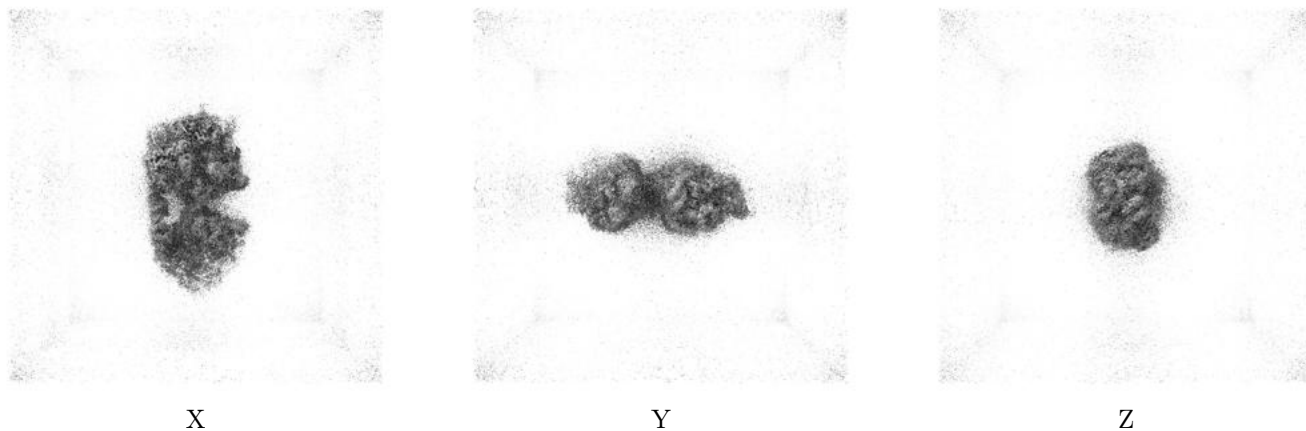
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
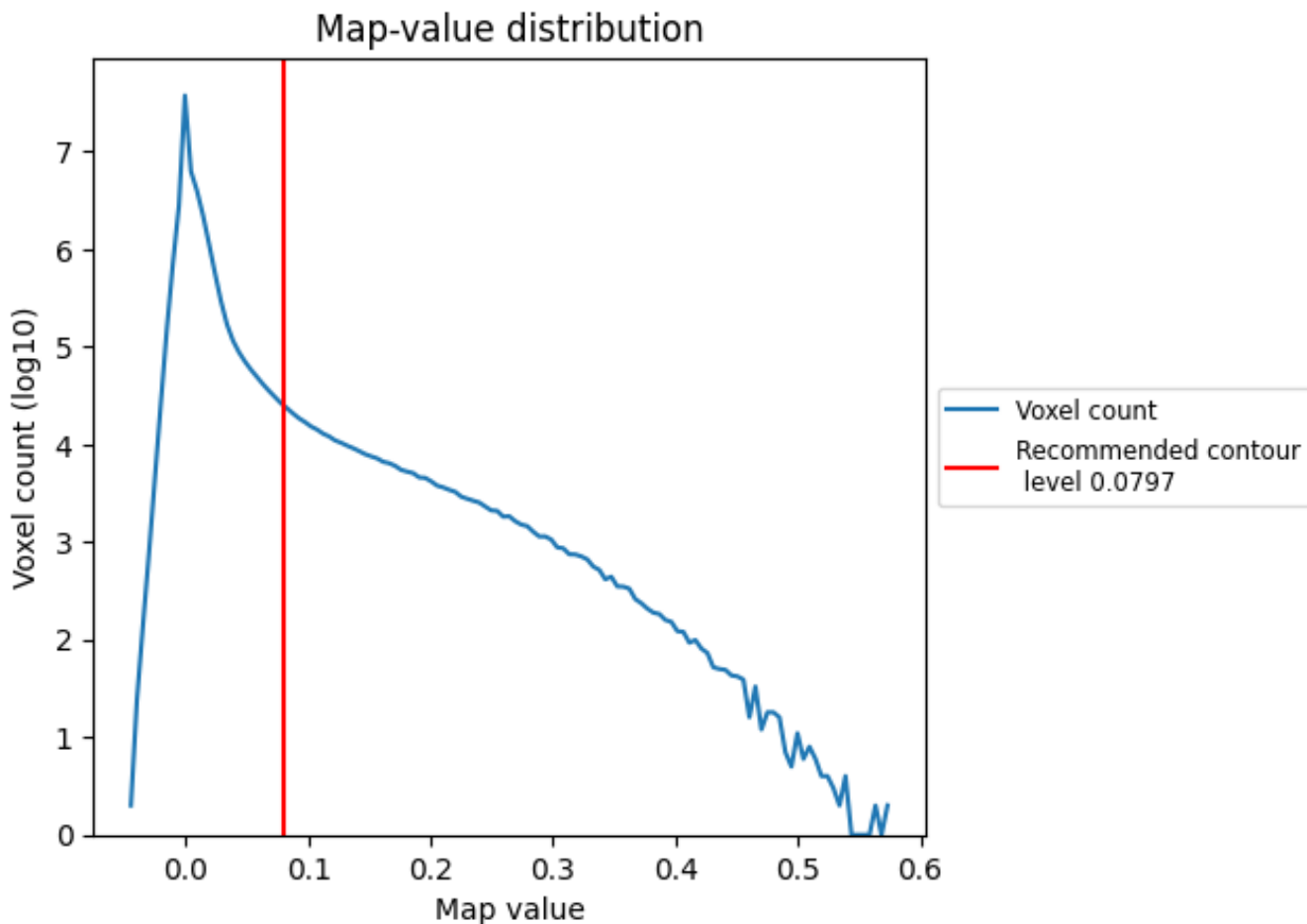
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
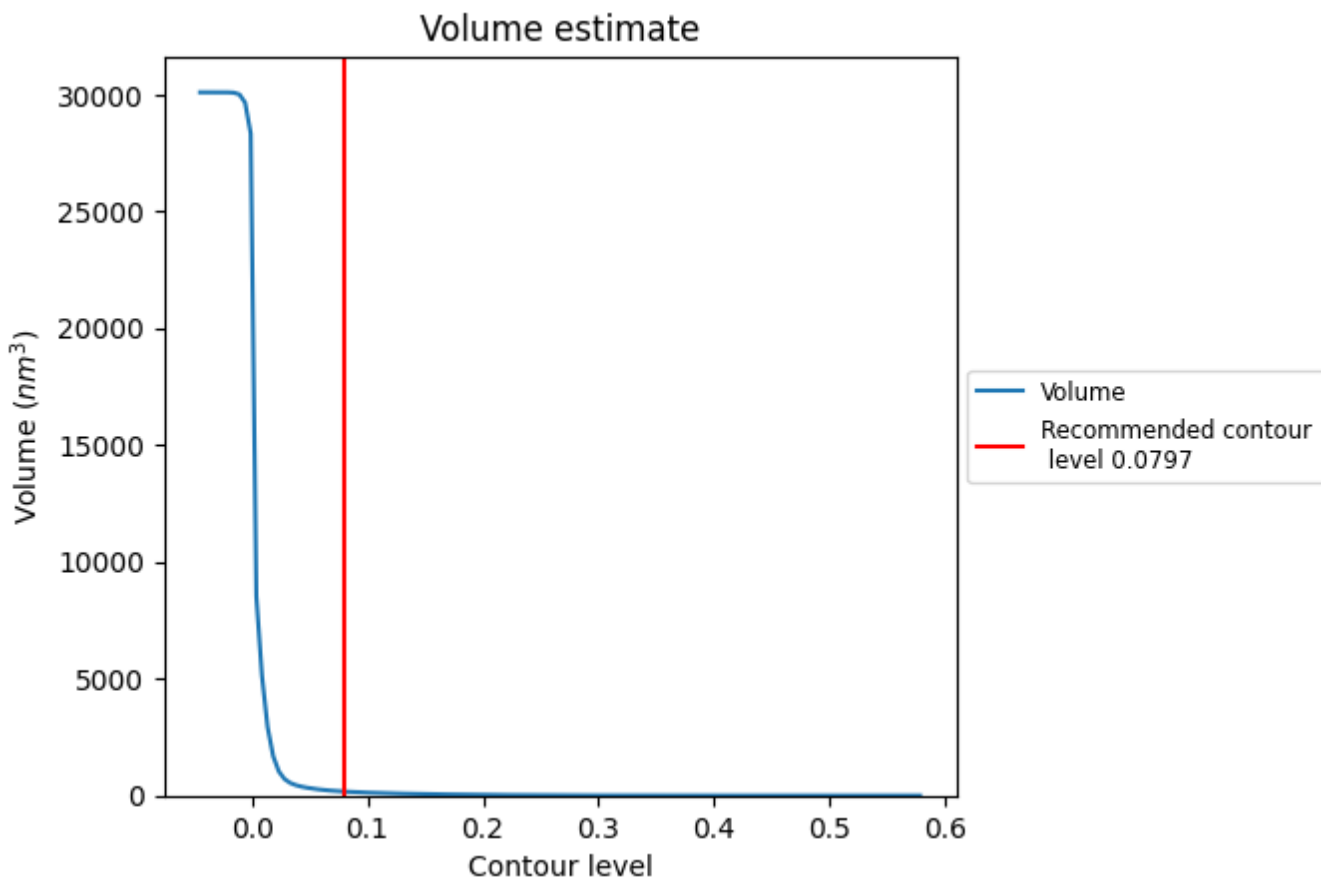
The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 156 kDa.

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 (i)
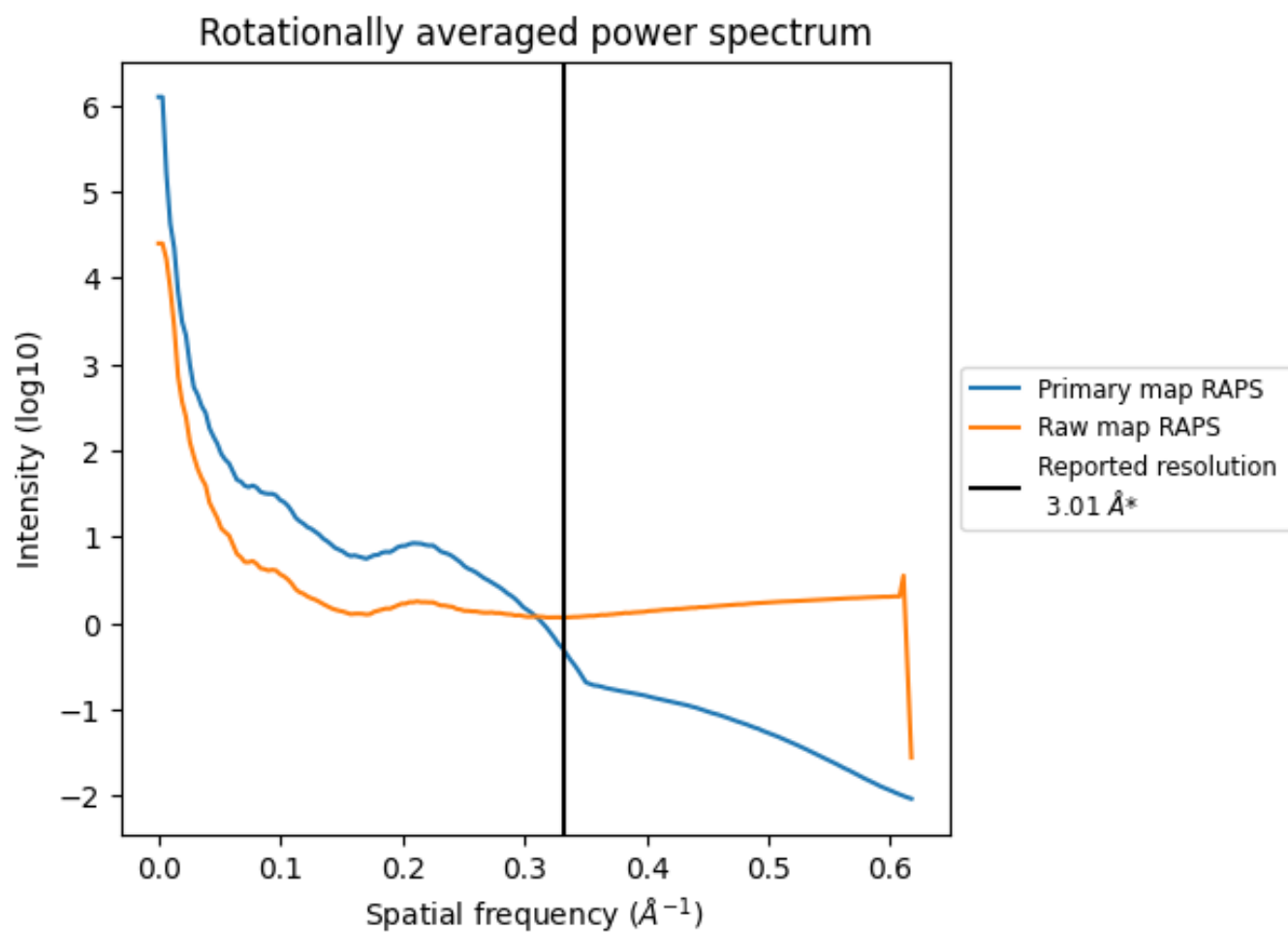
*Reported resolution corresponds to spatial frequency of 0.332 Å^{-1}

8　Fourier-Shell correlation ⓘ

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

8.1　FSC ⓘ
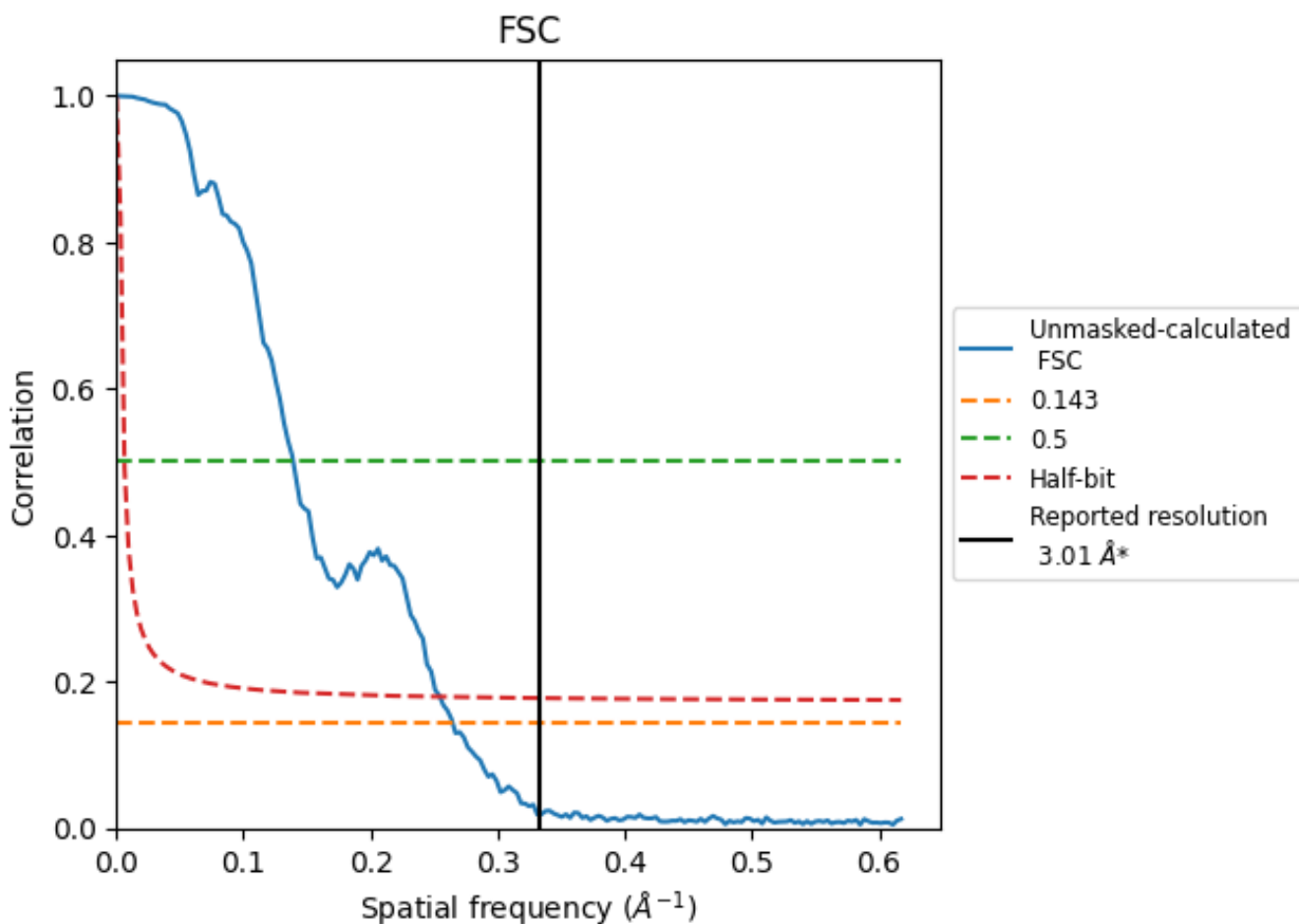
*Reported resolution corresponds to spatial frequency of 0.332 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
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　ⓘ

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 5.

9.1　Map-model overlay　ⓘ
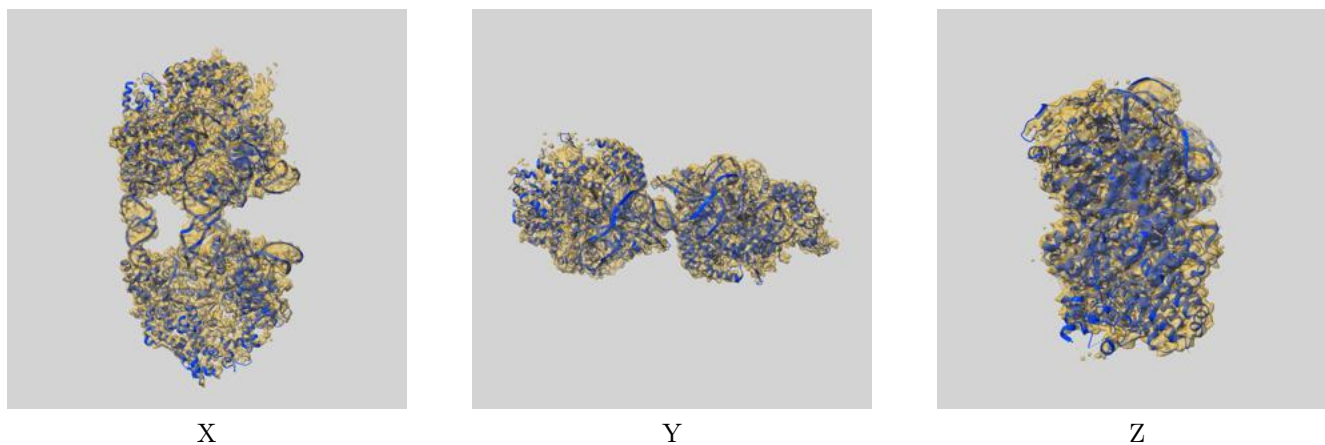
X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.0797 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 ⓘ

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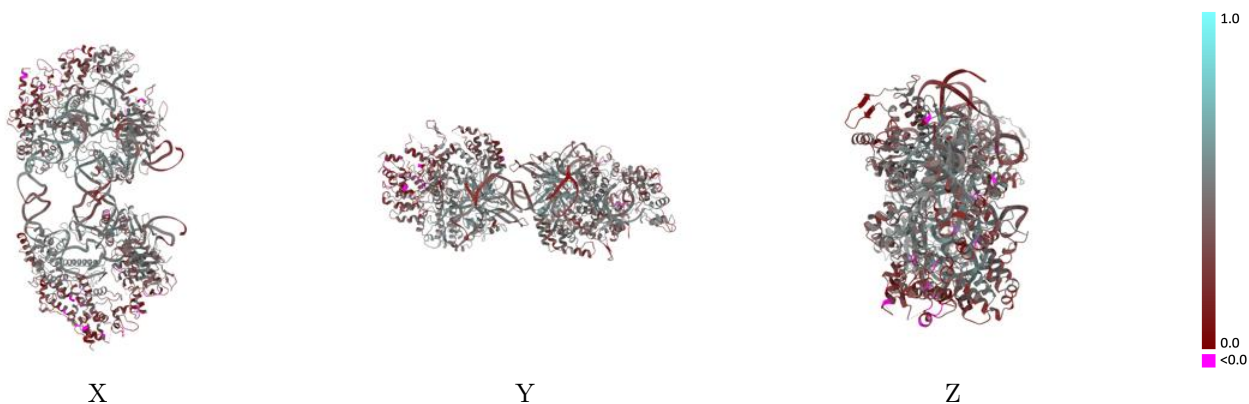
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
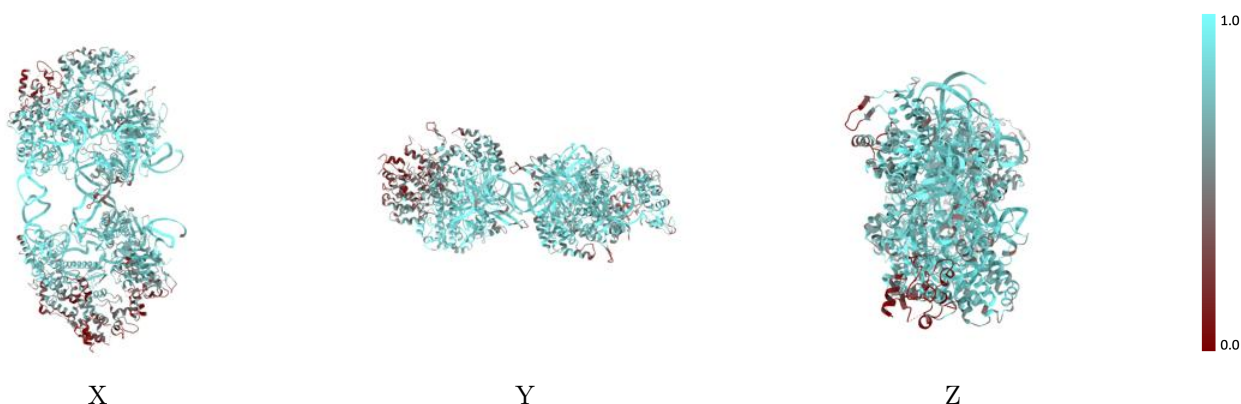
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0797).

9.4 Atom inclusion ⓘ
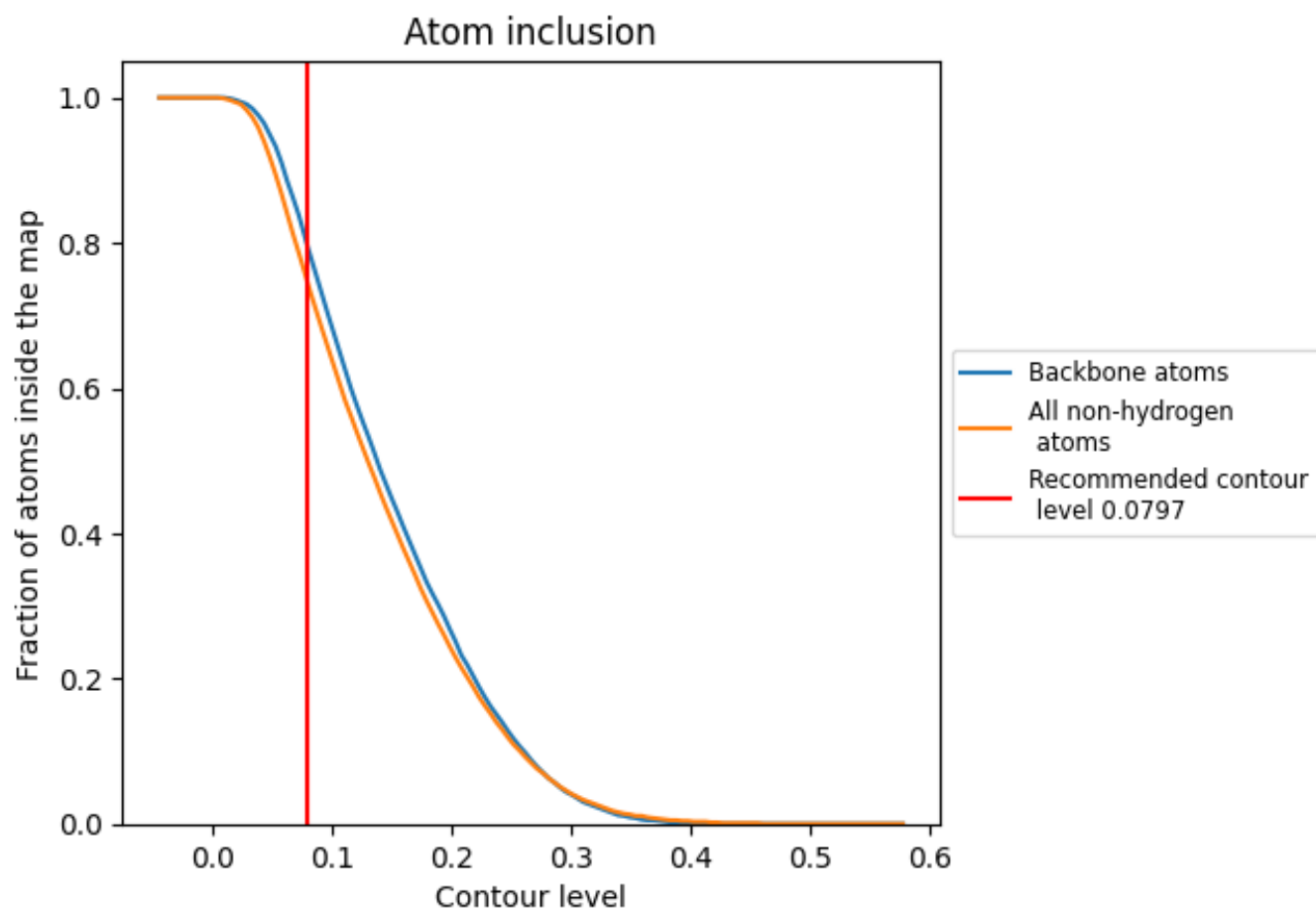
At the recommended contour level, 79% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

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