



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 04:09 PM UTC

PDB ID : 9DXG / pdb_00009dxg
EMDB ID : EMD-47287
Title : attP bound large serine integrase and RDF complex in the dimeric state (cleaved)
Authors : Shin, H.; Rice, P.A.; Olorunniji, F.J.
Deposited on : 2024-10-11
Resolution : 6.61 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

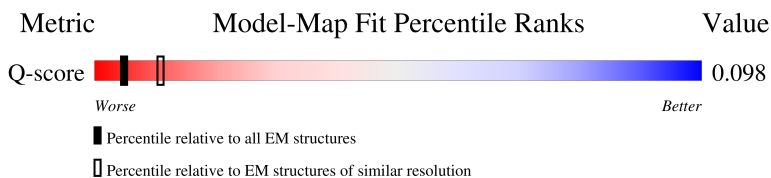
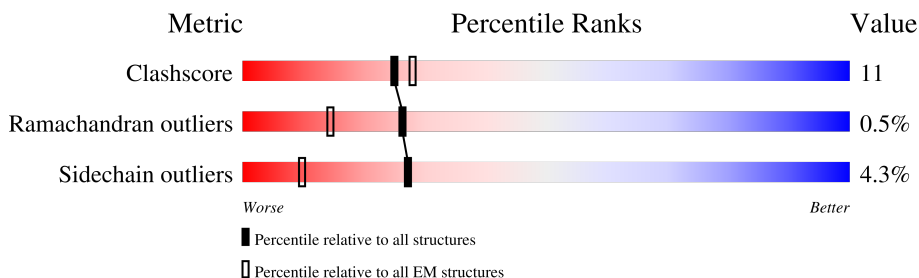
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 6.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	495 (6.11 - 7.10)

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	620	
1	B	620	
1	C	620	
1	D	620	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	34	<div><div></div><div>41%</div><div>44%</div><div>9%</div><div>6%</div></div>
2	G	34	<div><div></div><div>35%</div><div>47%</div><div>15%</div><div></div></div>
3	F	33	<div><div></div><div>33%</div><div>48%</div><div>15%</div><div></div></div>
3	H	33	<div><div></div><div>39%</div><div>39%</div><div>15%</div><div>6%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23754 atoms, of which 11336 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 Resolvase homolog YokA,SPbeta prophage-derived uncharacterized protein YotN.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	535	Total	C	H	N	O	S	0	0
			8782	2741	4428	753	841	19		
1	B	56	Total	C	H	N	O		0	0
			955	306	474	81	94			
1	C	535	Total	C	H	N	O	S	0	0
			8782	2741	4428	753	841	19		
1	D	56	Total	C	H	N	O		0	0
			955	306	474	81	94			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	THR	-	linker	UNP O32006
A	547	SER	-	linker	UNP O32006
A	548	GLY	-	linker	UNP O32006
A	549	SER	-	linker	UNP O32006
A	550	GLY	-	linker	UNP O32006
A	551	GLY	-	linker	UNP O32006
A	552	SER	-	linker	UNP O32006
A	553	GLY	-	linker	UNP O32006
A	554	GLY	-	linker	UNP O32006
A	555	SER	-	linker	UNP O32006
A	556	GLY	-	linker	UNP O32006
A	557	GLY	-	linker	UNP O32006
A	558	SER	-	linker	UNP O32006
A	559	GLY	-	linker	UNP O32006
A	560	ARG	-	linker	UNP O32006
A	561	SER	-	linker	UNP O32006
A	562	GLY	-	linker	UNP O32006
A	563	THR	-	linker	UNP O32006
B	-16	THR	-	linker	UNP O32006
B	-15	SER	-	linker	UNP O32006
B	-14	GLY	-	linker	UNP O32006

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	linker	UNP O32006
B	-12	GLY	-	linker	UNP O32006
B	-11	GLY	-	linker	UNP O32006
B	-10	SER	-	linker	UNP O32006
B	-9	GLY	-	linker	UNP O32006
B	-8	GLY	-	linker	UNP O32006
B	-7	SER	-	linker	UNP O32006
B	-6	GLY	-	linker	UNP O32006
B	-5	GLY	-	linker	UNP O32006
B	-4	SER	-	linker	UNP O32006
B	-3	GLY	-	linker	UNP O32006
B	-2	ARG	-	linker	UNP O32006
B	-1	SER	-	linker	UNP O32006
B	0	GLY	-	linker	UNP O32006
B	1	THR	-	linker	UNP O32006
C	546	THR	-	linker	UNP O32006
C	547	SER	-	linker	UNP O32006
C	548	GLY	-	linker	UNP O32006
C	549	SER	-	linker	UNP O32006
C	550	GLY	-	linker	UNP O32006
C	551	GLY	-	linker	UNP O32006
C	552	SER	-	linker	UNP O32006
C	553	GLY	-	linker	UNP O32006
C	554	GLY	-	linker	UNP O32006
C	555	SER	-	linker	UNP O32006
C	556	GLY	-	linker	UNP O32006
C	557	GLY	-	linker	UNP O32006
C	558	SER	-	linker	UNP O32006
C	559	GLY	-	linker	UNP O32006
C	560	ARG	-	linker	UNP O32006
C	561	SER	-	linker	UNP O32006
C	562	GLY	-	linker	UNP O32006
C	563	THR	-	linker	UNP O32006
D	-16	THR	-	linker	UNP O32006
D	-15	SER	-	linker	UNP O32006
D	-14	GLY	-	linker	UNP O32006
D	-13	SER	-	linker	UNP O32006
D	-12	GLY	-	linker	UNP O32006
D	-11	GLY	-	linker	UNP O32006
D	-10	SER	-	linker	UNP O32006
D	-9	GLY	-	linker	UNP O32006
D	-8	GLY	-	linker	UNP O32006

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	SER	-	linker	UNP O32006
D	-6	GLY	-	linker	UNP O32006
D	-5	GLY	-	linker	UNP O32006
D	-4	SER	-	linker	UNP O32006
D	-3	GLY	-	linker	UNP O32006
D	-2	ARG	-	linker	UNP O32006
D	-1	SER	-	linker	UNP O32006
D	0	GLY	-	linker	UNP O32006
D	1	THR	-	linker	UNP O32006

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	34	Total	C	H	N	O	P	0	0
			1087	337	393	110	213	34		
2	G	34	Total	C	H	N	O	P	0	0
			1087	337	393	110	213	34		

- Molecule 3 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	33	Total	C	H	N	O	P	0	0
			1052	326	373	130	190	33		
3	H	33	Total	C	H	N	O	P	0	0
			1052	326	373	130	190	33		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	



[illegible]

- Molecule 1: Resolvase homolog YokA, SPbeta prophage-derived uncharacterized protein YotN

Chain D:  7% . 91%

[illegible]

THR	ASN	SER	PHE	HIS	THR	SER	GLY	SER	GLY	SER	GLY	SER	GLY	SER	ARG	SER	GLY	THR	THR	GLU	P3	R6	Y23	S24	I25	R26	S34	N35	D38	E39	F40	Y41	F44	H47	L48	L49	A52	R55	F56
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 2: DNA (34-MER)

Chain E:  41% 44% 9% 6%

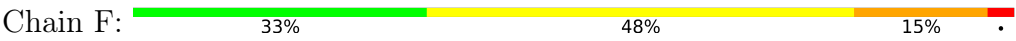
T-34
T-33
G-26
T-25
T-22
T-16
C-15
T-14
T-13
A-12
A-11
T-10
A-9
T-8
A-7
C-6
A-5
G-4
C-3
T-2
T-1

- Molecule 2: DNA (34-MER)

Chain G:  35% 47% 15%

T-34
T-33
T-32
G-26
T-25
A-24
G-23
T-22
T-16
C-15
T-14
T-13
A-12
A-11
T-10
A-9
T-8
A-7
C-6
A-5
G-4
C-3
T-2
T-1

- Molecule 3: DNA (33-MER)



● Molecule 3: DNA (33-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54766	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.960	Depositor
Minimum map value	-0.809	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	340.80002, 340.80002, 340.80002	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.13, 2.13, 2.13	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	13/4420 (0.3%)	1.61	57/5937 (1.0%)
1	B	0.79	0/489	1.44	4/654 (0.6%)
1	C	0.86	0/4420	1.56	49/5937 (0.8%)
1	D	0.80	0/489	1.48	2/654 (0.3%)
2	E	0.73	0/774	1.70	15/1193 (1.3%)
2	G	0.74	0/774	1.55	3/1193 (0.3%)
3	F	0.75	0/764	1.54	9/1176 (0.8%)
3	H	0.78	0/764	1.59	7/1176 (0.6%)
All	All	0.87	13/12894 (0.1%)	1.58	146/17920 (0.8%)

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	10
1	C	0	12
1	D	0	1
2	E	0	9
2	G	0	13
3	F	0	12
3	H	0	10
All	All	0	67

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	LYS	CA-CB	-11.25	1.35	1.53
1	A	279	ALA	CA-CB	9.19	1.69	1.53
1	A	478	ARG	CA-CB	-8.01	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ARG	N-CA	7.91	1.56	1.46
1	A	21	ARG	CA-C	7.24	1.62	1.52
1	A	22	SER	N-CA	7.07	1.54	1.45
1	A	179	ASN	N-CA	6.83	1.54	1.45
1	A	180	LYS	CB-CG	-6.72	1.32	1.52
1	A	182	THR	CB-OG1	-6.55	1.33	1.43
1	A	186	ASP	N-CA	6.12	1.52	1.45
1	A	180	LYS	CA-CB	-5.59	1.44	1.53
1	A	179	ASN	CA-C	-5.47	1.49	1.52
1	A	23	ARG	CA-CB	-5.08	1.44	1.53

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	SER	CA-C-N	13.21	141.74	120.60
1	A	22	SER	C-N-CA	13.21	141.74	120.60
1	A	23	ARG	N-CA-C	11.98	126.99	112.38
2	E	-2	DT	C4'-C3'-O3'	11.82	127.73	110.00
1	A	182	THR	N-CA-C	-11.46	92.88	109.96
2	E	-2	DT	O4'-C1'-N1	10.93	124.79	108.40
1	C	470	SER	N-CA-C	10.71	124.47	110.43
1	A	182	THR	N-CA-CB	10.67	126.36	109.51
1	A	179	ASN	N-CA-C	10.13	124.23	108.12
1	A	478	ARG	CB-CA-C	-9.87	96.11	112.00
1	A	475	ASN	N-CA-C	9.31	123.90	112.54
1	A	457	ASN	N-CA-C	8.83	122.02	111.33
3	H	3	DG	C2'-C3'-O3'	7.99	123.49	111.50
2	E	-2	DT	C2'-C3'-O3'	-7.97	99.54	111.50
1	A	186	ASP	CA-C-N	7.75	127.81	119.90
1	A	186	ASP	C-N-CA	7.75	127.81	119.90
1	C	502	ARG	CB-CA-C	7.67	122.92	110.88
1	C	457	ASN	N-CA-C	7.64	120.58	111.33
2	G	-15	DC	O3'-P-O5'	-7.59	92.62	104.00
1	A	140	LEU	N-CA-CB	-7.57	98.99	110.12
1	A	178	LEU	O-C-N	-7.57	112.94	123.01
2	G	-13	DT	C2'-C3'-O3'	7.39	122.59	111.50
3	H	9	DT	C4'-C3'-C2'	-7.34	91.39	102.40
1	A	474	SER	CA-C-N	7.29	132.90	120.72
1	A	474	SER	C-N-CA	7.29	132.90	120.72
1	C	452	PHE	CA-CB-CG	7.21	121.01	113.80
1	C	28	ARG	N-CA-C	7.18	119.97	111.71
1	A	279	ALA	N-CA-CB	-7.17	98.38	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	475	ASN	N-CA-C	7.14	121.09	112.38
1	C	161	TYR	CA-CB-CG	7.13	126.73	113.90
1	C	400	ASN	O-C-N	-6.80	115.07	122.07
1	A	32	THR	CB-CA-C	-6.75	99.48	110.08
1	A	135	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	C	388	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	C	190	ASP	CA-C-N	6.63	130.39	120.31
1	C	190	ASP	C-N-CA	6.63	130.39	120.31
3	F	3	DG	C4'-C3'-O3'	6.63	119.94	110.00
2	E	-2	DT	C5'-C4'-C3'	6.63	124.84	114.90
1	C	95	ARG	NE-CZ-NH2	6.56	125.10	119.20
1	C	299	LYS	CA-C-N	6.53	127.04	122.60
1	C	299	LYS	C-N-CA	6.53	127.04	122.60
2	E	-2	DT	C5'-C4'-O4'	-6.47	99.70	109.40
3	H	14	DA	C4'-C3'-O3'	-6.44	100.34	110.00
1	A	179	ASN	O-C-N	6.43	126.50	120.71
1	A	20	ARG	CA-C-N	6.38	133.73	121.54
1	A	20	ARG	C-N-CA	6.38	133.73	121.54
1	C	25	ASP	O-C-N	-6.37	114.74	122.25
1	C	233	ARG	NE-CZ-NH2	6.35	124.91	119.20
1	A	28	ARG	CD-NE-CZ	6.30	133.22	124.40
3	H	8	DA	C3'-C2'-C1'	6.29	111.03	101.60
1	A	139	GLU	CA-C-N	6.23	128.63	120.28
1	A	139	GLU	C-N-CA	6.23	128.63	120.28
3	F	15	DG	C3'-C2'-C1'	6.22	110.92	101.60
1	C	338	ASN	CA-CB-CG	6.17	118.77	112.60
3	F	9	DT	P-O3'-C3'	6.16	129.44	120.20
1	C	179	ASN	N-CA-C	6.15	121.18	113.43
1	C	300	VAL	N-CA-C	6.15	113.16	107.56
1	C	170	GLY	CA-C-N	-6.10	112.45	121.24
1	C	170	GLY	C-N-CA	-6.10	112.45	121.24
2	E	-15	DC	C3'-C2'-C1'	6.09	110.73	101.60
1	A	141	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	180	LYS	N-CA-C	-6.06	97.90	110.80
1	A	186	ASP	N-CA-C	-6.03	99.74	109.58
1	A	181	LYS	CB-CA-C	6.01	121.48	110.36
2	G	-14	DT	C5'-C4'-C3'	-5.96	105.95	114.90
1	A	161	TYR	CB-CA-C	5.96	120.98	110.85
2	E	-2	DT	N1-C1'-C2'	-5.95	104.58	113.50
1	C	194	VAL	CB-CA-C	5.90	119.52	111.97
3	F	2	DA	C5'-C4'-C3'	5.88	123.73	114.90
2	E	-2	DT	C6-N1-C1'	5.85	128.13	119.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	LEU	N-CA-C	5.85	121.02	111.37
1	A	200	ASN	CA-CB-CG	5.84	118.44	112.60
1	C	487	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	186	ASP	CA-CB-CG	-5.80	106.80	112.60
1	D	26	ARG	CD-NE-CZ	5.79	132.51	124.40
3	F	9	DT	C2'-C3'-O3'	5.77	120.16	111.50
1	C	362	ARG	NE-CZ-NH2	5.77	124.39	119.20
2	E	-2	DT	O5'-C5'-C4'	5.77	119.45	110.80
3	H	18	DA	C2'-C3'-O3'	5.72	120.08	111.50
1	A	262	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	25	ASP	N-CA-C	-5.64	105.68	113.18
1	A	151	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	A	179	ASN	CA-C-O	5.63	122.99	119.55
1	A	22	SER	CB-CA-C	5.61	121.30	109.79
1	D	26	ARG	NE-CZ-NH2	5.61	124.24	119.20
2	E	-2	DT	C6-C5-C7	-5.58	115.64	124.00
1	A	115	ARG	N-CA-C	5.56	119.36	112.24
1	B	6	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	C	479	ASN	CA-CB-CG	5.53	118.13	112.60
1	C	299	LYS	N-CA-C	5.49	117.61	110.53
1	A	362	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	A	155	THR	CA-C-N	5.46	125.89	119.94
1	A	155	THR	C-N-CA	5.46	125.89	119.94
3	F	3	DG	C4'-C3'-C2'	-5.46	94.21	102.40
1	C	236	GLN	N-CA-C	5.45	122.41	110.80
3	F	16	DA	C4'-C3'-O3'	5.45	118.17	110.00
1	A	79	ASP	CA-CB-CG	5.43	118.03	112.60
3	H	14	DA	C2'-C3'-O3'	5.42	119.63	111.50
1	C	533	ASN	CA-CB-CG	5.40	118.00	112.60
3	H	9	DT	P-O3'-C3'	5.40	128.29	120.20
1	A	136	ILE	CA-C-O	-5.39	115.80	121.41
1	A	338	ASN	CA-CB-CG	5.36	117.96	112.60
2	E	-1	DT	O5'-C5'-C4'	5.36	118.84	110.80
1	A	227	THR	N-CA-CB	5.36	117.93	110.11
1	C	404	LYS	CA-C-N	5.36	127.41	120.44
1	C	404	LYS	C-N-CA	5.36	127.41	120.44
1	B	26	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	C	273	GLN	OE1-CD-NE2	-5.34	117.26	122.60
2	E	-1	DT	N3-C4-O4	-5.34	114.59	122.60
1	A	238	THR	CB-CA-C	-5.32	101.81	110.85
1	C	178	LEU	N-CA-CB	-5.30	102.11	110.49
1	A	180	LYS	N-CA-CB	-5.29	101.56	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	ASN	N-CA-CB	-5.28	101.53	110.51
1	B	26	ARG	CD-NE-CZ	5.27	131.78	124.40
1	C	249	ILE	CB-CA-C	5.25	119.89	111.29
1	B	3	PRO	CA-N-CD	-5.24	104.67	112.00
1	C	18	TYR	N-CA-C	5.23	117.02	109.07
3	F	4	DC	C4'-C3'-O3'	-5.23	102.16	110.00
1	A	337	LYS	CA-C-N	5.21	128.47	120.82
1	A	337	LYS	C-N-CA	5.21	128.47	120.82
1	C	262	ASP	CA-C-N	5.20	131.00	121.85
1	C	262	ASP	C-N-CA	5.20	131.00	121.85
1	C	128	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	A	244	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	C	241	ALA	CA-C-N	5.17	127.28	120.60
1	C	241	ALA	C-N-CA	5.17	127.28	120.60
1	C	288	GLN	OE1-CD-NE2	-5.17	117.44	122.60
1	C	223	LEU	CA-C-N	5.16	129.67	122.08
1	C	223	LEU	C-N-CA	5.16	129.67	122.08
1	A	403	MET	N-CA-C	5.15	116.90	111.28
1	A	264	LYS	N-CA-CB	5.09	117.52	110.04
1	C	28	ARG	CD-NE-CZ	5.08	131.52	124.40
1	C	336	ARG	N-CA-C	5.08	121.76	114.39
2	E	-1	DT	N1-C1'-C2'	5.07	121.11	113.50
1	A	403	MET	CA-C-N	5.07	127.34	120.65
1	A	403	MET	C-N-CA	5.07	127.34	120.65
1	A	38	THR	N-CA-C	5.07	118.95	112.87
1	A	21	ARG	CA-C-N	5.06	130.53	122.59
1	A	21	ARG	C-N-CA	5.06	130.53	122.59
1	A	182	THR	O-C-N	-5.04	116.30	123.01
2	E	-16	DT	C3'-C2'-C1'	5.03	109.14	101.60
1	A	109	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	155	THR	CA-C-N	5.01	125.51	120.00
1	C	155	THR	C-N-CA	5.01	125.51	120.00
2	E	-10	DT	C4'-C3'-O3'	-5.00	102.49	110.00
3	F	19	DC	C2'-C3'-O3'	5.00	119.00	111.50

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	TYR	Sidechain
1	A	174	TYR	Sidechain
1	A	181	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	211	TYR	Sidechain
1	A	213	TYR	Sidechain
1	A	26	MET	Peptide
1	A	268	ARG	Sidechain
1	A	336	ARG	Sidechain
1	A	502	ARG	Sidechain
1	A	531	ARG	Sidechain
1	C	174	TYR	Sidechain
1	C	176	TYR	Sidechain
1	C	178	LEU	Peptide
1	C	211	TYR	Sidechain
1	C	213	TYR	Sidechain
1	C	23	ARG	Sidechain
1	C	233	ARG	Sidechain
1	C	236	GLN	Peptide
1	C	25	ASP	Mainchain
1	C	302	LEU	Peptide
1	C	436	TYR	Sidechain
1	C	441	PHE	Sidechain
1	D	6	ARG	Sidechain
2	E	-1	DT	Sidechain
2	E	-13	DT	Sidechain
2	E	-14	DT	Sidechain
2	E	-16	DT	Sidechain
2	E	-2	DT	Sidechain
2	E	-22	DT	Sidechain
2	E	-3	DC	Sidechain
2	E	-33	DT	Sidechain
2	E	-6	DC	Sidechain
3	F	12	DT	Sidechain
3	F	18	DA	Sidechain
3	F	19	DC	Sidechain
3	F	21	DT	Sidechain
3	F	23	DC	Sidechain
3	F	27	DA	Sidechain
3	F	29	DA	Sidechain
3	F	3	DG	Sidechain
3	F	33	DA	Sidechain
3	F	34	DA	Sidechain
3	F	8	DA	Sidechain
3	F	9	DT	Sidechain
2	G	-1	DT	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	G	-13	DT	Sidechain
2	G	-14	DT	Sidechain
2	G	-16	DT	Sidechain
2	G	-2	DT	Sidechain
2	G	-22	DT	Sidechain
2	G	-3	DC	Sidechain
2	G	-32	DT	Sidechain
2	G	-33	DT	Sidechain
2	G	-34	DT	Sidechain
2	G	-4	DG	Sidechain
2	G	-5	DA	Sidechain
2	G	-6	DC	Sidechain
3	H	12	DT	Sidechain
3	H	15	DG	Sidechain
3	H	2	DA	Sidechain
3	H	20	DT	Sidechain
3	H	21	DT	Sidechain
3	H	27	DA	Sidechain
3	H	29	DA	Sidechain
3	H	3	DG	Sidechain
3	H	6	DG	Sidechain
3	H	9	DT	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4354	4428	4424	111	0
1	B	481	474	474	12	0
1	C	4354	4428	4424	103	0
1	D	481	474	474	15	0
2	E	694	393	389	36	0
2	G	694	393	381	19	0
3	F	679	373	366	19	0
3	H	679	373	361	26	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
All	All	12418	11336	11293	250	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 11.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLY:HA2	1:A:279:ALA:HB1	1.34	1.06
1:A:165:GLY:CA	1:A:279:ALA:HB1	1.91	0.99
1:A:32:THR:HG23	1:C:161:TYR:CD1	2.07	0.89
1:C:157:ALA:HB1	1:C:161:TYR:CE2	2.12	0.84
1:A:518:GLY:HA2	3:F:25:DA:C2	2.14	0.81
2:G:-12:DA:H1'	2:G:-11:DA:C8	2.19	0.76
1:A:170:GLY:H	2:E:-4:DG:H21	1.35	0.74
1:A:475:ASN:HA	1:A:478:ARG:HB3	1.68	0.73
1:A:369:ALA:HB2	1:B:23:TYR:CG	2.22	0.73
1:A:518:GLY:HA2	3:F:25:DA:N3	2.04	0.72
1:A:99:GLY:HA2	1:A:140:LEU:HG	1.71	0.72
1:A:170:GLY:H	2:E:-4:DG:N2	1.88	0.72
1:C:170:GLY:HA2	2:G:-4:DG:N3	2.07	0.70
1:C:276:VAL:HG12	1:C:279:ALA:HB2	1.74	0.69
1:A:217:ALA:HB2	1:A:239:ILE:HG12	1.77	0.67
1:A:165:GLY:HA3	1:A:279:ALA:HB1	1.75	0.66
1:A:167:TRP:HB2	1:A:185:LEU:HG	1.79	0.64
1:C:167:TRP:C	1:C:168:ILE:HD13	2.24	0.63
3:F:5:DT:H2''	3:F:6:DG:C8	2.35	0.62
1:C:338:ASN:HB3	2:G:-26:DG:OP2	1.99	0.61
2:E:-12:DA:H1'	2:E:-11:DA:C8	2.35	0.61
1:A:27:GLU:HA	1:A:30:LYS:HE2	1.82	0.61
1:A:217:ALA:HB2	1:A:239:ILE:CG1	2.31	0.61
2:E:-3:DC:H2'	2:E:-2:DT:C5	2.35	0.60
1:C:165:GLY:CA	1:C:279:ALA:HB1	2.31	0.60
1:C:223:LEU:HD22	1:C:409:MET:HG3	1.83	0.60
3:H:9:DT:H2''	3:H:10:DA:H5'	1.85	0.59
1:A:167:TRP:CG	1:A:185:LEU:HD21	2.38	0.59
1:A:170:GLY:N	2:E:-4:DG:H21	1.99	0.59
1:C:295:LYS:HE3	1:C:295:LYS:HA	1.85	0.58
1:C:165:GLY:HA3	1:C:279:ALA:HB1	1.84	0.58
1:C:229:SER:HB3	3:H:8:DA:H4'	1.85	0.58
1:A:479:ASN:HB2	1:A:481:ILE:CD1	2.34	0.58
1:A:369:ALA:CB	1:B:23:TYR:CG	2.88	0.57
1:C:154:MET:HE3	3:H:2:DA:C2	2.40	0.57
2:E:-9:DA:C2	3:F:10:DA:C2	2.94	0.56
2:E:-2:DT:C5	2:E:-1:DT:C4	2.93	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:-3:DC:H2'	2:E:-2:DT:C4	2.41	0.56
1:C:369:ALA:HB2	1:D:23:TYR:CG	2.40	0.56
3:H:5:DT:H2''	3:H:6:DG:C8	2.40	0.56
1:A:348:VAL:HG21	2:E:-22:DT:C7	2.36	0.56
1:C:350:SER:HB2	1:C:360:TYR:CE2	2.42	0.55
3:H:7:DT:H2''	3:H:8:DA:C8	2.41	0.55
1:C:227:THR:HG21	3:H:9:DT:P	2.46	0.55
1:C:192:ALA:HA	1:C:283:ILE:HD11	1.88	0.55
1:C:167:TRP:O	1:C:168:ILE:HD13	2.07	0.55
1:A:448:LEU:HD11	1:A:452:PHE:CZ	2.42	0.54
1:C:174:TYR:CD1	1:C:228:PRO:HB3	2.42	0.54
1:A:170:GLY:HA2	2:E:-5:DA:C2	2.42	0.53
2:E:-3:DC:C2'	2:E:-2:DT:C5	2.91	0.53
1:A:167:TRP:CB	1:A:185:LEU:HG	2.38	0.53
1:A:217:ALA:HB1	1:A:234:TRP:O	2.09	0.53
1:A:166:LYS:HA	1:A:184:LYS:HA	1.90	0.53
1:C:157:ALA:HB1	1:C:161:TYR:CD2	2.44	0.53
1:A:518:GLY:CA	3:F:25:DA:C2	2.90	0.53
1:C:258:GLU:HB3	1:C:268:ARG:CZ	2.38	0.53
1:A:440:LEU:HD12	1:C:445:LYS:CE	2.39	0.53
1:A:99:GLY:HA2	1:A:140:LEU:CG	2.37	0.52
1:C:309:PHE:HB3	3:H:17:DT:H4'	1.90	0.52
1:A:321:SER:HB2	1:B:7:TYR:CE2	2.44	0.52
1:A:369:ALA:HB2	1:B:23:TYR:CB	2.38	0.52
1:A:309:PHE:HB3	3:F:17:DT:H4'	1.90	0.52
1:A:213:TYR:HB2	1:A:236:GLN:OE1	2.09	0.52
1:A:306:LYS:HE2	1:A:309:PHE:CZ	2.45	0.52
1:C:248:TYR:O	1:C:283:ILE:HG22	2.09	0.52
2:E:-1:DT:H3	3:F:2:DA:N6	2.07	0.52
1:C:163:ALA:HB2	1:C:274:ILE:HG12	1.90	0.51
1:C:264:LYS:HA	2:G:-8:DT:H71	1.92	0.51
1:A:114:LYS:O	1:A:116:LEU:HD23	2.11	0.51
1:D:40:PHE:CE1	1:D:44:PHE:HB2	2.45	0.51
1:A:216:ILE:HB	1:A:239:ILE:HG21	1.92	0.51
1:A:31:ARG:HB2	1:C:161:TYR:CD1	2.45	0.51
1:A:338:ASN:HB3	2:E:-26:DG:OP2	2.10	0.51
1:C:171:LEU:CD1	3:H:7:DT:H1'	2.41	0.51
1:A:518:GLY:HA2	3:F:25:DA:H2	1.72	0.51
1:C:7:VAL:HG11	1:C:51:ILE:HG23	1.90	0.51
2:E:-2:DT:C3'	2:E:-2:DT:C6	2.93	0.51
1:A:23:ARG:CG	3:F:2:DA:H2'	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:TYR:CD1	1:B:25:ILE:HG21	2.46	0.51
2:E:-3:DC:H2''	2:E:-2:DT:C6	2.46	0.51
1:A:32:THR:CG2	1:C:157:ALA:HA	2.40	0.50
1:C:346:TYR:CE1	2:G:-25:DT:H2'	2.46	0.50
2:G:-12:DA:C1'	2:G:-11:DA:C8	2.91	0.50
1:A:32:THR:HG23	1:C:161:TYR:CE1	2.45	0.50
1:A:154:MET:N	1:C:28:ARG:HH21	2.08	0.50
2:E:-2:DT:C6	2:E:-2:DT:H3'	2.46	0.50
2:G:-10:DT:H1'	2:G:-9:DA:H5'	1.93	0.50
1:C:283:ILE:HG23	1:C:284:ILE:HG12	1.94	0.50
1:A:172:ALA:HB2	1:A:178:LEU:H	1.77	0.50
1:A:369:ALA:HB2	1:B:23:TYR:CD2	2.46	0.50
1:C:392:MET:N	1:C:392:MET:HE2	2.27	0.49
1:C:479:ASN:HB2	1:C:481:ILE:CD1	2.42	0.49
1:A:170:GLY:HA2	2:E:-4:DG:C2	2.47	0.49
1:A:348:VAL:HG21	2:E:-22:DT:H71	1.93	0.49
1:C:171:LEU:HD12	3:H:7:DT:H1'	1.94	0.49
1:C:229:SER:CB	3:H:8:DA:H4'	2.41	0.49
3:F:5:DT:C2'	3:F:6:DG:C8	2.96	0.49
3:H:5:DT:C2'	3:H:6:DG:C8	2.95	0.49
1:A:32:THR:HG21	1:A:34:GLU:OE1	2.12	0.49
1:A:400:ASN:C	1:A:402:ASN:H	2.20	0.49
1:C:174:TYR:CD2	1:C:228:PRO:HD3	2.48	0.49
2:E:-7:DA:C2	3:F:8:DA:C2	3.00	0.49
2:E:-2:DT:H72	2:E:-1:DT:O4	2.13	0.49
1:C:171:LEU:HB3	3:H:7:DT:H4'	1.94	0.49
1:B:20:LYS:HB2	1:B:23:TYR:CE1	2.48	0.49
1:C:428:PHE:CZ	1:C:441:PHE:CE1	3.01	0.48
1:C:167:TRP:O	1:C:178:LEU:HD21	2.13	0.48
3:H:3:DG:H2'	3:H:4:DC:C6	2.48	0.48
1:C:228:PRO:HD2	3:H:8:DA:H5''	1.95	0.48
1:C:256:VAL:HG12	3:H:6:DG:OP1	2.12	0.48
1:C:99:GLY:CA	1:C:144:ARG:HG2	2.43	0.48
1:C:165:GLY:C	1:C:252:VAL:HG21	2.39	0.48
1:C:340:ASP:HB3	2:G:-26:DG:OP1	2.14	0.48
2:G:-13:DT:C2	2:G:-12:DA:C6	3.01	0.48
1:C:346:TYR:CD2	2:G:-24:DA:N7	2.82	0.47
1:A:161:TYR:CD2	1:A:166:LYS:HG3	2.50	0.47
1:A:16:LEU:HD22	1:A:85:TYR:CE2	2.49	0.47
1:A:80:LEU:HD11	1:A:88:ILE:HD11	1.95	0.47
1:C:223:LEU:HD22	1:C:409:MET:CG	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:PRO:CB	3:H:14:DA:H2	2.27	0.47
1:C:157:ALA:CB	1:C:161:TYR:CE2	2.92	0.47
1:C:163:ALA:HB2	1:C:274:ILE:CG1	2.45	0.47
3:H:9:DT:C2'	3:H:10:DA:H5'	2.44	0.47
1:A:99:GLY:CA	1:A:140:LEU:HG	2.43	0.47
1:A:245:ASN:HD21	1:A:247:VAL:HB	1.79	0.47
1:A:90:VAL:HG11	1:A:96:LEU:HG	1.97	0.47
2:E:-2:DT:C4	2:E:-1:DT:C4	3.02	0.47
1:A:518:GLY:CA	3:F:25:DA:H2	2.28	0.47
1:A:170:GLY:N	2:E:-4:DG:N2	2.58	0.47
1:A:502:ARG:CZ	1:A:502:ARG:HA	2.44	0.47
1:C:174:TYR:CE1	1:C:228:PRO:HB3	2.50	0.47
1:A:236:GLN:HG3	1:A:237:TYR:CD1	2.50	0.46
3:H:8:DA:C8	3:H:9:DT:H72	2.50	0.46
1:A:118:ILE:HD12	1:A:136:ILE:HD11	1.97	0.46
1:C:294:VAL:HG12	1:D:39:GLU:HG2	1.96	0.46
1:C:371:LEU:HD21	1:C:488:TYR:CE1	2.51	0.46
1:C:161:TYR:HB3	1:C:168:ILE:HD11	1.97	0.46
1:A:111:LEU:CD1	1:A:118:ILE:HD11	2.45	0.46
1:A:153:ARG:HE	1:C:28:ARG:NH1	2.14	0.46
1:A:227:THR:HG22	1:A:234:TRP:CD1	2.51	0.46
1:C:428:PHE:CE1	1:C:441:PHE:CE1	3.04	0.46
1:A:158:LYS:HG2	1:A:254:TYR:CE1	2.51	0.46
1:A:440:LEU:C	1:A:440:LEU:HD23	2.41	0.46
1:C:165:GLY:HA2	1:C:279:ALA:HB1	1.97	0.46
1:C:161:TYR:CZ	2:G:-2:DT:H4'	2.51	0.46
1:A:265:ARG:HG2	2:E:-8:DT:H72	1.98	0.45
1:A:436:TYR:HA	1:A:440:LEU:HD13	1.98	0.45
1:C:178:LEU:HD22	2:G:-3:DC:H4'	1.98	0.45
1:A:142:MET:HA	1:C:122:TYR:CZ	2.51	0.45
1:A:496:LYS:HZ3	1:B:54:GLU:CD	2.24	0.45
2:E:-3:DC:H2'	2:E:-2:DT:C7	2.47	0.45
2:E:-7:DA:N1	3:F:8:DA:C2	2.85	0.45
1:A:93:ILE:HD11	1:A:125:TYR:CE1	2.52	0.45
1:C:174:TYR:CD1	1:C:191:GLU:CD	2.95	0.45
1:C:524:PHE:CZ	1:D:23:TYR:HB3	2.52	0.45
1:A:28:ARG:HH21	1:C:157:ALA:HB2	1.82	0.45
1:C:90:VAL:HG11	1:C:96:LEU:HG	1.98	0.45
1:C:369:ALA:HA	1:D:23:TYR:CZ	2.52	0.45
2:G:-3:DC:H2'	2:G:-2:DT:C5	2.52	0.44
1:A:177:GLN:HG3	1:A:179:ASN:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:HA	1:C:206:LEU:H	1.82	0.44
1:A:170:GLY:HA2	2:E:-5:DA:H2	1.82	0.44
1:C:340:ASP:HB2	2:G:-26:DG:P	2.58	0.44
1:C:532:PHE:CD1	1:D:40:PHE:HB2	2.53	0.44
1:A:293:GLN:HA	1:A:296:ILE:HB	2.00	0.44
1:C:229:SER:HB3	3:H:8:DA:C4'	2.47	0.44
1:C:487:GLN:HG3	1:C:500:LEU:HD22	1.98	0.44
1:C:31:ARG:HH12	2:G:-3:DC:N4	2.15	0.44
2:E:-5:DA:C4	2:E:-4:DG:C5	3.06	0.44
1:A:373:TYR:CE2	1:A:528:PRO:HB2	2.52	0.43
1:A:392:MET:SD	1:B:42:LYS:HG2	2.58	0.43
1:C:220:LEU:HD13	1:C:234:TRP:CZ3	2.53	0.43
1:C:305:ASN:HA	3:H:16:DA:H1'	1.98	0.43
1:A:259:LYS:HD3	3:F:5:DT:H71	2.00	0.43
1:A:361:VAL:HG11	1:A:510:VAL:HG11	2.00	0.43
2:E:-3:DC:H2'	2:E:-2:DT:H73	2.01	0.43
1:A:15:ILE:CD1	1:A:51:ILE:HG21	2.48	0.43
1:A:175:GLY:H	1:A:191:GLU:HB3	1.82	0.43
1:A:254:TYR:CE2	1:A:255:LYS:HB2	2.53	0.43
1:A:346:TYR:CE1	2:E:-25:DT:H2'	2.53	0.43
1:C:48:LEU:HD11	1:C:89:ALA:CB	2.49	0.43
1:C:196:GLN:HA	1:C:284:ILE:HD11	2.00	0.43
1:A:80:LEU:HD22	1:A:116:LEU:HD21	2.01	0.43
1:A:186:ASP:HA	1:A:187:PRO:HD3	1.80	0.43
1:C:170:GLY:CA	2:G:-4:DG:N3	2.80	0.43
1:C:431:TYR:CD2	1:C:441:PHE:CG	3.06	0.43
1:A:406:LYS:HE3	1:A:465:LEU:HB3	2.01	0.42
1:C:162:ALA:HB1	1:C:254:TYR:HB2	2.01	0.42
1:A:413:LEU:HA	1:A:455:LEU:HD11	2.00	0.42
1:C:389:ILE:CD1	1:C:477:VAL:HG12	2.50	0.42
3:H:13:DA:C6	3:H:14:DA:C6	3.07	0.42
1:A:179:ASN:C	1:A:180:LYS:O	2.60	0.42
1:C:348:VAL:HG21	2:G:-22:DT:C7	2.49	0.42
1:A:199:PHE:CZ	1:A:243:LEU:HA	2.55	0.42
1:C:264:LYS:HG2	2:G:-9:DA:H3'	2.01	0.42
1:A:25:ASP:HA	1:A:28:ARG:H	1.84	0.42
1:A:178:LEU:HD23	2:E:-3:DC:H5''	2.01	0.42
1:A:440:LEU:HD12	1:C:445:LYS:HE3	2.02	0.42
2:E:-5:DA:C2	3:F:6:DG:N2	2.88	0.42
2:E:-2:DT:C6	2:E:-2:DT:O5'	2.73	0.42
1:A:175:GLY:H	1:A:191:GLU:CB	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:VAL:HG13	1:D:49:LEU:HA	2.01	0.42
3:F:3:DG:H2'	3:F:4:DC:C6	2.55	0.42
1:C:12:ILE:HG22	1:C:86:GLN:HB3	2.02	0.42
1:A:274:ILE:HD13	1:A:274:ILE:HA	1.94	0.42
1:A:503:MET:SD	1:B:47:HIS:HB2	2.60	0.42
1:C:175:GLY:N	1:C:191:GLU:HG3	2.35	0.42
1:A:73:PHE:CZ	1:A:77:LEU:HD21	2.55	0.42
1:A:535:ILE:HD12	1:B:30:GLN:HG2	2.01	0.42
1:C:336:ARG:O	1:C:337:LYS:C	2.61	0.42
1:C:525:GLU:HA	1:D:24:SER:HB2	2.02	0.42
1:A:150:THR:HA	1:A:153:ARG:CZ	2.50	0.41
1:A:259:LYS:HG2	3:F:5:DT:C7	2.50	0.41
1:C:154:MET:CE	3:H:2:DA:C2	3.03	0.41
2:E:-3:DC:C2'	2:E:-2:DT:C4	3.02	0.41
1:D:52:ALA:HA	1:D:55:ARG:HE	1.85	0.41
1:C:306:LYS:HE2	1:C:309:PHE:CE1	2.55	0.41
1:C:373:TYR:CD1	1:D:25:ILE:HG21	2.55	0.41
2:E:-12:DA:C1'	2:E:-11:DA:C8	3.03	0.41
1:A:28:ARG:HD3	1:C:157:ALA:HB2	2.02	0.41
1:A:167:TRP:CZ2	1:A:173:PRO:HD3	2.55	0.41
1:C:167:TRP:CZ3	1:C:247:VAL:HG21	2.55	0.41
1:C:389:ILE:HD12	1:C:477:VAL:HG12	2.01	0.41
1:C:488:TYR:CD1	1:C:488:TYR:C	2.97	0.41
3:H:14:DA:C2	3:H:15:DG:C4	3.08	0.41
1:A:265:ARG:N	2:E:-8:DT:H72	2.36	0.41
1:A:532:PHE:CG	1:B:40:PHE:HB2	2.56	0.41
2:G:-26:DG:H2'	2:G:-25:DT:H71	2.02	0.41
1:A:417:GLU:N	1:A:455:LEU:HD21	2.35	0.41
3:H:13:DA:C2	3:H:14:DA:C4	3.09	0.41
1:C:369:ALA:HB2	1:D:23:TYR:CD2	2.55	0.41
1:C:477:VAL:CG1	1:D:49:LEU:HA	2.50	0.41
1:A:93:ILE:HD12	1:A:139:GLU:HG3	2.03	0.40
1:A:99:GLY:HA2	1:A:140:LEU:CD1	2.51	0.40
1:C:201:ILE:CG1	1:C:206:LEU:HB2	2.52	0.40
1:A:23:ARG:HG3	3:F:2:DA:H2'	2.03	0.40
1:A:118:ILE:HD12	1:A:136:ILE:CD1	2.51	0.40
1:A:317:VAL:HG22	1:A:502:ARG:CZ	2.51	0.40
1:C:28:ARG:CZ	2:E:-1:DT:H5"	2.51	0.40
1:D:6:ARG:C	1:D:6:ARG:HD2	2.46	0.40
1:D:38:ASP:HA	1:D:41:TYR:CD2	2.56	0.40
1:A:80:LEU:HD11	1:A:88:ILE:CG1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD23	1:A:110:LEU:N	2.37	0.40
1:C:18:TYR:CG	1:C:19:LEU:N	2.90	0.40
1:C:385:LEU:HA	1:D:41:TYR:HB3	2.03	0.40
3:F:7:DT:H2''	3:F:8:DA:C8	2.55	0.40
1:A:236:GLN:HG3	1:A:237:TYR:CE1	2.56	0.40
1:C:93:ILE:CD1	1:C:118:ILE:HG21	2.51	0.40
1:C:235:ASN:ND2	3:H:9:DT:C5	2.90	0.40
3:H:13:DA:H1'	3:H:14:DA:H5''	2.03	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	533/620 (86%)	478 (90%)	52 (10%)	3 (1%)	21	59
1	B	54/620 (9%)	50 (93%)	4 (7%)	0	100	100
1	C	533/620 (86%)	475 (89%)	55 (10%)	3 (1%)	21	59
1	D	54/620 (9%)	47 (87%)	7 (13%)	0	100	100
All	All	1174/2480 (47%)	1050 (89%)	118 (10%)	6 (0%)	26	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	237	TYR
1	A	204	ASN
1	C	205	GLY
1	A	207	ASN
1	C	329	LYS
1	A	249	ILE

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	490/560 (88%)	467 (95%)	23 (5%)	23	45
1	B	51/560 (9%)	51 (100%)	0	100	100
1	C	490/560 (88%)	469 (96%)	21 (4%)	26	47
1	D	51/560 (9%)	49 (96%)	2 (4%)	28	49
All	All	1082/2240 (48%)	1036 (96%)	46 (4%)	27	47

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	31	ARG
1	A	110	LEU
1	A	116	LEU
1	A	133	MET
1	A	155	THR
1	A	158	LYS
1	A	171	LEU
1	A	183	SER
1	A	204	ASN
1	A	232	LYS
1	A	233	ARG
1	A	236	GLN
1	A	258	GLU
1	A	274	ILE
1	A	306	LYS
1	A	323	CYS
1	A	334	ARG
1	A	358	CYS
1	A	397	GLU
1	A	440	LEU
1	A	478	ARG
1	A	502	ARG
1	C	28	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	32	THR
1	C	133	MET
1	C	151	ARG
1	C	153	ARG
1	C	169	SER
1	C	174	TYR
1	C	191	GLU
1	C	197	LEU
1	C	201	ILE
1	C	202	PHE
1	C	204	ASN
1	C	236	GLN
1	C	260	THR
1	C	284	ILE
1	C	295	LYS
1	C	371	LEU
1	C	461	GLU
1	C	512	MET
1	C	516	ARG
1	C	532	PHE
1	D	35	ASN
1	D	47	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	222	ASN
1	A	388	HIS
1	A	456	GLN
1	A	460	ASN
1	A	469	GLN
1	A	533	ASN
1	C	5	ASN
1	C	45	ASN
1	C	219	HIS
1	C	244	GLN
1	C	293	GLN
1	C	425	ASN
1	C	456	GLN
1	C	463	ASN
1	D	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	47	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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](#)

There are no chain breaks in this entry.

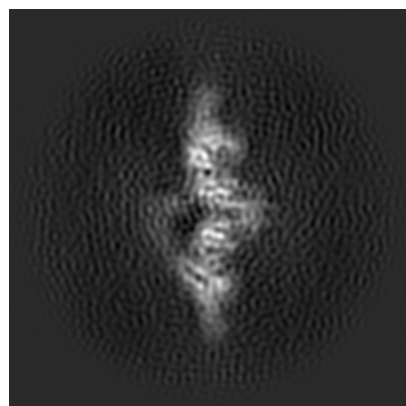
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47287. These allow visual inspection of the internal detail of the map and identification of artifacts.

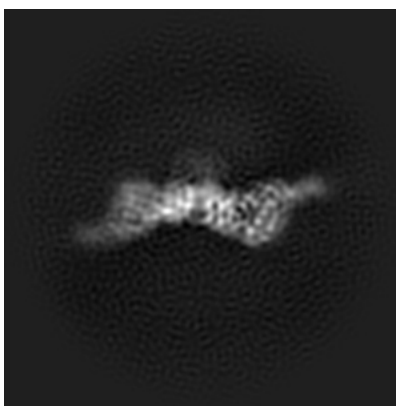
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

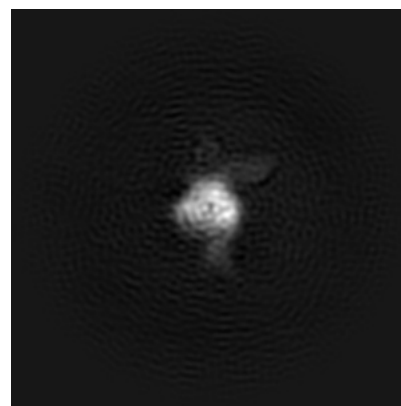
6.1.1 Primary map



X

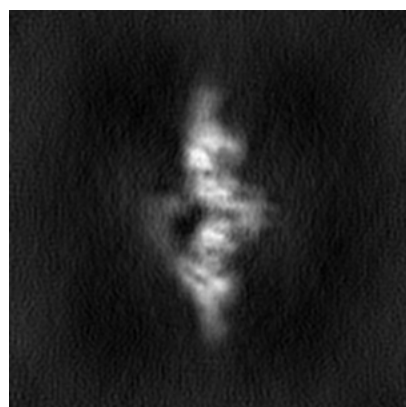


Y

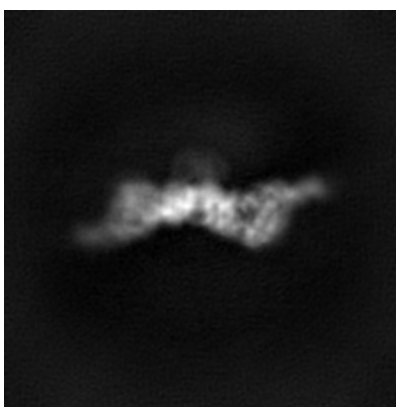


Z

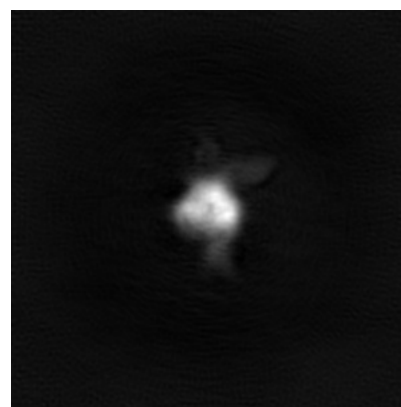
6.1.2 Raw map



X



Y

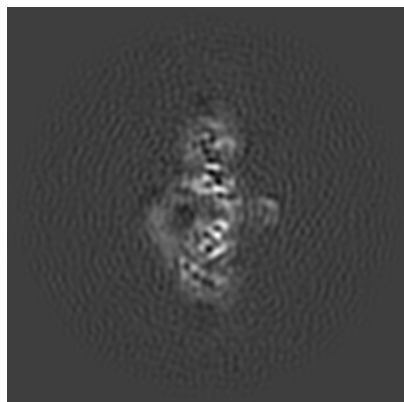


Z

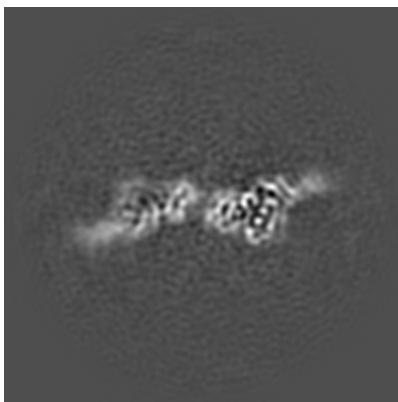
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

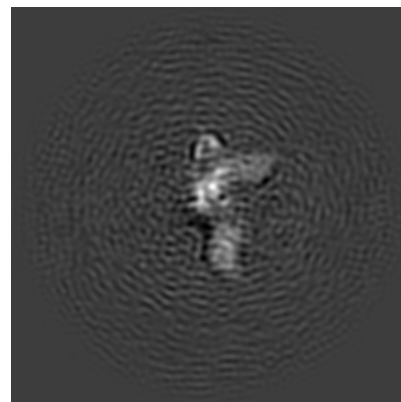
6.2.1 Primary map



X Index: 80

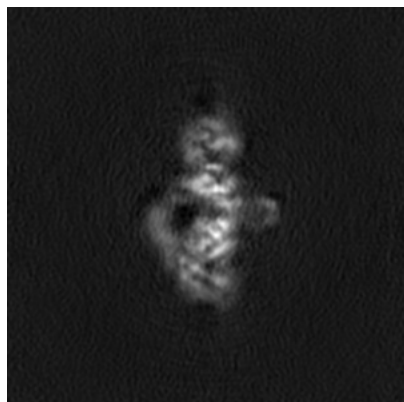


Y Index: 80

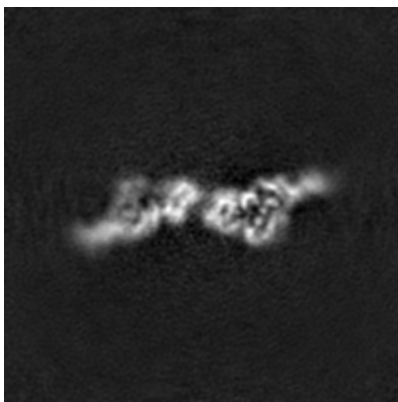


Z Index: 80

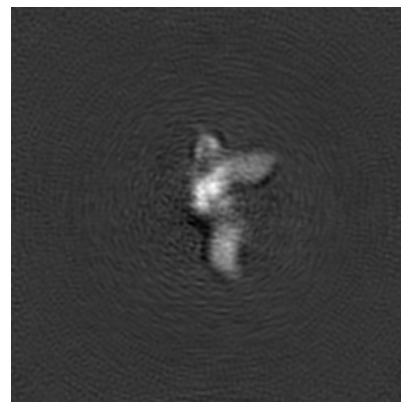
6.2.2 Raw map



X Index: 80



Y Index: 80

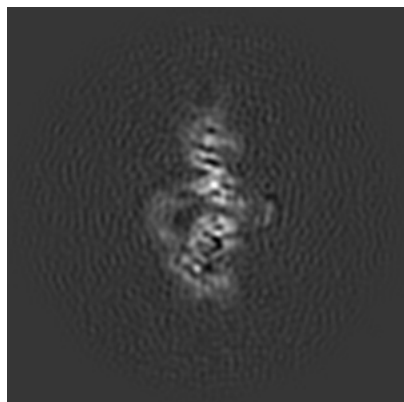


Z Index: 80

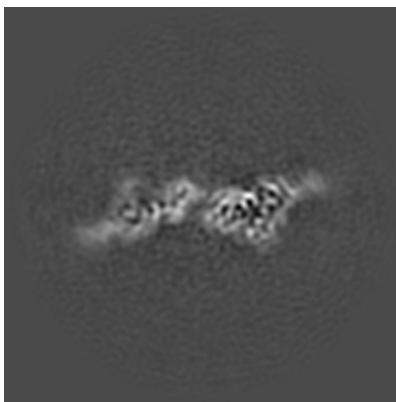
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

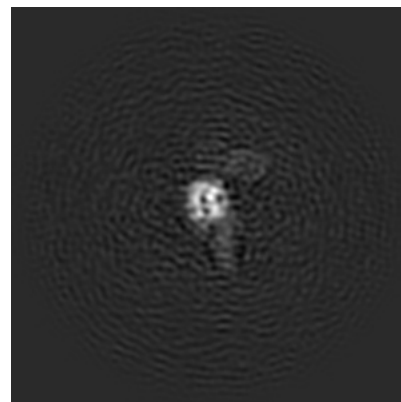
6.3.1 Primary map



X Index: 82

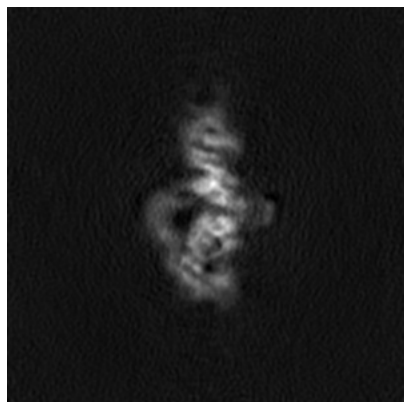


Y Index: 81

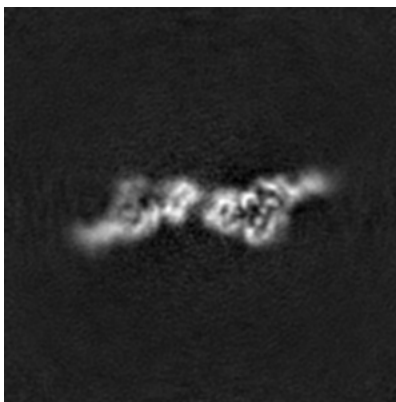


Z Index: 86

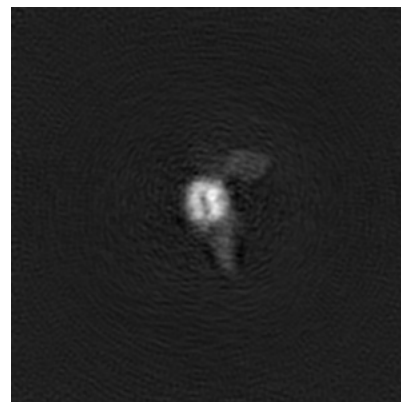
6.3.2 Raw map



X Index: 82



Y Index: 80

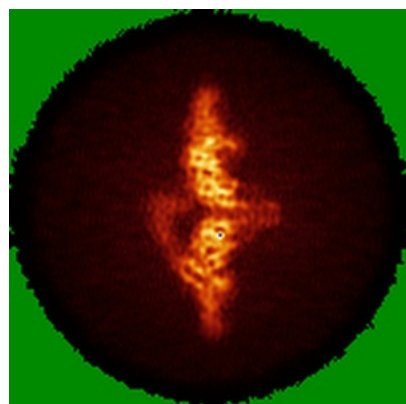


Z Index: 86

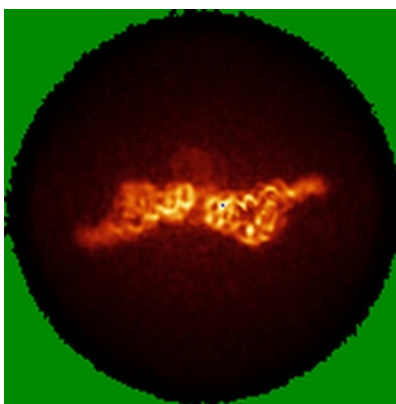
The images above show the largest variance slices of the map in three orthogonal directions.

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

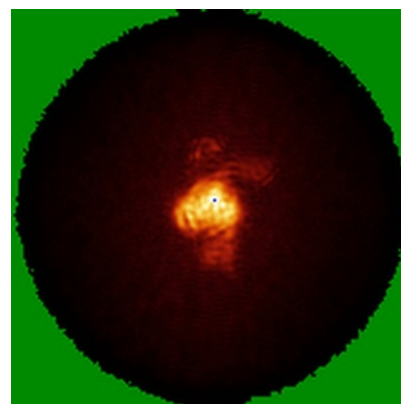
6.4.1 Primary map



X

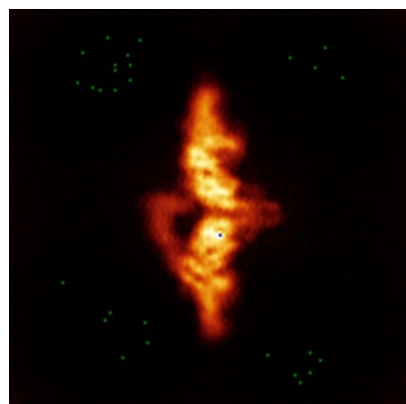


Y

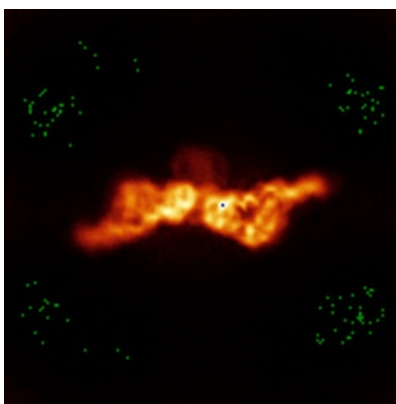


Z

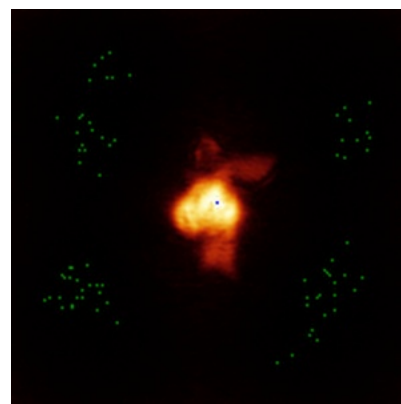
6.4.2 Raw map



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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

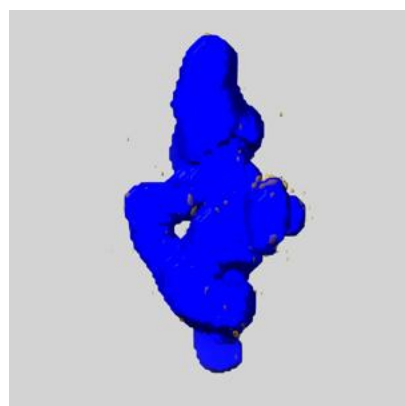
6.6 Mask visualisation [i](#)

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

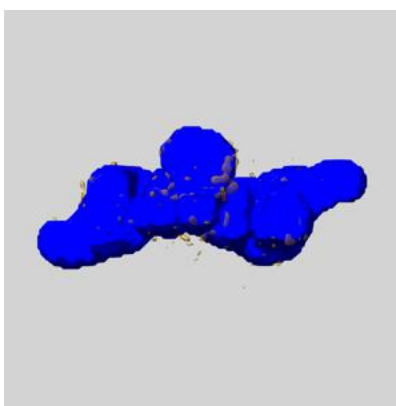
A mask typically either:

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

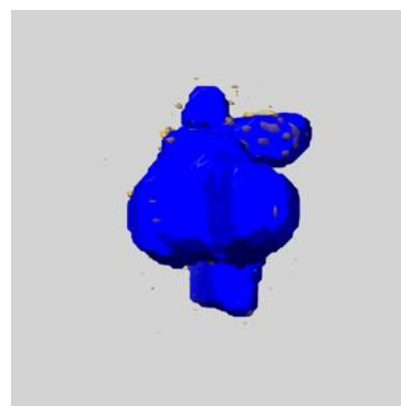
6.6.1 emd_47287_msk_1.map [i](#)



X



Y

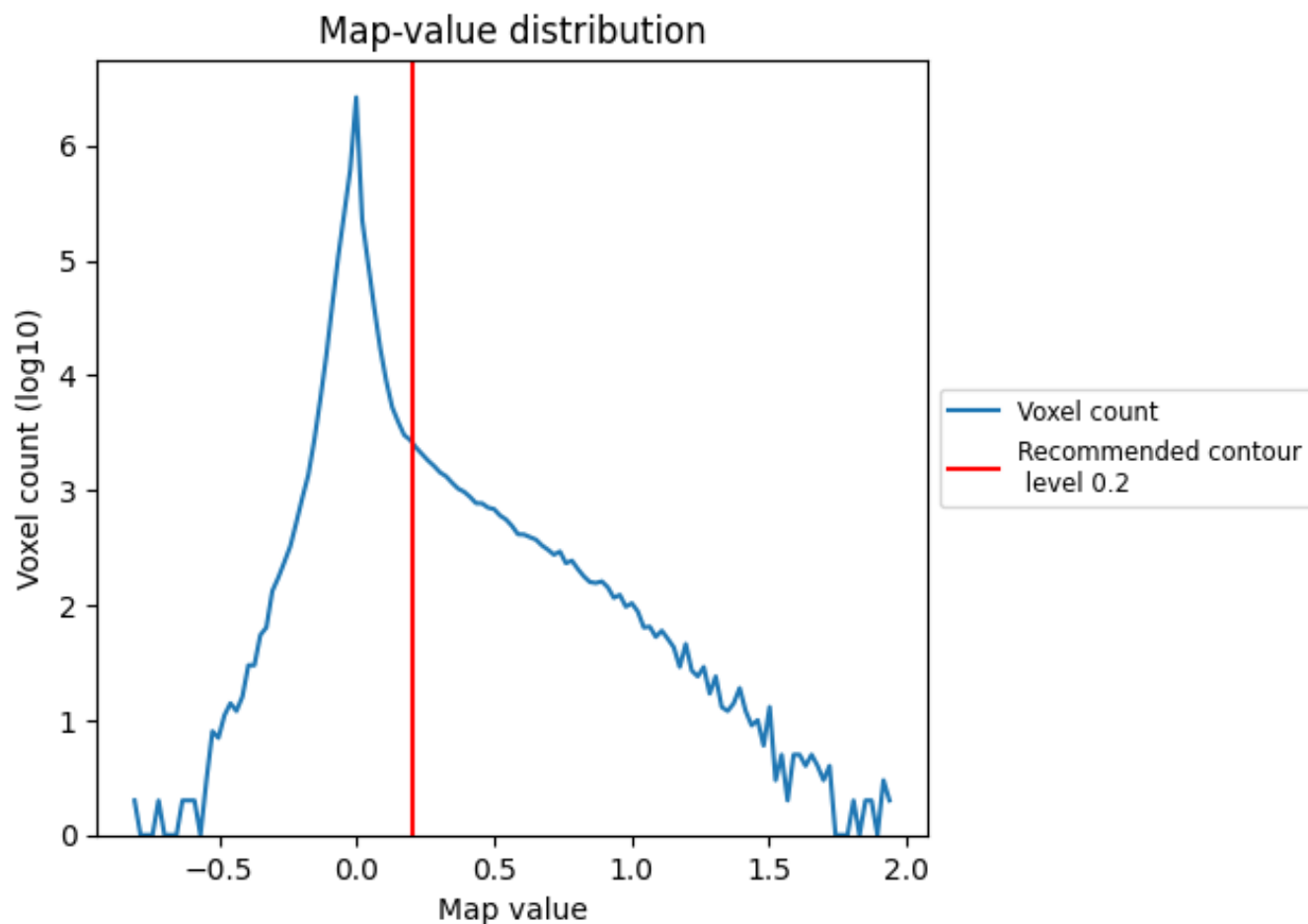


Z

7 Map analysis [i](#)

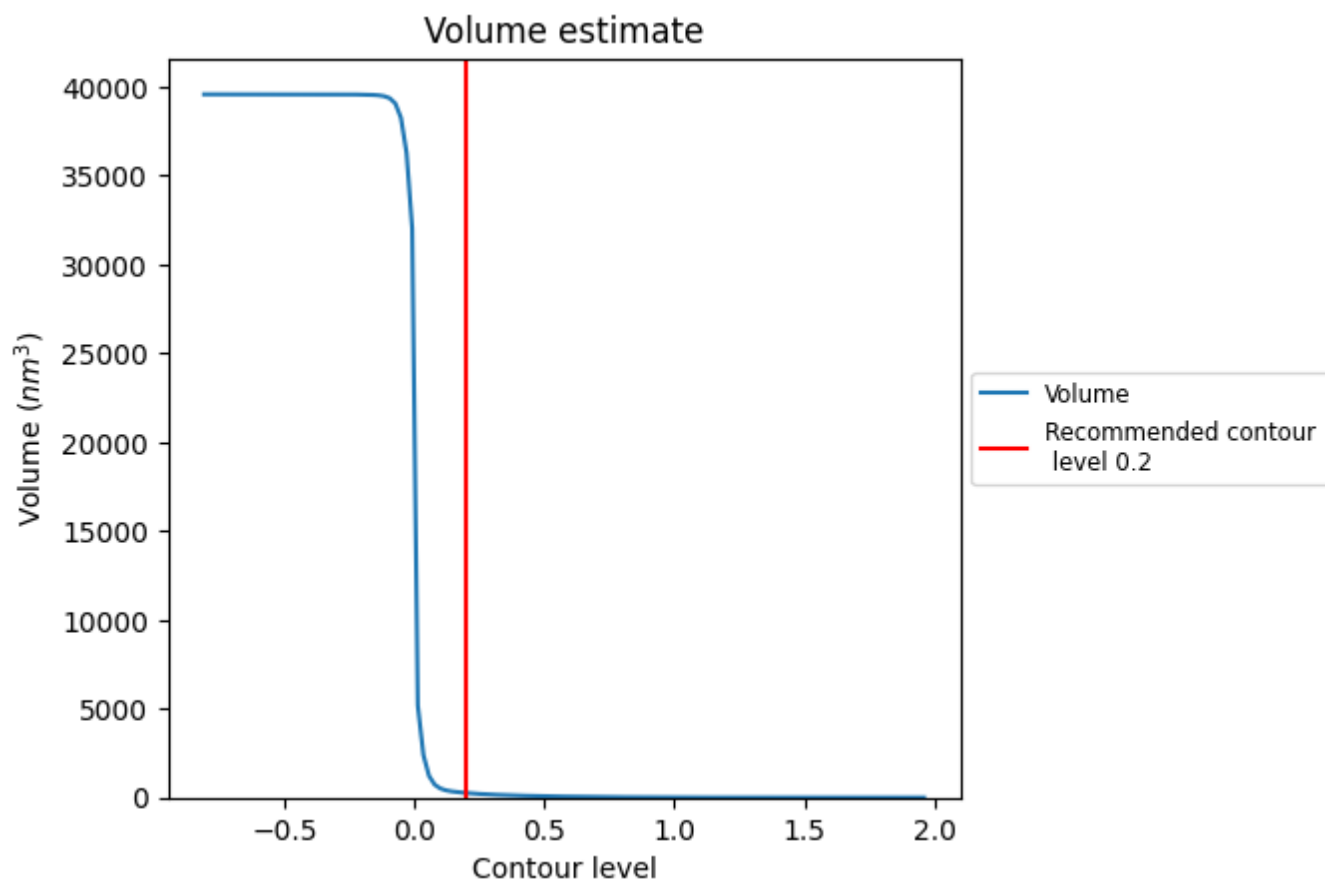
This section contains the results of statistical analysis of the map.

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.

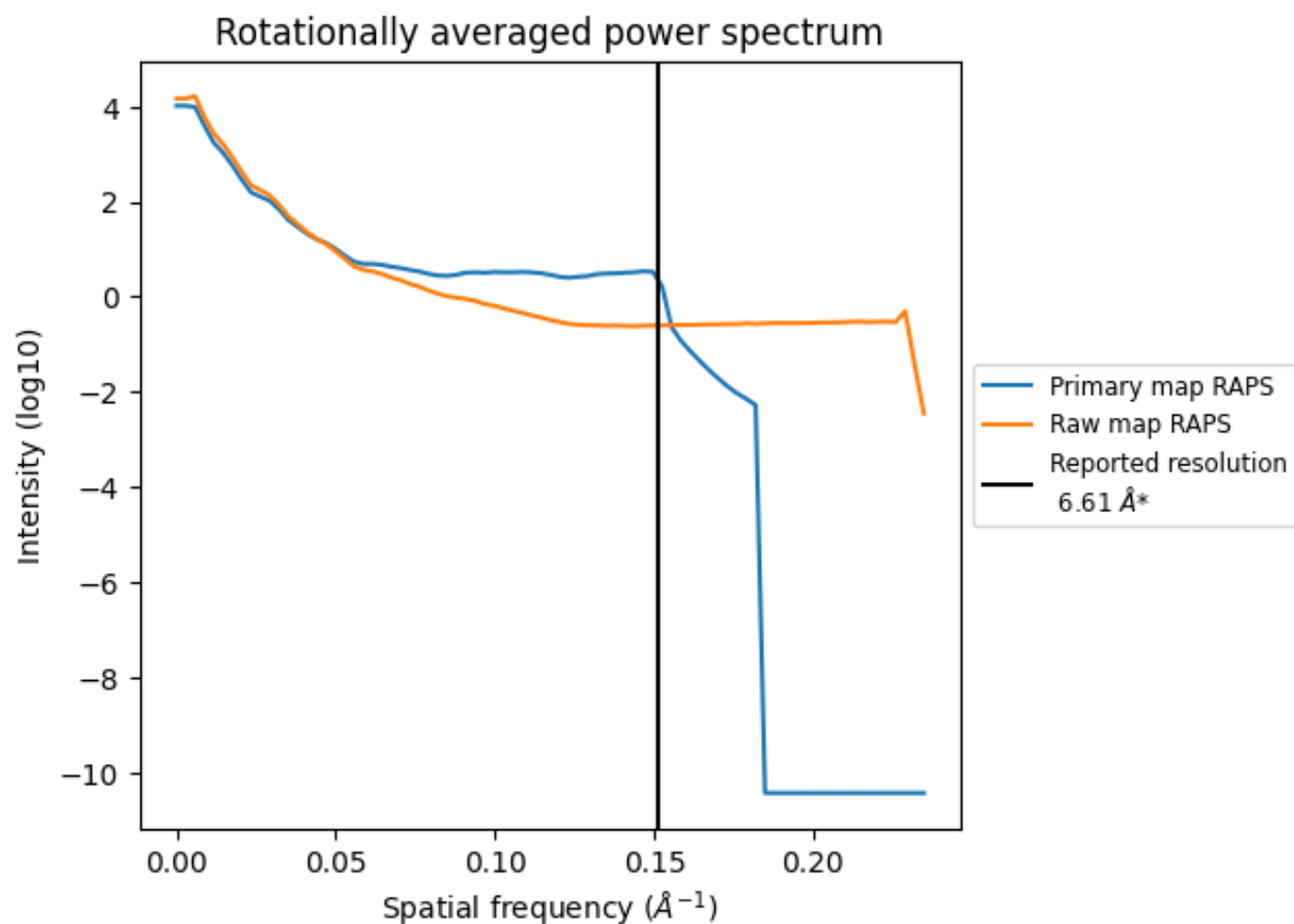
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 258 nm^3 ; this corresponds to an approximate mass of 233 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 ⓘ

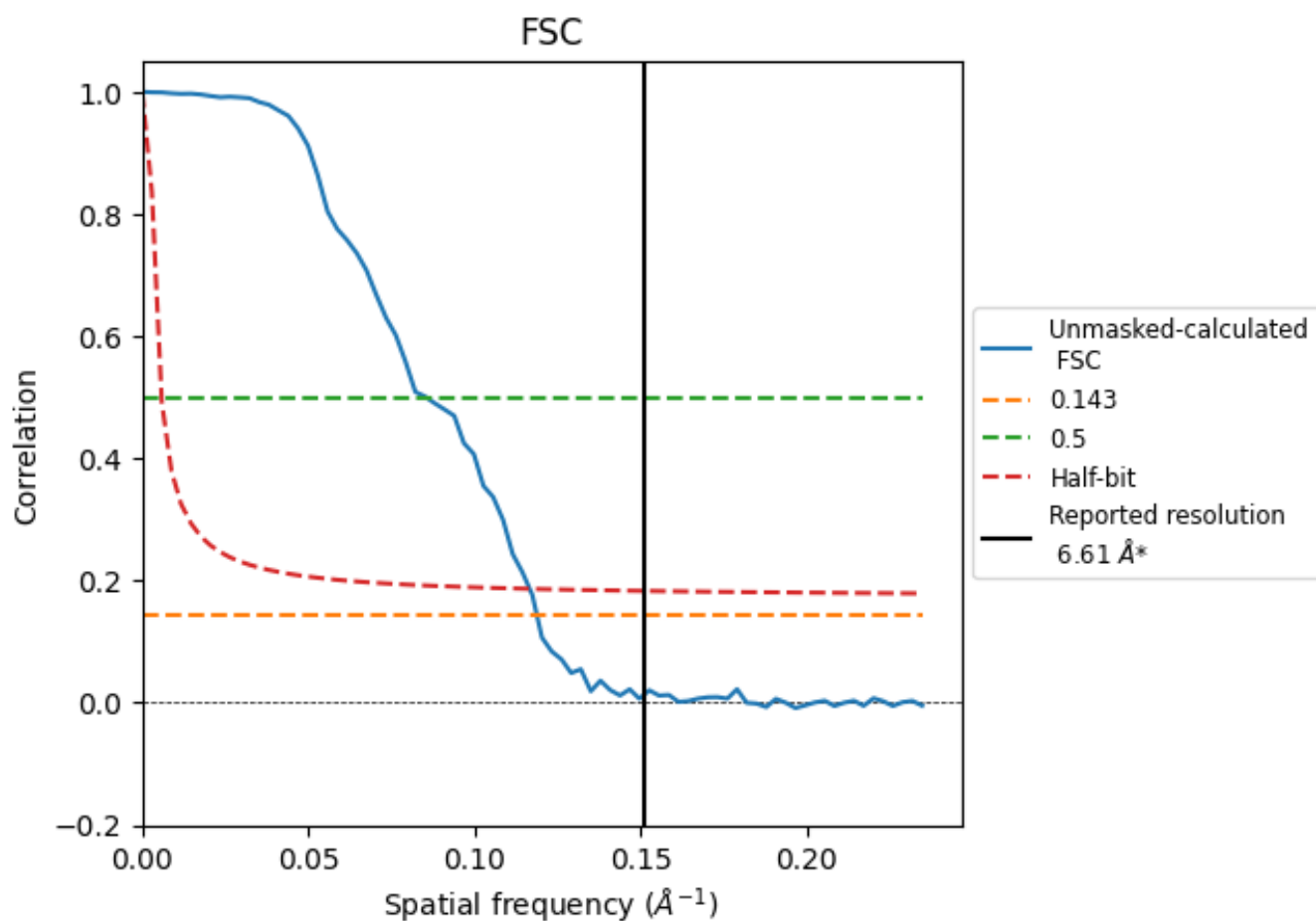


*Reported resolution corresponds to spatial frequency of 0.151 Å⁻¹

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 0.151 Å⁻¹

8.2 Resolution estimates [i](#)

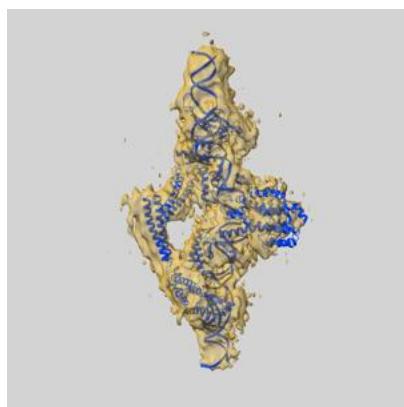
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.61	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.42	11.71	8.58

*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 8.42 differs from the reported value 6.61 by more than 10 %

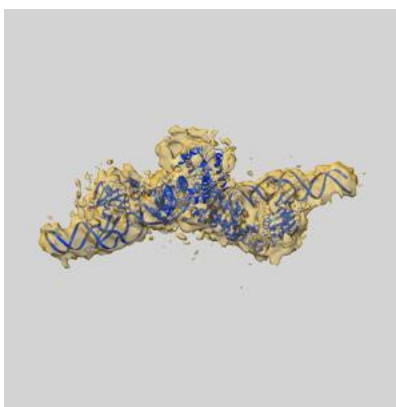
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47287 and PDB model 9DXG. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

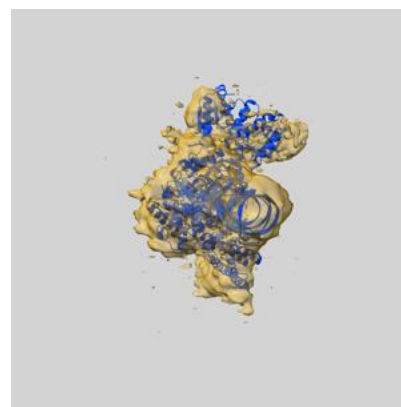
9.1 Map-model overlay [i](#)



X



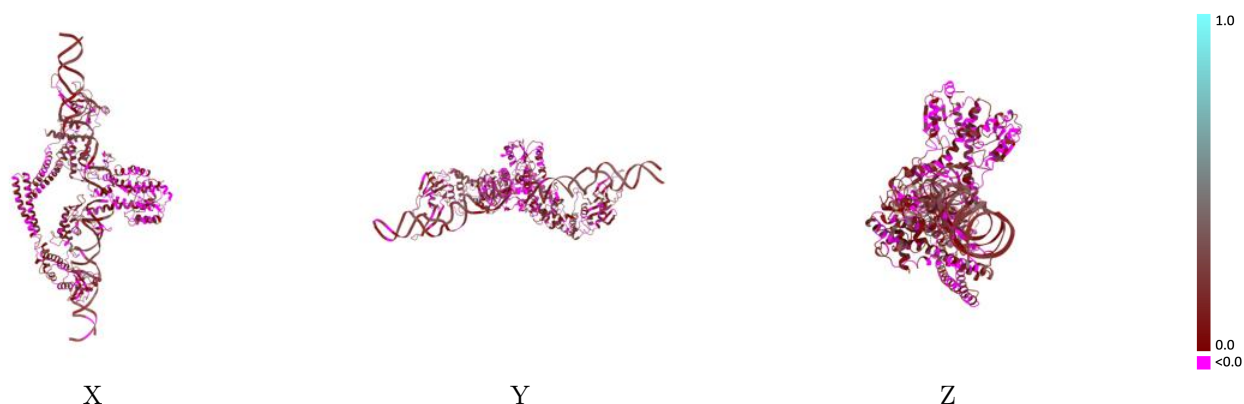
Y



Z

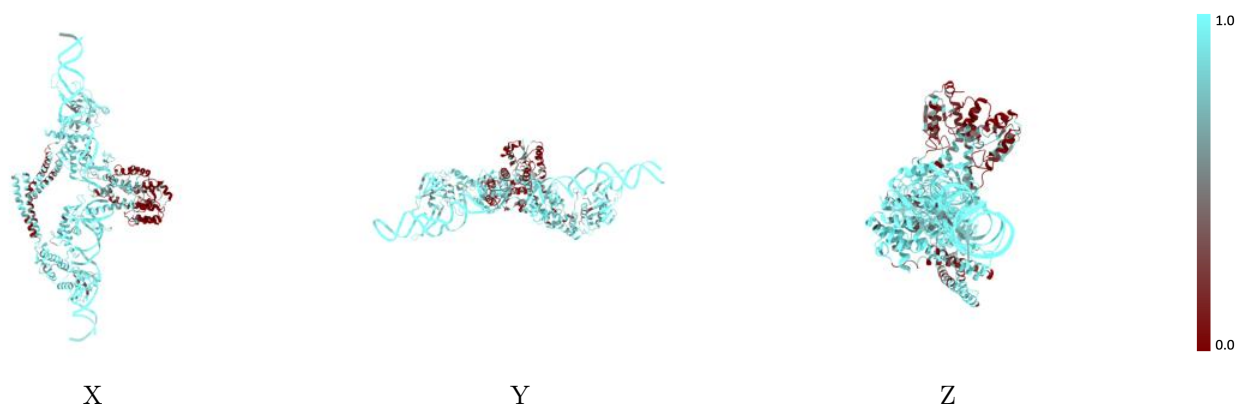
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



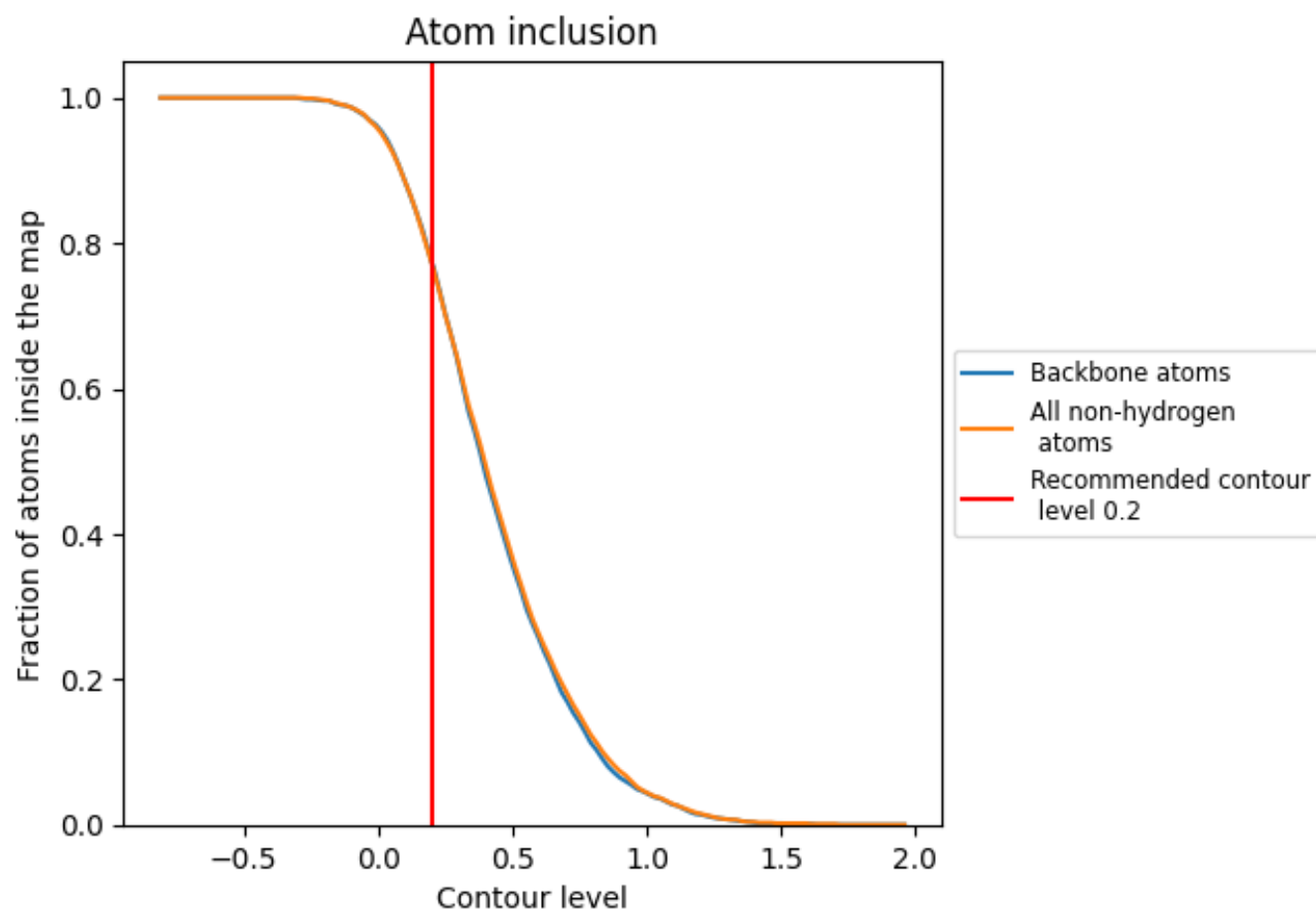
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 77% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7710	<div></div> 0.0980
A	<div></div> 0.7010	<div></div> 0.0640
B	<div></div> 0.9210	<div></div> 0.1240
C	<div></div> 0.6990	<div></div> 0.0740
D	<div></div> 0.9150	<div></div> 0.1130
E	<div></div> 0.9380	<div></div> 0.1630
F	<div></div> 0.9710	<div></div> 0.1740
G	<div></div> 0.9510	<div></div> 0.1970
H	<div></div> 0.9780	<div></div> 0.1920

1.0

0.0

<0.0