



# Full wwPDB EM Validation Report ⓘ

Nov 14, 2023 – 11:15 AM EST

PDB ID : 8FLJ  
EMDB ID : EMD-29280  
Title : Cas1-Cas2/3 integrase and IHF bound to CRISPR leader, repeat and foreign DNA  
Authors : Santiago-Frangos, A.; Henriques, W.S.; Wiegand, T.; Gauvin, C.; Buyukyoruk, M.; Neselu, K.; Eng, E.T.; Lander, G.C.; Wiedenheft, B.  
Deposited on : 2022-12-21  
Resolution : 3.48 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

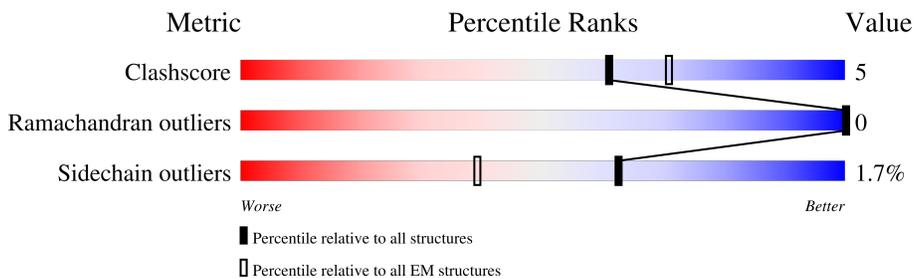
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.48 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.



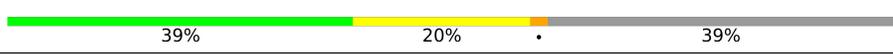
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	341	
1	B	341	
1	C	341	
1	D	341	
2	E	102	
2	G	102	
3	F	96	
3	H	96	

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Mol	Chain	Length	Quality of chain
4	I	139	 66% 34%
5	J	171	 68% 18% 13%
6	K	59	 39% 20% 39%
7	L	27	 70% 30%
8	M	1076	 83% 6% 10%
8	N	1076	 82% 6% 11%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 57091 atoms, of which 25297 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 Cas1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	310	4834	1540	2388	454	446	6	0	0
1	B	317	4940	1572	2442	462	458	6	0	0
1	C	303	4162	1376	1967	407	406	6	0	0
1	D	315	4920	1566	2434	460	454	6	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP Q02ML7
A	-15	TRP	-	expression tag	UNP Q02ML7
A	-14	SER	-	expression tag	UNP Q02ML7
A	-13	HIS	-	expression tag	UNP Q02ML7
A	-12	PRO	-	expression tag	UNP Q02ML7
A	-11	GLN	-	expression tag	UNP Q02ML7
A	-10	PHE	-	expression tag	UNP Q02ML7
A	-9	GLU	-	expression tag	UNP Q02ML7
A	-8	LYS	-	expression tag	UNP Q02ML7
A	-7	GLU	-	expression tag	UNP Q02ML7
A	-6	ASN	-	expression tag	UNP Q02ML7
A	-5	LEU	-	expression tag	UNP Q02ML7
A	-4	TYR	-	expression tag	UNP Q02ML7
A	-3	PHE	-	expression tag	UNP Q02ML7
A	-2	GLN	-	expression tag	UNP Q02ML7
A	-1	GLY	-	expression tag	UNP Q02ML7
A	0	SER	-	expression tag	UNP Q02ML7
B	-16	MET	-	expression tag	UNP Q02ML7
B	-15	TRP	-	expression tag	UNP Q02ML7
B	-14	SER	-	expression tag	UNP Q02ML7
B	-13	HIS	-	expression tag	UNP Q02ML7
B	-12	PRO	-	expression tag	UNP Q02ML7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLN	-	expression tag	UNP Q02ML7
B	-10	PHE	-	expression tag	UNP Q02ML7
B	-9	GLU	-	expression tag	UNP Q02ML7
B	-8	LYS	-	expression tag	UNP Q02ML7
B	-7	GLU	-	expression tag	UNP Q02ML7
B	-6	ASN	-	expression tag	UNP Q02ML7
B	-5	LEU	-	expression tag	UNP Q02ML7
B	-4	TYR	-	expression tag	UNP Q02ML7
B	-3	PHE	-	expression tag	UNP Q02ML7
B	-2	GLN	-	expression tag	UNP Q02ML7
B	-1	GLY	-	expression tag	UNP Q02ML7
B	0	SER	-	expression tag	UNP Q02ML7
C	-16	MET	-	expression tag	UNP Q02ML7
C	-15	TRP	-	expression tag	UNP Q02ML7
C	-14	SER	-	expression tag	UNP Q02ML7
C	-13	HIS	-	expression tag	UNP Q02ML7
C	-12	PRO	-	expression tag	UNP Q02ML7
C	-11	GLN	-	expression tag	UNP Q02ML7
C	-10	PHE	-	expression tag	UNP Q02ML7
C	-9	GLU	-	expression tag	UNP Q02ML7
C	-8	LYS	-	expression tag	UNP Q02ML7
C	-7	GLU	-	expression tag	UNP Q02ML7
C	-6	ASN	-	expression tag	UNP Q02ML7
C	-5	LEU	-	expression tag	UNP Q02ML7
C	-4	TYR	-	expression tag	UNP Q02ML7
C	-3	PHE	-	expression tag	UNP Q02ML7
C	-2	GLN	-	expression tag	UNP Q02ML7
C	-1	GLY	-	expression tag	UNP Q02ML7
C	0	SER	-	expression tag	UNP Q02ML7
D	-16	MET	-	expression tag	UNP Q02ML7
D	-15	TRP	-	expression tag	UNP Q02ML7
D	-14	SER	-	expression tag	UNP Q02ML7
D	-13	HIS	-	expression tag	UNP Q02ML7
D	-12	PRO	-	expression tag	UNP Q02ML7
D	-11	GLN	-	expression tag	UNP Q02ML7
D	-10	PHE	-	expression tag	UNP Q02ML7
D	-9	GLU	-	expression tag	UNP Q02ML7
D	-8	LYS	-	expression tag	UNP Q02ML7
D	-7	GLU	-	expression tag	UNP Q02ML7
D	-6	ASN	-	expression tag	UNP Q02ML7
D	-5	LEU	-	expression tag	UNP Q02ML7
D	-4	TYR	-	expression tag	UNP Q02ML7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	PHE	-	expression tag	UNP Q02ML7
D	-2	GLN	-	expression tag	UNP Q02ML7
D	-1	GLY	-	expression tag	UNP Q02ML7
D	0	SER	-	expression tag	UNP Q02ML7

- Molecule 2 is a protein called Integration host factor subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	E	94	Total	C	H	N	O	0	0
			680	276	216	94	94		
2	G	98	Total	C	H	N	O	0	0
			708	287	225	98	98		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP Q02NN5
E	2	PRO	-	expression tag	UNP Q02NN5
G	1	GLY	-	expression tag	UNP Q02NN5
G	2	PRO	-	expression tag	UNP Q02NN5

- Molecule 3 is a protein called Integration host factor subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	F	94	Total	C	H	N	O	0	0
			670	273	209	94	94		
3	H	94	Total	C	H	N	O	0	0
			670	273	209	94	94		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	GLY	-	expression tag	UNP Q02PW7
F	2	PRO	-	expression tag	UNP Q02PW7
H	1	GLY	-	expression tag	UNP Q02PW7
H	2	PRO	-	expression tag	UNP Q02PW7

- Molecule 4 is a DNA chain called CRISPR leader, sense strand of DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
4	I	139	4419	1361	1564	535	820	139	0	0

- Molecule 5 is a DNA chain called CRISPR leader and repeat, anti-sense strand of DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
5	J	148	4709	1450	1678	533	900	148	0	0

- Molecule 6 is a DNA chain called CRISPR repeat and prespacer, sense strand of DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	K	36	1145	352	408	128	221	36	0	0

- Molecule 7 is a DNA chain called Prespacer, anti-sense strand of DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	L	27	854	262	302	107	156	27	0	0

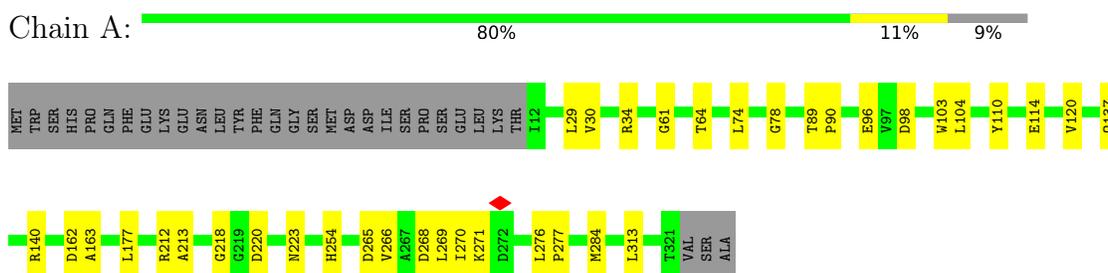
- Molecule 8 is a protein called CRISPR-associated nuclease/helicase Cas3 subtype I-F/YPEST.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	M	970	12232	4092	5636	1278	1205	21	0	0
8	N	954	12148	4057	5619	1259	1192	21	0	0

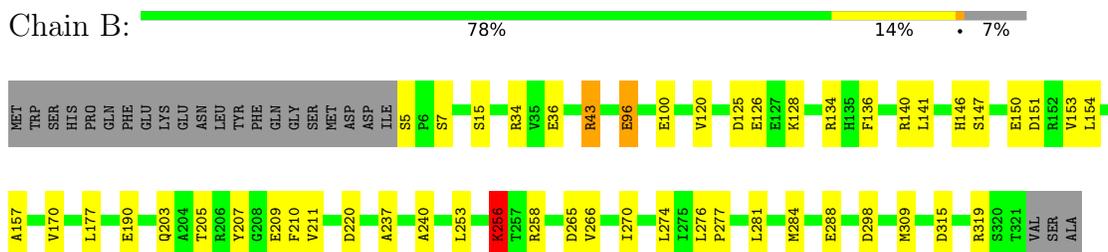
### 3 Residue-property plots [i](#)

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

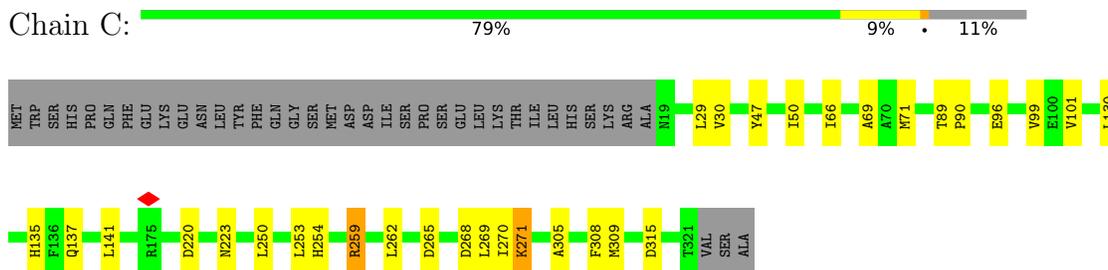
- Molecule 1: CRISPR-associated endonuclease Cas1



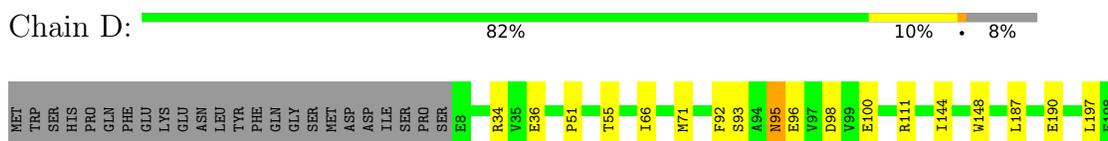
- Molecule 1: CRISPR-associated endonuclease Cas1



- Molecule 1: CRISPR-associated endonuclease Cas1

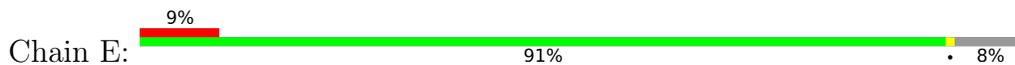


- Molecule 1: CRISPR-associated endonuclease Cas1

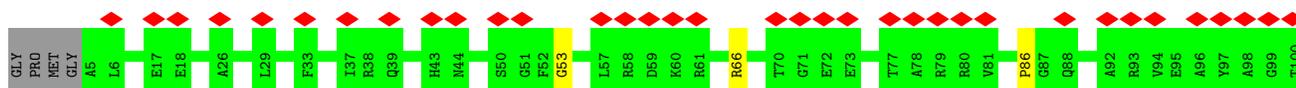




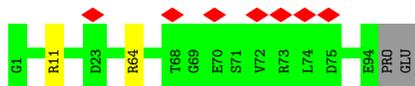
• Molecule 2: Integration host factor subunit alpha



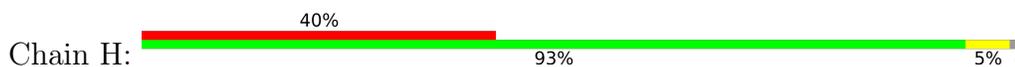
• Molecule 2: Integration host factor subunit alpha



• Molecule 3: Integration host factor subunit beta



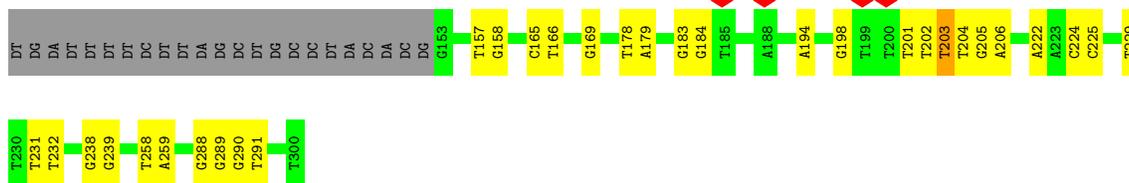
• Molecule 3: Integration host factor subunit beta



• Molecule 4: CRISPR leader, sense strand of DNA



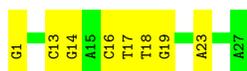
- Molecule 5: CRISPR leader and repeat, anti-sense strand of DNA



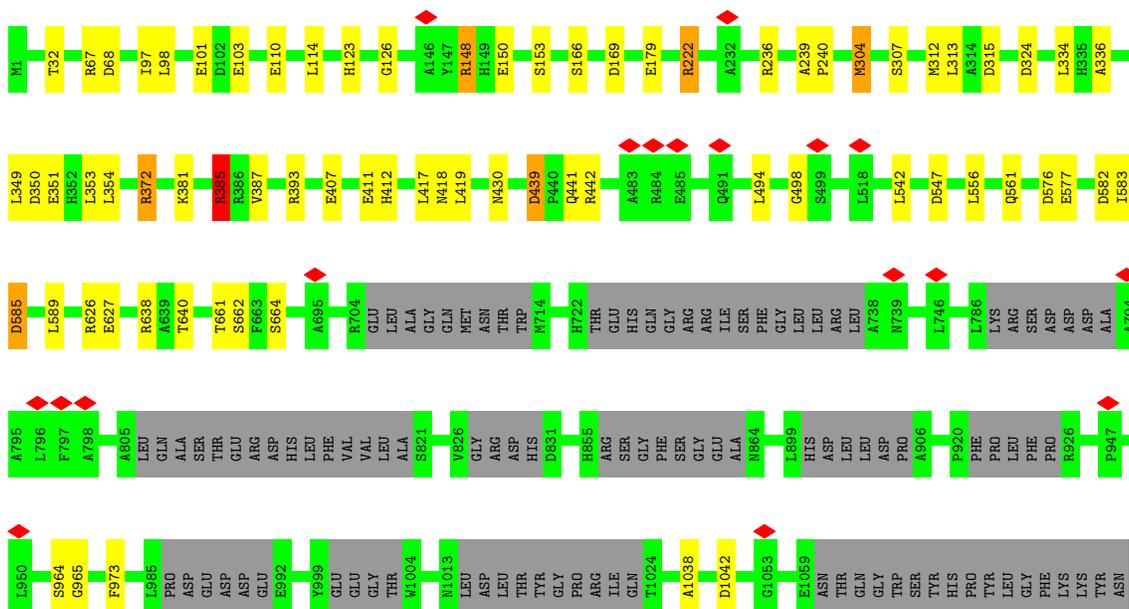
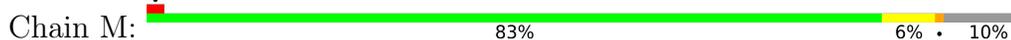
- Molecule 6: CRISPR repeat and prespacer, sense strand of DNA



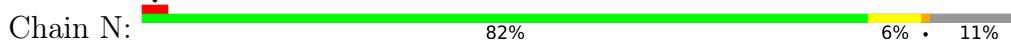
- Molecule 7: Prespacer, anti-sense strand of DNA



- Molecule 8: CRISPR-associated nuclease/helicase Cas3 subtype I-F/YPEST



- Molecule 8: CRISPR-associated nuclease/helicase Cas3 subtype I-F/YPEST





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	366794	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	69	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	46860	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	42.121	Depositor
Minimum map value	-22.553	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.6	Depositor
Map size (Å)	409.72803, 409.72803, 409.72803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	0.32	0/2498	0.59	1/3384 (0.0%)
1	B	0.40	1/2551 (0.0%)	0.60	2/3456 (0.1%)
1	C	0.35	1/2239 (0.0%)	0.68	5/3052 (0.2%)
1	D	0.33	0/2538	0.65	2/3438 (0.1%)
2	E	0.25	0/463	0.50	0/643
2	G	0.26	0/482	0.47	0/669
3	F	0.28	0/460	0.47	0/637
3	H	0.27	0/460	0.48	0/637
4	I	0.55	0/3208	0.91	0/4948
5	J	0.56	0/3395	0.97	1/5239 (0.0%)
6	K	0.61	0/824	0.99	1/1270 (0.1%)
7	L	0.65	0/620	0.90	1/953 (0.1%)
8	M	0.31	1/6702 (0.0%)	0.62	9/9133 (0.1%)
8	N	0.31	0/6637	0.61	7/9041 (0.1%)
All	All	0.40	3/33077 (0.0%)	0.72	29/46500 (0.1%)

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	C	0	1
3	F	0	2
3	H	0	3
8	M	0	1
8	N	0	2
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	GLU	CG-CD	-10.04	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	130	LEU	CG-CD2	-7.59	1.23	1.51
8	M	148	ARG	CB-CG	-5.02	1.39	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	67	ARG	CG-CD-NE	13.36	139.86	111.80
8	M	148	ARG	CG-CD-NE	-12.45	85.67	111.80
1	C	130	LEU	CA-CB-CG	10.51	139.46	115.30
8	M	385	ARG	CA-CB-CG	9.12	133.47	113.40
1	C	130	LEU	CB-CG-CD2	-9.10	95.52	111.00
1	C	130	LEU	CB-CG-CD1	8.75	125.87	111.00
1	C	271	LYS	CG-CD-CE	7.88	135.55	111.90
8	N	967	LEU	CB-CG-CD2	7.34	123.48	111.00
8	M	385	ARG	CG-CD-NE	7.24	127.00	111.80
8	M	304	MET	CG-SD-CE	7.16	111.65	100.20
1	A	104	LEU	CA-CB-CG	7.09	131.62	115.30
7	L	1	DG	OP1-P-OP2	-7.00	109.10	119.60
6	K	1	DG	OP1-P-OP2	-6.86	109.31	119.60
1	D	199	LYS	CD-CE-NZ	6.79	127.33	111.70
1	C	271	LYS	CD-CE-NZ	6.46	126.57	111.70
8	M	304	MET	CB-CG-SD	6.24	131.13	112.40
8	N	897	HIS	CB-CA-C	6.01	122.41	110.40
1	D	256	LYS	CG-CD-CE	5.88	129.55	111.90
8	N	458	GLN	CB-CG-CD	5.82	126.73	111.60
8	N	967	LEU	CB-CG-CD1	5.74	120.76	111.00
8	N	893	PRO	CA-N-CD	-5.73	103.48	111.50
8	M	67	ARG	CG-CD-NE	5.57	123.49	111.80
8	M	385	ARG	CB-CA-C	5.50	121.40	110.40
5	J	203	DT	O4'-C1'-N1	5.33	111.73	108.00
8	M	148	ARG	CB-CG-CD	5.25	125.25	111.60
1	B	96	GLU	CA-CB-CG	5.19	124.82	113.40
8	M	148	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	256	LYS	CA-CB-CG	5.08	124.57	113.40
8	N	65	ARG	CG-CD-NE	5.08	122.46	111.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	259	ARG	Sidechain
3	F	11	ARG	Peptide

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Mol	Chain	Res	Type	Group
3	F	64	ARG	Peptide
3	H	44	ARG	Peptide
3	H	53	PHE	Peptide
3	H	64	ARG	Peptide
8	M	372	ARG	Sidechain
8	N	372	ARG	Sidechain
8	N	65	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2446	2388	2409	24	0
1	B	2498	2442	2463	35	0
1	C	2195	1967	1987	18	0
1	D	2486	2434	2455	25	0
2	E	464	216	216	1	0
2	G	483	225	225	2	0
3	F	461	209	209	0	0
3	H	461	209	209	1	0
4	I	2855	1564	1564	42	0
5	J	3031	1678	1678	24	0
6	K	737	408	409	9	0
7	L	552	302	302	7	0
8	M	6596	5636	5634	50	0
8	N	6529	5619	5618	45	0
All	All	31794	25297	25378	264	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 (264) 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:D:96:GLU:N	1:D:96:GLU:OE1	2.08	0.87
8:M:582:ASP:OD1	8:M:583:ILE:N	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:407:GLU:OE1	8:N:407:GLU:N	2.09	0.85
4:I:107:DT:O2	5:J:194:DA:N7	2.10	0.84
1:C:305:ALA:O	1:C:309:MET:HG3	1.78	0.83
1:A:212:ARG:NH1	1:A:213:ALA:O	2.13	0.81
1:D:270:ILE:HD11	1:D:305:ALA:HB1	1.62	0.81
8:N:372:ARG:O	8:N:372:ARG:NH1	2.13	0.81
1:D:66:ILE:HD13	1:D:71:MET:SD	2.21	0.80
1:B:237:ALA:HA	1:B:309:MET:SD	2.22	0.79
8:M:412:HIS:O	8:M:626:ARG:NE	2.14	0.79
1:B:126:GLU:OE1	1:B:126:GLU:N	2.20	0.73
8:M:372:ARG:HD2	8:M:372:ARG:O	1.89	0.72
1:A:114:GLU:OE1	1:A:114:GLU:N	2.23	0.70
8:M:411:GLU:O	8:M:638:ARG:NH1	2.27	0.68
8:M:148:ARG:HH22	8:M:222:ARG:CZ	2.06	0.67
8:M:148:ARG:HH12	8:M:222:ARG:HD3	1.60	0.67
8:N:514:PHE:O	8:N:535:ARG:NH2	2.28	0.65
1:C:268:ASP:HA	1:C:271:LYS:HD3	1.77	0.65
1:D:34:ARG:NH1	1:D:36:GLU:OE2	2.30	0.65
8:M:407:GLU:N	8:M:407:GLU:OE1	2.30	0.65
8:N:577:GLU:N	8:N:577:GLU:OE1	2.30	0.64
1:B:5:SER:OG	1:B:7:SER:O	2.14	0.64
8:M:166:SER:N	8:M:169:ASP:OD2	2.29	0.64
8:N:385:ARG:NH1	8:N:386:ARG:O	2.30	0.63
8:N:63:TRP:CH2	8:N:65:ARG:HD3	2.34	0.63
8:N:462:ALA:O	8:N:466:ARG:HG3	1.99	0.63
8:M:32:THR:HG21	8:N:32:THR:HG21	1.81	0.62
1:A:162:ASP:OD1	1:A:163:ALA:N	2.33	0.62
1:C:137:GLN:O	1:C:141:LEU:HD22	2.00	0.62
8:M:372:ARG:HG2	8:M:442:ARG:NH2	2.16	0.61
1:A:34:ARG:NE	8:N:110:GLU:OE2	2.28	0.60
1:B:270:ILE:HD11	1:B:274:LEU:HD12	1.83	0.60
1:D:148:TRP:HZ3	1:D:200:LEU:HD11	1.66	0.60
1:B:96:GLU:N	1:B:96:GLU:OE1	2.35	0.59
1:A:254:HIS:ND1	1:A:265:ASP:OD1	2.29	0.59
1:D:306:LEU:HA	1:D:309:MET:HE2	1.83	0.59
8:M:179:GLU:N	8:M:179:GLU:OE1	2.36	0.59
1:A:89:THR:OG1	1:A:90:PRO:HD3	2.03	0.58
1:A:220:ASP:OD1	1:A:220:ASP:N	2.36	0.58
8:N:350:ASP:OD1	8:N:351:GLU:N	2.36	0.58
1:B:266:VAL:CG1	1:B:309:MET:SD	2.92	0.58
8:N:648:ASP:OD2	8:N:674:ARG:NH1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LEU:N	1:B:265:ASP:OD2	2.35	0.57
8:M:150:GLU:OE1	8:M:150:GLU:N	2.32	0.57
1:D:253:LEU:N	1:D:265:ASP:OD2	2.37	0.57
8:M:584:ASP:N	8:M:584:ASP:OD1	2.38	0.57
8:N:403:MET:SD	8:N:406:ARG:NH1	2.78	0.57
8:N:219:SER:O	8:N:219:SER:OG	2.20	0.56
1:C:96:GLU:OE1	1:C:96:GLU:N	2.39	0.56
8:N:372:ARG:C	8:N:372:ARG:HH11	2.09	0.56
8:N:561:GLN:N	8:N:561:GLN:OE1	2.39	0.56
8:M:148:ARG:NH1	8:M:222:ARG:HD3	2.20	0.56
8:M:964:SER:OG	8:M:965:GLY:N	2.39	0.56
8:M:577:GLU:OE2	8:M:577:GLU:N	2.40	0.55
8:M:123:HIS:NE2	8:M:315:ASP:OD2	2.38	0.55
8:N:545:THR:OG1	8:N:547:ASP:HB2	2.07	0.55
1:D:205:THR:HG22	1:D:284:MET:HG3	1.88	0.55
1:B:240:ALA:CB	1:B:309:MET:SD	2.95	0.55
1:C:253:LEU:N	1:C:265:ASP:OD2	2.35	0.55
1:B:209:GLU:N	1:B:209:GLU:OE1	2.41	0.54
1:D:95:ASN:OD1	1:D:96:GLU:OE1	2.26	0.54
8:N:648:ASP:OD1	8:N:649:GLU:N	2.40	0.54
1:D:111:ARG:N	1:D:111:ARG:HD2	2.22	0.54
8:N:641:GLU:OE1	8:N:641:GLU:N	2.41	0.54
4:I:114:DC:H2'	4:I:115:DA:C8	2.44	0.53
4:I:135:DA:H2'	4:I:136:DG:C1'	2.38	0.53
1:C:254:HIS:ND1	1:C:265:ASP:OD1	2.38	0.53
8:M:336:ALA:HB2	8:M:349:LEU:HD13	1.91	0.53
4:I:111:DA:H2''	4:I:112:DA:H8	1.74	0.52
1:D:187:LEU:HA	1:D:190:GLU:HG3	1.92	0.52
8:M:1038:ALA:O	8:M:1042:ASP:N	2.43	0.52
1:B:205:THR:HG22	1:B:205:THR:O	2.10	0.52
8:M:350:ASP:O	8:M:354:LEU:HG	2.09	0.52
1:C:30:VAL:O	8:M:103:GLU:HB2	2.10	0.51
1:B:205:THR:HG22	1:B:284:MET:HG3	1.93	0.51
5:J:165:DC:H2'	5:J:166:DT:C6	2.45	0.51
1:D:51:PRO:O	1:D:55:THR:HG23	2.11	0.51
1:B:266:VAL:HG11	1:B:309:MET:SD	2.51	0.51
4:I:136:DG:H2''	4:I:137:DC:C6	2.46	0.51
8:N:321:LEU:HD12	8:N:322:PRO:HD2	1.92	0.51
3:H:50:PHE:O	3:H:85:GLY:N	2.34	0.51
8:N:961:ALA:HB1	8:N:967:LEU:HD23	1.93	0.51
1:B:288:GLU:HA	1:B:288:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:871:ASN:O	8:N:874:SER:N	2.42	0.50
1:D:214:LYS:HD2	1:D:214:LYS:O	2.12	0.50
1:B:34:ARG:NH1	1:B:36:GLU:OE2	2.44	0.50
4:I:134:DG:C2	4:I:135:DA:C5	3.00	0.50
8:N:667:HIS:O	8:N:671:VAL:HG23	2.11	0.50
7:L:18:DT:H4'	7:L:19:DG:OP1	2.11	0.50
1:A:74:LEU:O	1:A:78:GLY:N	2.45	0.50
6:K:1:DG:C8	6:K:2:DT:H72	2.47	0.50
1:B:125:ASP:HB3	1:B:128:LYS:HG3	1.93	0.50
1:D:98:ASP:OD1	1:D:215:ARG:NH2	2.44	0.50
4:I:11:DC:H4'	4:I:12:DC:OP1	2.12	0.50
1:B:141:LEU:HD12	1:B:170:VAL:HG13	1.93	0.49
8:M:110:GLU:O	8:M:114:LEU:HD22	2.12	0.49
8:N:547:ASP:OD1	8:N:973:PHE:HE2	1.95	0.49
1:A:103:TRP:O	1:B:256:LYS:HB3	2.12	0.49
8:N:582:ASP:OD1	8:N:582:ASP:C	2.50	0.49
1:B:146:HIS:ND1	1:B:150:GLU:OE1	2.43	0.49
1:B:240:ALA:HB3	1:B:309:MET:SD	2.52	0.49
1:B:266:VAL:HG13	1:B:309:MET:HG3	1.94	0.49
1:C:99:VAL:HG23	1:C:101:VAL:HG13	1.95	0.49
8:M:239:ALA:HB3	8:M:240:PRO:HD3	1.95	0.49
8:N:585:ASP:OD1	8:N:973:PHE:CD1	2.66	0.49
1:D:144:ILE:HD11	1:D:197:LEU:HD22	1.94	0.48
1:B:100:GLU:N	1:B:100:GLU:OE1	2.46	0.48
1:A:96:GLU:HA	1:A:96:GLU:OE2	2.14	0.48
4:I:133:DG:C2	4:I:134:DG:C4	3.01	0.48
5:J:290:DG:H2'	5:J:291:DT:H72	1.95	0.48
8:N:455:LEU:HD11	8:N:459:THR:HB	1.95	0.48
1:A:218:GLY:HA3	1:A:223:ASN:HD22	1.77	0.48
2:E:51:GLY:N	4:I:35:DA:OP1	2.46	0.48
4:I:75:DG:C2	4:I:76:DG:C5	3.02	0.48
8:M:148:ARG:HH22	8:M:222:ARG:NE	2.11	0.48
1:A:284:MET:SD	1:A:284:MET:C	2.92	0.48
1:D:92:PHE:CD1	1:D:93:SER:N	2.82	0.48
7:L:16:DC:C6	7:L:17:DT:H72	2.48	0.48
1:B:96:GLU:OE1	1:B:96:GLU:CA	2.59	0.48
1:B:298:ASP:OD2	8:N:69:HIS:NE2	2.40	0.48
1:A:120:VAL:HG21	1:B:120:VAL:CG2	2.43	0.48
4:I:97:DA:C2	5:J:205:DG:C2	3.02	0.48
1:A:266:VAL:O	1:A:269:LEU:HD12	2.13	0.48
4:I:104:DG:C2	5:J:198:DG:C2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:288:DG:C2	5:J:289:DG:C5	3.03	0.47
8:M:68:ASP:O	8:M:68:ASP:OD2	2.32	0.47
8:M:418:ASN:ND2	8:M:430:ASN:OD1	2.45	0.47
1:B:151:ASP:OD1	1:B:153:VAL:N	2.47	0.47
1:C:269:LEU:O	1:C:270:ILE:HD13	2.14	0.47
1:D:200:LEU:HD12	1:D:201:ALA:N	2.29	0.47
1:D:214:LYS:HD2	1:D:215:ARG:HG2	1.95	0.47
1:D:220:ASP:OD1	1:D:220:ASP:C	2.53	0.47
8:M:494:LEU:O	8:M:498:GLY:N	2.48	0.47
8:N:940:LEU:O	8:N:940:LEU:HD12	2.15	0.47
1:C:66:ILE:HD13	1:C:71:MET:SD	2.55	0.47
4:I:27:DT:C6	4:I:28:DT:H72	2.50	0.47
1:C:269:LEU:HD21	1:C:308:PHE:CE2	2.50	0.47
4:I:113:DT:H4'	4:I:114:DC:OP2	2.14	0.47
8:M:324:ASP:N	8:M:351:GLU:OE2	2.44	0.47
8:M:661:THR:O	8:M:664:SER:OG	2.29	0.47
6:K:20:DA:H2'	6:K:21:DG:C8	2.50	0.46
4:I:122:DT:H1'	4:I:123:DA:C5	2.49	0.46
8:N:547:ASP:OD1	8:N:973:PHE:CE2	2.68	0.46
4:I:113:DT:H2''	4:I:114:DC:C6	2.51	0.46
8:M:126:GLY:N	8:M:153:SER:OG	2.42	0.46
1:A:212:ARG:NH2	6:K:26:DA:N7	2.63	0.46
2:G:66:ARG:O	4:I:115:DA:N3	2.49	0.46
4:I:11:DC:H2''	4:I:12:DC:O5'	2.16	0.46
4:I:107:DT:C2	5:J:194:DA:N7	2.83	0.46
4:I:133:DG:C2	5:J:169:DG:C2	3.03	0.46
1:A:30:VAL:O	8:N:103:GLU:HB2	2.16	0.46
4:I:108:DC:C2	4:I:109:DG:C5	3.04	0.46
1:D:100:GLU:OE1	1:D:100:GLU:N	2.49	0.46
1:D:268:ASP:OD1	1:D:268:ASP:N	2.48	0.45
8:N:642:ILE:N	8:N:642:ILE:HD12	2.32	0.45
8:N:216:LEU:HD11	8:N:307:SER:HB2	1.98	0.45
1:D:92:PHE:CD1	1:D:92:PHE:C	2.90	0.45
1:D:95:ASN:OD1	1:D:95:ASN:N	2.46	0.45
4:I:124:DT:O3'	4:I:125:DA:C8	2.70	0.45
8:M:97:ILE:HG22	8:M:98:LEU:N	2.31	0.45
8:N:641:GLU:HG2	8:N:641:GLU:O	2.17	0.45
7:L:18:DT:H2''	7:L:19:DG:O5'	2.17	0.45
5:J:203:DT:H2''	5:J:204:DT:H72	1.98	0.45
8:M:582:ASP:OD1	8:M:582:ASP:C	2.55	0.45
8:N:887:PHE:O	8:N:936:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:118:DC:H2'	4:I:119:DG:C8	2.52	0.45
4:I:135:DA:H2'	4:I:136:DG:O4'	2.16	0.45
8:M:304:MET:O	8:M:307:SER:OG	2.25	0.45
4:I:92:DA:H2''	4:I:93:DA:C8	2.52	0.45
4:I:111:DA:H2''	4:I:112:DA:C8	2.52	0.44
4:I:113:DT:H2''	4:I:114:DC:C5	2.52	0.44
8:M:585:ASP:OD1	8:M:973:PHE:CD1	2.70	0.44
6:K:27:DT:O2	6:K:27:DT:O4'	2.35	0.44
8:M:417:LEU:HB3	8:M:419:LEU:HD23	1.99	0.44
1:B:140:ARG:NH1	1:B:190:GLU:OE1	2.39	0.44
8:N:477:LEU:HD23	8:N:548:HIS:CG	2.53	0.44
1:A:120:VAL:HG21	1:B:120:VAL:HG21	1.98	0.44
8:N:14:LEU:HD21	8:N:18:ARG:CZ	2.48	0.44
8:M:349:LEU:O	8:M:353:LEU:HD23	2.18	0.44
4:I:8:DC:H2''	4:I:9:DG:C8	2.53	0.44
4:I:73:DG:N2	5:J:229:DT:O2	2.50	0.44
5:J:157:DT:H2''	5:J:158:DG:C8	2.52	0.44
8:N:312:MET:O	8:N:313:LEU:C	2.51	0.44
8:N:467:LEU:O	8:N:469:LEU:HD23	2.18	0.44
1:B:315:ASP:O	1:B:319:ARG:N	2.45	0.44
5:J:183:DG:C6	5:J:184:DG:C6	3.06	0.44
8:M:334:LEU:CB	8:M:349:LEU:HD23	2.48	0.44
1:A:276:LEU:HB3	1:A:277:PRO:HD3	1.99	0.43
5:J:203:DT:H2''	5:J:204:DT:C7	2.48	0.43
8:N:10:GLU:HB2	8:N:56:ASN:HB3	2.00	0.43
1:B:134:ARG:NH1	1:B:177:LEU:O	2.51	0.43
7:L:18:DT:C2'	7:L:19:DG:C8	3.01	0.43
8:M:627:GLU:HG3	8:M:640:THR:HG21	2.01	0.43
6:K:11:DT:H2'	6:K:12:DT:C7	2.49	0.43
6:K:29:DT:H2'	6:K:30:DT:H72	1.99	0.43
1:B:207:TYR:OH	1:B:220:ASP:OD2	2.30	0.43
1:B:276:LEU:HB3	1:B:277:PRO:HD3	2.01	0.43
7:L:17:DT:H2'	7:L:18:DT:H71	2.01	0.43
7:L:23:DA:H4'	7:L:23:DA:OP1	2.19	0.43
8:N:119:ALA:O	8:N:123:HIS:N	2.52	0.43
8:N:546:ILE:HD11	8:N:575:LEU:HD22	2.00	0.43
5:J:178:DT:O3'	5:J:179:DA:C8	2.71	0.43
5:J:203:DT:H1'	5:J:204:DT:C6	2.53	0.43
8:M:439:ASP:OD1	8:M:441:GLN:N	2.51	0.43
1:A:137:GLN:CB	1:A:177:LEU:HD21	2.49	0.43
1:D:187:LEU:O	1:D:190:GLU:OE2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:NE	1:B:43:ARG:HA	2.34	0.43
1:A:61:GLY:O	1:A:64:THR:HG22	2.18	0.42
8:M:372:ARG:HG2	8:M:442:ARG:CZ	2.49	0.42
1:C:89:THR:HG23	1:C:90:PRO:HD3	2.01	0.42
1:A:266:VAL:HG22	1:A:313:LEU:HD11	2.02	0.42
7:L:13:DC:H2''	7:L:14:DG:C8	2.54	0.42
8:M:236:ARG:O	8:M:240:PRO:HD2	2.19	0.42
1:B:151:ASP:OD1	1:B:154:LEU:N	2.43	0.42
1:C:220:ASP:OD1	1:C:223:ASN:ND2	2.48	0.42
5:J:222:DA:OP1	8:M:393:ARG:HD3	2.19	0.42
4:I:99:DA:H2''	4:I:100:DA:C8	2.55	0.42
4:I:135:DA:H2'	4:I:136:DG:H1'	2.02	0.42
4:I:14:DT:H2'	4:I:15:DT:H72	2.02	0.42
5:J:258:DT:H2''	5:J:259:DA:C8	2.54	0.42
8:M:350:ASP:OD1	8:M:351:GLU:N	2.53	0.42
1:C:30:VAL:HG11	1:C:69:ALA:HB1	2.01	0.42
1:C:47:TYR:O	1:C:50:ILE:HG13	2.20	0.42
4:I:92:DA:H1'	4:I:93:DA:C8	2.55	0.42
8:M:101:GLU:OE1	8:M:372:ARG:NH1	2.45	0.42
1:B:157:ALA:HB1	1:B:281:LEU:HD21	2.02	0.41
1:C:250:LEU:O	1:C:262:LEU:HD12	2.20	0.41
8:N:411:GLU:O	8:N:638:ARG:NH1	2.53	0.41
1:D:111:ARG:N	1:D:111:ARG:CD	2.84	0.41
4:I:120:DG:C2'	4:I:121:DT:H72	2.51	0.41
5:J:231:DT:H4'	5:J:232:DT:OP1	2.20	0.41
8:M:387:VAL:HG11	8:M:393:ARG:HA	2.02	0.41
6:K:12:DT:C6	6:K:13:DT:H72	2.55	0.41
8:M:439:ASP:OD1	8:M:442:ARG:N	2.43	0.41
8:N:110:GLU:HA	8:N:110:GLU:OE1	2.20	0.41
8:N:610:LEU:HD13	8:N:615:VAL:HG12	2.02	0.41
1:A:140:ARG:HD2	1:A:268:ASP:OD1	2.20	0.41
4:I:108:DC:H1'	4:I:109:DG:C8	2.55	0.41
8:M:547:ASP:OD1	8:M:547:ASP:N	2.53	0.41
5:J:205:DG:C4	5:J:206:DA:C8	3.08	0.41
5:J:224:DC:C2	5:J:225:DC:C5	3.09	0.41
1:C:135:HIS:NE2	1:C:315:ASP:OD2	2.49	0.41
4:I:28:DT:C2'	4:I:29:DT:H71	2.51	0.41
4:I:101:DA:C2	5:J:201:DT:O2	2.73	0.41
4:I:26:DA:C2'	4:I:27:DT:H71	2.51	0.41
5:J:205:DG:H4'	5:J:206:DA:OP1	2.21	0.41
1:B:210:PHE:CG	1:B:211:VAL:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:53:GLY:HA3	2:G:86:PRO:HA	2.02	0.40
4:I:18:DT:H2'	4:I:19:DT:H72	2.03	0.40
8:M:312:MET:O	8:M:313:LEU:C	2.58	0.40
8:N:10:GLU:OE2	8:N:10:GLU:HA	2.21	0.40
6:K:11:DT:H2'	6:K:12:DT:H72	2.04	0.40
1:A:270:ILE:O	1:A:271:LYS:C	2.60	0.40
1:C:89:THR:CG2	1:C:90:PRO:HD3	2.50	0.40
5:J:201:DT:H2''	5:J:202:DT:C6	2.56	0.40
5:J:238:DG:H4'	5:J:239:DG:OP1	2.21	0.40
1:A:98:ASP:N	1:A:98:ASP:OD1	2.54	0.40
6:K:34:DT:N3	6:K:35:DG:O6	2.53	0.40
8:M:381:LYS:O	8:M:385:ARG:HB3	2.21	0.40
4:I:23:DA:C4	4:I:24:DC:C5	3.10	0.40
4:I:25:DG:C2	4:I:26:DA:C4	3.10	0.40
4:I:124:DT:H1'	4:I:125:DA:N7	2.36	0.40
8:M:222:ARG:HG2	8:M:556:LEU:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/341 (90%)	292 (95%)	16 (5%)	0	100	100
1	B	315/341 (92%)	297 (94%)	18 (6%)	0	100	100
1	C	301/341 (88%)	290 (96%)	11 (4%)	0	100	100
1	D	313/341 (92%)	300 (96%)	13 (4%)	0	100	100
2	E	92/102 (90%)	90 (98%)	2 (2%)	0	100	100
2	G	96/102 (94%)	94 (98%)	2 (2%)	0	100	100
3	F	92/96 (96%)	88 (96%)	4 (4%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	92/96 (96%)	85 (92%)	7 (8%)	0	100	100
8	M	946/1076 (88%)	905 (96%)	41 (4%)	0	100	100
8	N	930/1076 (86%)	895 (96%)	35 (4%)	0	100	100
All	All	3485/3912 (89%)	3336 (96%)	149 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	248/277 (90%)	246 (99%)	2 (1%)	81	92
1	B	255/277 (92%)	248 (97%)	7 (3%)	44	72
1	C	190/277 (69%)	188 (99%)	2 (1%)	73	88
1	D	253/277 (91%)	250 (99%)	3 (1%)	71	87
8	M	494/885 (56%)	485 (98%)	9 (2%)	59	81
8	N	498/885 (56%)	488 (98%)	10 (2%)	55	79
All	All	1938/2878 (67%)	1905 (98%)	33 (2%)	62	82

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	110	TYR
1	B	15	SER
1	B	43	ARG
1	B	136	PHE
1	B	147	SER
1	B	203	GLN
1	B	256	LYS
1	B	258	ARG
1	C	29	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	259	ARG
1	D	95	ASN
1	D	214	LYS
1	D	296	CYS
8	M	222	ARG
8	M	385	ARG
8	M	439	ASP
8	M	542	LEU
8	M	561	GLN
8	M	576	ASP
8	M	585	ASP
8	M	589	LEU
8	M	662	SER
8	N	14	LEU
8	N	43	ASP
8	N	65	ARG
8	N	158	GLU
8	N	250	ASP
8	N	385	ARG
8	N	386	ARG
8	N	582	ASP
8	N	585	ASP
8	N	916	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

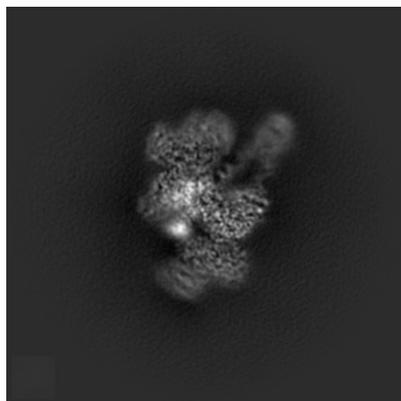
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29280. These allow visual inspection of the internal detail of the map and identification of artifacts.

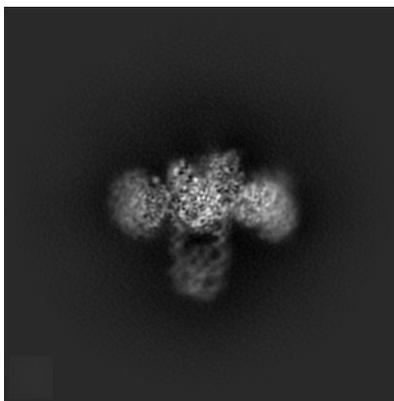
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

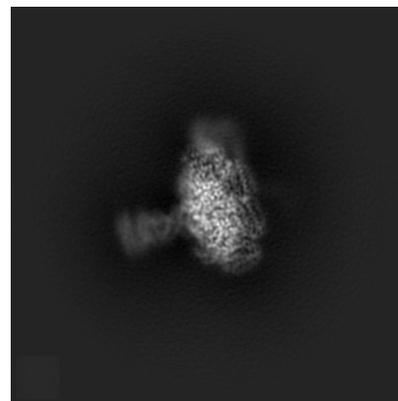
#### 6.1.1 Primary map



X

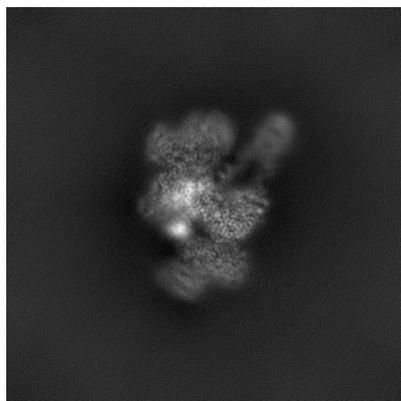


Y

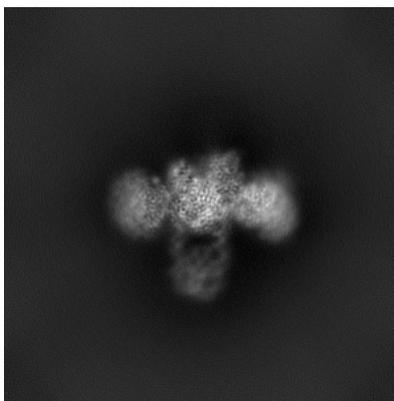


Z

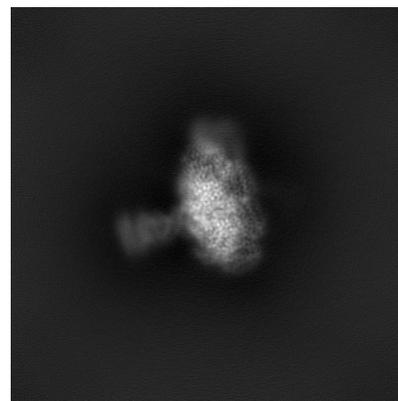
#### 6.1.2 Raw map



X



Y

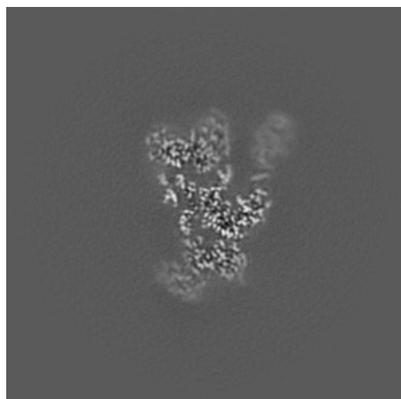


Z

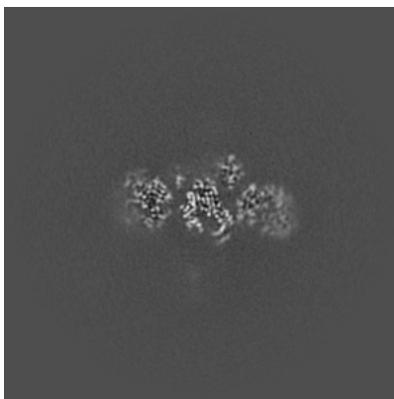
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

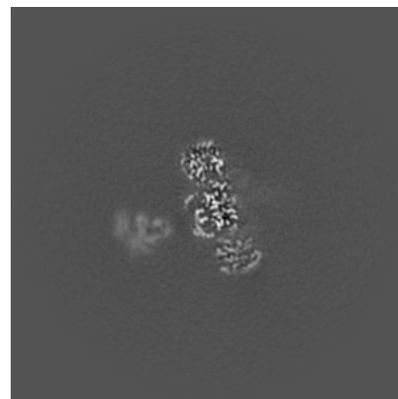
### 6.2.1 Primary map



X Index: 192

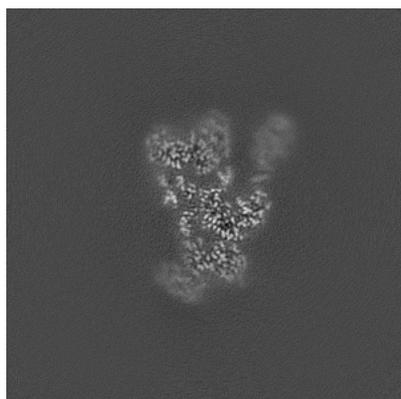


Y Index: 192

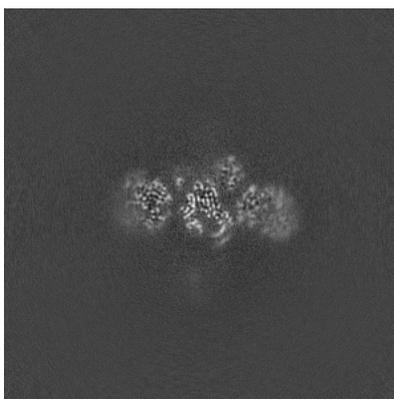


Z Index: 192

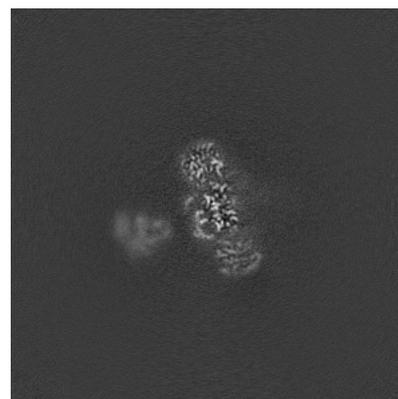
### 6.2.2 Raw map



X Index: 192



Y Index: 192

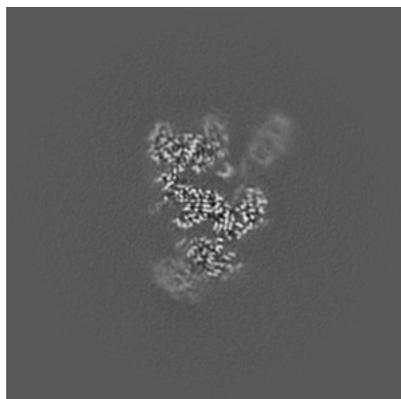


Z Index: 192

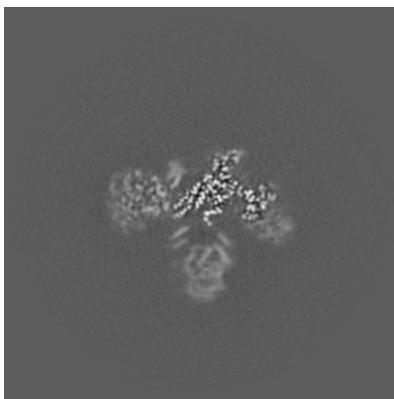
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 198

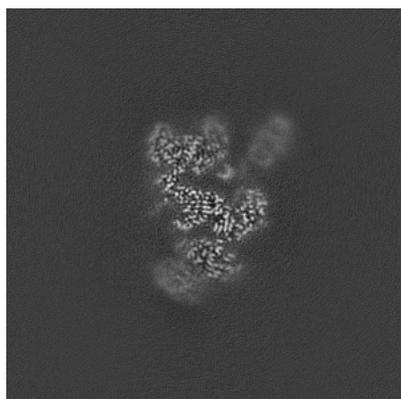


Y Index: 174

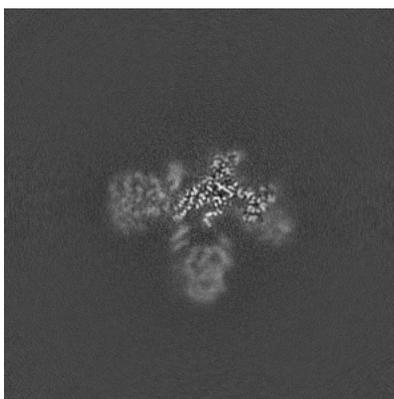


Z Index: 187

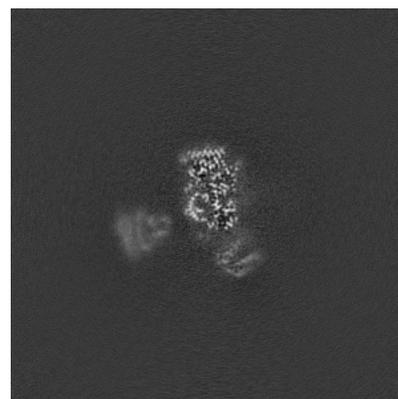
### 6.3.2 Raw map



X Index: 198



Y Index: 173

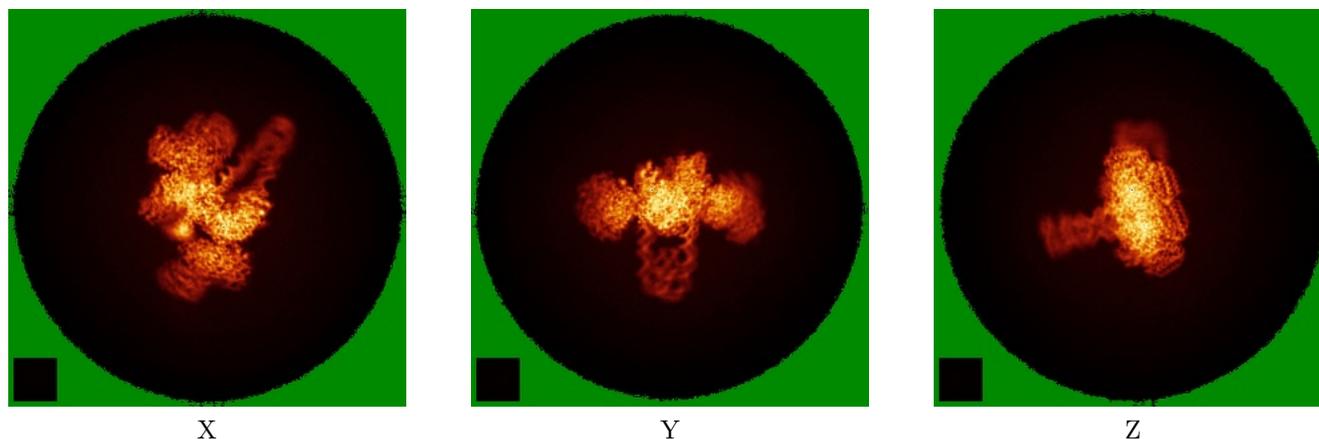


Z Index: 187

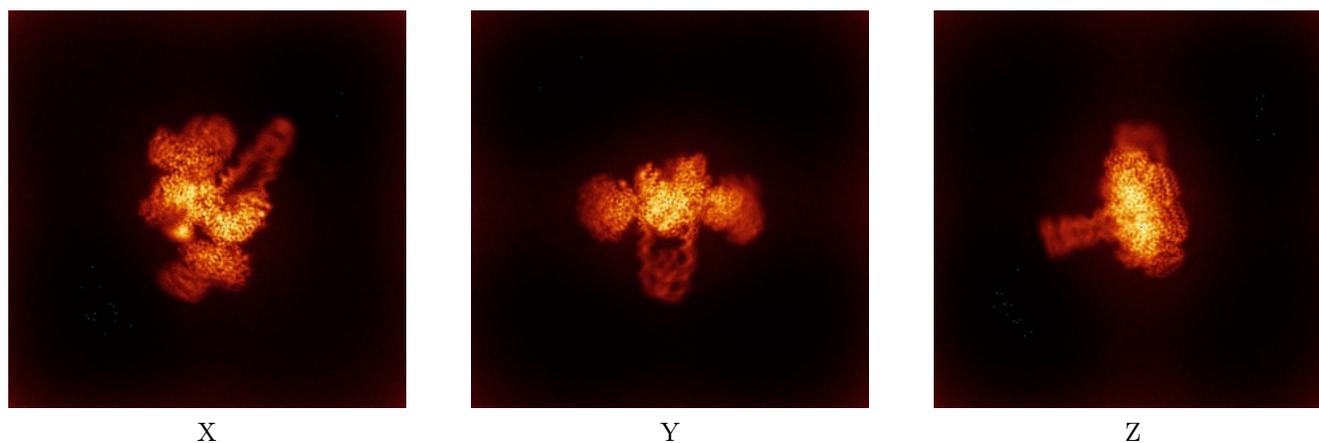
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



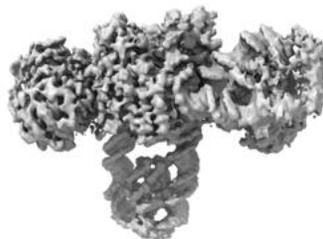
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.6. 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.

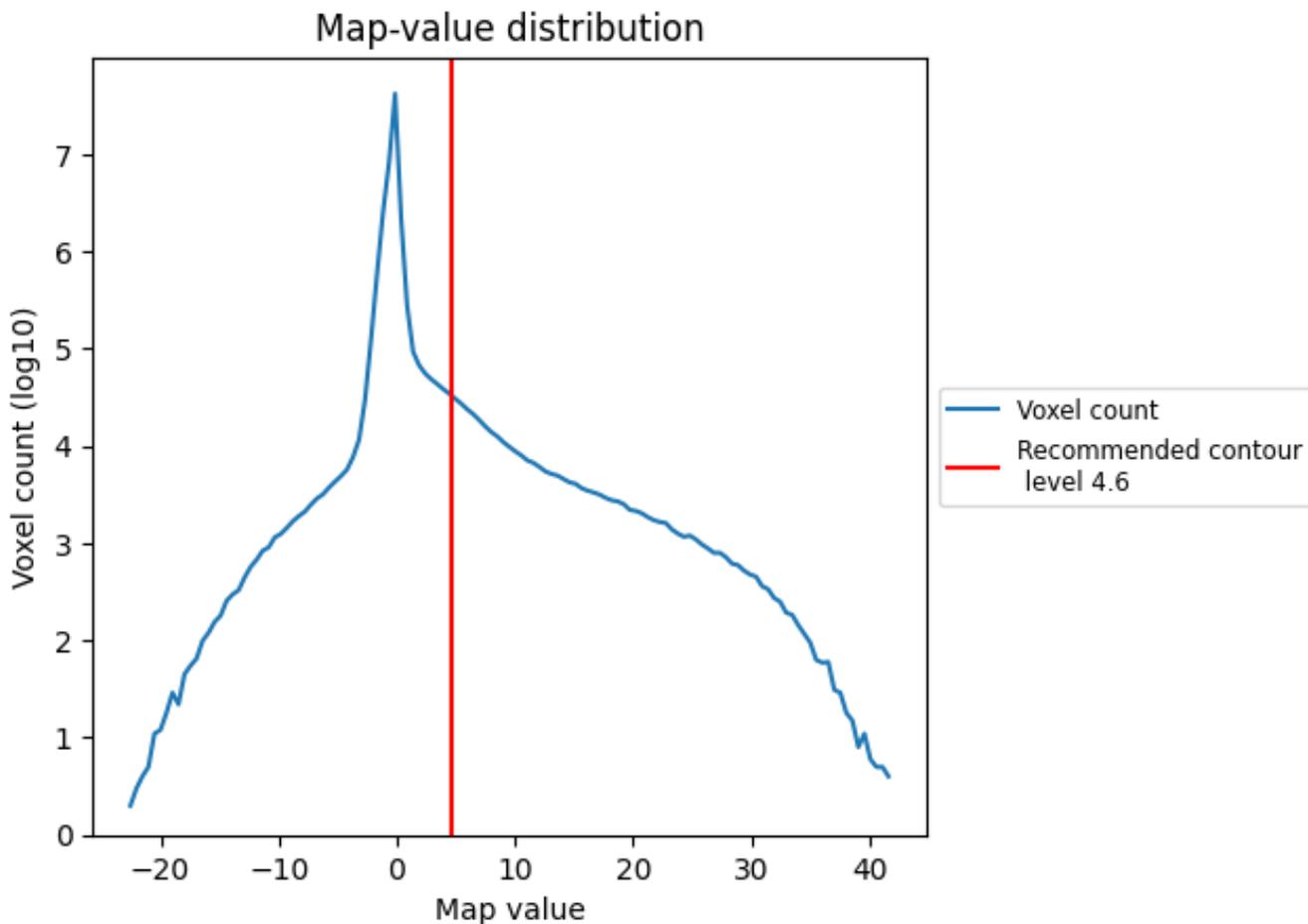
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

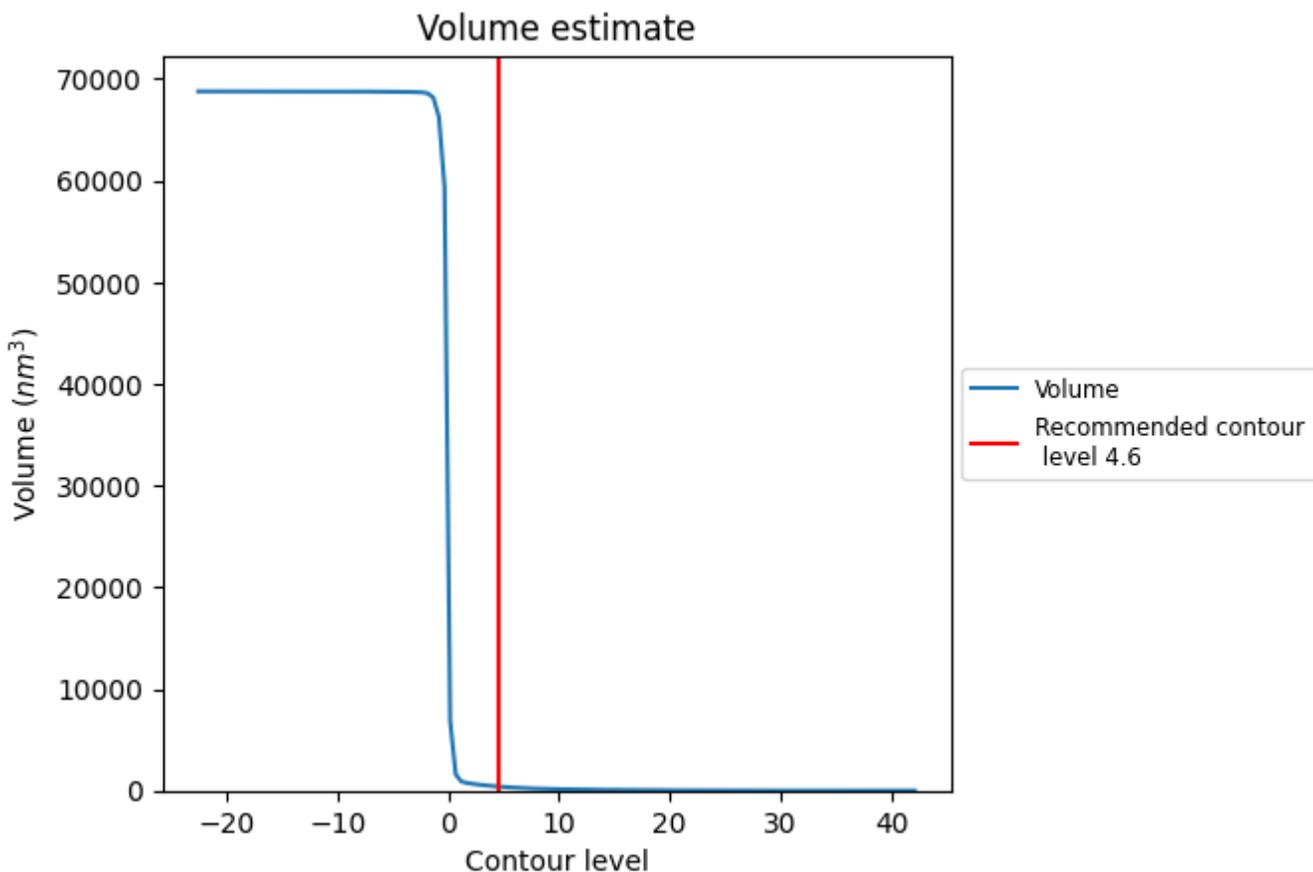
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

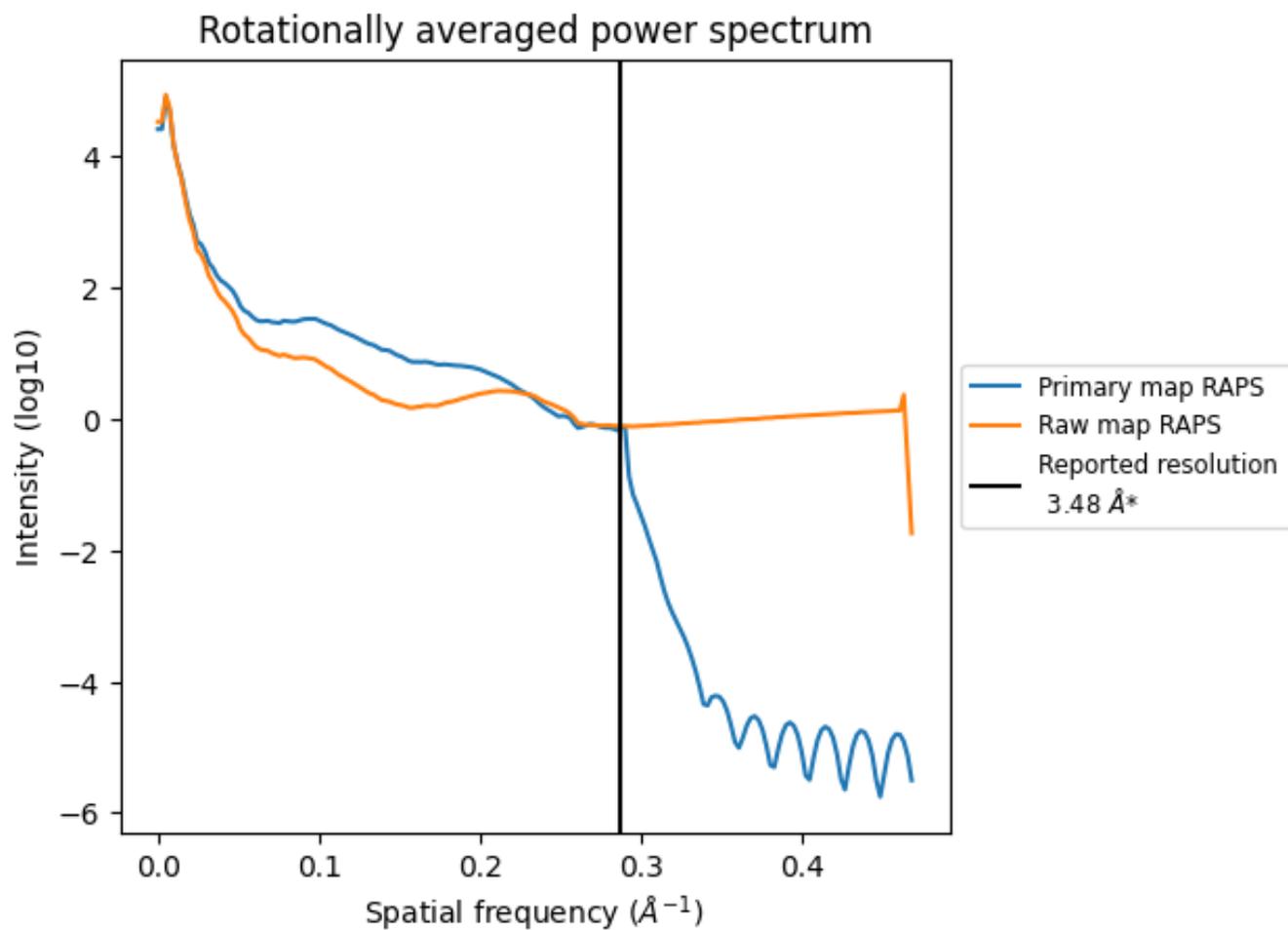
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 395 nm<sup>3</sup>; this corresponds to an approximate mass of 357 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](#)

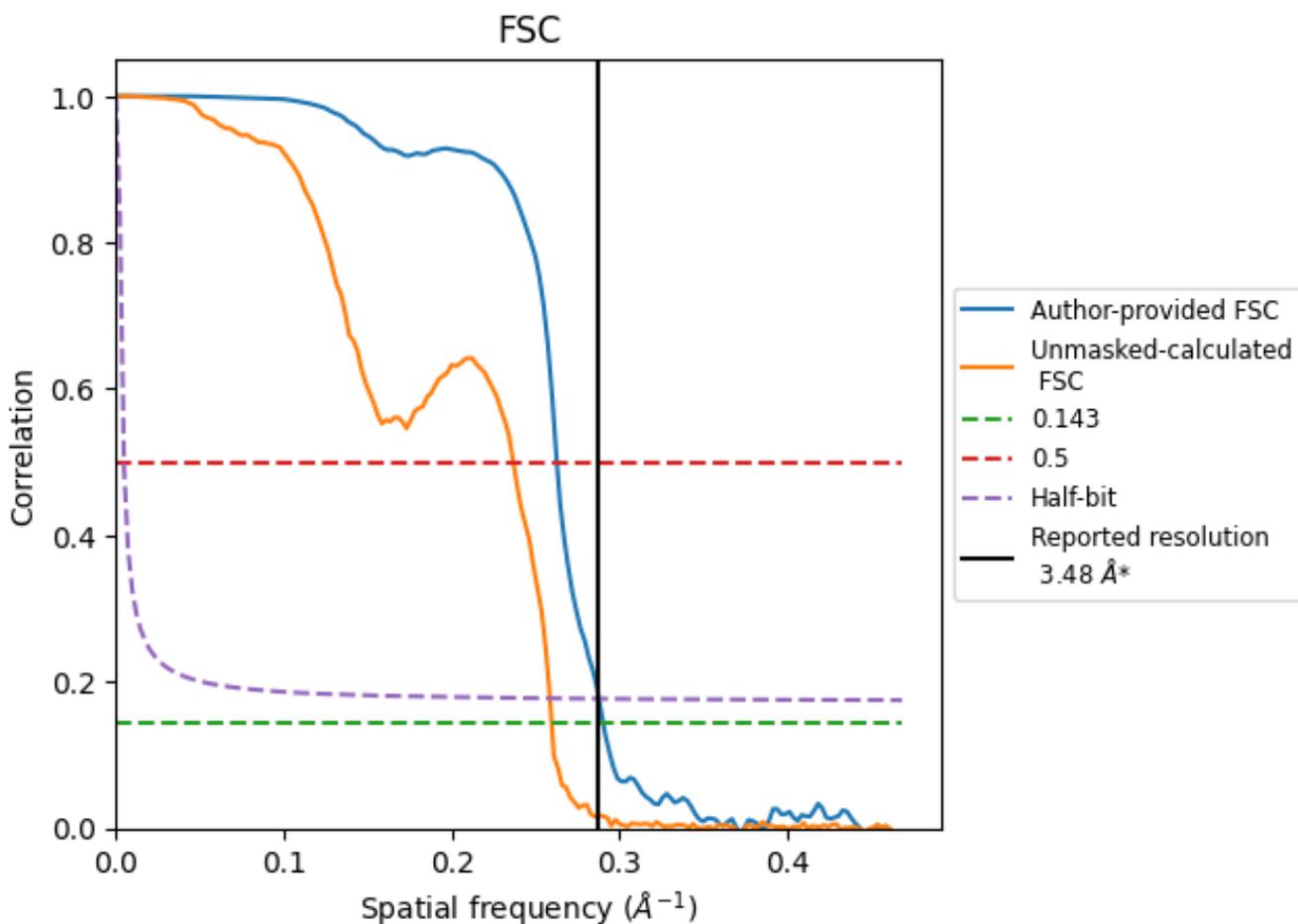


\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>

## 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 0.287 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

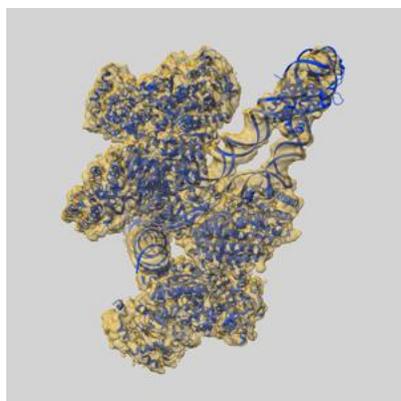
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	3.44	3.81	3.47
Unmasked-calculated*	3.85	4.22	3.87

\*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 3.85 differs from the reported value 3.48 by more than 10 %

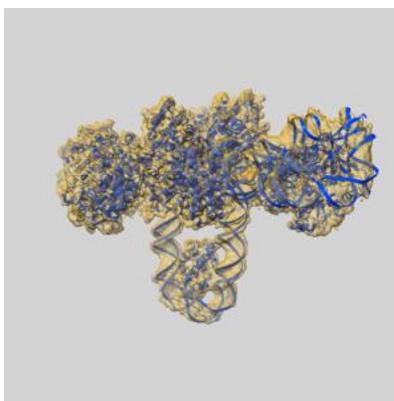
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29280 and PDB model 8FLJ. Per-residue inclusion information can be found in section 3 on page 8.

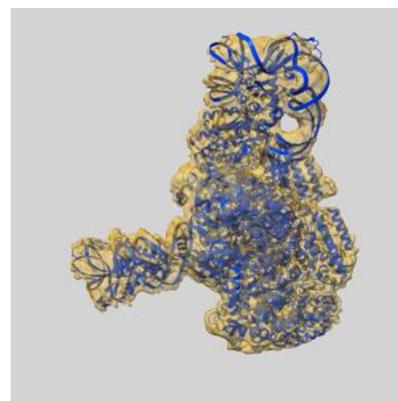
### 9.1 Map-model overlay [i](#)



X



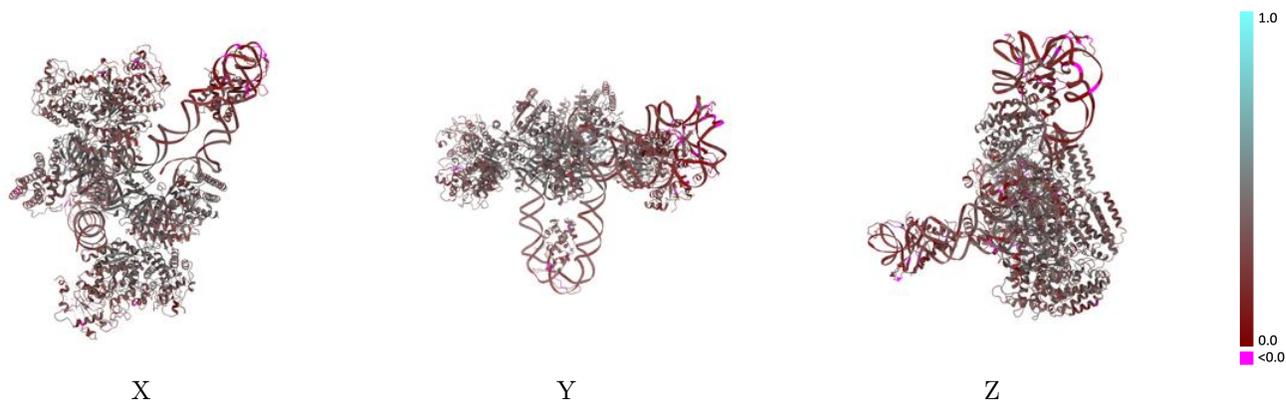
Y



Z

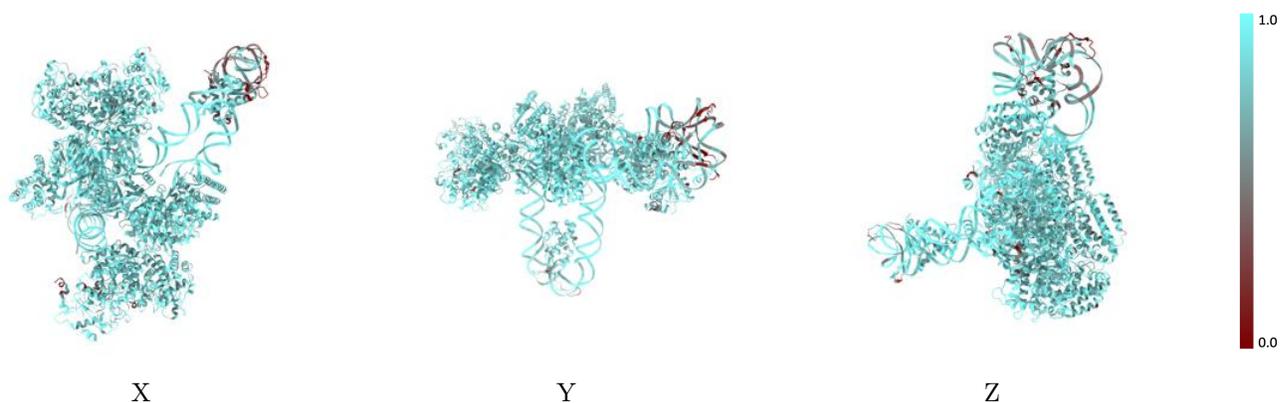
The images above show the 3D surface view of the map at the recommended contour level 4.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



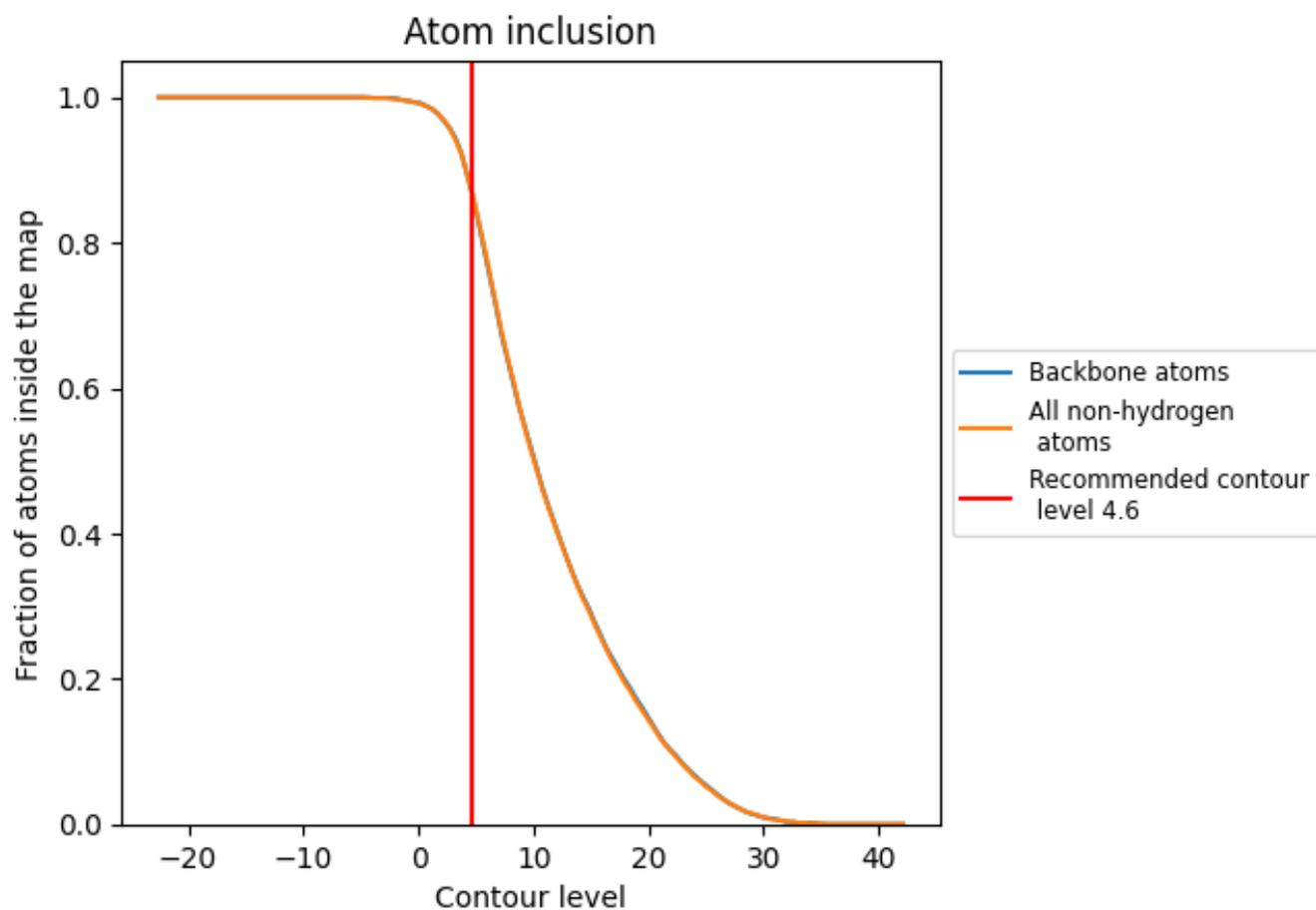
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (4.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.3500
A	 0.9080	 0.4170
B	 0.8980	 0.4080
C	 0.8900	 0.3880
D	 0.8930	 0.3950
E	 0.8430	 0.2240
F	 0.8680	 0.2150
G	 0.5670	 0.1760
H	 0.5770	 0.1970
I	 0.8850	 0.2630
J	 0.8740	 0.2530
K	 0.9470	 0.3820
L	 0.9660	 0.4000
M	 0.8860	 0.3590
N	 0.8750	 0.3790

