Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 05:43 PM JST

PDB ID	:	6IFU
EMDB ID	:	EMD-9657
Title	:	Cryo-EM structure of type III-A Csm-CTR2-dsDNA complex
Authors	:	You, L.; Ma, J.; Wang, J.; Zhang, X.; Wang, Y.
Deposited on	:	2018-09-21
Resolution	:	3.05 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 (i) 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 (i)) were used in the production of this report:

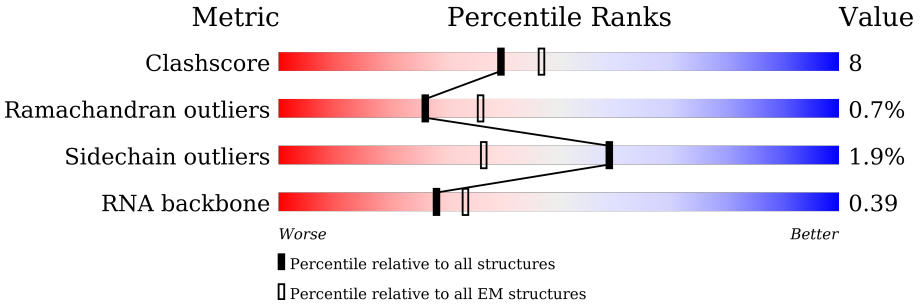
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.05 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
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	758	19% 76% 16% • 7%
2	B	126	9% 79% 17% • •
2	C	126	5% 76% 19% • •
3	D	220	8% 73% 23% • •
3	E	220	• 74% 23% • •
3	F	220	• 68% 24% • 6%
4	G	299	7% 67% 21% • 9%

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Mol	Chain	Length	Quality of chain
5	H	357	13% 74% 20%
6	I	36	22% 36% 28% 8% 6%
7	J	50	32% 12% 10% 44%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18750 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Type III-A CRISPR-associated protein Csm1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	706	5561	3578	933	1033	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	HIS	engineered mutation	UNP A0A2U2M0F3

- Molecule 2 is a protein called Type III-A CRISPR-associated protein Csm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	121	975	631	164	178	2	0	0
2	C	121	975	631	164	178	2	0	0

- Molecule 3 is a protein called Type III-A CRISPR-associated RAMP protein Csm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	217	1695	1075	291	327	2	0	0
3	E	216	1690	1072	290	326	2	0	0
3	F	207	1626	1033	279	312	2	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	33	ASN	ASP	engineered mutation	UNP A0A2U2M035
E	33	ASN	ASP	engineered mutation	UNP A0A2U2M035
F	33	ASN	ASP	engineered mutation	UNP A0A2U2M035

- Molecule 4 is a protein called Type III-A CRISPR-associated RAMP protein Csm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	272	2163	1387	349	422	5	0	0

- Molecule 5 is a protein called Type III-A CRISPR-associated RAMP protein Csm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	341	2744	1765	469	503	7	0	0

- Molecule 6 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	I	34	715	321	123	237	34	0	0

- Molecule 7 is a RNA chain called CTR2.

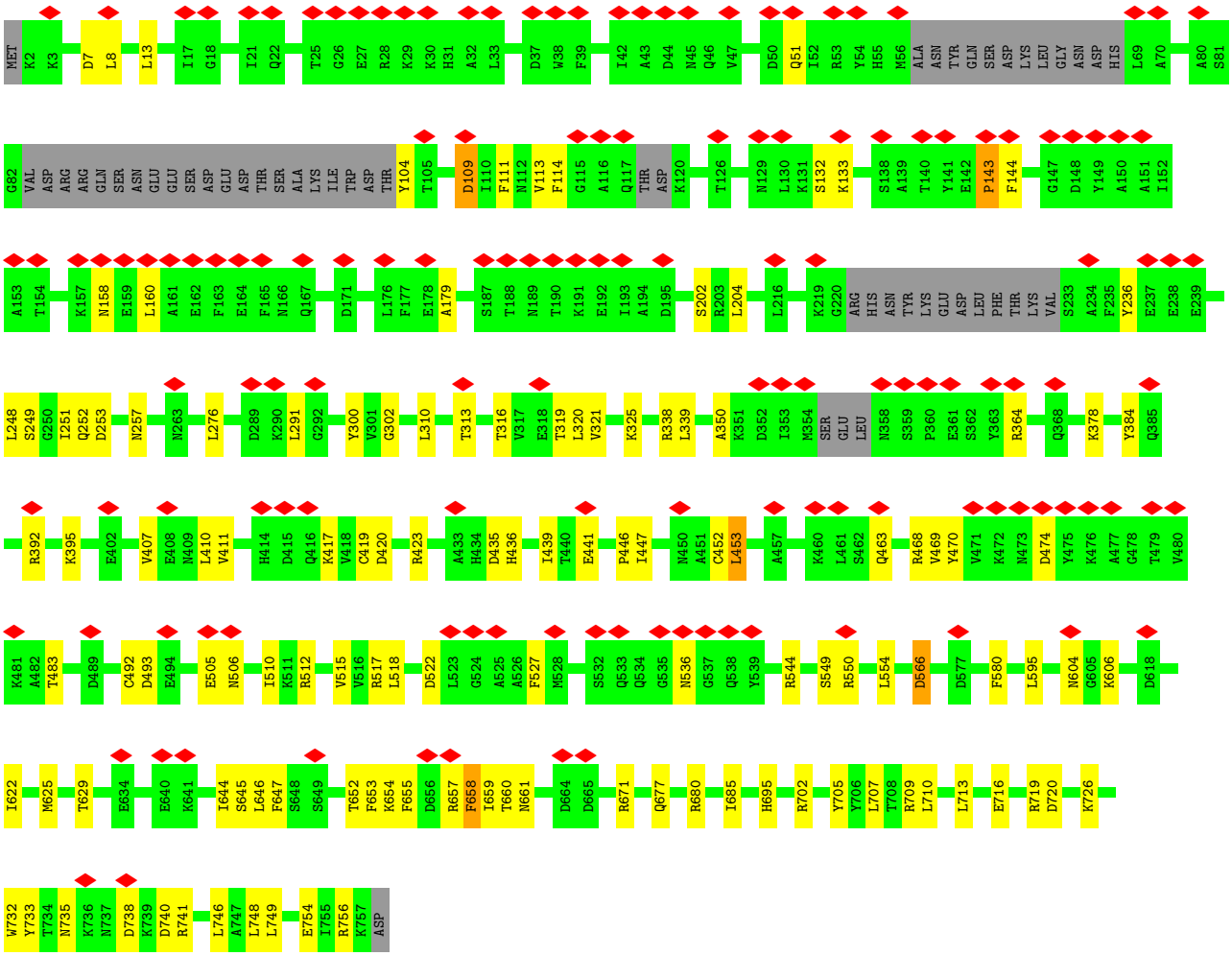
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	J	28	606	271	116	191	28	0	0

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.

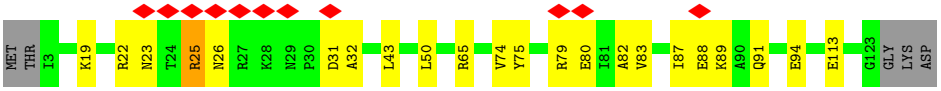
- Molecule 1: Type III-A CRISPR-associated protein Csm1

Chain A:



- Molecule 2: Type III-A CRISPR-associated protein Csm2

Chain B:

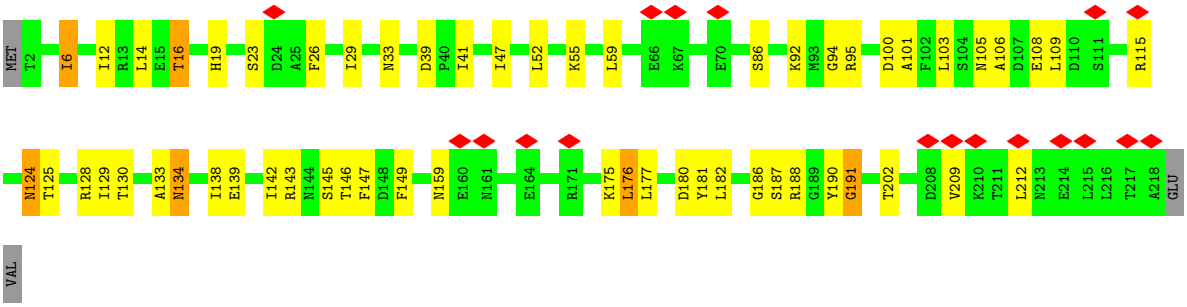


• Molecule 2: Type III-A CRISPR-associated protein Csm2

Chain C:

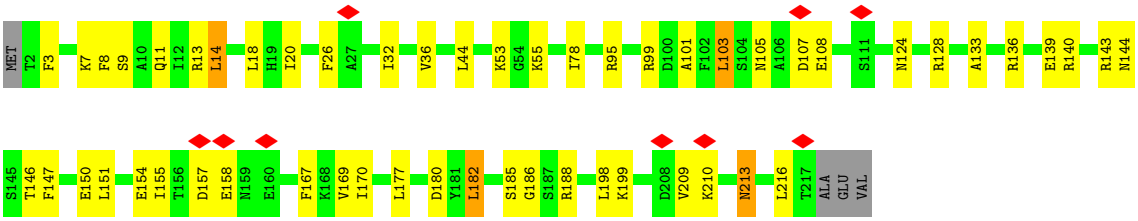
• Molecule 3: Type III-A CRISPR-associated RAMP protein Csm3

Chain D:



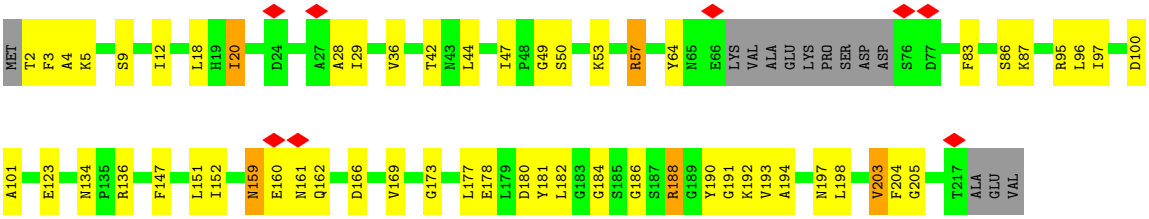
• Molecule 3: Type III-A CRISPR-associated RAMP protein Csm3

Chain E:



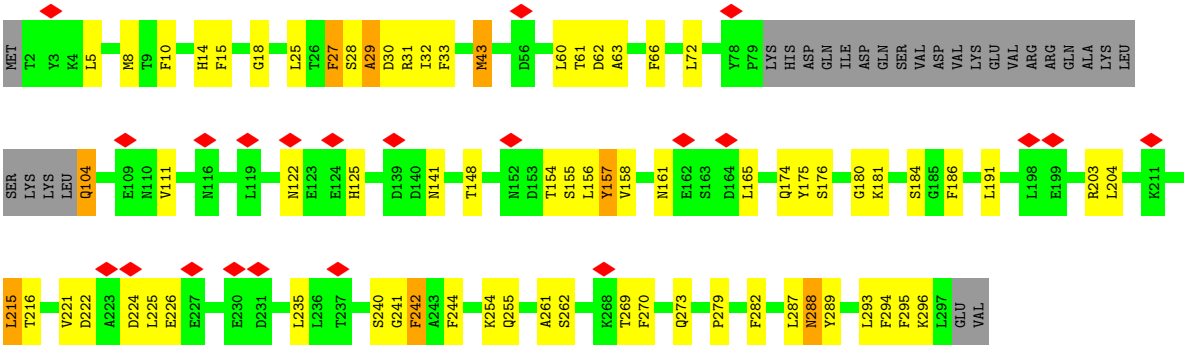
• Molecule 3: Type III-A CRISPR-associated RAMP protein Csm3

Chain F:



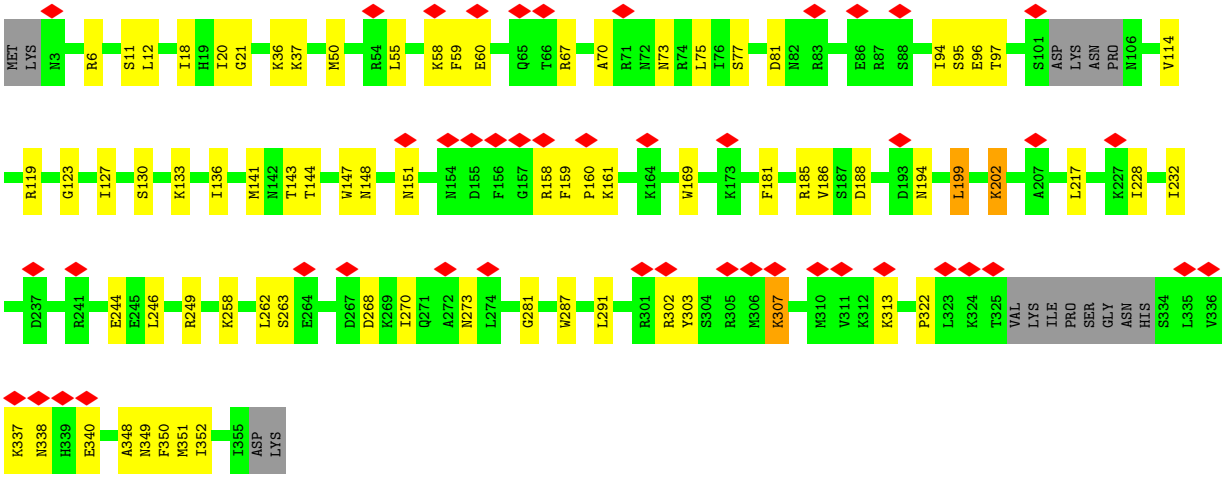
• Molecule 4: Type III-A CRISPR-associated RAMP protein Csm4

Chain G:



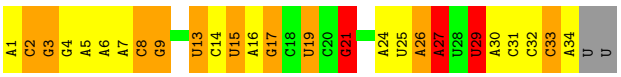
- Molecule 5: Type III-A CRISPR-associated RAMP protein Csm5

Chain H:



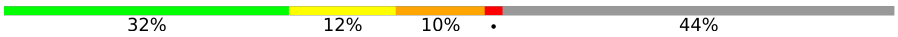
- Molecule 6: crRNA

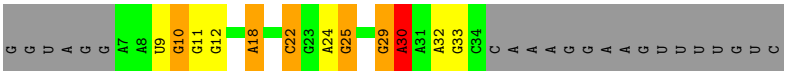
Chain I:



- Molecule 7: CTR2

Chain J:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75887	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.590	Depositor
Minimum map value	-0.325	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.076	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	0.47	0/5673	0.68	7/7657 (0.1%)
2	B	0.56	0/989	0.65	0/1334
2	C	0.62	0/989	0.74	1/1334 (0.1%)
3	D	0.64	0/1720	0.80	0/2316
3	E	0.66	0/1715	0.80	0/2309
3	F	0.65	0/1649	0.81	1/2218 (0.0%)
4	G	0.58	0/2213	0.82	4/2994 (0.1%)
5	H	0.53	1/2805 (0.0%)	0.76	4/3774 (0.1%)
6	I	1.59	1/797 (0.1%)	1.73	22/1237 (1.8%)
7	J	1.42	2/680 (0.3%)	1.24	1/1059 (0.1%)
All	All	0.68	4/19230 (0.0%)	0.85	40/26232 (0.2%)

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	3
3	D	0	4
3	E	0	3
3	F	0	3
4	G	0	6
5	H	0	3
All	All	0	22

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	30	A	N9-C4	-7.46	1.33	1.37
5	H	307	LYS	CA-CB	5.99	1.67	1.53
7	J	22	C	N3-C4	-5.83	1.29	1.33
6	I	17	G	N9-C8	-5.46	1.34	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	27	A	O4'-C1'-N9	11.23	117.19	108.20
6	I	14	C	N1-C2-O2	11.17	125.60	118.90
6	I	14	C	N3-C2-O2	-10.46	114.58	121.90
6	I	8	C	N3-C2-O2	-10.38	114.64	121.90
5	H	199	LEU	CA-CB-CG	9.85	137.94	115.30
6	I	14	C	C2-N1-C1'	9.76	129.54	118.80
6	I	21	G	O4'-C1'-N9	9.52	115.81	108.20
6	I	8	C	C2-N1-C1'	9.45	129.19	118.80
6	I	8	C	N1-C2-O2	9.38	124.53	118.90
6	I	8	C	C6-N1-C2	-9.26	116.59	120.30
6	I	9	G	O4'-C1'-N9	9.11	115.49	108.20
6	I	9	G	N3-C4-N9	-6.83	121.90	126.00
6	I	14	C	C6-N1-C1'	-6.83	112.61	120.80
1	A	143	PRO	N-CA-CB	6.75	111.40	103.30
7	J	30	A	O5'-P-OP1	-6.72	99.65	105.70
6	I	9	G	N9-C4-C5	6.59	108.03	105.40
1	A	710	LEU	CB-CG-CD1	-6.28	100.33	111.00
6	I	14	C	C6-N1-C2	-6.15	117.84	120.30
1	A	160	LEU	CA-CB-CG	6.09	129.31	115.30
2	C	85	ASP	CB-CG-OD1	6.06	123.75	118.30
6	I	13	U	O4'-C1'-N1	6.05	113.04	108.20
5	H	75	LEU	CA-CB-CG	6.03	129.17	115.30
6	I	29	U	C5-C6-N1	6.01	125.70	122.70
4	G	5	LEU	CA-CB-CG	5.97	129.04	115.30
3	F	18	LEU	CB-CG-CD1	-5.76	101.21	111.00
4	G	215	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	713	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	658	PHE	N-CA-C	-5.63	95.80	111.00
1	A	453	LEU	CA-CB-CG	5.58	128.14	115.30
6	I	8	C	C6-N1-C1'	-5.54	114.16	120.80
4	G	43	MET	CA-CB-CG	5.45	122.57	113.30
6	I	9	G	C6-C5-N7	5.43	133.66	130.40
5	H	12	LEU	CA-CB-CG	5.29	127.48	115.30
4	G	157	TYR	CA-CB-CG	5.23	123.34	113.40
6	I	19	U	O4'-C1'-N1	5.17	112.33	108.20
5	H	263	SER	C-N-CA	5.07	134.36	121.70
1	A	310	LEU	CB-CG-CD2	-5.03	102.44	111.00
6	I	33	C	P-O3'-C3'	5.02	125.72	119.70
6	I	9	G	N1-C6-O6	-5.02	116.89	119.90
6	I	29	U	C6-N1-C2	-5.01	117.99	121.00

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ASP	Peptide
1	A	505	GLU	Peptide
1	A	566	ASP	Peptide
3	D	16	THR	Peptide
3	D	191	GLY	Peptide
3	D	23	SER	Peptide
3	D	94	GLY	Peptide
3	E	128	ARG	Peptide
3	E	157	ASP	Peptide
3	E	185	SER	Peptide
3	F	20	ILE	Peptide
3	F	203	VAL	Peptide
3	F	28	ALA	Peptide
4	G	15	PHE	Peptide
4	G	240	SER	Peptide
4	G	241	GLY	Peptide
4	G	27	PHE	Peptide
4	G	28	SER	Peptide
4	G	43	MET	Peptide
5	H	159	PHE	Peptide
5	H	20	ILE	Peptide
5	H	340	GLU	Peptide

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	5561	0	5361	73	0
2	B	975	0	977	12	0
2	C	975	0	977	16	0
3	D	1695	0	1709	43	0
3	E	1690	0	1704	32	0
3	F	1626	0	1641	35	0
4	G	2163	0	2090	46	0
5	H	2744	0	2739	42	0
6	I	715	0	366	21	0
7	J	606	0	303	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18750	0	17867	280	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 8.

All (280) 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:677:GLN:HE22	1:A:680:ARG:H	1.32	0.77
3:D:124:ASN:HD21	3:D:133:ALA:HB1	1.52	0.74
3:F:123:GLU:HB2	3:F:136:ARG:HB2	1.70	0.73
4:G:174:GLN:HE21	4:G:191:LEU:H	1.40	0.70
3:D:59:LEU:HB3	3:D:176:LEU:HD22	1.74	0.68
1:A:732:TRP:HB2	1:A:740:ASP:HB3	1.76	0.67
5:H:77:SER:O	5:H:81:ASP:HB2	1.97	0.65
3:D:47:ILE:HB	3:D:101:ALA:HB3	1.78	0.64
3:E:13:ARG:HG2	3:E:146:THR:HG22	1.79	0.63
5:H:144:THR:OG1	5:H:249:ARG:NH2	2.31	0.63
4:G:29:ALA:H	4:G:62:ASP:HB3	1.64	0.62
3:E:188:ARG:NH1	6:I:19:U:OP2	2.33	0.62
1:A:109:ASP:HB3	1:A:111:PHE:H	1.65	0.61
3:E:7:LYS:NZ	3:E:9:SER:OG	2.33	0.61
3:E:136:ARG:NH2	6:I:19:U:O2'	2.34	0.61
5:H:273:ASN:O	5:H:349:ASN:ND2	2.32	0.61
4:G:14:HIS:HB3	4:G:180:GLY:HA3	1.82	0.61
3:F:101:ALA:HB1	3:F:147:PHE:HB3	1.83	0.61
2:C:27:ARG:HA	2:C:30:PRO:HB3	1.82	0.61
4:G:62:ASP:OD1	4:G:62:ASP:N	2.34	0.61
2:B:74:VAL:HG11	5:H:60:GLU:HG3	1.82	0.60
1:A:395:LYS:O	4:G:255:GLN:NE2	2.34	0.60
5:H:133:LYS:NZ	5:H:181:PHE:O	2.32	0.60
3:E:44:LEU:HD13	3:E:103:LEU:HD12	1.83	0.60
3:F:188:ARG:NH2	6:I:13:U:OP2	2.34	0.60
3:E:198:LEU:HB3	3:E:216:LEU:HD23	1.83	0.60
4:G:255:GLN:HE21	4:G:279:PRO:HA	1.66	0.60
5:H:70:ALA:HB2	7:J:10:G:H5'	1.83	0.59
1:A:257:ASN:HD22	1:A:338:ARG:HH21	1.49	0.59
1:A:419:CYS:SG	1:A:420:ASP:N	2.75	0.59
3:D:129:ILE:HD12	3:D:130:THR:HG23	1.84	0.59
1:A:114:PHE:HB2	1:A:606:LYS:HE3	1.83	0.59
3:D:125:THR:OG1	6:I:25:U:O2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:95:ARG:NH2	3:F:166:ASP:OD2	2.35	0.59
3:E:105:ASN:HB2	3:E:108:GLU:HB3	1.85	0.59
3:F:42:THR:HG22	3:F:44:LEU:HD13	1.83	0.59
1:A:756:ARG:NH2	7:J:30:A:OP1	2.36	0.58
5:H:97:THR:HG23	5:H:322:PRO:HD3	1.84	0.58
5:H:287:TRP:NE1	5:H:313:LYS:O	2.32	0.58
3:F:136:ARG:NH2	6:I:13:U:O2'	2.37	0.58
3:F:169:VAL:O	3:F:173:GLY:N	2.36	0.58
4:G:27:PHE:HB2	4:G:31:ARG:HD2	1.85	0.58
2:B:80:GLU:HG2	2:B:82:ALA:H	1.69	0.58
4:G:31:ARG:NH2	6:I:4:G:OP1	2.37	0.58
3:D:100:ASP:OD2	3:E:140:ARG:NH2	2.29	0.58
3:E:101:ALA:HB1	3:E:147:PHE:HB3	1.86	0.57
5:H:141:MET:HB3	5:H:291:LEU:HD21	1.86	0.57
3:F:181:TYR:HB2	3:F:191:GLY:HA3	1.86	0.57
4:G:215:LEU:HD22	4:G:295:PHE:HB2	1.86	0.57
5:H:127:ILE:HD12	5:H:228:ILE:HG21	1.85	0.57
1:A:249:SER:OG	1:A:378:LYS:NZ	2.37	0.57
1:A:300:TYR:HD2	1:A:302:GLY:H	1.51	0.57
1:A:707:LEU:HB3	1:A:726:LYS:HG3	1.87	0.57
2:C:22:ARG:NH1	2:C:31:ASP:O	2.36	0.57
3:D:186:GLY:H	3:D:190:TYR:HB2	1.70	0.57
3:D:101:ALA:HB1	3:D:147:PHE:HB3	1.86	0.56
1:A:179:ALA:HB2	1:A:474:ASP:HB2	1.87	0.56
3:F:20:ILE:H	3:F:36:VAL:HG23	1.69	0.56
4:G:221:VAL:HA	4:G:273:GLN:HE21	1.69	0.56
4:G:29:ALA:N	4:G:62:ASP:HB3	2.20	0.56
3:D:95:ARG:HD3	3:D:159:ASN:HD21	1.70	0.56
4:G:221:VAL:O	4:G:225:LEU:N	2.38	0.56
1:A:738:ASP:OD1	1:A:741:ARG:NH2	2.37	0.56
4:G:72:LEU:HD12	4:G:111:VAL:HG21	1.87	0.56
1:A:446:PRO:HA	1:A:452:CYS:HA	1.87	0.56
4:G:63:ALA:HB1	4:G:156:LEU:HB3	1.88	0.56
4:G:242:PHE:O	4:G:254:LYS:NZ	2.38	0.56
5:H:258:LYS:HA	5:H:262:LEU:HB2	1.87	0.55
1:A:671:ARG:NH2	1:A:754:GLU:OE2	2.36	0.55
3:E:53:LYS:HD3	3:F:188:ARG:HB3	1.86	0.55
3:D:188:ARG:NH1	6:I:25:U:OP2	2.39	0.55
2:B:22:ARG:NH2	2:B:31:ASP:O	2.39	0.55
3:E:32:ILE:HG21	3:E:139:GLU:HB2	1.88	0.55
3:D:33:ASN:HD22	7:J:18:A:H5"	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6:ARG:NH1	5:H:244:GLU:OE2	2.38	0.54
5:H:143:THR:O	5:H:249:ARG:NH2	2.41	0.54
3:D:128:ARG:NH2	6:I:26:A:OP2	2.41	0.54
3:F:97:ILE:HB	3:F:152:ILE:HB	1.89	0.53
5:H:55:LEU:HD22	5:H:58:LYS:HD2	1.90	0.53
3:F:12:ILE:HG23	3:F:147:PHE:HB2	1.89	0.53
3:D:12:ILE:HB	3:D:147:PHE:HB2	1.90	0.53
3:D:130:THR:O	5:H:302:ARG:NH1	2.42	0.53
5:H:202:LYS:HD2	5:H:217:LEU:HD23	1.90	0.53
1:A:518:LEU:HD21	1:A:595:LEU:HD13	1.91	0.52
2:B:25:ARG:NH1	2:B:26:ASN:OD1	2.43	0.52
3:D:16:THR:OG1	5:H:188:ASP:OD2	2.27	0.52
3:D:19:HIS:ND1	3:D:139:GLU:O	2.40	0.52
3:F:57:ARG:NH2	6:I:7:A:OP1	2.41	0.52
3:D:105:ASN:HB2	3:D:108:GLU:HB3	1.92	0.52
3:F:4:ALA:HA	3:F:205:GLY:HA3	1.91	0.52
3:D:12:ILE:O	3:D:146:THR:HA	2.10	0.52
3:D:180:ASP:OD1	5:H:185:ARG:NH1	2.40	0.52
4:G:125:HIS:HB3	4:G:154:THR:HG21	1.91	0.52
2:C:47:THR:HG21	2:C:112:MET:HG3	1.91	0.52
3:D:181:TYR:HB2	3:D:191:GLY:HA3	1.91	0.52
3:D:6:ILE:HG22	3:D:202:THR:HG22	1.92	0.52
3:E:8:PHE:O	3:E:150:GLU:HA	2.11	0.52
1:A:7:ASP:O	1:A:51:GLN:NE2	2.43	0.51
1:A:735:ASN:ND2	1:A:740:ASP:OD2	2.37	0.51
6:I:15:U:O4	7:J:29:G:N2	2.44	0.51
3:E:14:LEU:HD13	3:E:18:LEU:HD23	1.93	0.51
5:H:18:ILE:HD11	5:H:348:ALA:HB2	1.93	0.51
1:A:468:ARG:NH1	1:A:483:THR:OG1	2.44	0.50
3:D:209:VAL:HG12	3:D:212:LEU:HD12	1.93	0.50
1:A:645:SER:HA	1:A:652:THR:HA	1.93	0.50
3:E:20:ILE:H	3:E:36:VAL:HG23	1.74	0.50
1:A:104:TYR:HE2	1:A:144:PHE:HA	1.76	0.50
4:G:62:ASP:OD2	4:G:262:SER:OG	2.28	0.50
3:F:53:LYS:HE3	3:F:83:PHE:HD1	1.76	0.50
3:F:97:ILE:HD13	4:G:176:SER:HA	1.94	0.50
1:A:705:TYR:O	1:A:709:ARG:HB2	2.12	0.50
3:D:109:LEU:HD13	3:D:142:ILE:HD11	1.94	0.50
1:A:654:LYS:HB3	1:A:657:ARG:HG2	1.94	0.49
3:F:2:THR:N	3:F:160:GLU:OE2	2.45	0.49
1:A:316:THR:HA	1:A:319:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:GLU:OE2	1:A:719:ARG:NH1	2.43	0.49
1:A:13:LEU:O	1:A:202:SER:OG	2.30	0.49
1:A:236:TYR:HA	1:A:350:ALA:HB3	1.93	0.49
3:F:184:GLY:O	3:F:186:GLY:N	2.46	0.49
4:G:288:ASN:N	6:I:1:A:OP2	2.46	0.49
3:E:8:PHE:HB2	3:E:151:LEU:HB2	1.95	0.49
3:E:124:ASN:ND2	6:I:21:G:N3	2.61	0.48
3:F:86:SER:HB3	6:I:6:A:H1'	1.94	0.48
4:G:30:ASP:OD2	4:G:288:ASN:ND2	2.46	0.48
3:D:55:LYS:HZ3	3:D:182:LEU:H	1.61	0.48
1:A:392:ARG:NH1	4:G:222:ASP:OD2	2.46	0.48
3:E:3:PHE:HA	3:E:155:ILE:O	2.13	0.48
5:H:119:ARG:NH2	5:H:123:GLY:O	2.46	0.48
1:A:709:ARG:NH2	7:J:25:G:OP1	2.47	0.48
1:A:439:ILE:HD13	1:A:453:LEU:HD23	1.94	0.48
3:D:187:SER:HB2	5:H:133:LYS:HZ2	1.78	0.48
3:E:11:GLN:HG3	3:E:146:THR:HB	1.94	0.48
3:F:96:LEU:HD22	3:F:151:LEU:HD21	1.94	0.48
1:A:653:PHE:HE2	1:A:746:LEU:HD13	1.79	0.48
3:E:55:LYS:NZ	3:E:180:ASP:OD2	2.36	0.48
1:A:658:PHE:O	1:A:661:ASN:N	2.40	0.48
1:A:746:LEU:HA	1:A:749:LEU:HD12	1.96	0.48
3:D:55:LYS:HG3	3:D:182:LEU:HA	1.95	0.48
4:G:181:LYS:HB2	4:G:186:PHE:HD2	1.77	0.48
3:E:78:ILE:HD11	3:E:169:VAL:HG21	1.96	0.47
5:H:37:LYS:HA	5:H:95:SER:HA	1.95	0.47
3:E:167:PHE:HD1	3:E:170:ILE:HD12	1.79	0.47
2:C:40:LEU:HG	2:C:116:VAL:HG22	1.95	0.47
4:G:18:GLY:HA2	6:I:3:G:C8	2.48	0.47
5:H:158:ARG:H	5:H:160:PRO:HG3	1.80	0.47
1:A:411:VAL:O	1:A:423:ARG:NH1	2.47	0.47
1:A:253:ASP:O	1:A:257:ASN:ND2	2.47	0.47
1:A:435:ASP:HA	1:A:470:TYR:HE1	1.80	0.47
4:G:203:ARG:HG2	4:G:296:LYS:HB2	1.95	0.47
5:H:268:ASP:HA	5:H:337:LYS:HB3	1.97	0.47
3:D:86:SER:O	3:D:92:LYS:NZ	2.46	0.47
4:G:203:ARG:HG2	4:G:296:LYS:HE2	1.96	0.47
2:B:19:LYS:HG2	2:B:89:LYS:HD2	1.97	0.47
5:H:67:ARG:O	5:H:73:ASN:ND2	2.45	0.47
6:I:16:A:H2'	6:I:17:G:C8	2.50	0.47
1:A:522:ASP:OD1	1:A:522:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:95:ARG:HA	3:E:154:GLU:HG2	1.96	0.47
1:A:510:ILE:HG12	1:A:512:ARG:HG2	1.97	0.47
2:B:43:LEU:HD11	2:B:83:VAL:HG13	1.96	0.47
3:D:16:THR:H	3:D:143:ARG:HG3	1.80	0.46
1:A:251:ILE:H	1:A:251:ILE:HG13	1.52	0.46
3:D:125:THR:HB	3:D:134:ASN:HB3	1.97	0.46
1:A:251:ILE:HG22	1:A:276:LEU:HD13	1.97	0.46
3:D:177:LEU:HD22	3:D:182:LEU:HG	1.96	0.46
3:F:177:LEU:HD22	3:F:182:LEU:HB2	1.96	0.46
4:G:204:LEU:HB3	4:G:293:LEU:HD11	1.96	0.46
1:A:622:ILE:HA	1:A:625:MET:HB3	1.98	0.46
2:B:75:TYR:CZ	2:B:79:ARG:HD2	2.51	0.46
2:B:91:GLN:HB3	2:B:94:GLU:HB2	1.97	0.46
3:E:177:LEU:HD22	3:E:182:LEU:HG	1.96	0.46
1:A:113:VAL:HG21	1:A:544:ARG:HD3	1.96	0.46
2:B:50:LEU:HD11	2:B:65:ARG:HG2	1.98	0.46
3:D:6:ILE:HA	3:D:202:THR:HA	1.98	0.46
3:F:2:THR:OG1	3:F:3:PHE:N	2.47	0.46
6:I:4:G:H2'	6:I:5:A:C8	2.49	0.46
2:B:87:ILE:HD12	2:B:88:GLU:HG2	1.97	0.46
5:H:114:VAL:HG11	5:H:199:LEU:HD22	1.98	0.46
1:A:439:ILE:HD12	1:A:447:ILE:HD11	1.98	0.46
1:A:756:ARG:HH12	7:J:29:G:H3'	1.81	0.46
4:G:32:ILE:HG23	4:G:60:LEU:HD11	1.97	0.46
1:A:685:ILE:HG23	1:A:748:LEU:HD22	1.98	0.45
5:H:186:VAL:HG22	5:H:232:ILE:HG12	1.99	0.45
1:A:441:GLU:O	1:A:463:GLN:NE2	2.49	0.45
2:C:7:GLU:O	2:C:9:TYR:N	2.47	0.45
1:A:709:ARG:HG3	2:C:120:LYS:HE2	1.99	0.45
2:B:113:GLU:HB3	3:D:29:ILE:HD12	1.98	0.45
3:D:39:ASP:OD2	3:E:143:ARG:NH2	2.48	0.45
1:A:291:LEU:HD11	1:A:316:THR:HG22	1.97	0.45
1:A:550:ARG:O	1:A:554:LEU:N	2.48	0.45
5:H:302:ARG:NH2	5:H:303:TYR:OH	2.35	0.45
3:F:5:LYS:HD3	4:G:175:TYR:HB2	1.99	0.45
4:G:235:LEU:HB3	4:G:261:ALA:HB2	1.99	0.45
2:C:4:LEU:HD12	2:C:107:ARG:HE	1.81	0.44
2:C:51:PHE:HB2	2:C:109:CYS:HB3	1.98	0.44
3:E:199:LYS:HA	3:E:213:ASN:HD21	1.81	0.44
5:H:262:LEU:HG	5:H:270:ILE:HD12	1.99	0.44
3:D:177:LEU:HD13	3:D:182:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:65:ARG:HD2	3:D:26:PHE:CG	2.52	0.44
3:E:99:ARG:HD2	3:F:192:LYS:HD2	1.99	0.44
5:H:21:GLY:HA2	6:I:27:A:H3'	2.00	0.44
5:H:148:ASN:O	5:H:151:ASN:ND2	2.51	0.44
1:A:492:CYS:SG	1:A:493:ASP:N	2.88	0.44
1:A:527:PHE:HE1	1:A:549:SER:HB2	1.83	0.44
3:F:49:GLY:N	3:F:100:ASP:OD1	2.40	0.44
5:H:36:LYS:HB3	5:H:96:GLU:HG2	2.00	0.44
2:C:65:ARG:HD2	3:D:26:PHE:CD2	2.53	0.44
2:C:66:ILE:HD11	2:C:105:LEU:HD22	1.99	0.44
4:G:141:ASN:OD1	4:G:141:ASN:N	2.50	0.44
4:G:287:LEU:N	6:I:1:A:OP2	2.50	0.44
1:A:8:LEU:HA	1:A:51:GLN:HE22	1.82	0.44
5:H:77:SER:O	5:H:81:ASP:CB	2.64	0.44
5:H:94:ILE:HD11	5:H:199:LEU:HD23	1.99	0.44
5:H:141:MET:HA	5:H:147:TRP:HE3	1.82	0.43
1:A:248:LEU:HD21	1:A:339:LEU:HD13	1.99	0.43
2:C:68:TYR:HD2	3:D:26:PHE:HD1	1.66	0.43
1:A:316:THR:O	1:A:320:LEU:HB2	2.18	0.43
3:E:13:ARG:HH21	3:E:144:ASN:HB3	1.83	0.43
3:F:12:ILE:HA	3:F:194:ALA:O	2.19	0.43
3:F:87:LYS:H	3:F:87:LYS:HG2	1.65	0.43
3:D:188:ARG:HB3	5:H:130:SER:HB3	2.00	0.43
4:G:244:PHE:N	6:I:2:C:OP2	2.43	0.43
5:H:352:ILE:H	5:H:352:ILE:HG13	1.53	0.43
3:F:50:SER:HB3	4:G:184:SER:HB3	1.99	0.43
3:F:64:TYR:CZ	3:F:169:VAL:HG22	2.54	0.43
1:A:517:ARG:HG2	1:A:580:PHE:HD1	1.83	0.43
4:G:33:PHE:CD2	4:G:289:TYR:HB2	2.53	0.43
1:A:248:LEU:HD22	1:A:251:ILE:HG23	2.01	0.43
1:A:410:LEU:HB3	1:A:417:LYS:HD2	2.01	0.43
3:F:47:ILE:HB	3:F:101:ALA:HB3	2.01	0.42
4:G:224:ASP:OD2	4:G:270:PHE:HB2	2.19	0.42
1:A:407:VAL:HA	1:A:410:LEU:HD11	2.01	0.42
4:G:25:LEU:HA	4:G:148:THR:HG21	2.02	0.42
1:A:658:PHE:O	1:A:660:THR:N	2.53	0.42
2:C:66:ILE:O	2:C:69:LEU:HB2	2.20	0.42
4:G:61:THR:HA	4:G:216:THR:HG22	2.01	0.42
4:G:10:PHE:CE2	4:G:156:LEU:HD12	2.54	0.42
3:E:209:VAL:O	3:E:213:ASN:N	2.48	0.42
5:H:119:ARG:HH22	5:H:194:ASN:HD22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:268:ASP:HB3	5:H:338:ASN:HB3	2.02	0.42
1:A:251:ILE:HD12	1:A:252:GLN:HG2	2.02	0.42
5:H:50:MET:HE1	5:H:59:PHE:CG	2.54	0.42
5:H:136:ILE:HG23	5:H:246:LEU:HD21	2.02	0.42
1:A:644:ILE:HB	1:A:655:PHE:CZ	2.55	0.42
4:G:288:ASN:H	6:I:1:A:P	2.42	0.42
1:A:644:ILE:HG12	1:A:646:LEU:HD22	2.02	0.41
3:E:133:ALA:O	7:J:22:C:O2'	2.31	0.41
4:G:8:MET:HE3	4:G:158:VAL:HG13	2.02	0.41
1:A:515:VAL:HG12	1:A:629:THR:HG21	2.02	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.92	0.41
3:D:138:ILE:HG21	3:D:138:ILE:HD13	1.83	0.41
3:F:159:ASN:O	3:F:162:GLN:N	2.43	0.41
4:G:174:GLN:HE21	4:G:191:LEU:N	2.13	0.41
2:C:44:LEU:HD22	2:C:116:VAL:HG21	2.03	0.41
1:A:720:ASP:N	1:A:720:ASP:OD1	2.53	0.41
3:D:14:LEU:HD12	3:D:145:SER:HB2	2.01	0.41
3:E:107:ASP:N	3:E:107:ASP:OD1	2.52	0.41
3:D:41:ILE:HD13	3:E:144:ASN:HB2	2.02	0.41
3:F:186:GLY:HA2	3:F:190:TYR:HB2	2.03	0.41
4:G:269:THR:HG23	4:G:294:PHE:CE2	2.55	0.41
2:C:40:LEU:HD13	2:C:86:LEU:HD21	2.02	0.41
3:F:9:SER:O	3:F:198:LEU:HA	2.21	0.41
3:F:178:GLU:HG2	3:F:194:ALA:HA	2.03	0.41
2:B:23:ASN:HD22	2:B:32:ALA:HB3	1.85	0.41
3:D:52:LEU:HD13	3:D:149:PHE:HE1	1.86	0.41
4:G:104:GLN:HG2	4:G:122:ASN:HB2	2.03	0.40
5:H:11:SER:O	5:H:350:PHE:HA	2.21	0.40
1:A:702:ARG:HB3	3:E:26:PHE:HE2	1.86	0.40
2:C:65:ARG:HD3	2:C:65:ARG:HA	1.82	0.40
3:D:103:LEU:HD12	3:D:106:ALA:HB2	2.04	0.40
1:A:257:ASN:ND2	1:A:338:ARG:HH21	2.16	0.40
1:A:436:HIS:CE1	1:A:469:VAL:HG12	2.56	0.40
4:G:279:PRO:HG2	4:G:282:PHE:CD1	2.57	0.40
1:A:132:SER:OG	1:A:133:LYS:N	2.54	0.40
1:A:321:VAL:HG12	1:A:325:LYS:HE2	2.04	0.40
1:A:384:TYR:CZ	4:G:226:GLU:HB2	2.56	0.40
1:A:646:LEU:HB3	1:A:647:PHE:H	1.51	0.40
1:A:695:HIS:HD2	1:A:733:TYR:CZ	2.38	0.40
3:F:203:VAL:O	3:F:205:GLY:N	2.54	0.40
4:G:66:PHE:HB3	4:G:155:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:29:U:H2'	6:I:30:A:C8	2.57	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	694/758 (92%)	598 (86%)	92 (13%)	4 (1%)	25	55
2	B	119/126 (94%)	107 (90%)	12 (10%)	0	100	100
2	C	119/126 (94%)	109 (92%)	8 (7%)	2 (2%)	9	32
3	D	215/220 (98%)	181 (84%)	34 (16%)	0	100	100
3	E	214/220 (97%)	187 (87%)	24 (11%)	3 (1%)	11	36
3	F	203/220 (92%)	178 (88%)	23 (11%)	2 (1%)	15	45
4	G	268/299 (90%)	219 (82%)	47 (18%)	2 (1%)	22	52
5	H	335/357 (94%)	272 (81%)	61 (18%)	2 (1%)	25	55
All	All	2167/2326 (93%)	1851 (85%)	301 (14%)	15 (1%)	26	52

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	A	659	ILE
2	C	8	ASN
3	E	158	GLU
3	F	204	PHE
2	C	7	GLU
4	G	29	ALA
3	E	186	GLY
1	A	566	ASP

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Mol	Chain	Res	Type
3	F	29	ILE
5	H	202	LYS
4	G	242	PHE
1	A	313	THR
3	E	182	LEU
5	H	281	GLY

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	561/650 (86%)	556 (99%)	5 (1%)	78	90
2	B	99/112 (88%)	98 (99%)	1 (1%)	76	89
2	C	99/112 (88%)	98 (99%)	1 (1%)	76	89
3	D	182/188 (97%)	176 (97%)	6 (3%)	38	67
3	E	182/188 (97%)	178 (98%)	4 (2%)	52	76
3	F	175/188 (93%)	167 (95%)	8 (5%)	27	57
4	G	237/263 (90%)	232 (98%)	5 (2%)	53	77
5	H	290/312 (93%)	286 (99%)	4 (1%)	67	84
All	All	1825/2013 (91%)	1791 (98%)	34 (2%)	59	79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	364	ARG
1	A	506	ASN
1	A	536	ASN
1	A	604	ASN
2	B	25	ARG
2	C	102	ARG
3	D	6	ILE
3	D	115	ARG

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Mol	Chain	Res	Type
3	D	124	ASN
3	D	134	ASN
3	D	175	LYS
3	D	176	LEU
3	E	14	LEU
3	E	103	LEU
3	E	210	LYS
3	E	213	ASN
3	F	57	ARG
3	F	134	ASN
3	F	159	ASN
3	F	161	ASN
3	F	180	ASP
3	F	188	ARG
3	F	193	VAL
3	F	197	ASN
4	G	104	GLN
4	G	157	TYR
4	G	161	ASN
4	G	165	LEU
4	G	288	ASN
5	H	161	LYS
5	H	169	TRP
5	H	307	LYS
5	H	351	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	158	ASN
1	A	257	ASN
1	A	297	ASN
1	A	391	ASN
1	A	506	ASN
1	A	536	ASN
1	A	604	ASN
1	A	675	ASN
1	A	677	GLN
1	A	695	HIS
2	B	23	ASN
3	D	124	ASN

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Mol	Chain	Res	Type
3	D	134	ASN
3	E	19	HIS
3	F	11	GLN
3	F	134	ASN
3	F	144	ASN
3	F	161	ASN
3	F	197	ASN
4	G	14	HIS
4	G	161	ASN
4	G	174	GLN
4	G	284	HIS
4	G	288	ASN
5	H	273	ASN
5	H	294	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	I	33/36 (91%)	12 (36%)	2 (6%)
7	J	27/50 (54%)	11 (40%)	1 (3%)
All	All	60/86 (69%)	23 (38%)	3 (5%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	I	2	C
6	I	3	G
6	I	8	C
6	I	9	G
6	I	15	U
6	I	21	G
6	I	24	A
6	I	27	A
6	I	29	U
6	I	31	C
6	I	32	C
6	I	34	A
7	J	9	U
7	J	10	G
7	J	11	G
7	J	12	G

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Mol	Chain	Res	Type
7	J	18	A
7	J	24	A
7	J	25	G
7	J	29	G
7	J	30	A
7	J	32	A
7	J	33	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	I	26	A
6	I	33	C
7	J	9	U

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.

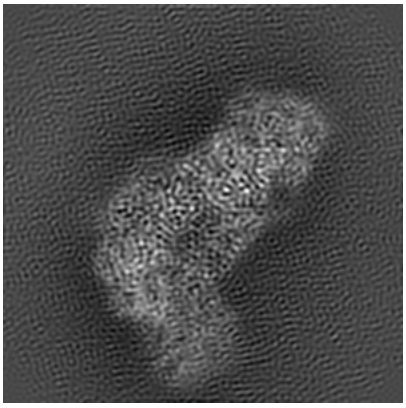
6 Map visualisation (i)

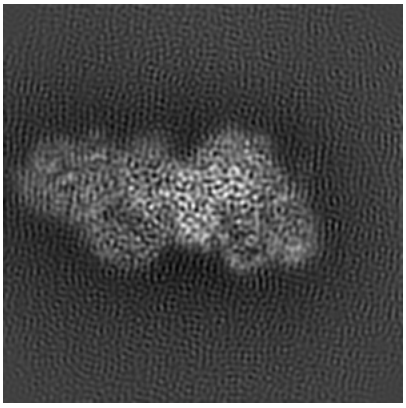
This section contains visualisations of the EMDB entry EMD-9657. These allow visual inspection of the internal detail of the map and identification of artifacts.

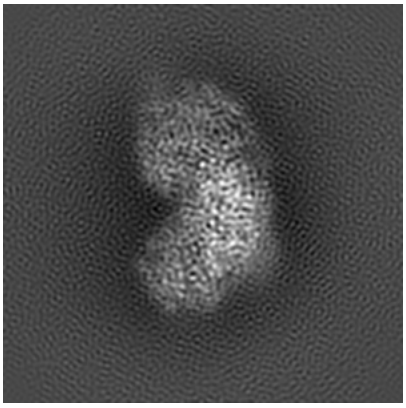
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

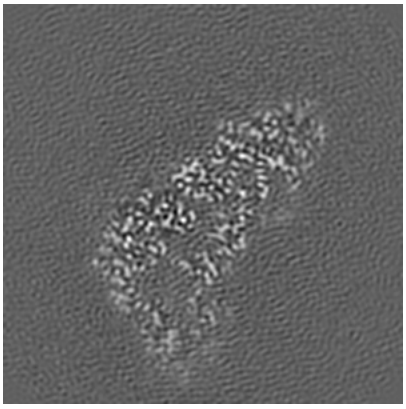

Y

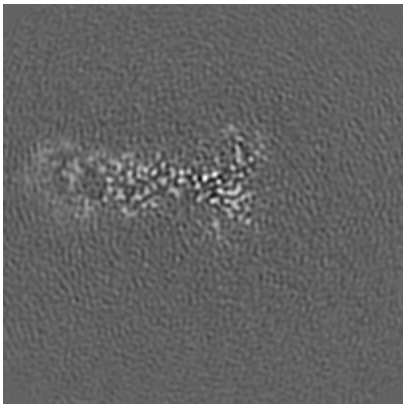

Z

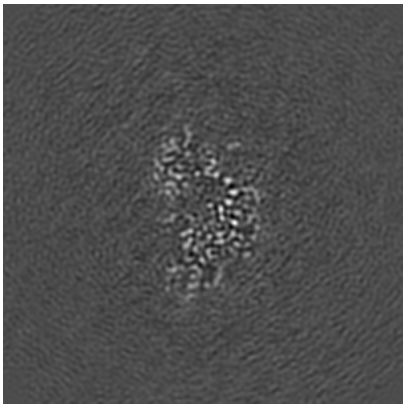
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 100

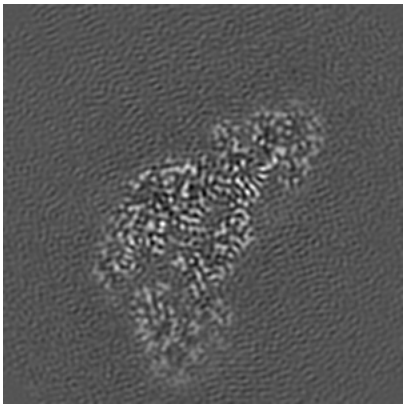

Y Index: 100

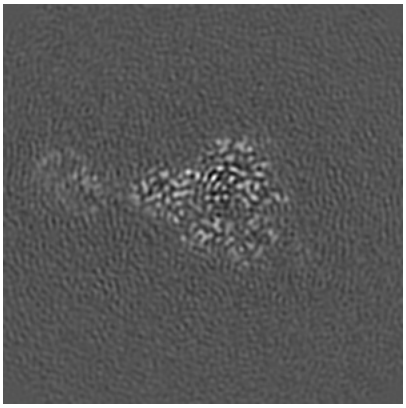

Z Index: 100

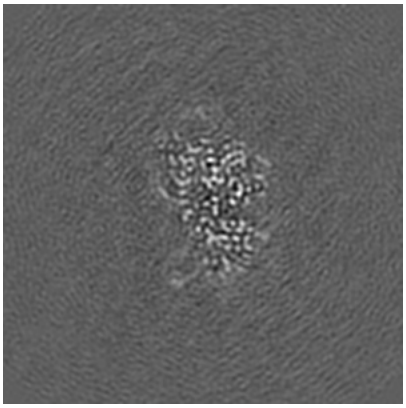
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 104

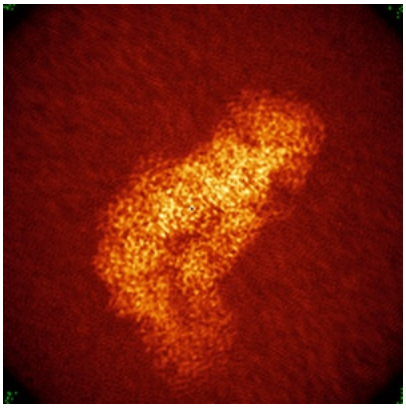

Y Index: 110

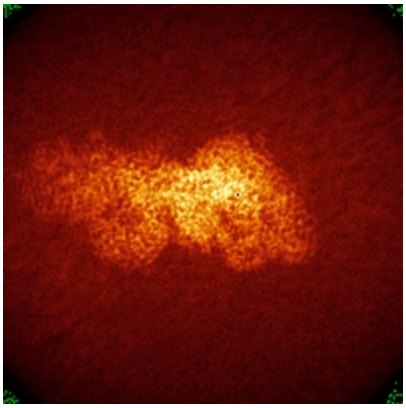

Z Index: 106

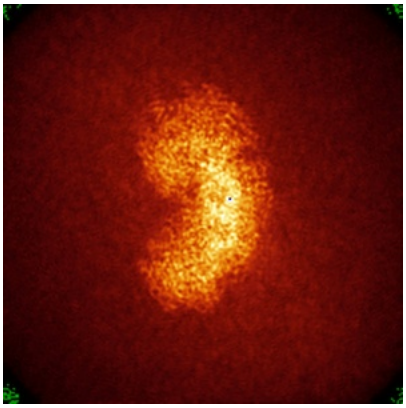
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

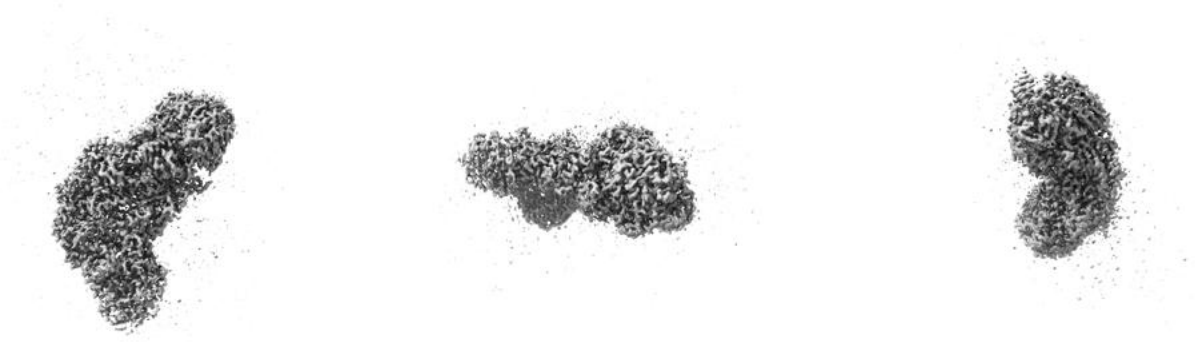

Y


Z

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

6.5 Orthogonal surface views (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 0.076. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

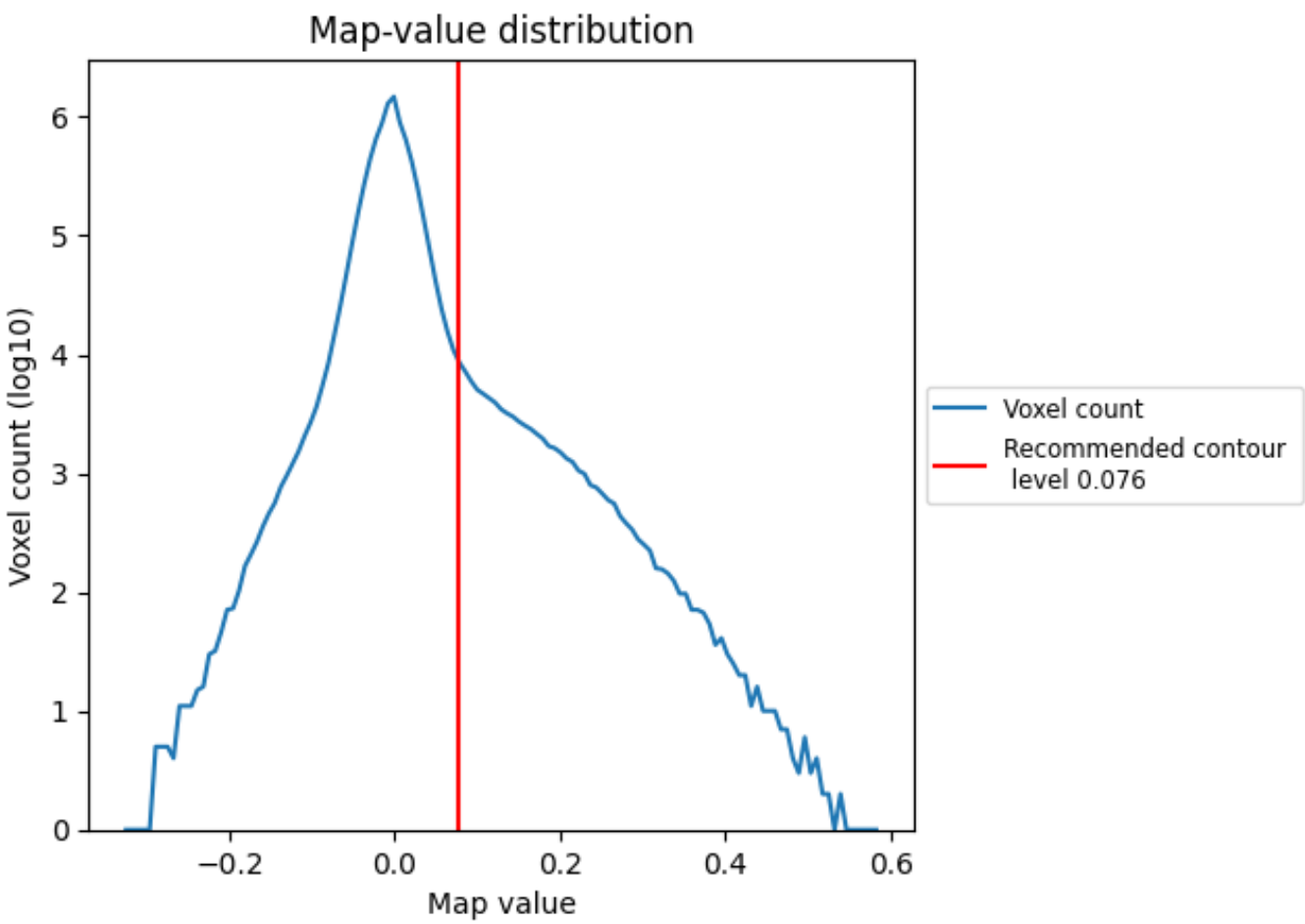
6.6 Mask visualisation (i)

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

7 Map analysis (i)

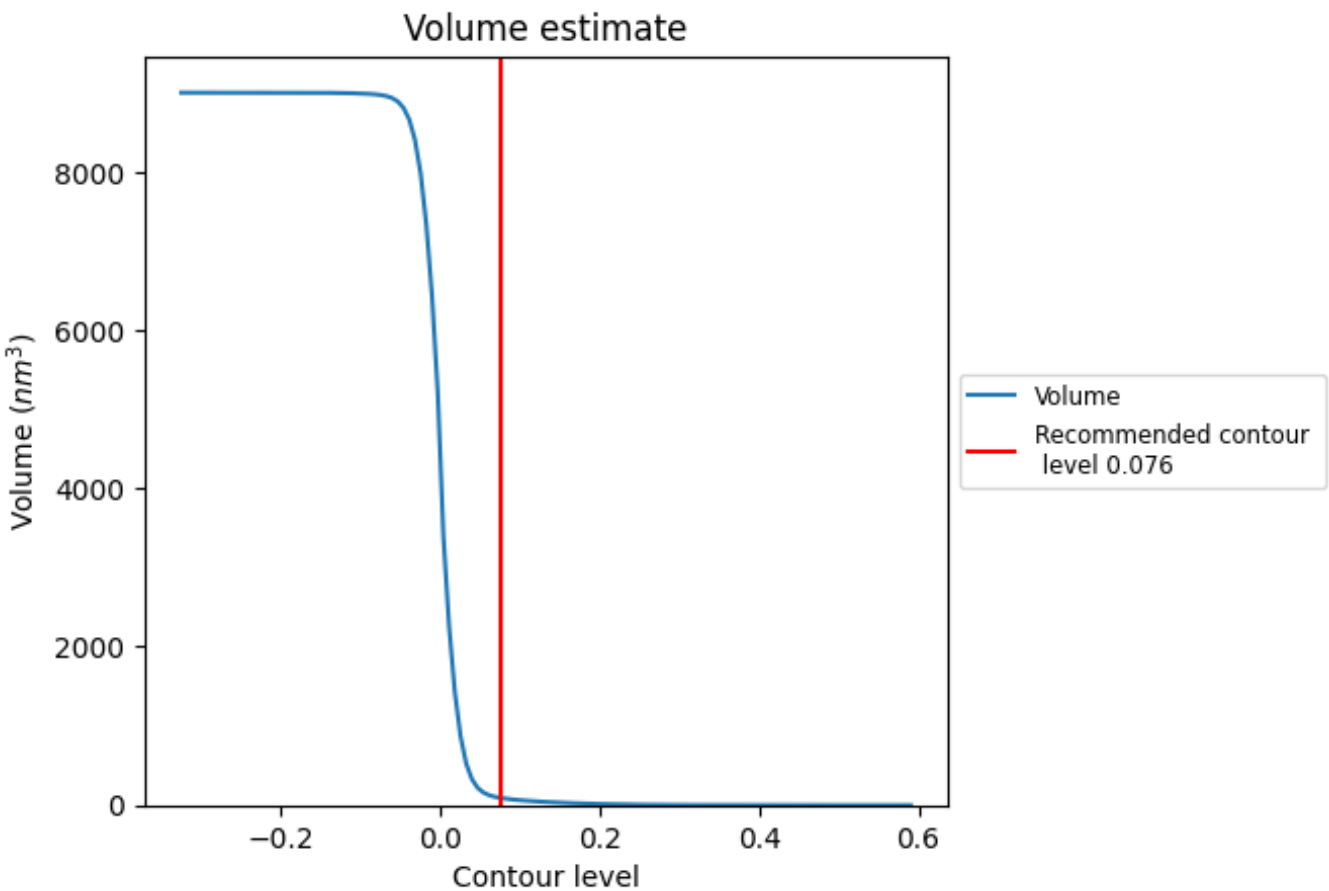
This section contains the results of statistical analysis of the map.

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.

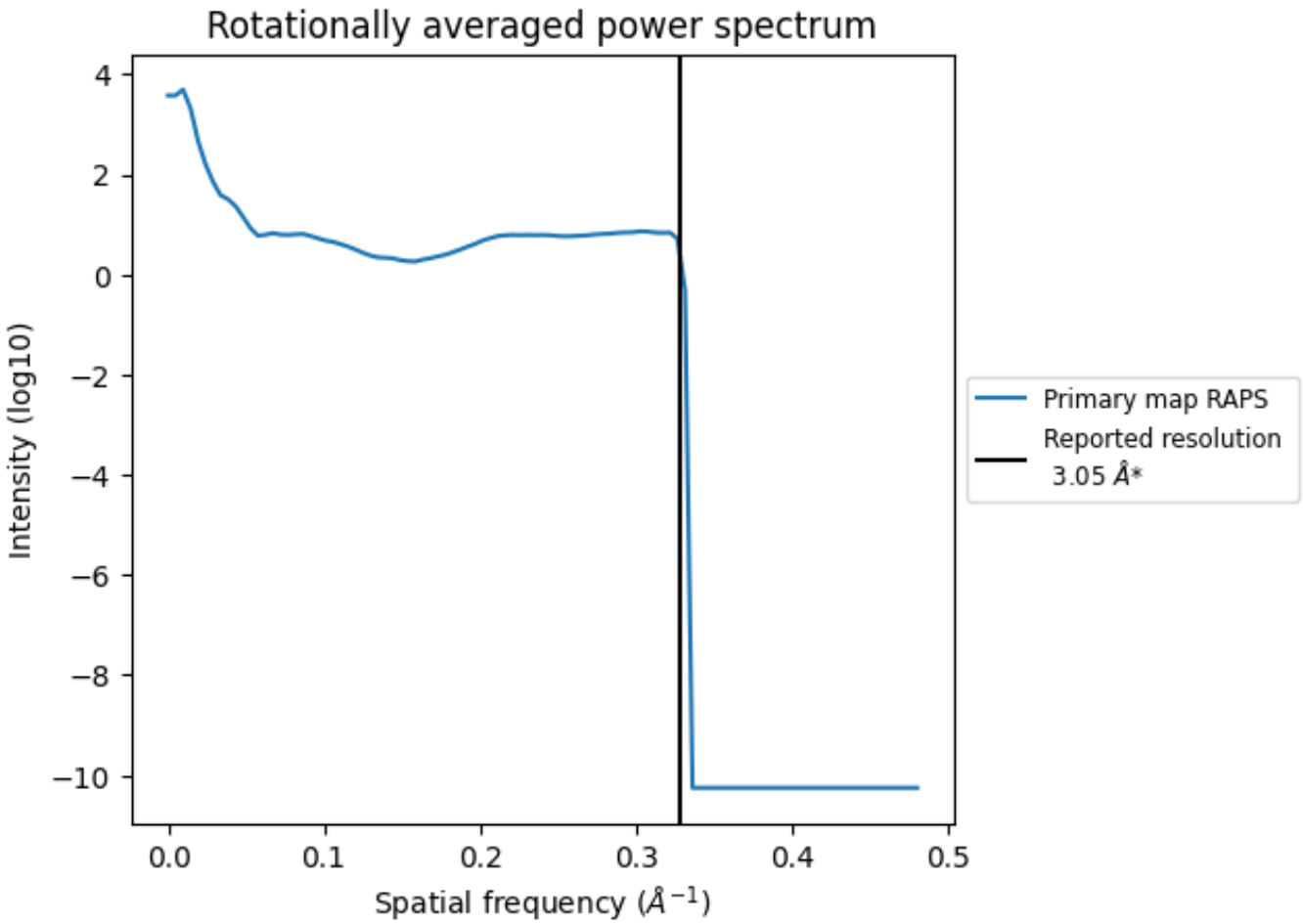
7.2 Volume estimate (i)



The volume at the recommended contour level is 91 nm^3; this corresponds to an approximate mass of 82 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 0.328 Å^{-1}

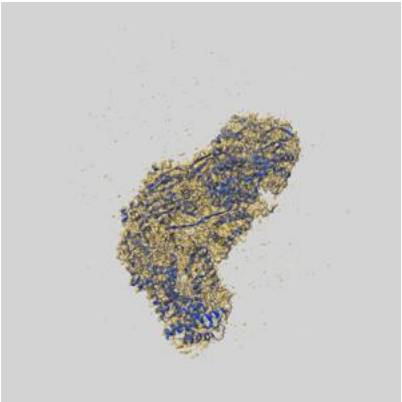
8 Fourier-Shell correlation (i)

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

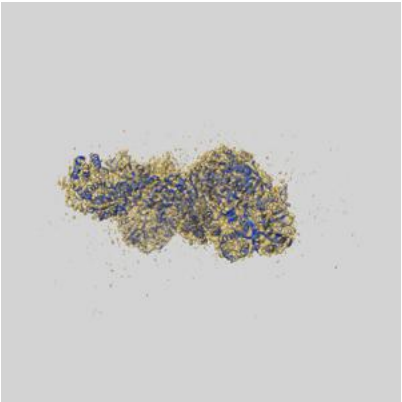
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9657 and PDB model 6IFU. Per-residue inclusion information can be found in section 3 on page 6.

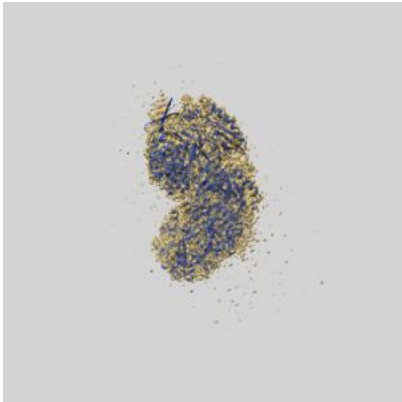
9.1 Map-model overlay (i)



X



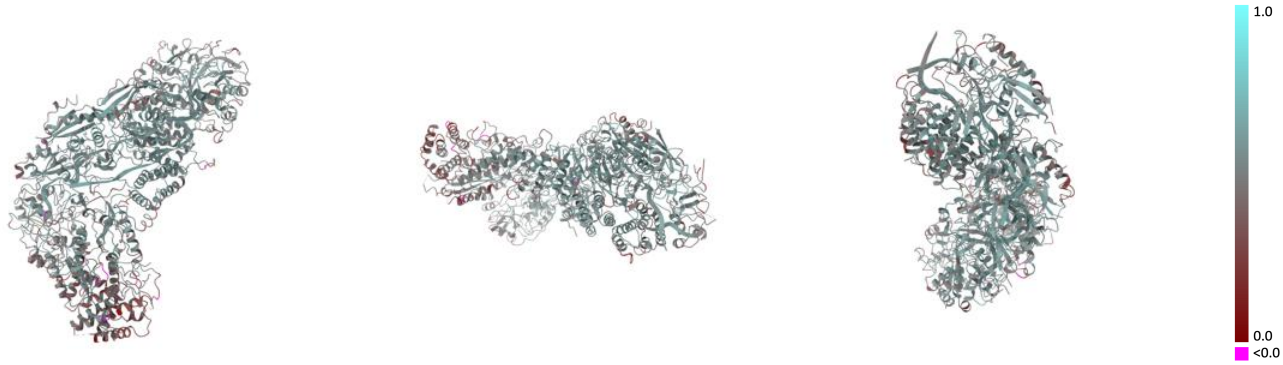
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.076 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.

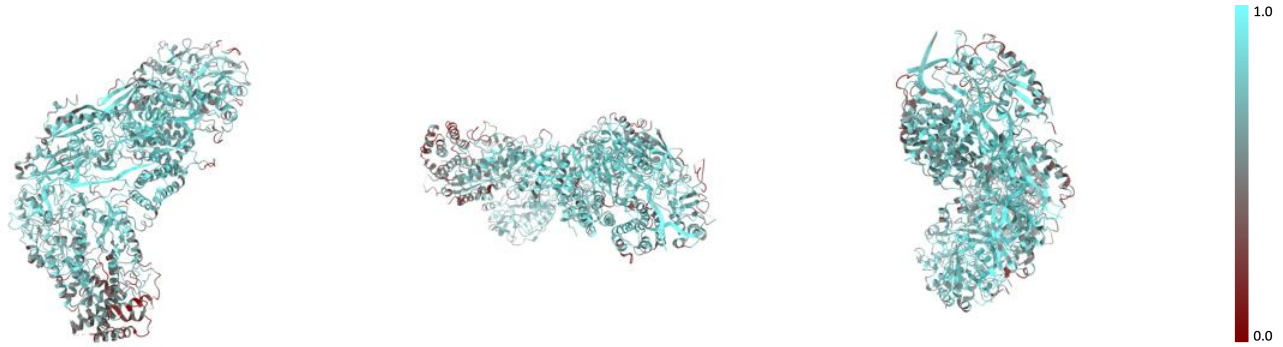
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

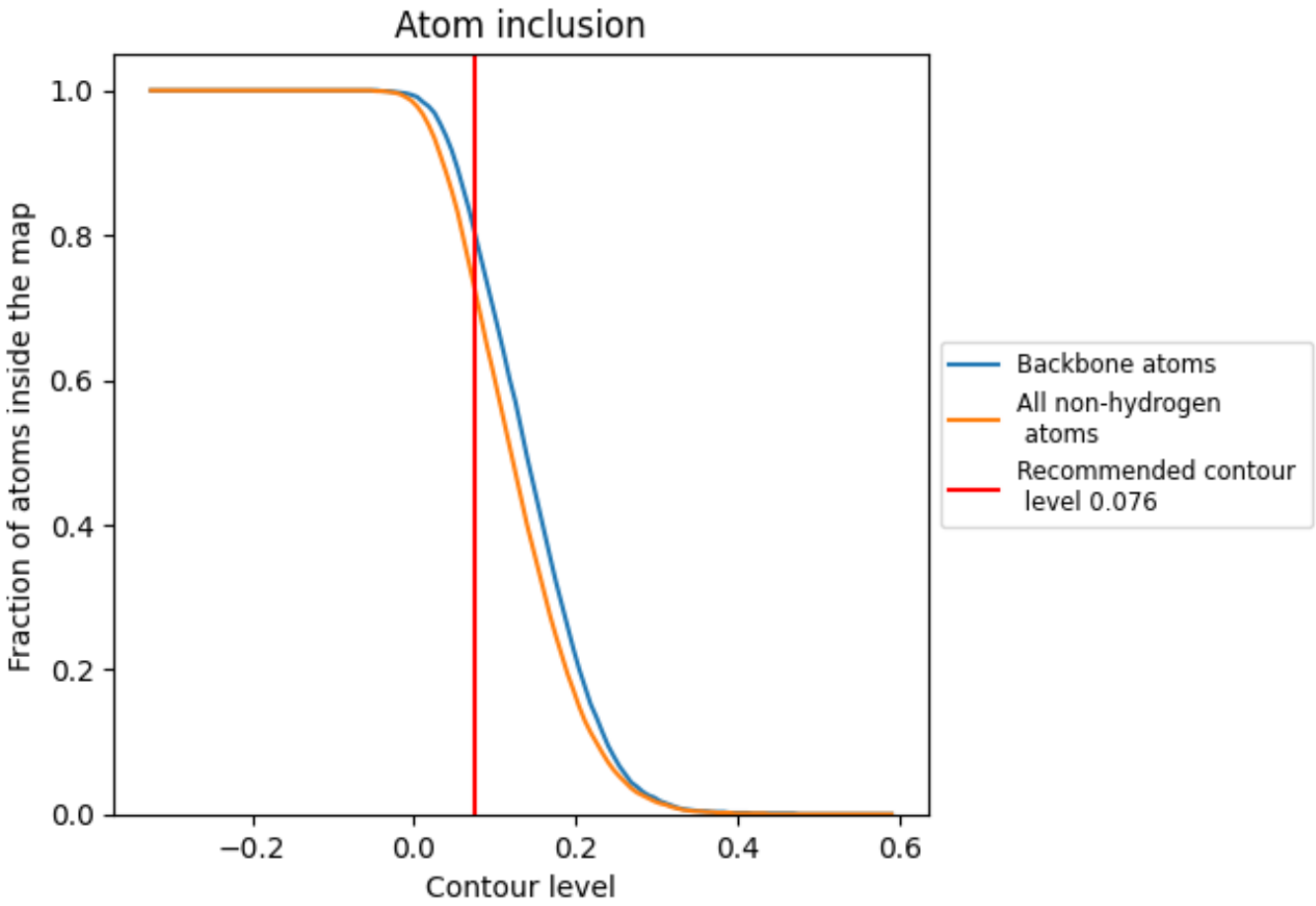
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.076).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.076) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.5080
A	0.6280	0.4510
B	0.7130	0.5010
C	0.7730	0.5460
D	0.7600	0.5310
E	0.7820	0.5520
F	0.7820	0.5440
G	0.7440	0.5120
H	0.6660	0.5050
I	0.9390	0.5930
J	0.9210	0.5900