Full wwPDB EM Validation Report (i)

Mar 3, 2024 – 02:15 PM EST

PDB ID	:	6B45
EMDB ID	:	EMD-7049
Title	:	Cryo-EM structure of Type I-F CRISPR crRNA-guided Csy surveillance complex
Authors	:	Guo, T.W.; Bartesaghi, A.; Yang, H.; Falconieri, V.; Rao, P.; Merk, A.; Fox, T.; Earl, L.; Patel, D.J.; Subramaniam, S.
Deposited on	:	2017-09-25
Resolution	:	3.50 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:

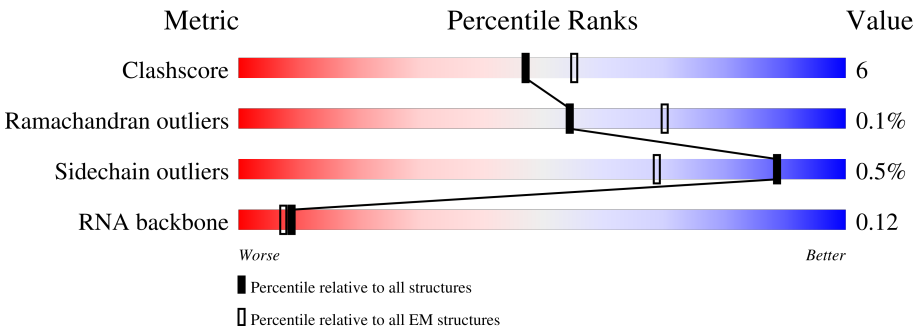
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	436	85%; 91%; 6%; •
2	B	329	77%; 71%; 21%; 7%
3	C	344	69%; 68%; 17%; 15%
3	D	344	49%; 77%; 19%; •
3	E	344	30%; 82%; 15%; •
3	F	344	24%; 83%; 13%; • •
3	G	344	24%; 82%; 15%; •

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Mol	Chain	Length	Quality of chain
3	H	344	43% 81% 16%
4	L	189	99% 97%
5	M	60	38% 20% 60% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	424	2079	1145	473	461	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q02ML9
A	0	SER	-	expression tag	UNP Q02ML9

- Molecule 2 is a protein called CRISPR-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	305	2374	1504	440	425	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP Q02MM0
B	0	ALA	-	expression tag	UNP Q02MM0

- Molecule 3 is a protein called CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	293	2272	1430	409	431	2	0	0
3	D	333	2554	1603	466	483	2	0	0
3	E	334	2561	1611	466	482	2	0	0
3	F	335	2566	1614	467	483	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	333	2557	1608	466	481	2	0	0
			Total	C	N	O	S		
3	H	333	2554	1603	466	483	2	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP Q02MM1
C	0	ALA	-	expression tag	UNP Q02MM1
D	-1	MET	-	initiating methionine	UNP Q02MM1
D	0	ALA	-	expression tag	UNP Q02MM1
E	-1	MET	-	initiating methionine	UNP Q02MM1
E	0	ALA	-	expression tag	UNP Q02MM1
F	-1	MET	-	initiating methionine	UNP Q02MM1
F	0	ALA	-	expression tag	UNP Q02MM1
G	-1	MET	-	initiating methionine	UNP Q02MM1
G	0	ALA	-	expression tag	UNP Q02MM1
H	-1	MET	-	initiating methionine	UNP Q02MM1
H	0	ALA	-	expression tag	UNP Q02MM1

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	L	189	758	380	189	189	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	MET	-	initiating methionine	UNP Q02MM2
L	0	ALA	-	expression tag	UNP Q02MM2

- Molecule 5 is a RNA chain called Pseudomonas aeruginosa strain SMC4485 CRISPR repeat sequence.

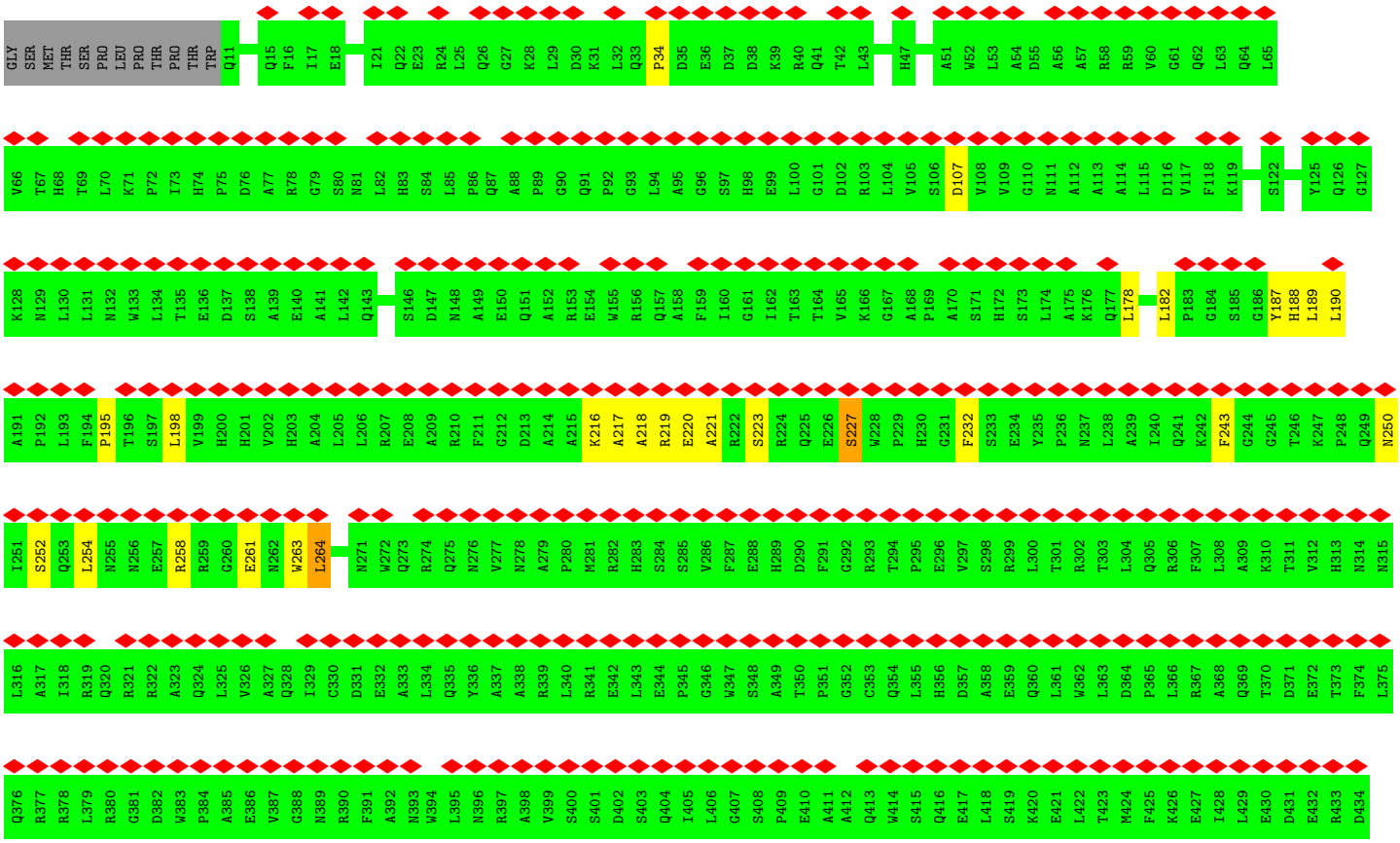
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	M	60	1272	569	223	421	59	0	0

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.

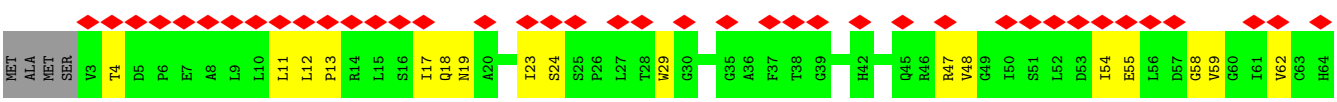
- Molecule 1: CRISPR-associated protein Csy1

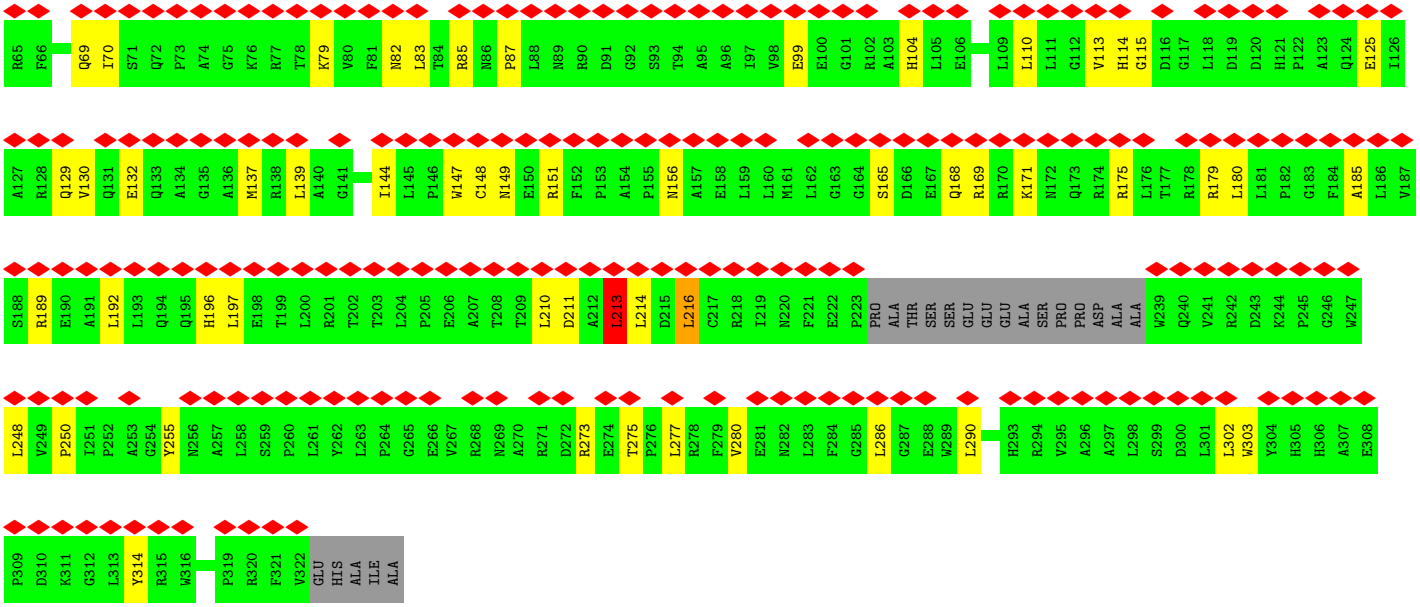
Chain A: 85% 91% 6%



- Molecule 2: CRISPR-associated protein Csy2

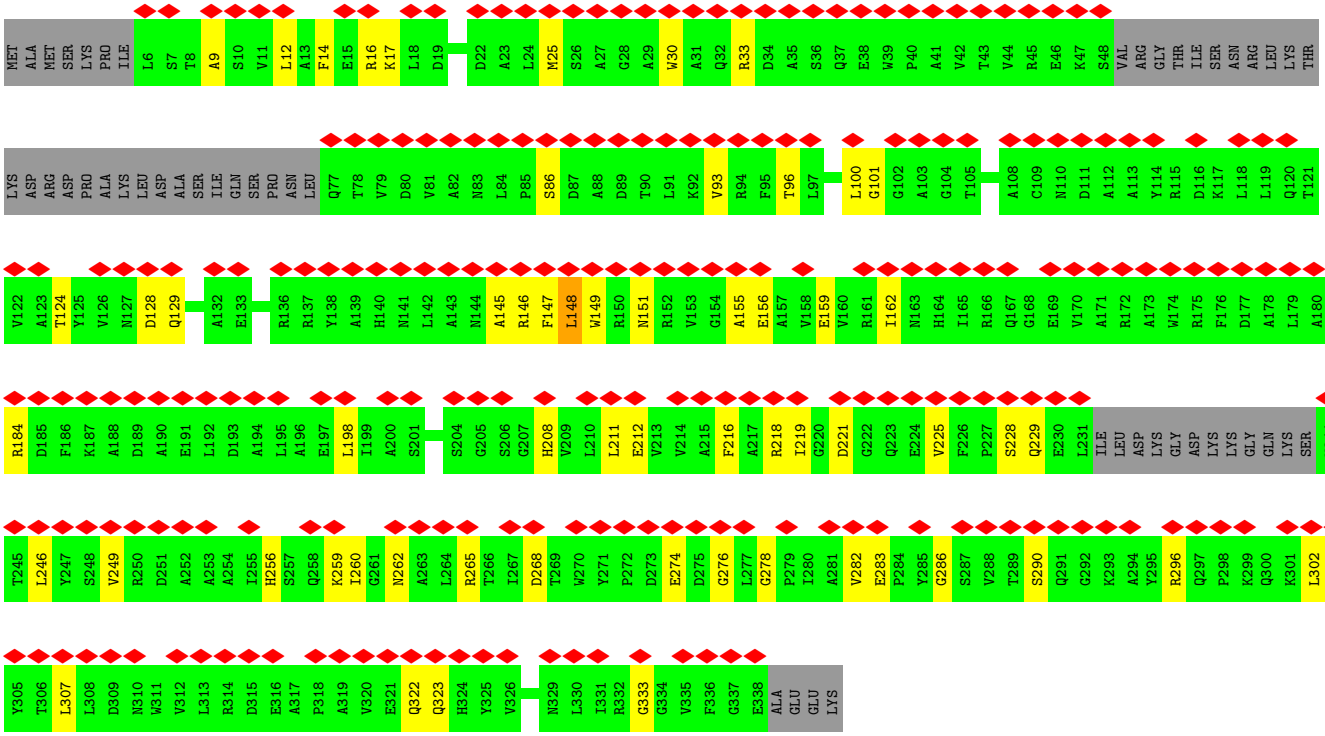
Chain B: 77% 71% 21% 7%





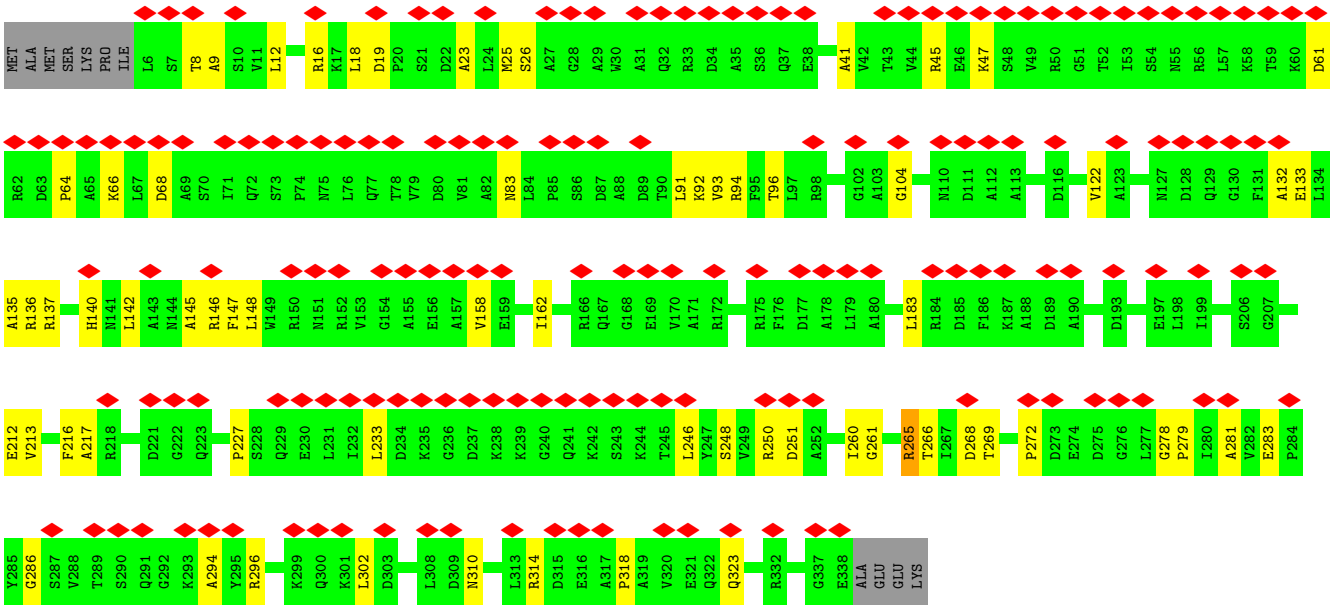
- Molecule 3: CRISPR-associated protein Csy3

Chain C:



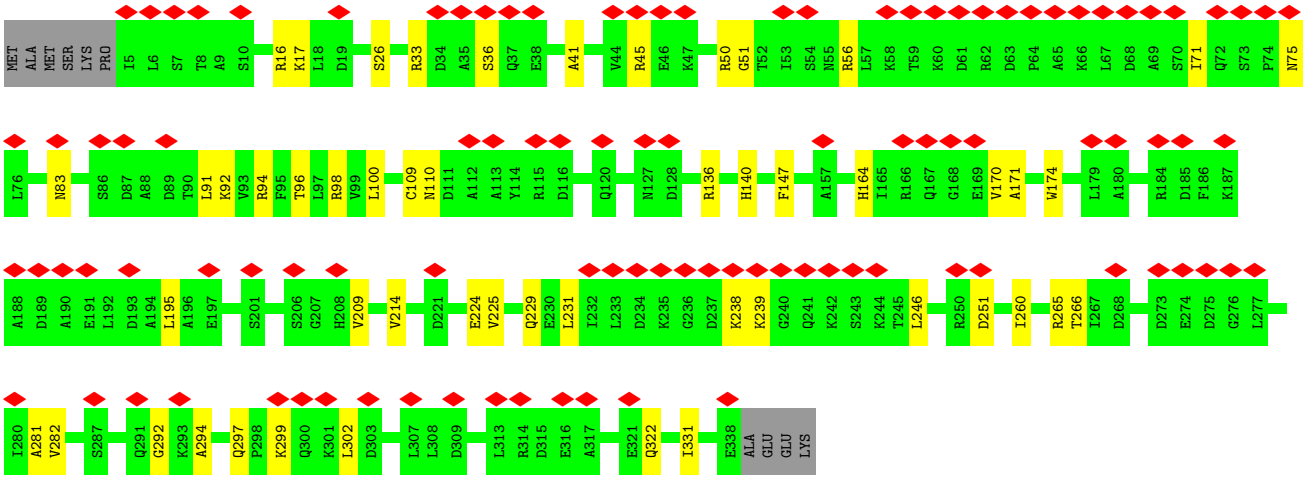
- Molecule 3: CRISPR-associated protein Csy3

Chain D:



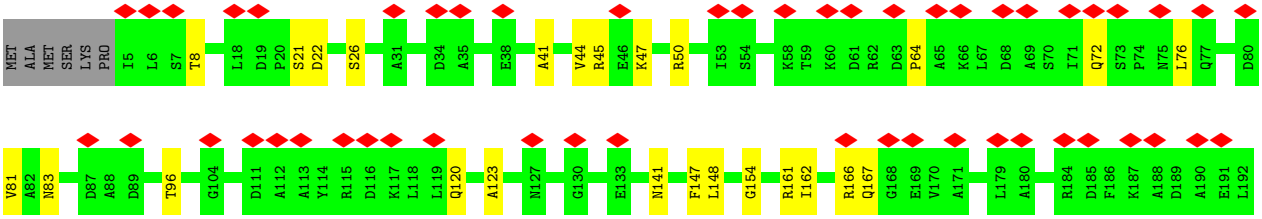
- Molecule 3: CRISPR-associated protein Csy3

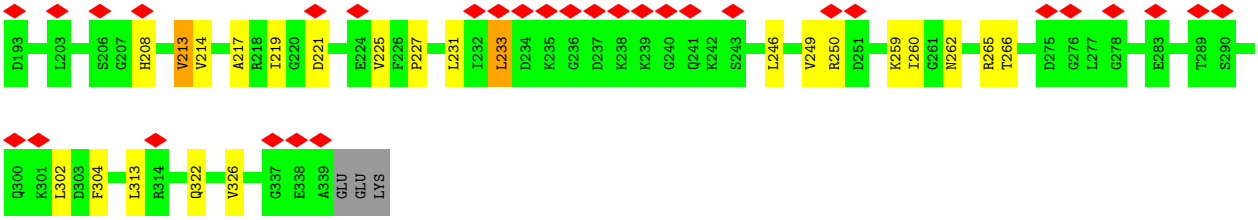
Chain E:



- Molecule 3: CRISPR-associated protein Csy3

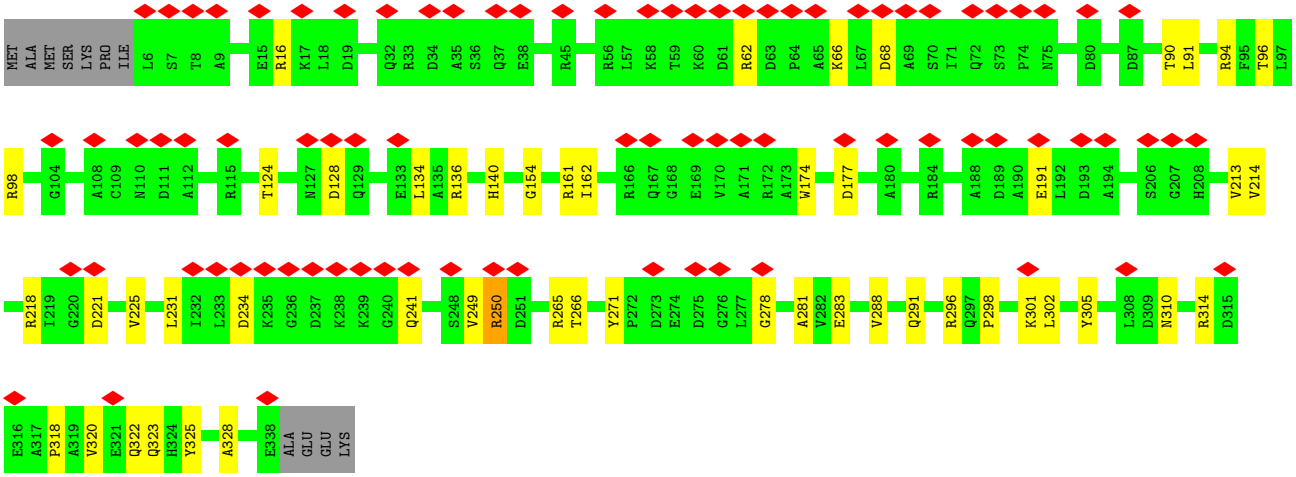
Chain F:





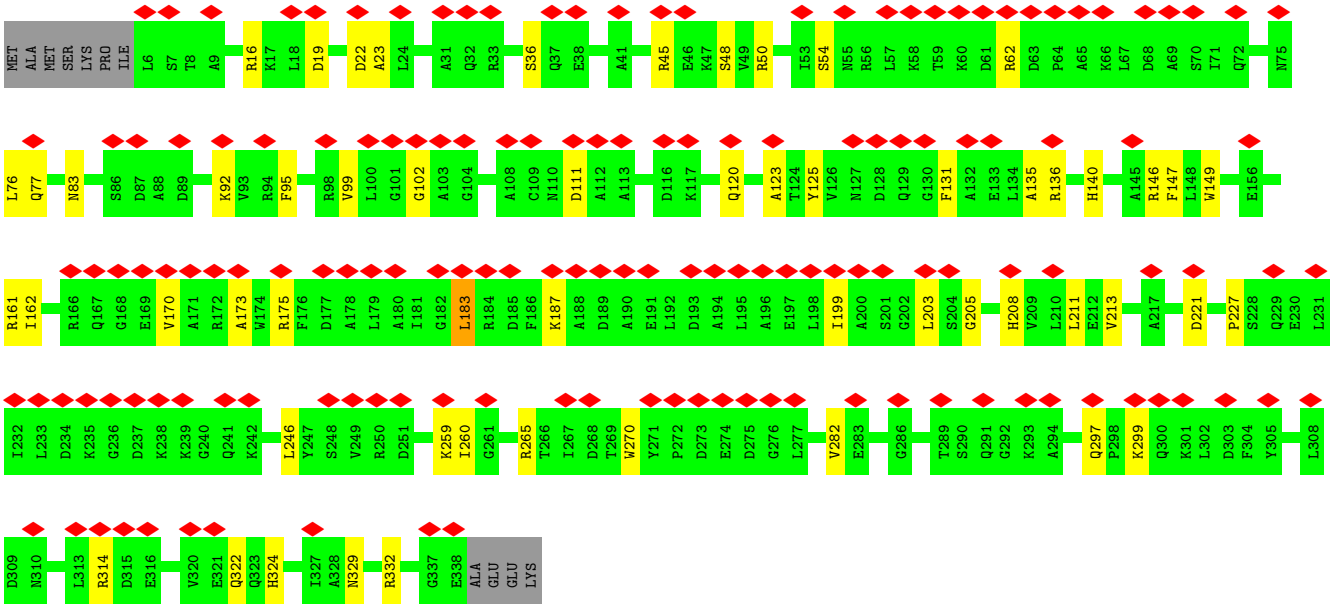
• Molecule 3: CRISPR-associated protein Csy3

Chain G:



• Molecule 3: CRISPR-associated protein Csy3

Chain H:



• Molecule 4: CRISPR-associated endonuclease Cas6/Csy4

Chain L: 99% 97%

M-1 A0 M1 D2 H3 Y4 L5 D6 I7 R8 L9 R10 P11 D12 P13 E14 F15 P16 P17 A18 Q19 L20 M21 S22 V23 L24 F25 G26 K27 L28 H29 Q30 A31 L32 V33 A34 Q35 G36 G37 D38 R39 I40 G41 V42 S43 F44 P45 D46 L47 D48 E49 S50 R51 S52 R53 L54 G55 E56 R57 L58

R59 I60 H61 A62 S63 A64 D65 D66 L67 R68 A69 L70 L71 A72 R73 P74 W75 L76 E77 G78 L79 R80 D81 H82 L83 Q84 F85 G86 E87 P88 A89 V90 V91 P92 H93 P94 T95 P96 Y97 R98 Q99 V100 S101 R102 V103 Q104 A105 K106 S107 N108 P109 E110 R111 L112 R113 R114 R115 L116 M117 R118

R119 H120 D121 L122 S123 E124 E125 E126 A127 R128 K129 R130 I131 P132 D133 T134 V135 A136 R137 A138 L139 D140 L141 P142 F143 V144 T145 L146 R147 S148 Q149 S150 T151 G152 Q153 H154 F155 R156 L157 F158 I159 R160 H161 G162 P163 L164 Q165 V166 T167 A168 E169 E170 G171 G172 F173 T174 C175 Y176 G177 L178

S179 K180 G181 G182 F183 V184 P185 W186 F187

- Molecule 5: Pseudomonas aeruginosa strain SMC4485 CRISPR repeat sequence

Chain M: 38% 20% 60% 20%

C1 U2 A6 A7 A8 U9 A12 C13 G14 G15 C16 G17 G18 G19 C20 U21 U22 G23 A24 U25 G26 U27 G30 C31 G32 U33 C34 U35 A36 C37 C38 U39 G40 G41 U42 U43 C44 A45 C46 U47 G48 C49 C50 G51 U52 G53 U54 A55 G56 G57 C58 A59 G60

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31488	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 ($e^-/Å^2$)	40	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	10.087	Depositor
Minimum map value	-7.702	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.714	Depositor
Recommended contour level	2.9	Depositor
Map size (Å)	199.92, 199.92, 199.92	wwPDB
Map dimensions	238, 238, 238	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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	0.26	0/2104	0.56	3/2715 (0.1%)
2	B	0.31	0/2431	0.63	2/3310 (0.1%)
3	C	0.30	0/2315	0.65	3/3143 (0.1%)
3	D	0.33	0/2601	0.63	1/3532 (0.0%)
3	E	0.34	0/2608	0.62	1/3540 (0.0%)
3	F	0.35	0/2613	0.63	1/3547 (0.0%)
3	G	0.34	0/2604	0.60	0/3533
3	H	0.32	0/2601	0.61	1/3532 (0.0%)
4	L	0.24	0/757	0.51	0/946
5	M	0.49	0/1420	1.14	14/2212 (0.6%)
All	All	0.33	0/22054	0.67	26/30010 (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	A	0	2
2	B	0	1
3	C	0	1
3	G	0	1
All	All	0	5

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	58	C	N1-C2-O2	9.05	124.33	118.90
5	M	58	C	C2-N1-C1'	8.86	128.54	118.80
5	M	58	C	C6-N1-C2	-7.23	117.41	120.30
5	M	58	C	N3-C2-O2	-7.20	116.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	46	C	C6-N1-C2	-7.05	117.48	120.30
3	D	18	LEU	CA-CB-CG	6.80	130.95	115.30
5	M	60	G	C4-N9-C1'	6.44	134.88	126.50
1	A	189	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	264	LEU	CA-CB-CG	6.09	129.30	115.30
5	M	46	C	C5-C6-N1	6.08	124.04	121.00
5	M	58	C	C5-C6-N1	5.96	123.98	121.00
5	M	46	C	N1-C2-O2	5.92	122.45	118.90
5	M	58	C	C6-N1-C1'	-5.73	113.92	120.80
3	E	251	ASP	CB-CG-OD1	5.71	123.44	118.30
3	C	198	LEU	CA-CB-CG	5.56	128.08	115.30
5	M	60	G	N3-C4-C5	-5.54	125.83	128.60
5	M	60	G	N3-C4-N9	5.53	129.32	126.00
3	F	233	LEU	CA-CB-CG	5.50	127.94	115.30
3	H	183	LEU	CA-CB-CG	5.48	127.91	115.30
2	B	213	LEU	CA-CB-CG	5.41	127.75	115.30
5	M	60	G	C8-N9-C1'	-5.25	120.18	127.00
5	M	46	C	C2-N1-C1'	5.20	124.52	118.80
3	C	148	LEU	CA-CB-CG	5.15	127.14	115.30
2	B	277	LEU	CA-CB-CG	5.08	126.99	115.30
3	C	307	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	254	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	SER	Peptide
1	A	263	TRP	Peptide
2	B	12	LEU	Peptide
3	C	249	VAL	Peptide
3	G	301	LYS	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	2079	0	1094	17	0
2	B	2374	0	2345	53	0
3	C	2272	0	2232	39	0
3	D	2554	0	2522	40	0
3	E	2561	0	2542	35	0
3	F	2566	0	2547	31	0
3	G	2557	0	2542	31	0
3	H	2554	0	2522	38	0
4	L	758	0	209	5	0
5	M	1272	0	644	24	0
All	All	21547	0	19199	261	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 6.

All (261) 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)
3:H:199:ILE:O	3:H:203:LEU:HB2	1.85	0.77
3:C:148:LEU:HB2	3:C:151:ASN:HB3	1.68	0.75
3:C:124:THR:O	3:C:128:ASP:HB2	1.88	0.73
1:A:221:ALA:HB1	1:A:227:SER:HB2	1.71	0.72
4:L:-1:MET:CB	4:L:183:PHE:C	2.58	0.71
3:G:302:LEU:HB3	3:G:322:GLN:HE22	1.57	0.69
3:F:162:ILE:HG12	3:F:213:VAL:HG12	1.77	0.66
3:E:238:LYS:HG2	3:E:239:LYS:HG3	1.78	0.66
2:B:189:ARG:HB3	2:B:192:LEU:HB3	1.79	0.64
3:D:283:GLU:HB3	3:D:286:GLY:HA2	1.81	0.63
3:G:298:PRO:HB2	3:H:62:ARG:HD3	1.80	0.63
3:C:9:ALA:HB3	3:C:12:LEU:HD12	1.80	0.62
2:B:23:ILE:HA	2:B:29:TRP:HA	1.82	0.62
3:G:161:ARG:HB2	3:G:214:VAL:HB	1.80	0.62
3:C:296:ARG:HH12	3:C:322:GLN:HE22	1.47	0.61
3:D:310:ASN:OD1	3:D:314:ARG:NH2	2.34	0.61
3:G:265:ARG:NH2	5:M:14:G:OP2	2.33	0.60
3:D:16:ARG:HB2	5:M:30:G:H5”	1.82	0.60
3:G:90:THR:HA	3:G:218:ARG:HA	1.84	0.60
2:B:69:GLN:HB3	2:B:82:ASN:HB2	1.83	0.60
2:B:83:LEU:HD21	2:B:99:GLU:HG2	1.84	0.59
3:C:162:ILE:HD11	3:C:211:LEU:HB3	1.85	0.59
3:C:129:GLN:NE2	3:C:323:GLN:OE1	2.35	0.59
4:L:-1:MET:CB	4:L:183:PHE:CA	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:GLY:HA3	2:B:302:LEU:HB3	1.84	0.59
2:B:156:ASN:OD1	2:B:179:ARG:NH2	2.36	0.59
3:C:16:ARG:NH1	5:M:37:C:OP1	2.36	0.59
3:E:98:ARG:NH1	3:F:219:ILE:O	2.36	0.59
2:B:85:ARG:NH2	5:M:9:U:O2	2.36	0.58
3:E:17:LYS:HG3	3:E:100:LEU:HB2	1.84	0.58
3:H:136:ARG:O	3:H:140:HIS:ND1	2.33	0.58
3:D:146:ARG:NH2	3:D:183:LEU:O	2.37	0.58
3:E:16:ARG:HD3	5:M:24:A:H5'	1.85	0.57
2:B:11:LEU:O	2:B:156:ASN:ND2	2.37	0.57
2:B:197:LEU:HB2	2:B:210:LEU:HD22	1.85	0.57
3:E:96:THR:HG21	3:F:221:ASP:HB3	1.86	0.57
2:B:214:LEU:HD22	2:B:248:LEU:HD13	1.86	0.57
2:B:273:ARG:NH1	3:H:111:ASP:OD1	2.37	0.57
3:D:272:PRO:HD3	3:D:302:LEU:HD12	1.85	0.57
3:G:234:ASP:OD1	3:G:241:GLN:NE2	2.36	0.57
3:D:248:SER:O	3:E:45:ARG:NH2	2.38	0.57
3:C:25:MET:HG2	3:C:93:VAL:HG12	1.85	0.56
3:E:109:CYS:SG	3:E:110:ASN:N	2.77	0.56
3:C:14:PHE:HB2	3:C:333:GLY:HA2	1.86	0.56
1:A:218:ALA:HB2	1:A:232:PHE:HB2	1.87	0.56
2:B:59:VAL:HG22	2:B:303:TRP:HB2	1.88	0.56
3:D:266:THR:HA	3:D:281:ALA:HA	1.87	0.56
3:E:265:ARG:NH1	3:E:282:VAL:O	2.39	0.56
2:B:70:ILE:HD12	2:B:79:LYS:HD3	1.87	0.56
3:G:231:LEU:HD21	3:H:76:LEU:HB3	1.88	0.56
3:H:131:PHE:O	3:H:135:ALA:N	2.37	0.56
3:E:94:ARG:HG3	3:E:214:VAL:HG22	1.88	0.55
3:D:61:ASP:OD2	3:D:66:LYS:NZ	2.40	0.55
3:C:184:ARG:HD3	3:C:278:GLY:HA3	1.88	0.55
3:H:147:PHE:HB2	3:H:260:ILE:HG13	1.88	0.55
3:C:155:ALA:HA	3:C:219:ILE:HA	1.89	0.55
3:D:96:THR:HG22	3:D:212:GLU:HG2	1.89	0.55
2:B:148:CYS:SG	2:B:149:ASN:N	2.80	0.55
3:C:124:THR:O	3:C:128:ASP:CB	2.54	0.55
3:E:51:GLY:O	3:E:75:ASN:ND2	2.40	0.55
3:G:271:TYR:HB3	3:G:296:ARG:HE	1.72	0.55
2:B:165:SER:O	2:B:169:ARG:N	2.39	0.55
3:E:147:PHE:HB2	3:E:260:ILE:HG13	1.89	0.55
3:E:164:HIS:HD2	3:E:171:ALA:HB3	1.73	0.54
3:H:99:VAL:HG11	3:H:203:LEU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:LYS:O	2:B:175:ARG:HB2	2.07	0.54
1:A:216:LYS:NZ	1:A:220:GLU:OE1	2.37	0.53
2:B:11:LEU:HD23	2:B:110:LEU:HB3	1.90	0.53
3:C:265:ARG:HH22	5:M:37:C:H4'	1.73	0.53
3:F:47:LYS:HE2	3:F:81:VAL:HG21	1.89	0.53
1:A:195:PRO:HB2	1:A:198:LEU:HB2	1.89	0.53
3:H:162:ILE:HD11	3:H:211:LEU:HB3	1.91	0.53
3:D:132:ALA:HA	3:D:135:ALA:HB3	1.91	0.53
4:L:6:ASP:H	4:L:86:GLY:HA3	1.74	0.53
3:C:290:SER:OG	4:L:12:ASP:O	2.24	0.52
2:B:18:GLN:HE22	3:H:22:ASP:H	1.57	0.52
3:F:148:LEU:HD13	3:F:217:ALA:HB2	1.92	0.52
3:D:261:GLY:O	3:D:265:ARG:NE	2.41	0.52
3:F:96:THR:HG21	3:G:221:ASP:HB2	1.92	0.52
3:E:36:SER:O	3:E:92:LYS:NZ	2.32	0.52
3:H:146:ARG:NH2	3:H:183:LEU:O	2.42	0.52
3:H:162:ILE:HD13	3:H:213:VAL:HG22	1.91	0.52
3:C:151:ASN:HA	3:C:225:VAL:HB	1.92	0.52
3:E:231:LEU:HD11	3:F:76:LEU:HB3	1.92	0.52
2:B:125:GLU:OE2	2:B:129:GLN:NE2	2.43	0.52
3:H:297:GLN:HG2	3:H:299:LYS:H	1.75	0.51
3:E:292:GLY:O	3:F:72:GLN:NE2	2.43	0.51
3:F:208:HIS:NE2	3:G:154:GLY:O	2.43	0.51
3:H:36:SER:O	3:H:92:LYS:NZ	2.37	0.51
3:H:227:PRO:HG2	3:H:246:LEU:HD22	1.93	0.51
3:C:33:ARG:HB2	3:C:216:PHE:HZ	1.76	0.51
3:C:147:PHE:HB2	3:C:260:ILE:HG13	1.92	0.51
3:E:136:ARG:O	3:E:140:HIS:ND1	2.39	0.51
3:D:25:MET:HG2	3:D:93:VAL:HG22	1.93	0.50
3:G:124:THR:O	3:G:128:ASP:HB2	2.11	0.50
2:B:165:SER:HB3	2:B:168:GLN:HB2	1.92	0.50
3:C:274:GLU:OE1	3:C:276:GLY:N	2.44	0.50
3:C:283:GLU:HG2	3:C:286:GLY:HA2	1.94	0.49
3:D:294:ALA:HB2	3:E:71:ILE:HD11	1.93	0.49
2:B:17:ILE:HG22	2:B:144:ILE:HG12	1.95	0.49
2:B:189:ARG:HH21	2:B:290:LEU:HD21	1.77	0.49
3:F:45:ARG:NH2	3:F:83:ASN:OD1	2.45	0.49
3:C:256:HIS:HD2	3:D:47:LYS:HD2	1.76	0.49
3:G:231:LEU:HD13	3:H:48:SER:HB2	1.94	0.49
3:D:45:ARG:NH2	3:D:83:ASN:OD1	2.46	0.49
1:A:258:ARG:NH1	1:A:261:GLU:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:ILE:HG12	3:D:213:VAL:HG12	1.94	0.49
1:A:187:TYR:O	2:B:275:THR:OG1	2.31	0.48
2:B:192:LEU:O	2:B:196:HIS:CB	2.61	0.48
3:E:294:ALA:O	3:E:297:GLN:NE2	2.34	0.48
3:D:137:ARG:HH22	3:D:269:THR:HG23	1.78	0.48
2:B:13:PRO:HD3	2:B:156:ASN:HD21	1.78	0.48
3:E:299:LYS:HB2	3:F:64:PRO:HB3	1.95	0.48
3:E:83:ASN:HA	3:E:224:GLU:HA	1.95	0.48
3:E:91:LEU:HD13	3:E:225:VAL:HG11	1.96	0.48
3:H:45:ARG:HH21	3:H:83:ASN:HB2	1.77	0.48
3:H:125:TYR:HH	3:H:324:HIS:HD1	1.61	0.48
5:M:49:C:H2'	5:M:56:G:H22	1.77	0.48
2:B:185:ALA:N	2:B:290:LEU:O	2.45	0.48
3:D:9:ALA:HB3	3:D:12:LEU:HD12	1.95	0.48
2:B:55:GLU:HB3	2:B:114:HIS:HB2	1.95	0.48
3:F:147:PHE:HB2	3:F:260:ILE:HG13	1.95	0.48
3:F:259:LYS:NZ	5:M:22:U:OP1	2.47	0.48
3:D:250:ARG:NH1	3:D:251:ASP:OD2	2.47	0.48
3:D:136:ARG:O	3:D:140:HIS:ND1	2.38	0.48
3:H:23:ALA:HB2	3:H:95:PHE:HB3	1.95	0.48
3:E:50:ARG:O	5:M:31:C:O2'	2.32	0.48
3:E:164:HIS:H	3:E:170:VAL:HG23	1.79	0.48
2:B:17:ILE:HD13	2:B:139:LEU:HD21	1.95	0.47
3:D:23:ALA:HB1	3:D:93:VAL:HG13	1.96	0.47
1:A:219:ARG:O	1:A:223:SER:HB3	2.13	0.47
2:B:192:LEU:O	2:B:196:HIS:HB3	2.12	0.47
3:G:68:ASP:OD1	3:G:68:ASP:N	2.39	0.47
3:G:266:THR:HA	3:G:281:ALA:HA	1.96	0.47
3:C:14:PHE:O	5:M:35:U:O2'	2.32	0.47
3:C:259:LYS:NZ	5:M:40:G:OP1	2.38	0.47
3:G:162:ILE:HG12	3:G:213:VAL:HG22	1.96	0.47
3:G:271:TYR:OH	3:G:278:GLY:O	2.26	0.47
2:B:62:VAL:HG11	2:B:180:LEU:HD11	1.96	0.47
3:F:225:VAL:HG23	3:F:227:PRO:HD3	1.97	0.47
3:C:17:LYS:HG3	3:C:100:LEU:HB3	1.97	0.47
3:C:219:ILE:HD13	3:C:225:VAL:HG11	1.97	0.47
3:G:174:TRP:HD1	3:G:191:GLU:HG3	1.80	0.47
3:H:120:GLN:HA	3:H:123:ALA:HB3	1.96	0.47
3:C:146:ARG:NH1	3:C:183:LEU:O	2.48	0.47
3:F:265:ARG:NH2	5:M:20:C:OP2	2.48	0.47
3:D:104:GLY:HA3	3:D:122:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:VAL:HG12	2:B:115:GLY:H	1.80	0.47
3:H:265:ARG:NH2	5:M:8:A:OP2	2.48	0.47
3:D:93:VAL:HG21	3:D:148:LEU:HD21	1.97	0.46
3:D:158:VAL:HG12	3:D:217:ALA:HA	1.95	0.46
3:F:166:ARG:HG3	3:F:167:GLN:HG2	1.98	0.46
3:D:133:GLU:HA	3:D:136:ARG:HG2	1.98	0.46
2:B:87:PRO:HD3	5:M:7:A:H1'	1.98	0.46
2:B:47:ARG:NH1	2:B:137:MET:SD	2.89	0.46
3:G:310:ASN:HA	3:G:314:ARG:HB2	1.98	0.46
3:H:102:GLY:H	3:H:205:GLY:HA2	1.81	0.46
2:B:85:ARG:O	5:M:7:A:O2'	2.33	0.45
3:F:50:ARG:N	5:M:27:U:OP2	2.45	0.45
3:D:8:THR:HG21	3:E:56:ARG:HH12	1.81	0.45
3:G:96:THR:HG21	3:H:221:ASP:HB3	1.97	0.45
3:H:149:TRP:CD1	3:H:259:LYS:HE2	2.52	0.45
1:A:178:LEU:HD22	5:M:2:U:H5"	1.99	0.45
3:D:91:LEU:HG	3:D:93:VAL:HG23	1.98	0.45
3:D:145:ALA:HB1	3:D:148:LEU:HD12	1.98	0.45
3:G:249:VAL:HG12	3:G:250:ARG:H	1.82	0.45
3:H:16:ARG:HB3	3:H:19:ASP:HB3	1.99	0.45
3:C:156:GLU:HB3	3:C:218:ARG:HB2	1.98	0.45
3:C:229:GLN:HB3	3:C:246:LEU:HG	1.99	0.45
3:G:177:ASP:N	3:G:177:ASP:OD1	2.47	0.45
3:D:142:LEU:HD22	3:D:213:VAL:HG11	2.00	0.45
1:A:107:ASP:O	1:A:252:SER:OG	2.32	0.44
3:G:62:ARG:HA	3:G:66:LYS:HE2	1.99	0.44
1:A:182:LEU:HD21	1:A:188:HIS:HD2	1.81	0.44
3:E:174:TRP:CD2	3:E:195:LEU:HD12	2.53	0.44
1:A:243:PHE:O	1:A:250:ASN:ND2	2.41	0.44
3:F:302:LEU:HD21	3:F:322:GLN:HE22	1.82	0.44
3:H:50:ARG:HB3	5:M:14:G:H3'	1.99	0.44
2:B:196:HIS:HE1	2:B:214:LEU:HD21	1.83	0.44
3:E:302:LEU:HD22	3:E:322:GLN:HE22	1.83	0.44
3:G:91:LEU:HD13	3:G:225:VAL:HG11	1.98	0.44
1:A:217:ALA:O	1:A:221:ALA:CB	2.66	0.44
3:G:16:ARG:NH2	5:M:13:C:OP2	2.50	0.44
3:H:329:ASN:HA	3:H:332:ARG:HB3	1.99	0.44
3:E:26:SER:HA	3:E:41:ALA:HA	2.00	0.44
3:F:304:PHE:HE1	3:F:326:VAL:HG13	1.83	0.44
3:D:64:PRO:O	3:D:68:ASP:HB3	2.17	0.43
3:D:278:GLY:HA3	3:D:279:PRO:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:THR:HB	2:B:114:HIS:HE1	1.82	0.43
2:B:213:LEU:HA	2:B:216:LEU:HD21	2.00	0.43
3:D:26:SER:HA	3:D:41:ALA:HA	2.01	0.43
3:E:17:LYS:HB2	3:E:331:ILE:HG23	2.00	0.43
3:F:21:SER:OG	3:F:22:ASP:N	2.52	0.43
3:F:161:ARG:HB2	3:F:214:VAL:HB	1.99	0.43
2:B:85:ARG:HB3	5:M:8:A:H3'	2.00	0.43
3:C:268:ASP:HB2	3:C:282:VAL:HG12	2.00	0.43
3:D:227:PRO:HG2	3:D:246:LEU:HD22	2.01	0.43
3:G:283:GLU:O	3:G:325:TYR:OH	2.34	0.43
2:B:147:TRP:HB3	2:B:151:ARG:HD2	2.00	0.43
3:C:86:SER:OG	3:C:221:ASP:OD2	2.26	0.43
3:D:147:PHE:HB2	3:D:260:ILE:HG13	2.01	0.43
3:E:100:LEU:HD22	3:F:154:GLY:HA3	2.01	0.43
2:B:18:GLN:NE2	3:H:22:ASP:H	2.16	0.42
2:B:18:GLN:NE2	3:H:22:ASP:OD1	2.52	0.42
2:B:48:VAL:HG11	2:B:130:VAL:HG22	2.00	0.42
3:C:101:GLY:HA3	3:C:208:HIS:HE1	1.84	0.42
3:H:22:ASP:OD1	3:H:22:ASP:N	2.50	0.42
1:A:190:LEU:HD11	2:B:314:TYR:HD2	1.83	0.42
3:C:96:THR:HA	3:C:212:GLU:HA	2.01	0.42
3:E:229:GLN:HA	3:E:246:LEU:HA	2.01	0.42
3:F:8:THR:HB	3:F:313:LEU:HD11	2.01	0.42
3:H:140:HIS:NE2	3:H:187:LYS:O	2.53	0.42
3:C:228:SER:HB2	3:C:259:LYS:HD3	2.01	0.42
3:D:233:LEU:HD21	3:E:239:LYS:HD2	2.02	0.42
3:D:268:ASP:OD2	3:D:296:ARG:NH1	2.52	0.42
3:F:249:VAL:HG12	3:F:250:ARG:H	1.83	0.42
3:E:164:HIS:HE1	3:E:209:VAL:HG12	1.84	0.42
3:F:262:ASN:HB2	5:M:20:C:H5'	2.00	0.42
2:B:54:ILE:HA	2:B:115:GLY:HA3	2.01	0.42
3:E:266:THR:HA	3:E:281:ALA:HA	2.01	0.42
3:G:136:ARG:O	3:G:140:HIS:ND1	2.52	0.42
3:G:318:PRO:HD2	3:G:323:GLN:HE21	1.84	0.42
4:L:-1:MET:CB	4:L:184:VAL:N	2.82	0.42
2:B:211:ASP:HB3	2:B:250:PRO:HG3	2.01	0.42
3:C:101:GLY:HA3	3:C:208:HIS:CE1	2.54	0.42
3:F:231:LEU:HD11	3:F:233:LEU:HD23	2.01	0.42
3:F:120:GLN:HA	3:F:123:ALA:HB3	2.02	0.42
3:G:288:VAL:HB	3:G:291:GLN:HB2	2.01	0.42
2:B:255:TYR:HB3	2:B:280:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:270:TRP:HB3	3:H:322:GLN:HG3	2.02	0.42
1:A:217:ALA:O	1:A:221:ALA:HB2	2.20	0.42
3:D:19:ASP:OD1	3:D:19:ASP:N	2.53	0.41
3:H:77:GLN:OE1	5:M:13:C:N4	2.53	0.41
3:H:282:VAL:HG12	3:H:329:ASN:HB3	2.02	0.41
1:A:190:LEU:HD13	2:B:280:VAL:HG21	2.02	0.41
2:B:132:GLU:OE2	3:H:208:HIS:NE2	2.50	0.41
3:E:265:ARG:NH2	5:M:26:G:OP2	2.53	0.41
3:C:149:TRP:CD1	3:C:259:LYS:HE2	2.55	0.41
3:H:161:ARG:HD2	3:H:175:ARG:HE	1.84	0.41
3:C:30:TRP:CD2	3:C:218:ARG:HD2	2.55	0.41
3:C:262:ASN:ND2	5:M:38:C:OP2	2.54	0.41
3:F:259:LYS:HE3	3:F:259:LYS:HB2	1.89	0.41
3:F:141:ASN:ND2	3:F:266:THR:O	2.41	0.41
3:G:134:LEU:HD11	3:G:328:ALA:HB2	2.03	0.41
1:A:190:LEU:HD22	2:B:280:VAL:HB	2.03	0.41
2:B:19:ASN:H	2:B:104:HIS:CD2	2.39	0.41
3:C:159:GLU:HB3	3:C:216:PHE:HD2	1.86	0.41
2:B:213:LEU:HD22	2:B:216:LEU:HD11	2.02	0.41
3:C:145:ALA:HB1	3:C:148:LEU:HD21	2.02	0.41
3:D:92:LYS:HG3	3:D:216:PHE:HE1	1.85	0.41
3:D:318:PRO:HG2	3:D:323:GLN:HG2	2.01	0.41
3:F:26:SER:HA	3:F:41:ALA:HA	2.03	0.41
3:F:44:VAL:HG13	3:F:246:LEU:HD12	2.02	0.41
3:H:170:VAL:HG11	3:H:173:ALA:HB2	2.03	0.41
2:B:23:ILE:HG13	2:B:24:SER:H	1.86	0.41
3:G:305:TYR:OH	3:H:54:SER:O	2.30	0.41
3:C:296:ARG:NH1	3:C:302:LEU:O	2.54	0.40
3:E:33:ARG:HA	3:E:36:SER:HB3	2.02	0.40
3:D:318:PRO:O	3:D:323:GLN:NE2	2.54	0.40
3:G:134:LEU:HD12	3:G:134:LEU:HA	1.94	0.40
1:A:264:LEU:HD21	2:B:23:ILE:HG22	2.03	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	422/436 (97%)	355 (84%)	66 (16%)	1 (0%)	47	81
2	B	301/329 (92%)	266 (88%)	35 (12%)	0	100	100
3	C	287/344 (83%)	255 (89%)	32 (11%)	0	100	100
3	D	331/344 (96%)	297 (90%)	34 (10%)	0	100	100
3	E	332/344 (96%)	292 (88%)	40 (12%)	0	100	100
3	F	333/344 (97%)	302 (91%)	31 (9%)	0	100	100
3	G	331/344 (96%)	295 (89%)	34 (10%)	2 (1%)	25	64
3	H	331/344 (96%)	297 (90%)	34 (10%)	0	100	100
4	L	187/189 (99%)	143 (76%)	44 (24%)	0	100	100
All	All	2855/3018 (95%)	2502 (88%)	350 (12%)	3 (0%)	54	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	320	VAL
3	G	250	ARG
1	A	34	PRO

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	78/366 (21%)	78 (100%)	0	100	100
2	B	245/271 (90%)	242 (99%)	3 (1%)	71	87
3	C	230/274 (84%)	230 (100%)	0	100	100
3	D	258/274 (94%)	256 (99%)	2 (1%)	81	91
3	E	259/274 (94%)	259 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	259/274 (94%)	258 (100%)	1 (0%)	91	96
3	G	259/274 (94%)	257 (99%)	2 (1%)	81	91
3	H	258/274 (94%)	257 (100%)	1 (0%)	91	96
All	All	1846/2281 (81%)	1837 (100%)	9 (0%)	89	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	213	LEU
2	B	216	LEU
2	B	286	LEU
3	D	94	ARG
3	D	265	ARG
3	F	213	VAL
3	G	94	ARG
3	G	98	ARG
3	H	314	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
2	B	18	GLN
2	B	114	HIS
3	C	140	HIS
3	C	208	HIS
3	C	322	GLN
3	E	164	HIS
3	E	300	GLN
3	E	310	ASN
3	E	322	GLN
3	F	223	GLN
3	F	322	GLN
3	G	310	ASN
3	G	322	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	M	59/60 (98%)	38 (64%)	0

All (38) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	M	6	A
5	M	7	A
5	M	9	U
5	M	12	A
5	M	15	G
5	M	16	C
5	M	17	G
5	M	19	G
5	M	20	C
5	M	21	U
5	M	23	G
5	M	27	U
5	M	32	G
5	M	33	U
5	M	36	A
5	M	37	C
5	M	38	C
5	M	39	U
5	M	40	G
5	M	41	G
5	M	42	U
5	M	43	U
5	M	44	C
5	M	45	A
5	M	46	C
5	M	48	G
5	M	49	C
5	M	50	C
5	M	51	G
5	M	52	U
5	M	53	G
5	M	54	U
5	M	55	A
5	M	56	G
5	M	57	G
5	M	58	C
5	M	59	A
5	M	60	G

There are no RNA pucker outliers to report.

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.

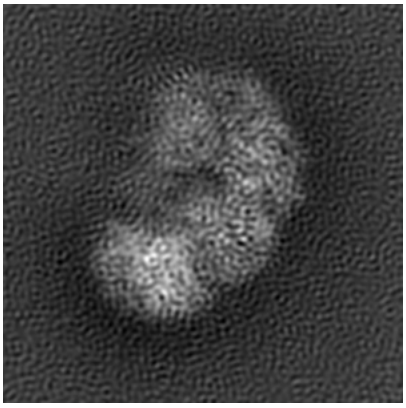
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7049. These allow visual inspection of the internal detail of the map and identification of artifacts.

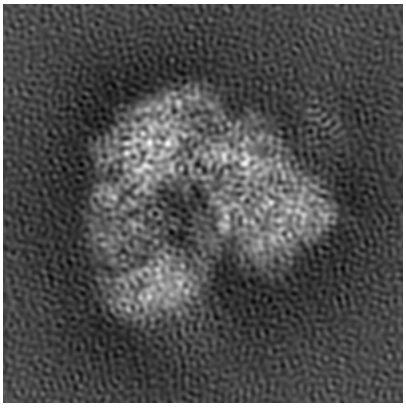
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

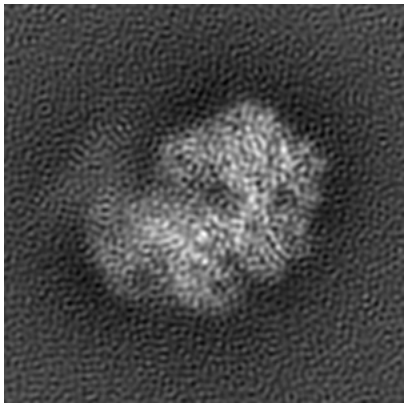
6.1.1 Primary map



X



Y

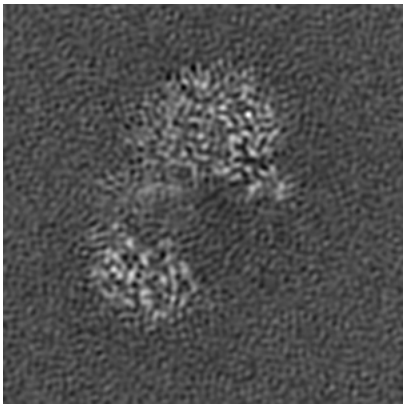


Z

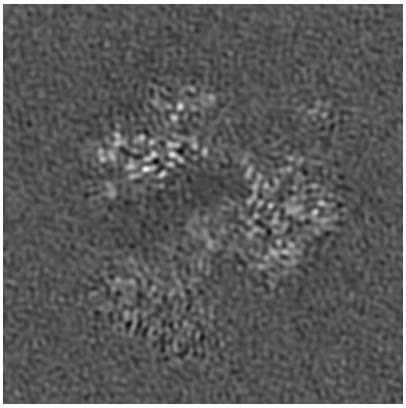
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

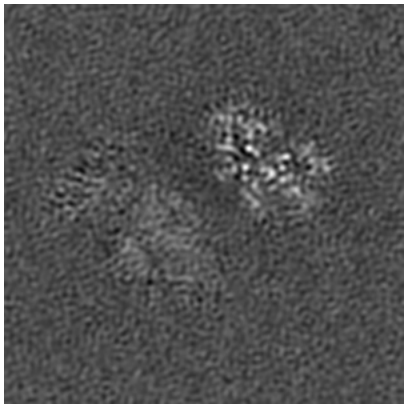
6.2.1 Primary map



X Index: 119



Y Index: 119

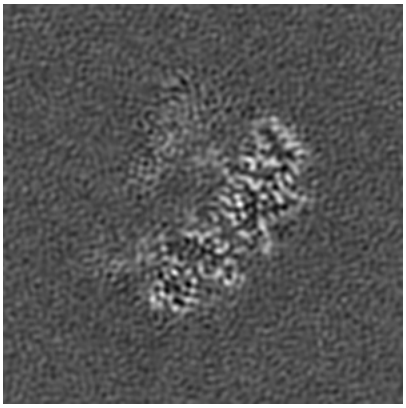


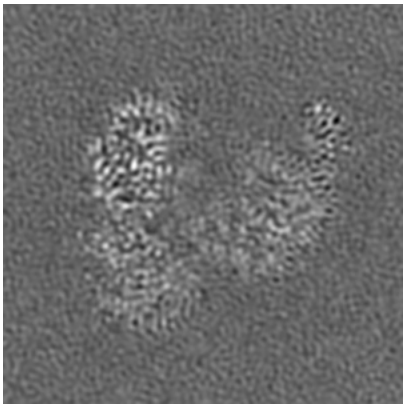
Z Index: 119

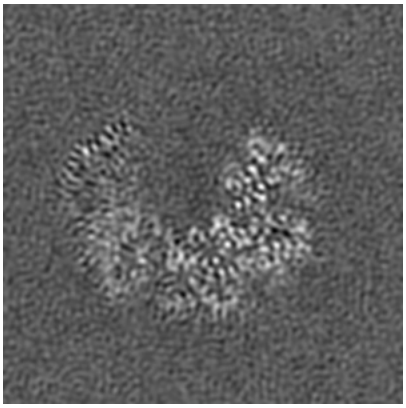
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 143

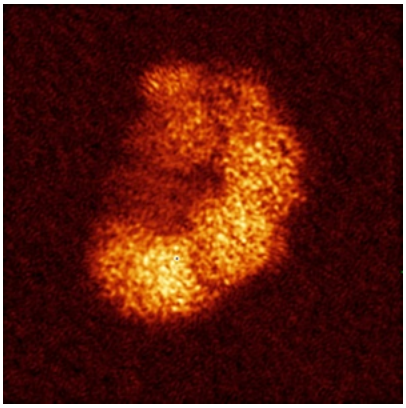

Y Index: 102

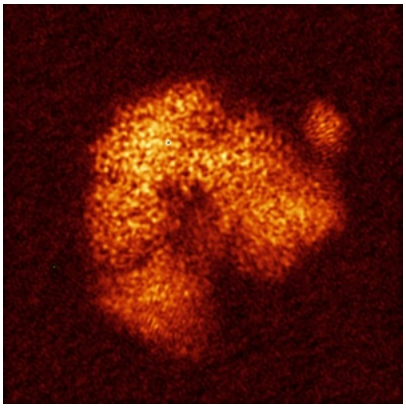

Z Index: 86

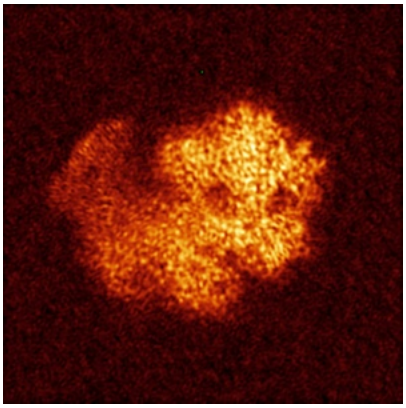
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (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 2.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

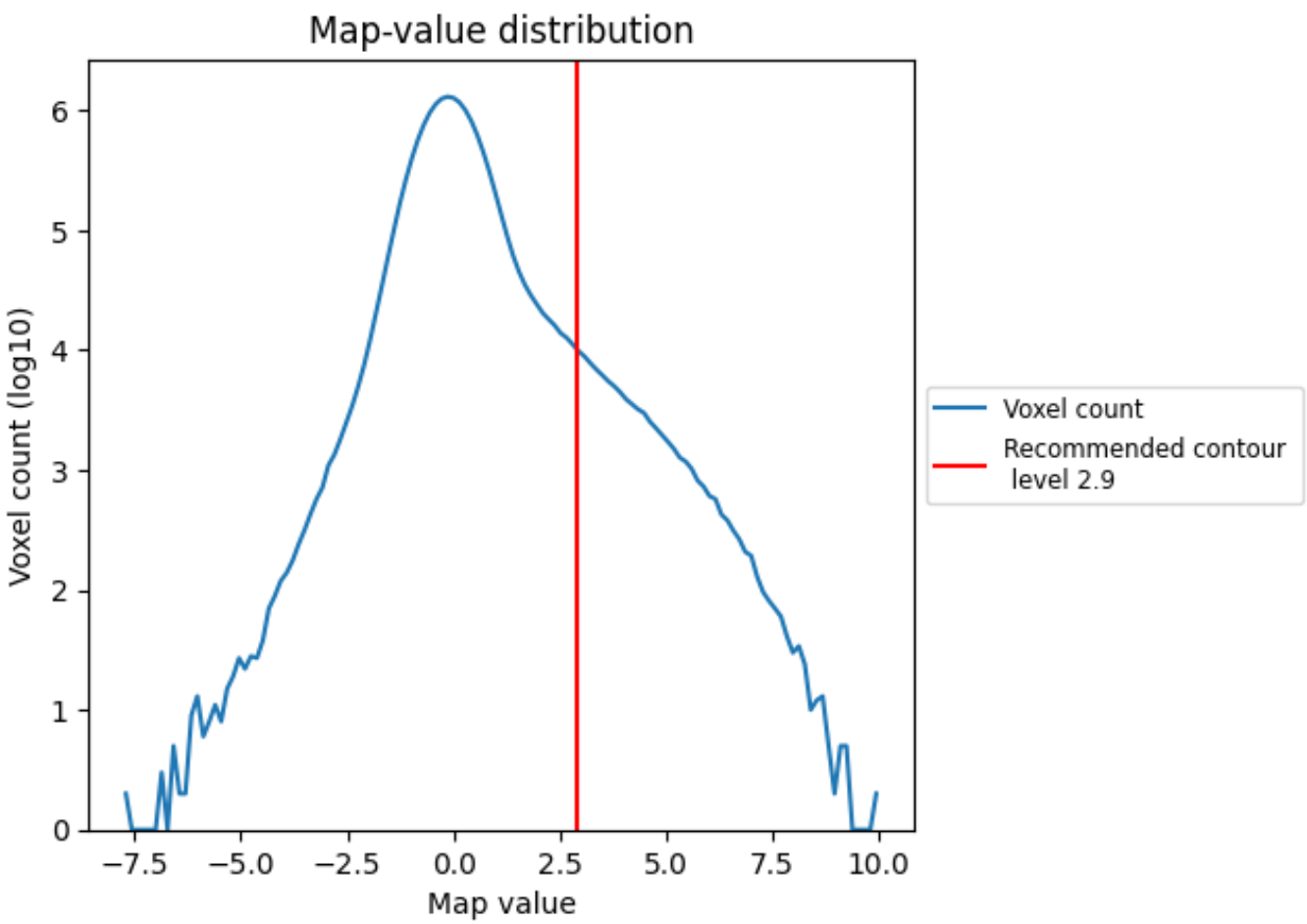
6.6 Mask visualisation (i)

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

7 Map analysis (i)

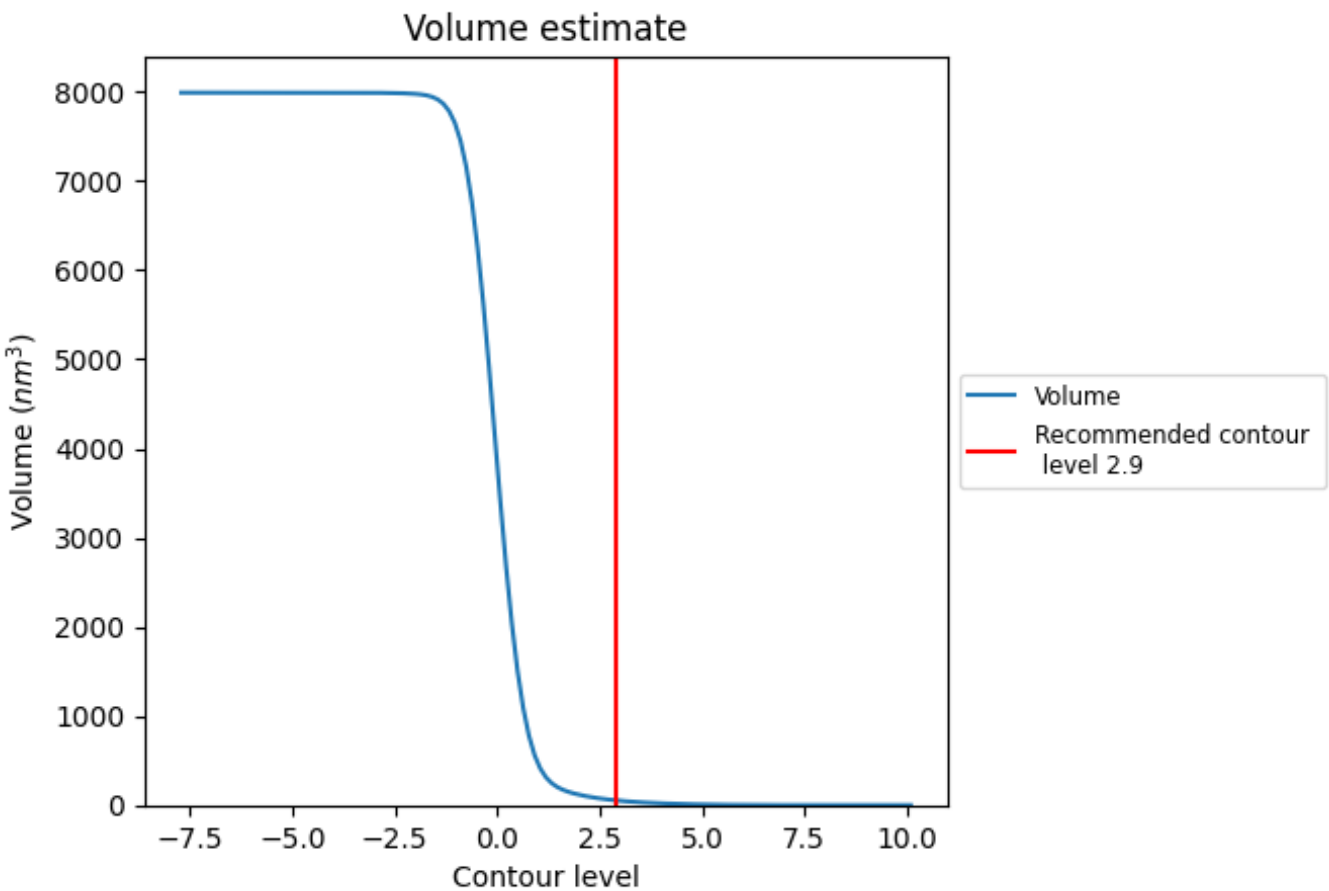
This section contains the results of statistical analysis of the map.

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.

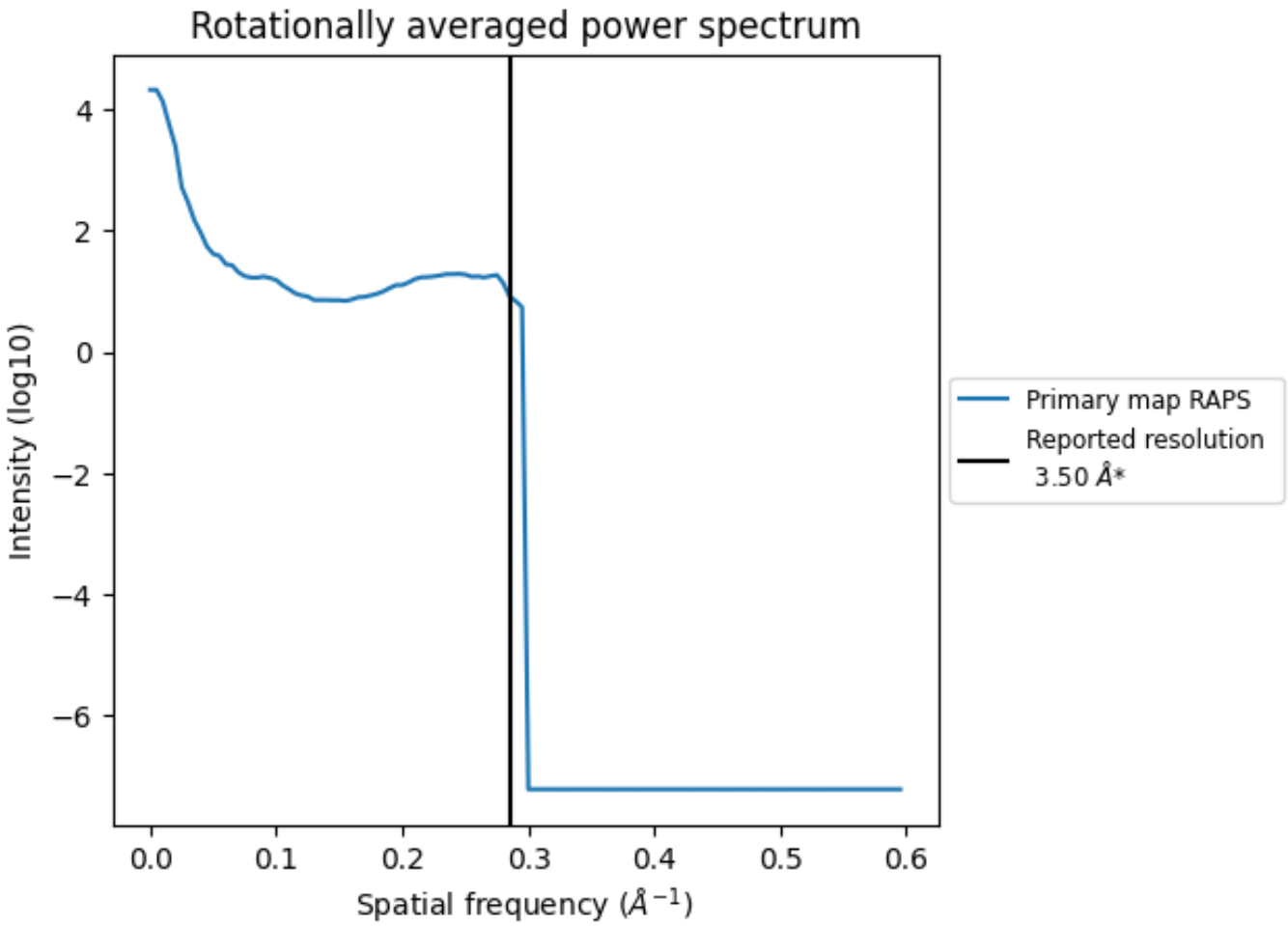
7.2 Volume estimate (i)



The volume at the recommended contour level is 54 nm^3; this corresponds to an approximate mass of 48 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 0.286 Å^{-1}

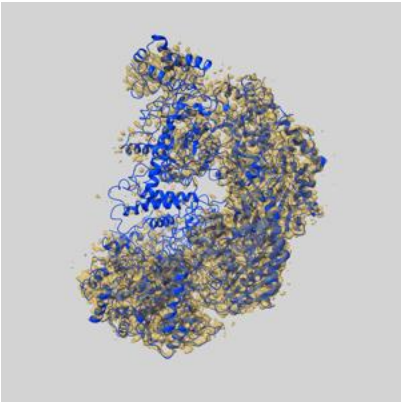
8 Fourier-Shell correlation (i)

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

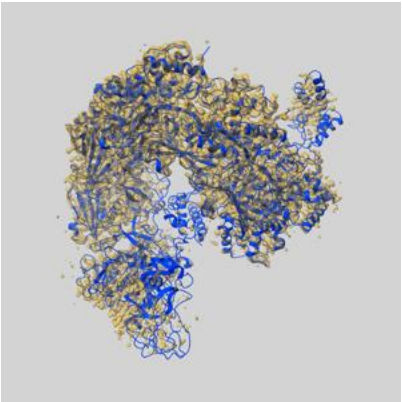
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7049 and PDB model 6B45. Per-residue inclusion information can be found in section 3 on page 6.

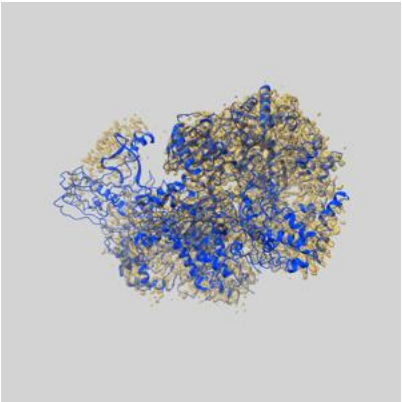
9.1 Map-model overlay (i)



X



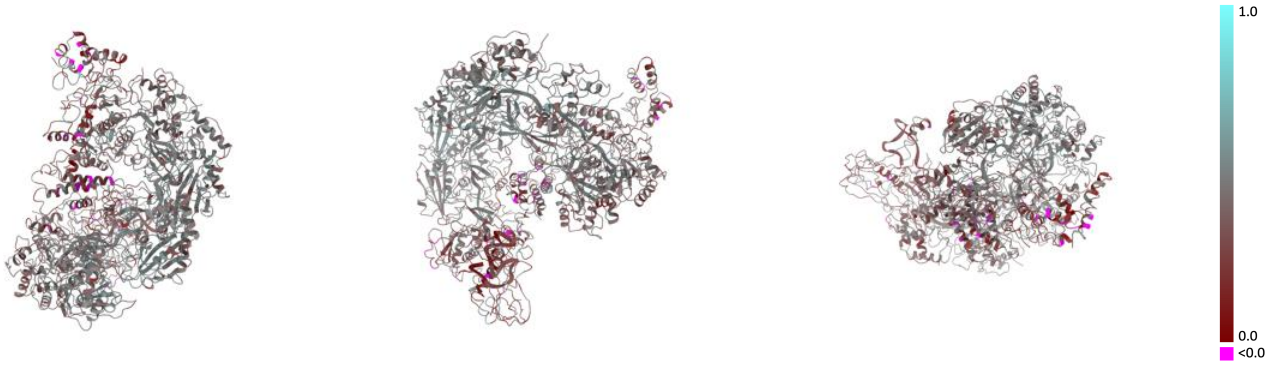
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.9 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.

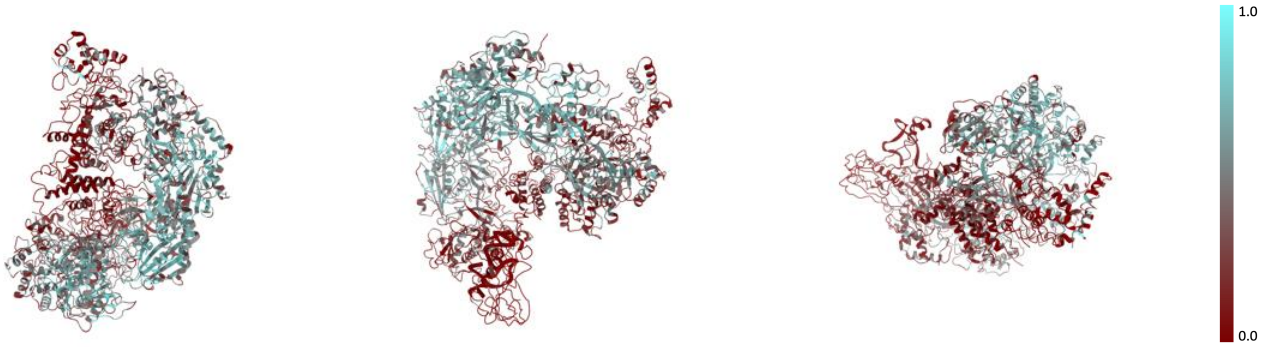
9.2 Q-score mapped to coordinate model (i)



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.

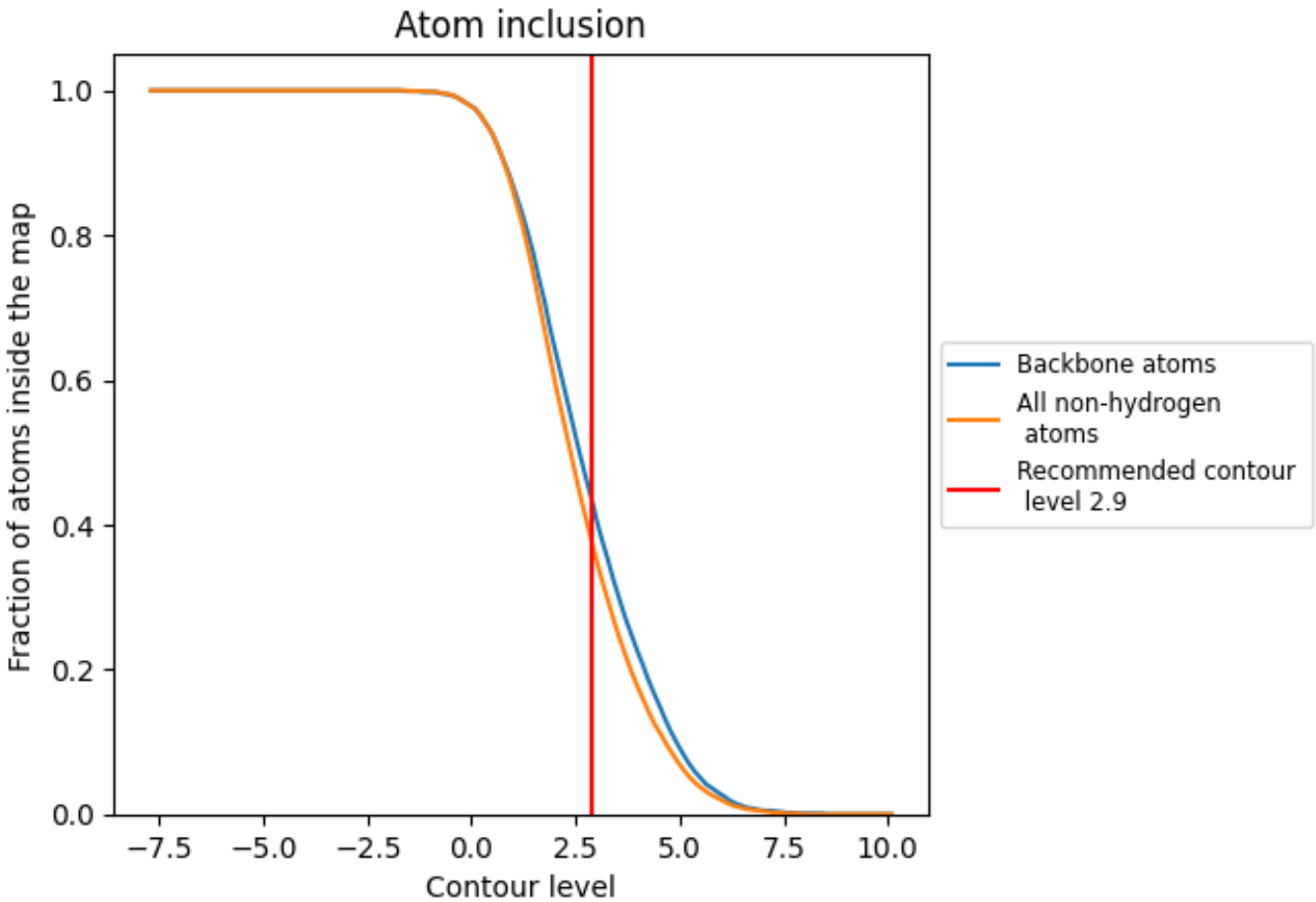
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.9).

9.4 Atom inclusion (i)



At the recommended contour level, 43% of all backbone atoms, 37% 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 (2.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3740	0.4130
A	0.1170	0.3450
B	0.2240	0.3760
C	0.2020	0.3490
D	0.3990	0.4170
E	0.5040	0.4550
F	0.5540	0.4640
G	0.5520	0.4670
H	0.4360	0.4380
L	0.0260	0.3330
M	0.4410	0.3960