



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:49 AM UTC

PDB ID : 8G9U / pdb_00008g9u
EMDB ID : EMD-29879
Title : Exploiting Activation and Inactivation Mechanisms in Type I-C CRISPR-Cas3
for Genome Editing Applications
Authors : Hu, C.; Nam, K.H.; Ke, A.
Deposited on : 2023-02-22
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

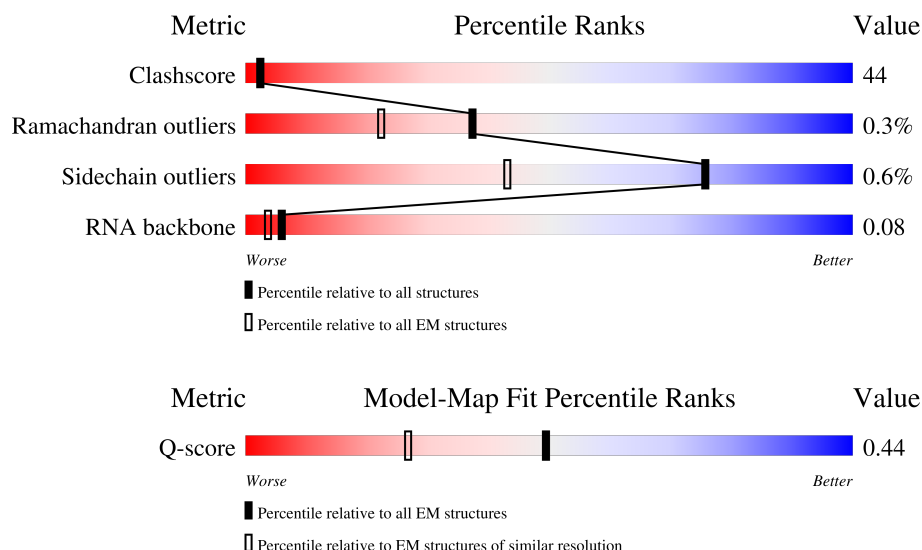
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



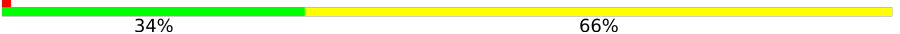
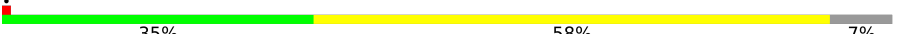
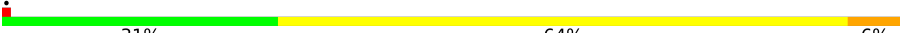
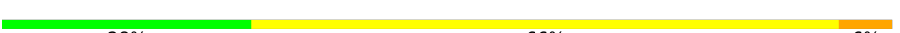
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	P	771	
2	A	283	
2	B	283	

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Mol	Chain	Length	Quality of chain
2	C	283	 30% 69%
2	D	283	 34% 66%
2	E	283	 37% 63%
2	F	283	 40% 55%
2	M	283	 35% 58% 7%
3	G	124	 31% 64% 6%
3	I	124	 28% 66% 6%
3	J	124	 30% 65% 6%
4	H	582	 37% 62%
5	K	43	 21% 79%
6	L	53	 26% 74%
7	N	205	 35% 65%
8	O	20	 20% 80%
9	Q	20	 30% 70%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PO4	P	803	-	-	X	-
11	PO4	P	804	-	-	X	-
11	PO4	Q	101	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 33546 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 Cas3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	757	Total	C	N	O	S	1	0
			5855	3716	1037	1084	18		

- Molecule 2 is a protein called CRISPR-associated protein, Csd2 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	B	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	D	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	C	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	E	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
2	F	271	Total	C	N	O	S	0	0
			2173	1360	391	411	11		
2	M	264	Total	C	N	O	S	0	0
			2110	1318	379	402	11		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	GLY	-	expression tag	UNP D0W8X6
B	284	GLY	-	expression tag	UNP D0W8X6
D	284	GLY	-	expression tag	UNP D0W8X6
C	284	GLY	-	expression tag	UNP D0W8X6
E	284	GLY	-	expression tag	UNP D0W8X6
F	284	GLY	-	expression tag	UNP D0W8X6
M	284	GLY	-	expression tag	UNP D0W8X6

- Molecule 3 is a protein called Phage associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
3	G	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
3	J	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		

- Molecule 4 is a protein called CRISPR-associated protein, Csd1 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	582	Total	C	N	O	S	0	0
			4555	2889	800	849	17		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	190	ALA	VAL	conflict	UNP D0W8X5
H	239	ALA	ILE	conflict	UNP D0W8X5
H	242	ILE	VAL	conflict	UNP D0W8X5
H	260	GLY	SER	conflict	UNP D0W8X5
H	271	THR	ALA	conflict	UNP D0W8X5
H	296	ASN	LYS	conflict	UNP D0W8X5
H	299	ALA	GLU	conflict	UNP D0W8X5
H	306	ALA	THR	conflict	UNP D0W8X5
H	317	CYS	GLN	conflict	UNP D0W8X5
H	322	GLU	LYS	conflict	UNP D0W8X5
H	323	ASP	GLU	conflict	UNP D0W8X5

- Molecule 5 is a RNA chain called crRNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	43	Total	C	N	O	P	0	0
			916	408	161	304	43		

- Molecule 6 is a DNA chain called Traget strand DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	53	Total	C	N	O	P	0	0
			1093	515	211	314	53		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	7	DA	-	expression tag	GB 1394359882
L	8	DG	-	expression tag	GB 1394359882

- Molecule 7 is a protein called pre-crRNA processing endonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	205	Total	C	N	O	S	0	0
			1674	1067	289	306	12		

- Molecule 8 is a DNA chain called proximal nontarget strand DNA (5'-D(P*AP*TP*GP*A P*AP*CP*TP*TP*CP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	20	Total	C	N	O	P	0	0
			414	198	87	109	20		

- Molecule 9 is a DNA chain called Distal nontarget DNA (5'-D(P*TP*TP*AP*TP*AP*TP*TP*AP*AP*TP*AP*TP*TP*AP*TP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	20	Total	C	N	O	P	0	0
			408	200	64	124	20		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	P	2	Total	Mg	0
			2	2	

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).

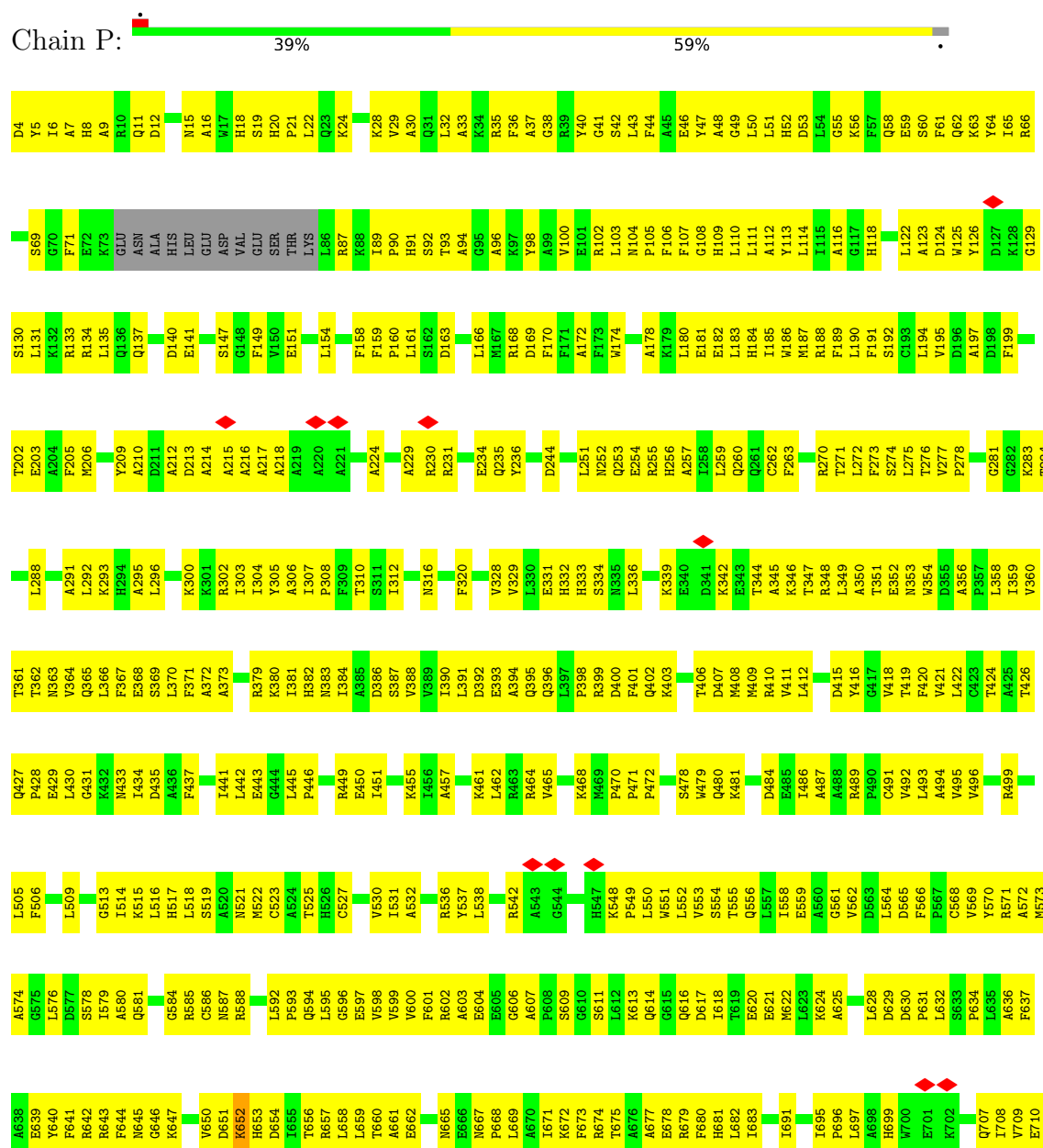


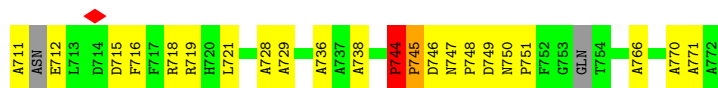
Mol	Chain	Residues	Atoms			AltConf
11	P	1	Total	O	P	0
			5	4	1	
11	P	1	Total	O	P	0
			5	4	1	
11	O	1	Total	O	P	0
			5	4	1	
11	Q	1	Total	O	P	0
			5	4	1	

3 Residue-property plots

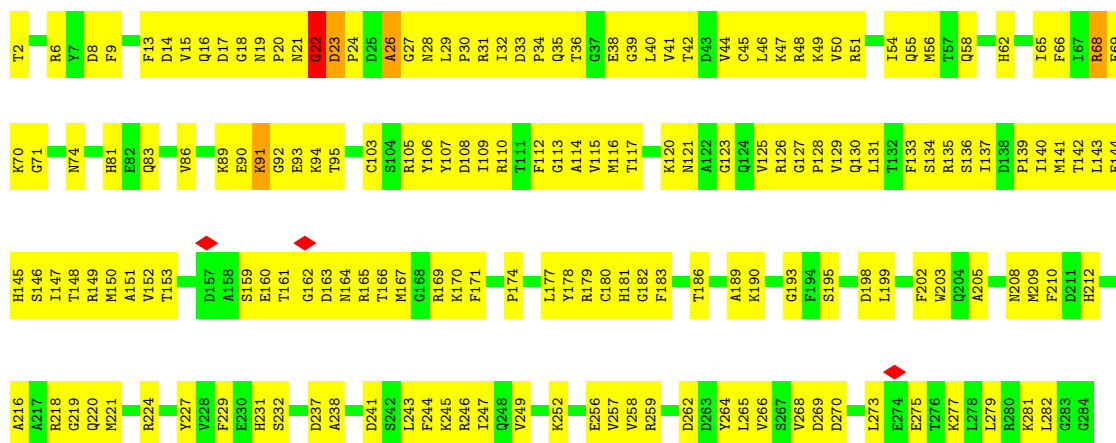
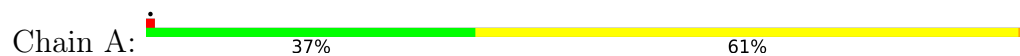
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Cas3

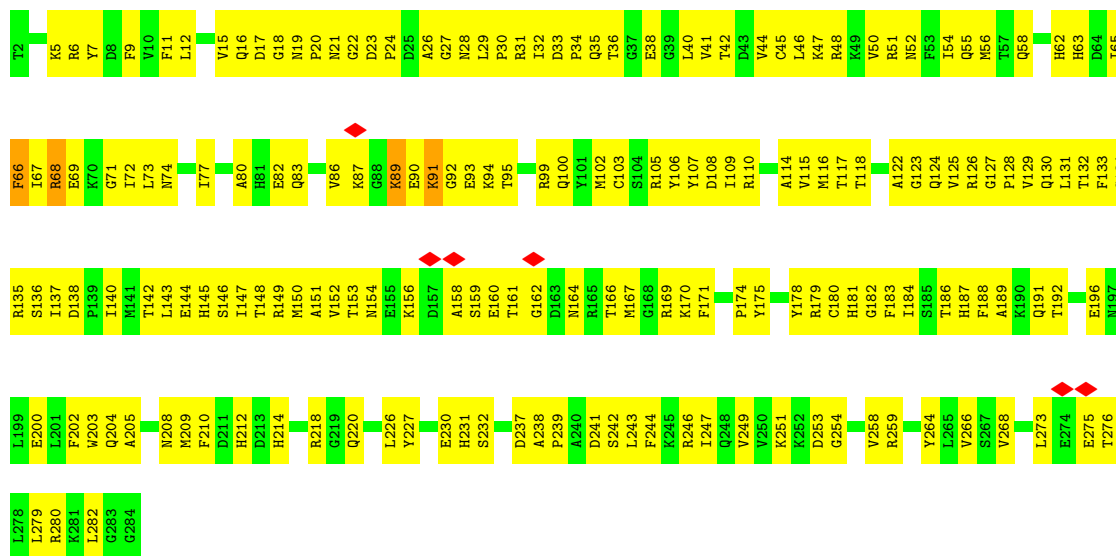




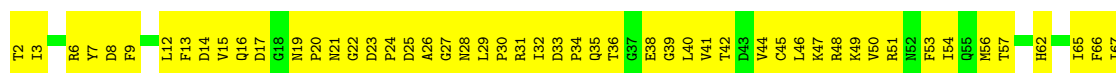
- Molecule 2: CRISPR-associated protein, Csd2 family

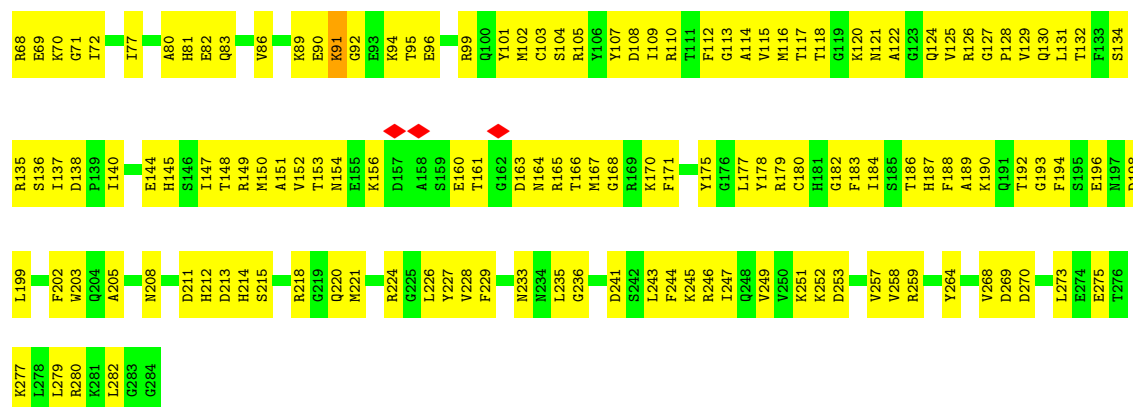


- Molecule 2: CRISPR-associated protein, Csd2 family



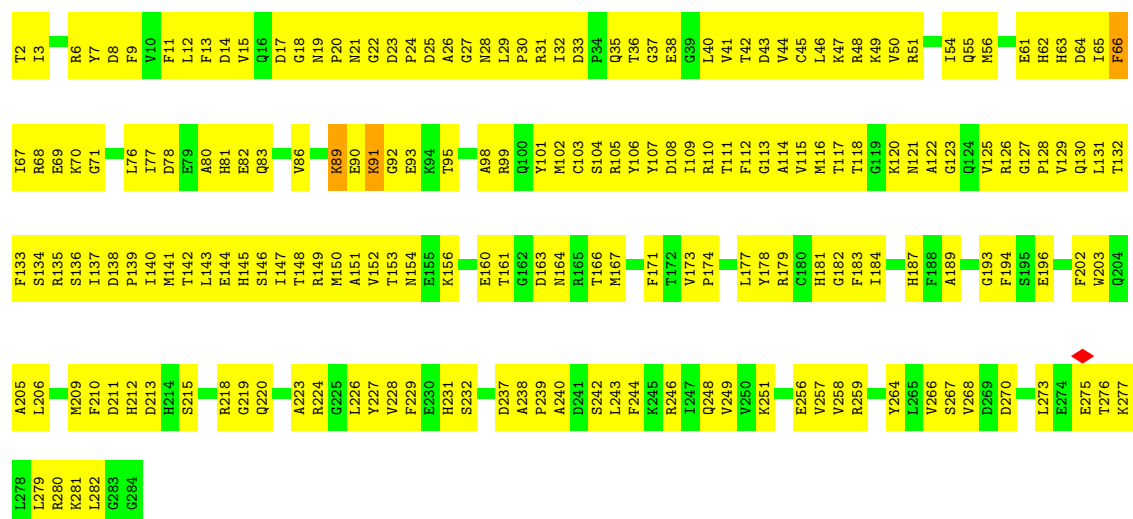
- Molecule 2: CRISPR-associated protein, Csd2 family





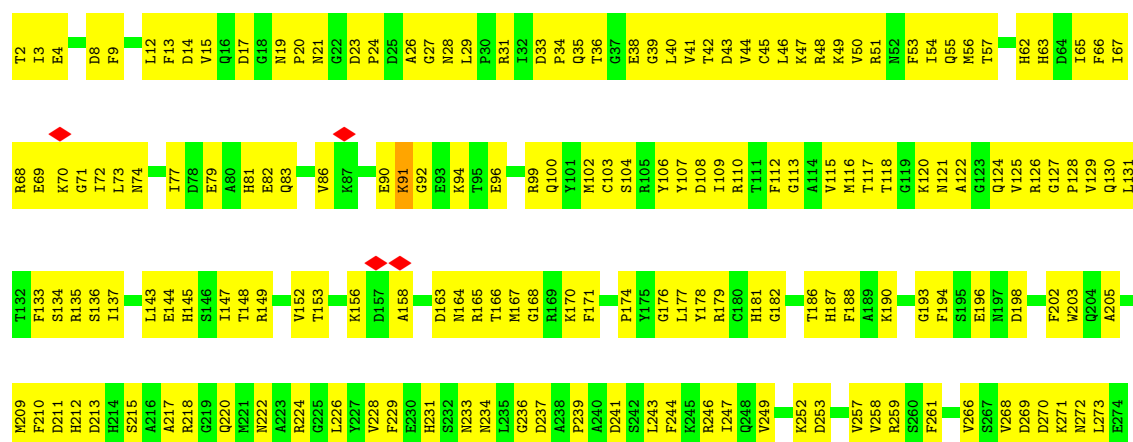
• Molecule 2: CRISPR-associated protein, Csd2 family

Chain C: 30% 69%



• Molecule 2: CRISPR-associated protein, Csd2 family

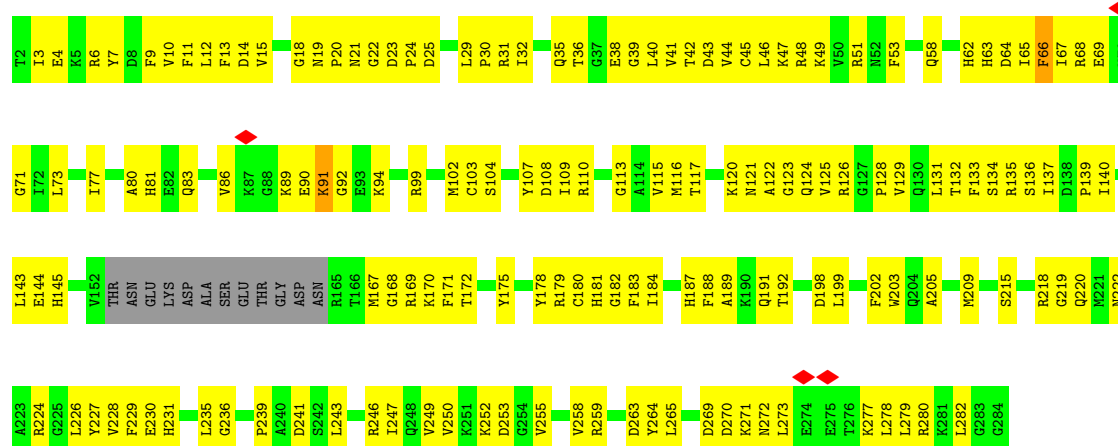
Chain E: 37% 63%



E275
L276
K277
L278
L279
R280
K281
L282
G284

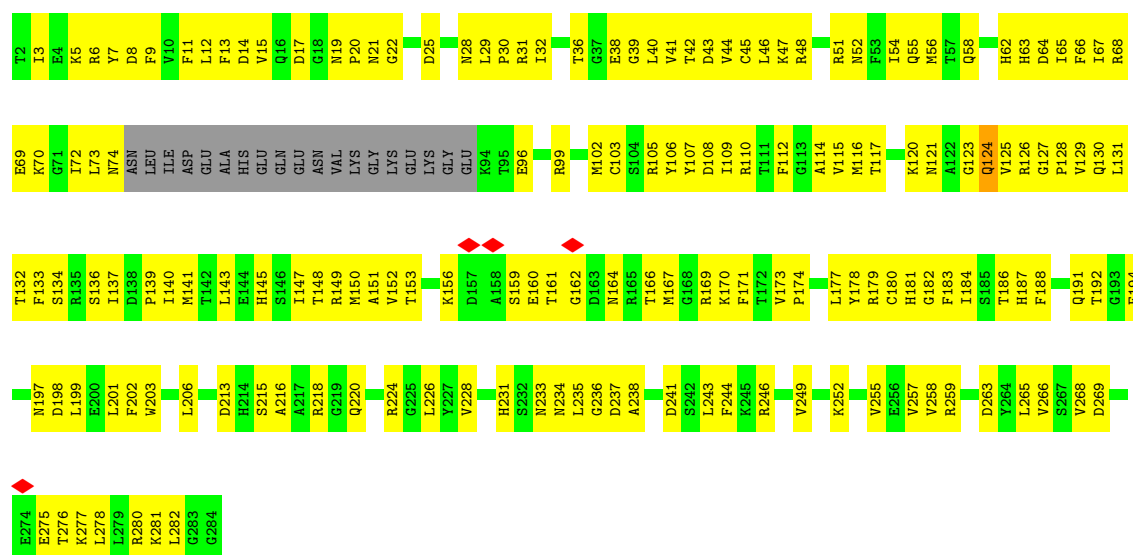
• Molecule 2: CRISPR-associated protein, Csd2 family

Chain F:  40% 55%

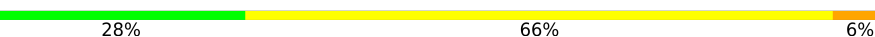


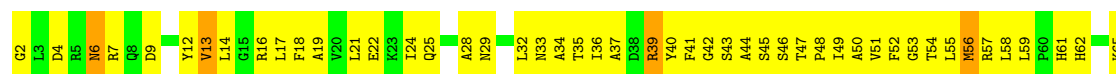
• Molecule 2: CRISPR-associated protein, Csd2 family

Chain M:  35% 58% 7%



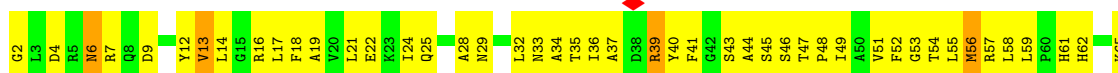
• Molecule 3: Phage associated protein

Chain I:  28% 66% 6%

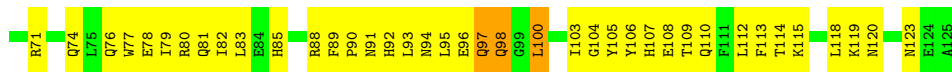
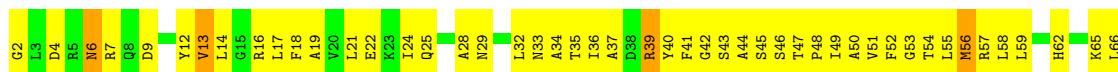




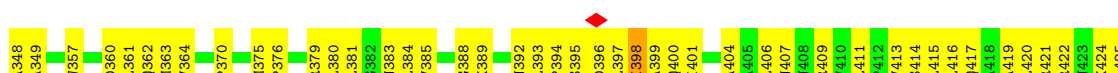
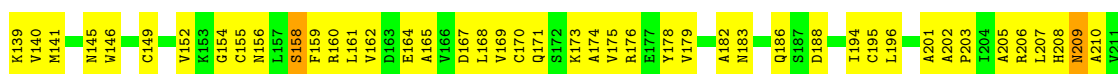
• Molecule 3: Phage associated protein



• Molecule 3: Phage associated protein

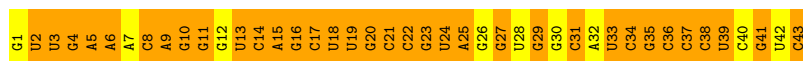


• Molecule 4: CRISPR-associated protein, Csd1 family





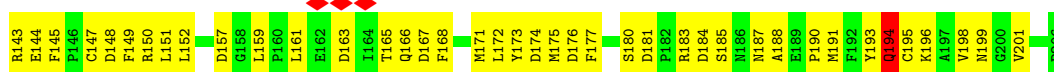
• Molecule 5: crRNA (43-MER)



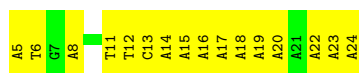
• Molecule 6: Target strand DNA (53-MER)



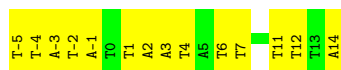
• Molecule 7: pre-crRNA processing endonuclease



• Molecule 8: proximal nontarget strand DNA (5'-D(P*AP*TP*GP*AP*AP*CP*TP*TP*CP*A P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



• Molecule 9: Distal nontarget DNA (5'-D(P*TP*TP*AP*TP*AP*TP*TP*AP*AP*TP*AP*TP *TP*AP*TP*AP*TP*TP*TP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	307088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	67000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.947	Depositor
Minimum map value	-0.276	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.111	Depositor
Map size (Å)	381.30002, 381.30002, 381.30002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.271, 1.271, 1.271	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	P	0.32	0/5983	0.55	0/8111
2	A	0.59	0/2303	0.70	2/3101 (0.1%)
2	B	0.57	0/2303	0.66	0/3101
2	C	0.57	0/2303	0.64	0/3101
2	D	0.58	0/2303	0.66	0/3101
2	E	0.51	0/2303	0.62	0/3101
2	F	0.35	0/2214	0.54	0/2979
2	M	0.53	0/2150	0.60	0/2896
3	G	0.54	0/1030	0.64	0/1392
3	I	0.54	0/1030	0.64	0/1392
3	J	0.54	0/1030	0.64	0/1392
4	H	0.50	0/4644	0.66	2/6277 (0.0%)
5	K	0.65	0/1022	0.59	0/1591
6	L	0.57	0/1228	0.44	0/1894
7	N	0.46	0/1712	0.68	3/2307 (0.1%)
8	O	0.31	0/468	0.33	0/719
9	Q	0.36	0/455	0.52	1/700 (0.1%)
All	All	0.50	0/34481	0.61	8/47155 (0.0%)

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	P	0	4
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	1
2	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	M	0	1
3	G	0	1
3	I	0	1
3	J	0	1
4	H	0	5
7	N	0	1
All	All	0	23

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	22	GLY	CA-C-N	-8.14	101.94	121.80
2	A	22	GLY	C-N-CA	-8.14	101.94	121.80
7	N	195	CYS	N-CA-C	-7.03	95.83	110.80
9	Q	-5	DT	C2'-C3'-O3'	-6.60	101.60	111.50
7	N	195	CYS	CA-C-N	5.92	133.55	122.84

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	22	GLY	Peptide
1	P	606	GLY	Peptide
1	P	652	LYS	Peptide
1	P	654	ASP	Peptide
1	P	744	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	5855	0	5783	474	0
2	A	2261	0	2193	243	0
2	B	2261	0	2193	236	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2261	0	2193	240	0
2	D	2261	0	2193	235	0
2	E	2261	0	2193	225	0
2	F	2173	0	2120	166	0
2	M	2110	0	2050	223	0
3	G	1007	0	992	116	0
3	I	1007	0	992	132	0
3	J	1007	0	992	143	0
4	H	4555	0	4558	438	0
5	K	916	0	464	178	0
6	L	1093	0	592	97	0
7	N	1674	0	1663	178	0
8	O	414	0	224	24	0
9	Q	408	0	233	20	0
10	P	2	0	0	0	0
11	O	5	0	0	1	0
11	P	10	0	0	13	0
11	Q	5	0	0	2	0
All	All	33546	0	31628	2826	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 44.

The worst 5 of 2826 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:P:56:LYS:HZ3	11:P:804:PO4:P	1.75	1.08
4:H:370:PRO:HB2	11:Q:101:PO4:O2	1.52	1.08
1:P:56:LYS:NZ	11:P:804:PO4:O1	1.94	0.99
1:P:180:LEU:HD21	4:H:289:ILE:HG23	1.46	0.96
2:C:126:ARG:HH21	5:K:14:C:H41	1.13	0.95

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	752/771 (98%)	627 (83%)	123 (16%)	2 (0%)	36	70
2	A	281/283 (99%)	223 (79%)	55 (20%)	3 (1%)	11	43
2	B	281/283 (99%)	223 (79%)	56 (20%)	2 (1%)	18	53
2	C	281/283 (99%)	233 (83%)	47 (17%)	1 (0%)	30	65
2	D	281/283 (99%)	229 (82%)	51 (18%)	1 (0%)	30	65
2	E	281/283 (99%)	231 (82%)	49 (17%)	1 (0%)	30	65
2	F	267/283 (94%)	218 (82%)	48 (18%)	1 (0%)	30	65
2	M	260/283 (92%)	214 (82%)	46 (18%)	0	100	100
3	G	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
3	I	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
3	J	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
4	H	580/582 (100%)	477 (82%)	102 (18%)	1 (0%)	43	76
7	N	203/205 (99%)	163 (80%)	39 (19%)	1 (0%)	24	60
All	All	3833/3911 (98%)	3180 (83%)	640 (17%)	13 (0%)	37	70

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	745	PRO
2	A	91	LYS
2	D	91	LYS
2	C	91	LYS
2	E	91	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	588/601 (98%)	588 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	245/245 (100%)	245 (100%)	0	100	100
2	B	245/245 (100%)	245 (100%)	0	100	100
2	C	245/245 (100%)	245 (100%)	0	100	100
2	D	245/245 (100%)	245 (100%)	0	100	100
2	E	245/245 (100%)	245 (100%)	0	100	100
2	F	235/245 (96%)	235 (100%)	0	100	100
2	M	229/245 (94%)	229 (100%)	0	100	100
3	G	104/104 (100%)	98 (94%)	6 (6%)	18	51
3	I	104/104 (100%)	98 (94%)	6 (6%)	18	51
3	J	104/104 (100%)	98 (94%)	6 (6%)	18	51
4	H	475/475 (100%)	475 (100%)	0	100	100
7	N	182/182 (100%)	182 (100%)	0	100	100
All	All	3246/3285 (99%)	3228 (99%)	18 (1%)	76	88

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	39	ARG
3	J	100	LEU
3	J	98	GLN
3	G	39	ARG
3	J	13	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	181	HIS
7	N	89	GLN
2	F	83	GLN
7	N	68	ASN
3	J	33	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	K	42/43 (97%)	33 (78%)	3 (7%)

5 of 33 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	K	2	U
5	K	3	U
5	K	4	G
5	K	5	A
5	K	6	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	K	4	G
5	K	9	A
5	K	14	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	PO4	Q	101	-	4,4,4	0.75	0	6,6,6	0.46	0
11	PO4	P	803	-	4,4,4	0.96	0	6,6,6	0.44	0
11	PO4	O	101	-	4,4,4	0.89	0	6,6,6	0.46	0
11	PO4	P	804	10	4,4,4	1.27	0	6,6,6	0.31	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

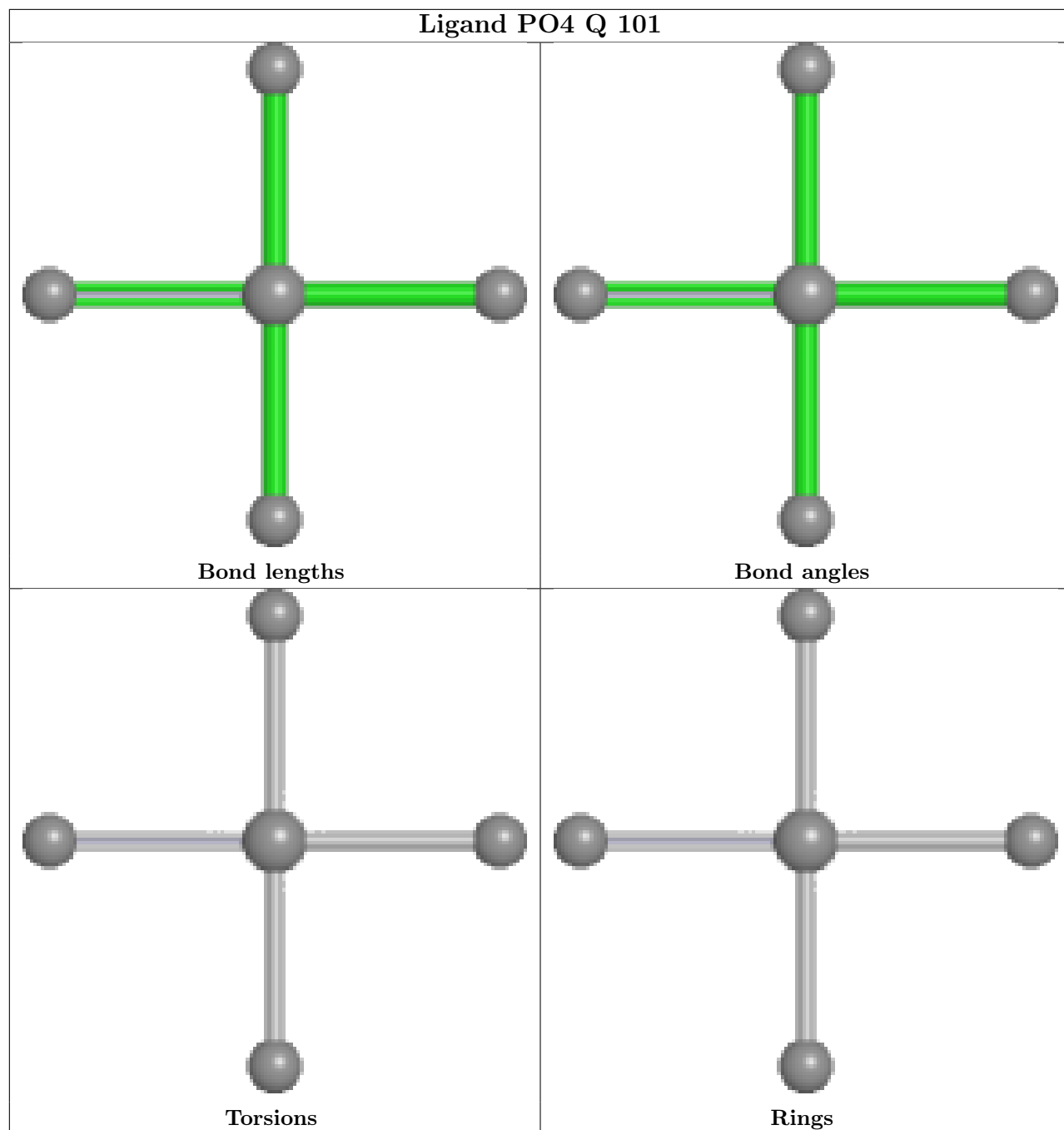
There are no torsion outliers.

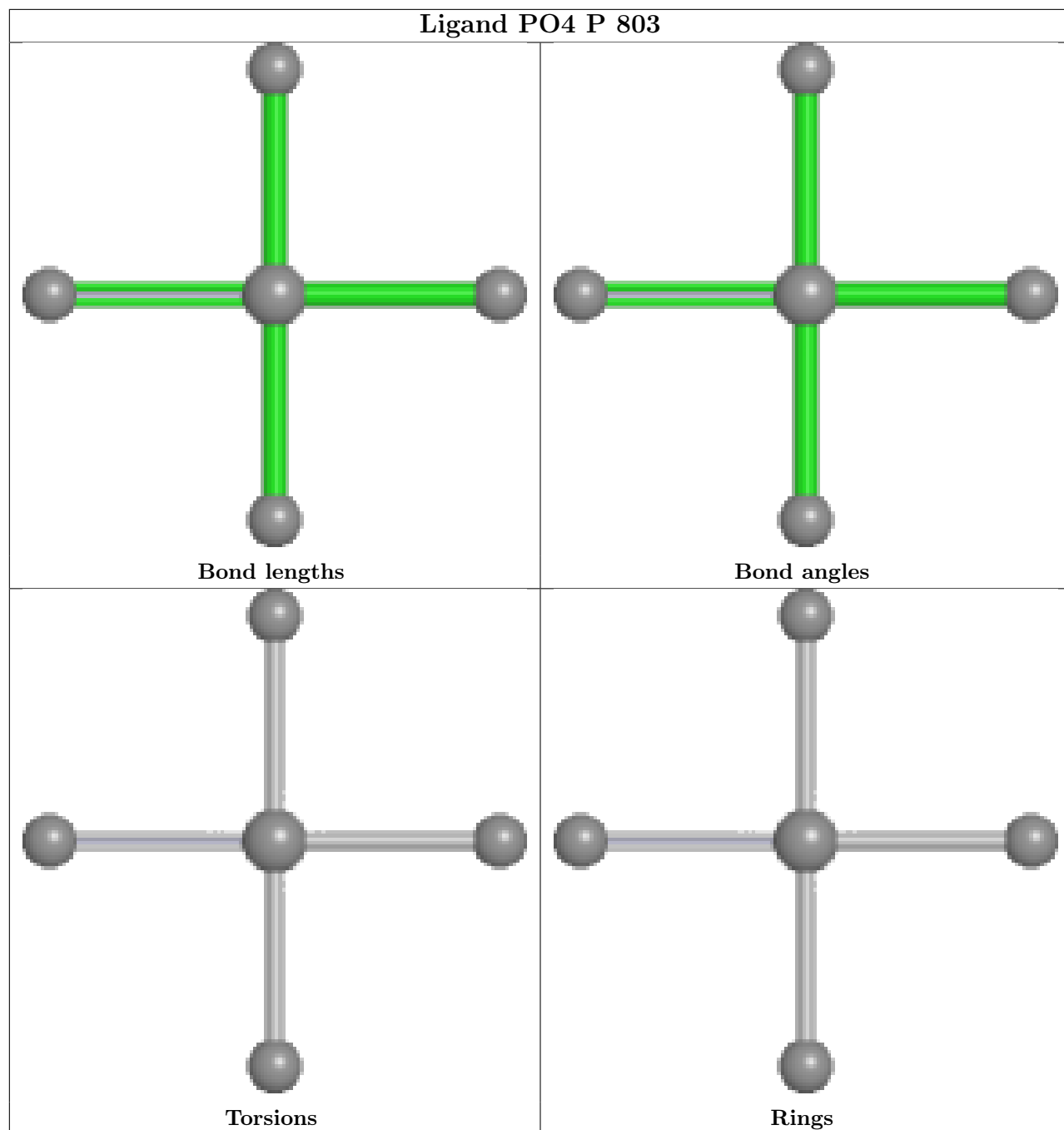
There are no ring outliers.

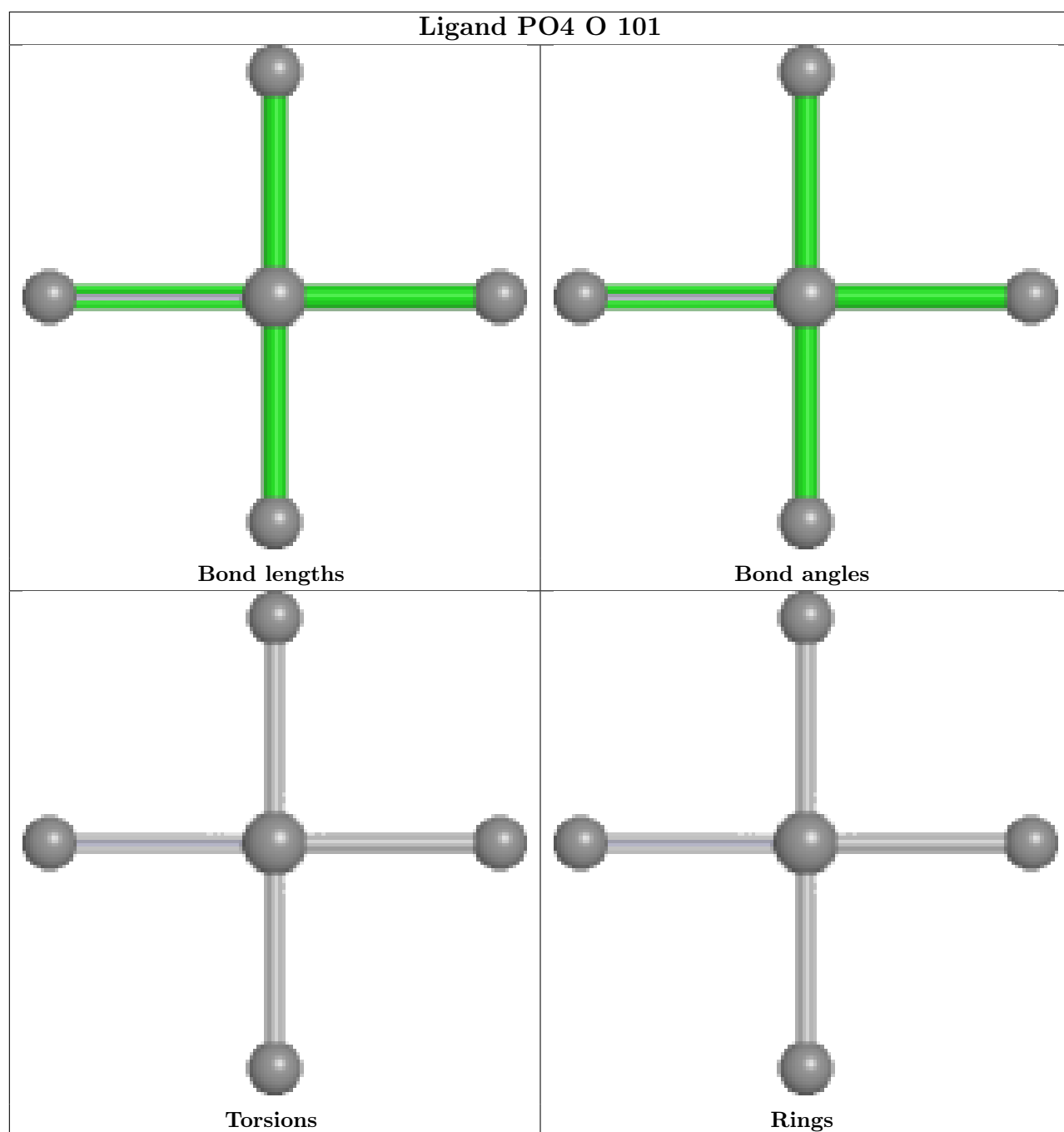
4 monomers are involved in 16 short contacts:

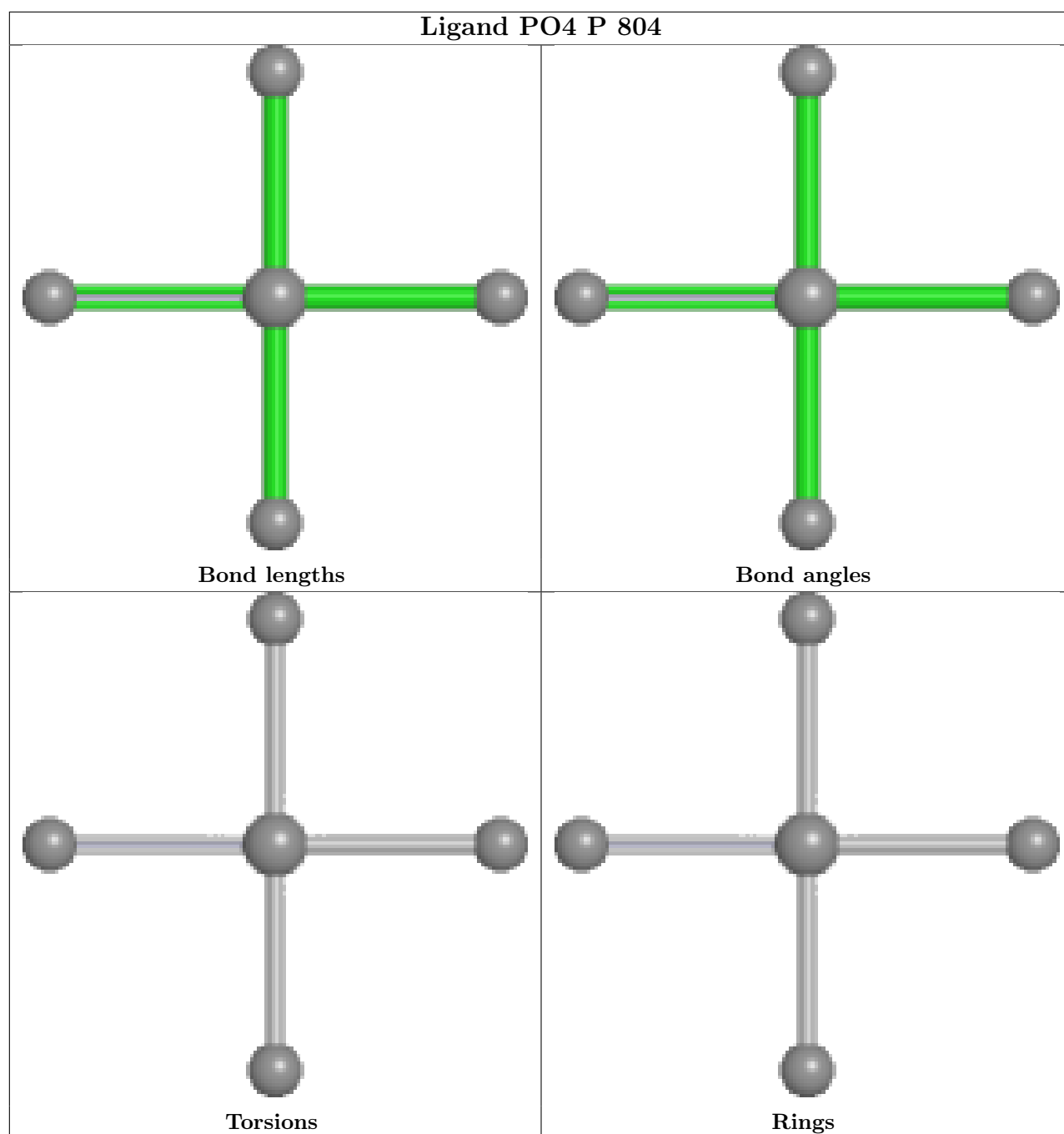
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Q	101	PO4	2	0
11	P	803	PO4	9	0
11	O	101	PO4	1	0
11	P	804	PO4	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	759:LEU	C	760:ALA	N	6.63

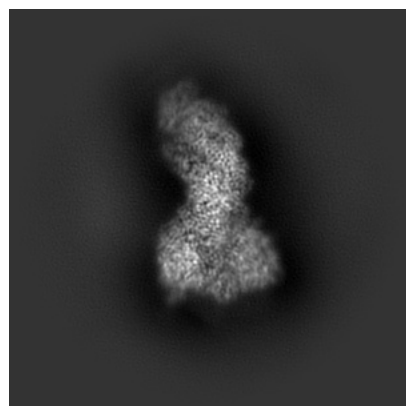
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29879. These allow visual inspection of the internal detail of the map and identification of artifacts.

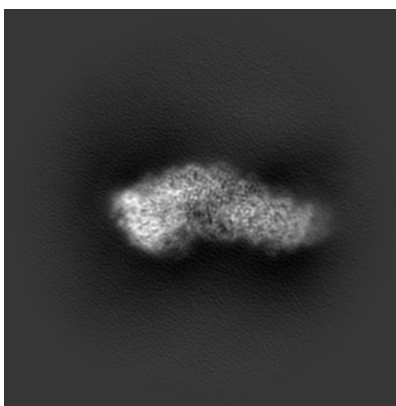
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

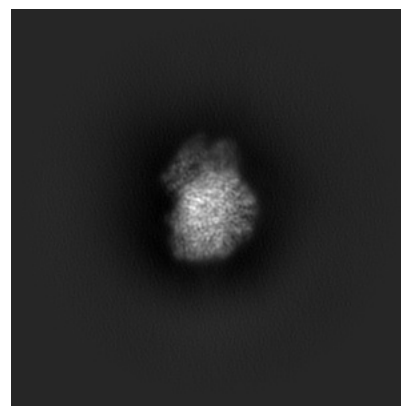
6.1.1 Primary map



X

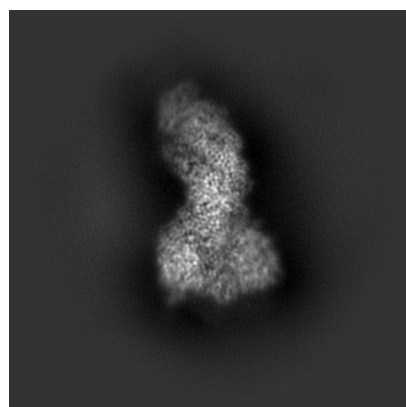


Y

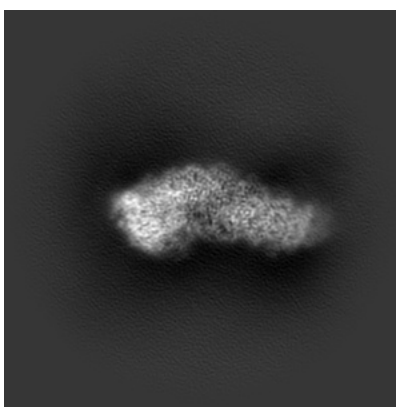


Z

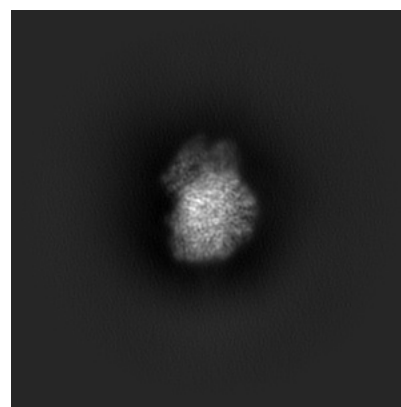
6.1.2 Raw map



X



Y

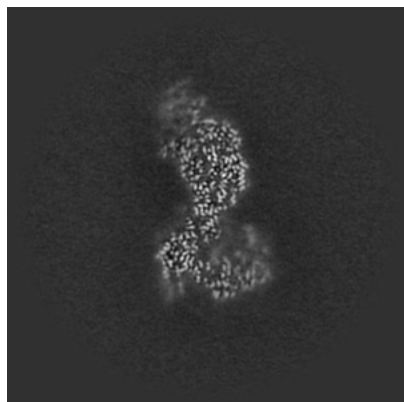


Z

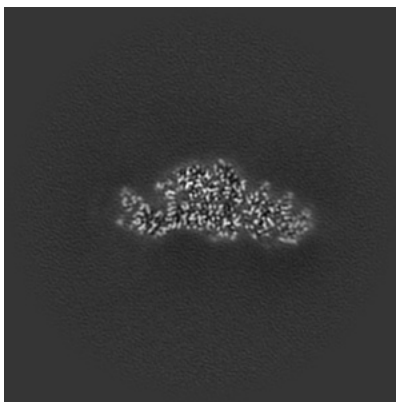
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

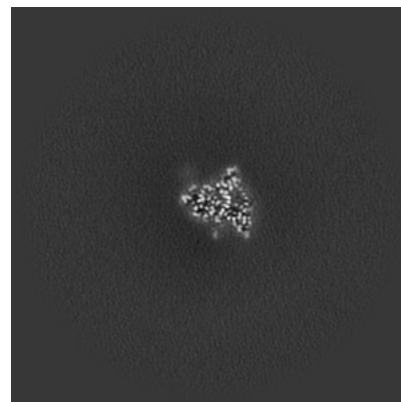
6.2.1 Primary map



X Index: 150

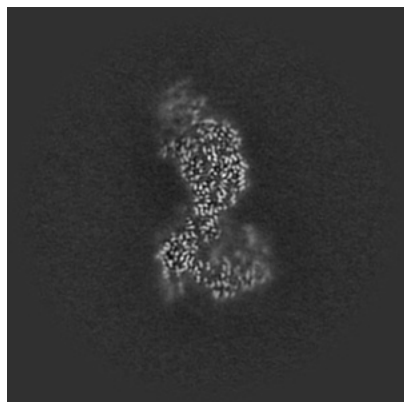


Y Index: 150

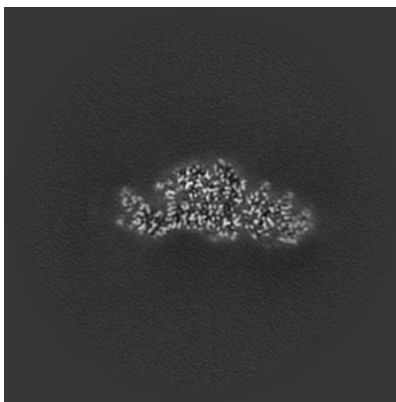


Z Index: 150

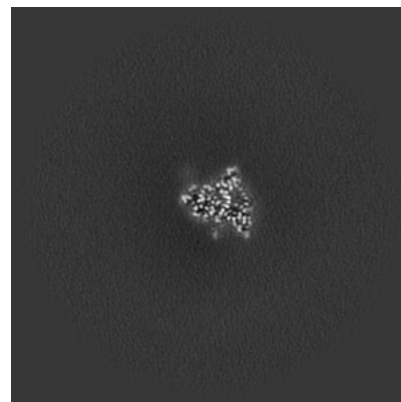
6.2.2 Raw map



X Index: 150



Y Index: 150

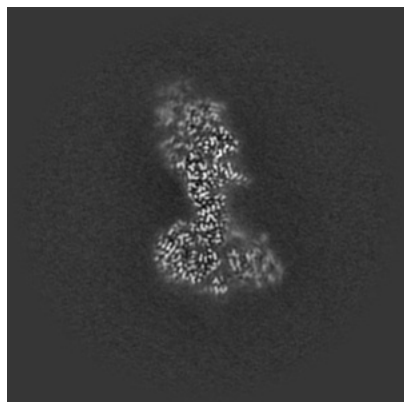


Z Index: 150

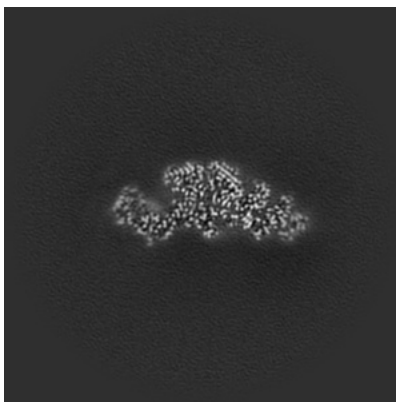
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

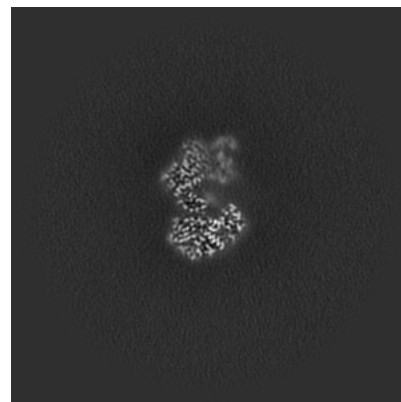
6.3.1 Primary map



X Index: 141

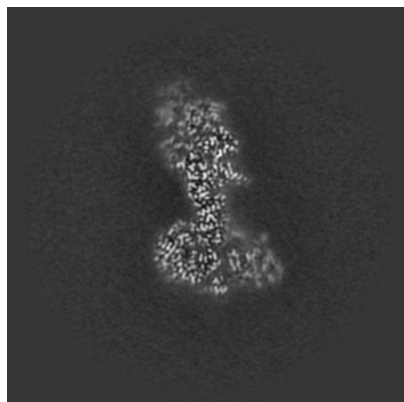


Y Index: 155

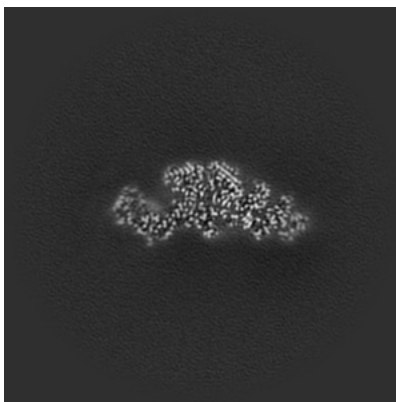


Z Index: 115

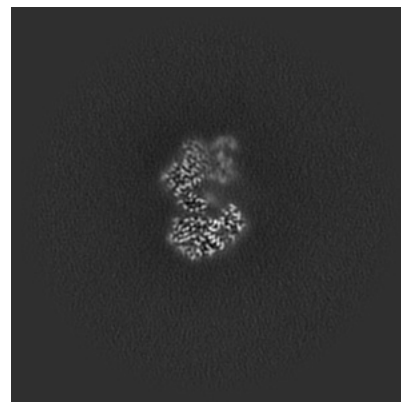
6.3.2 Raw map



X Index: 141



Y Index: 155

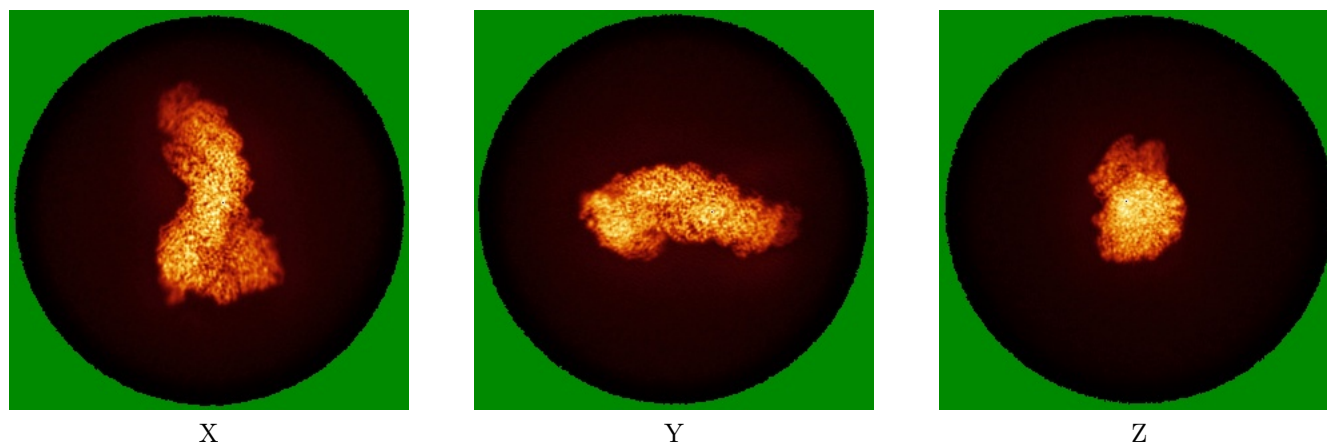


Z Index: 115

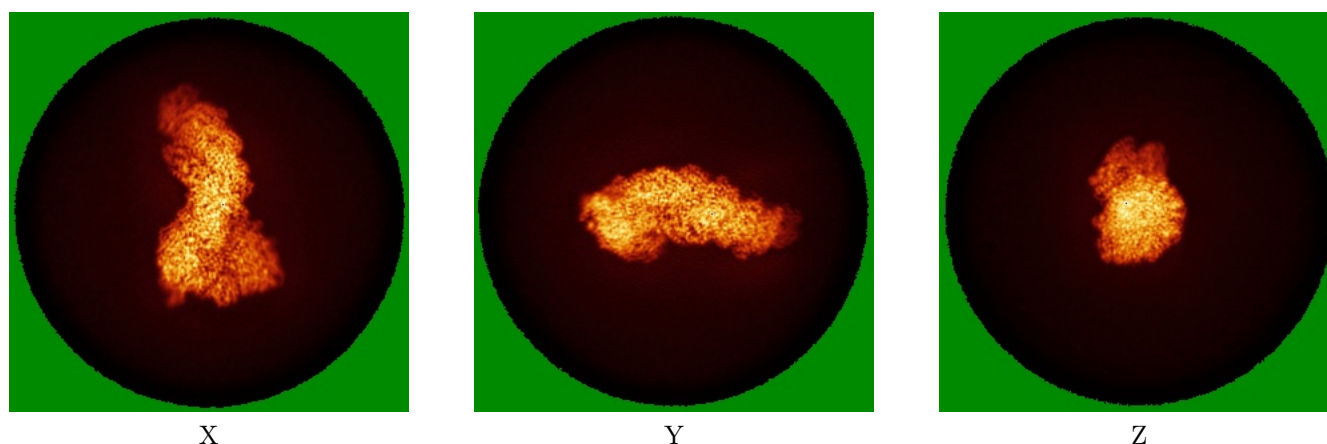
The images above show the largest variance slices of the map in three orthogonal directions.

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](#)

This section was not generated.

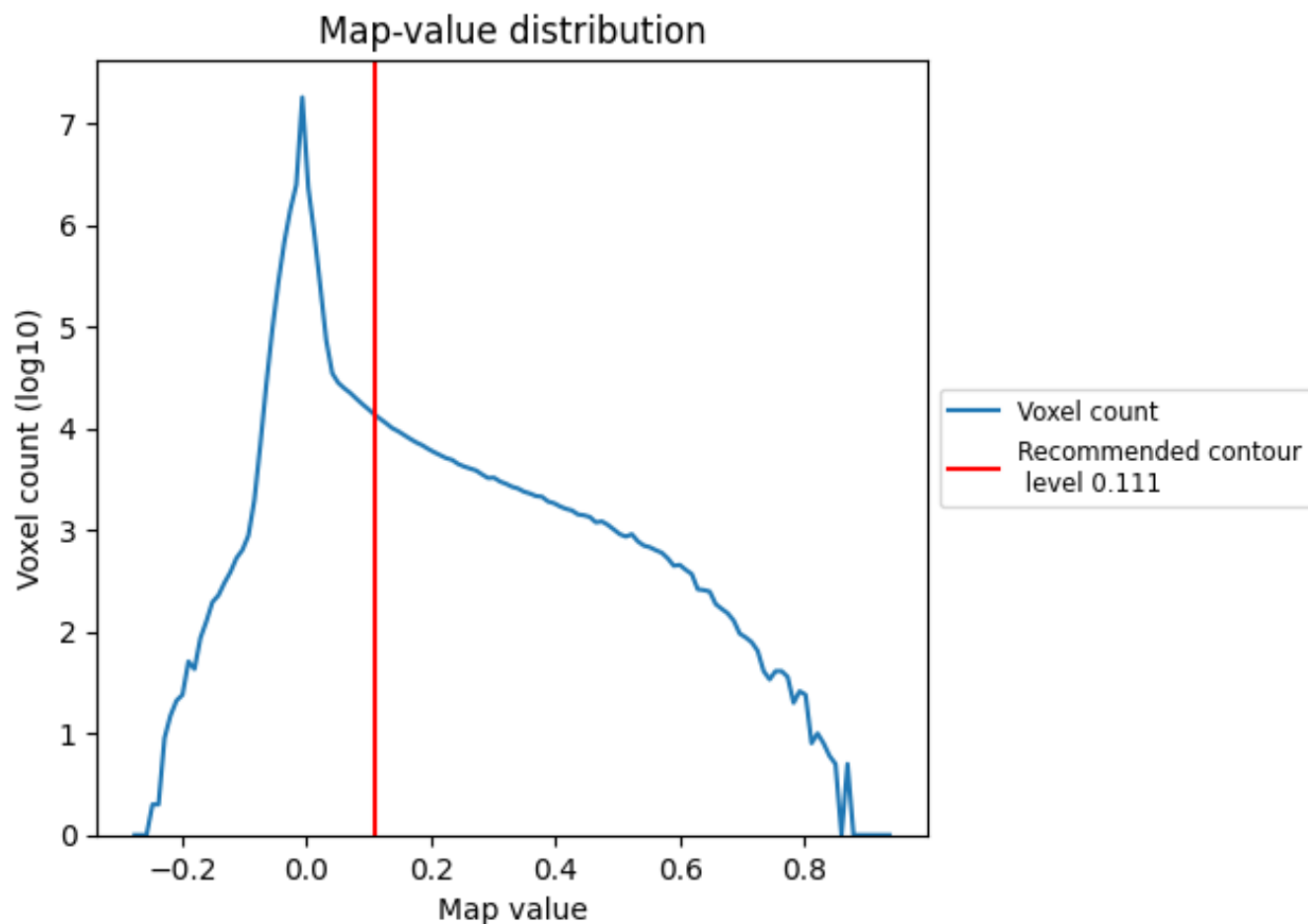
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

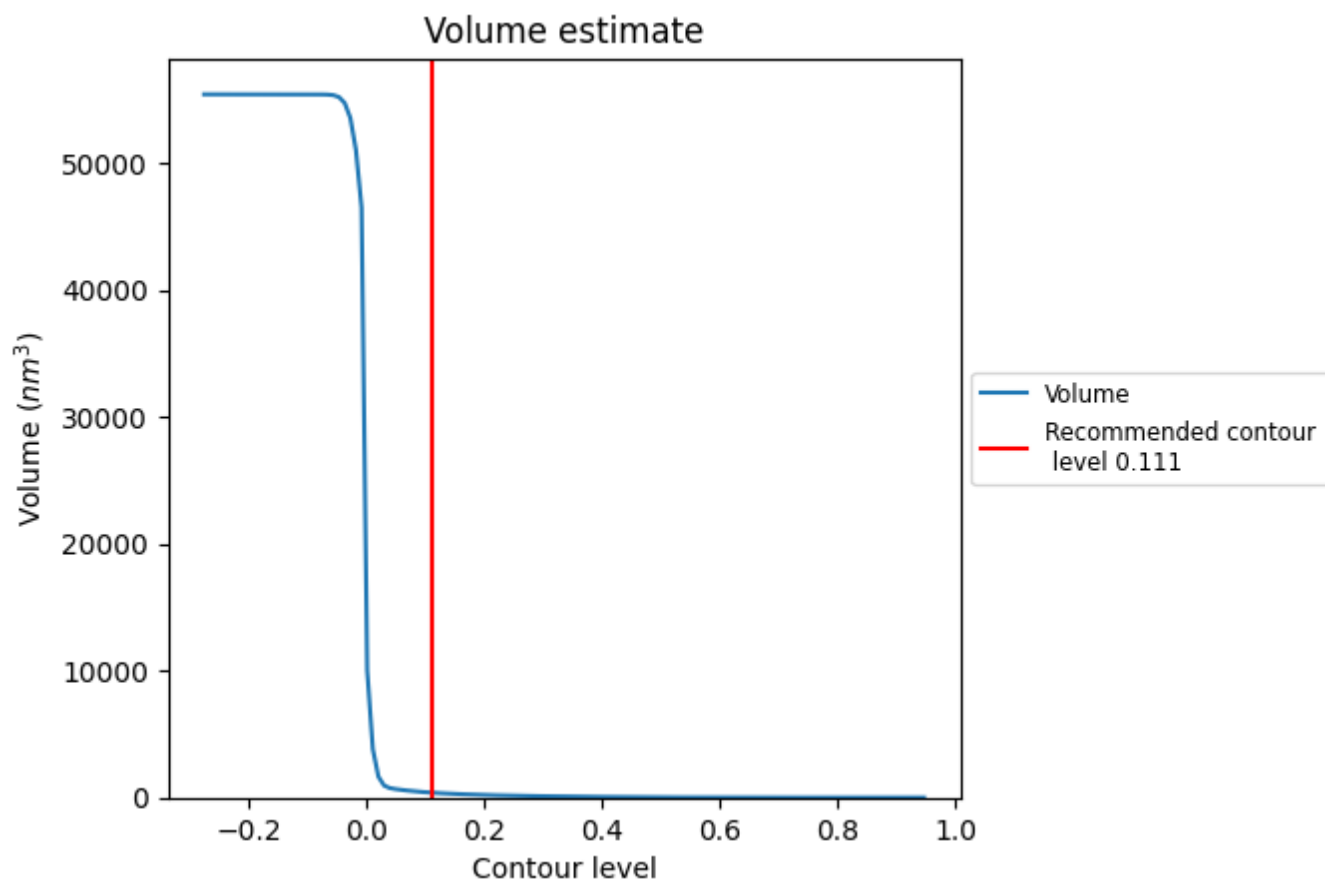
This section contains the results of statistical analysis of the map.

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.

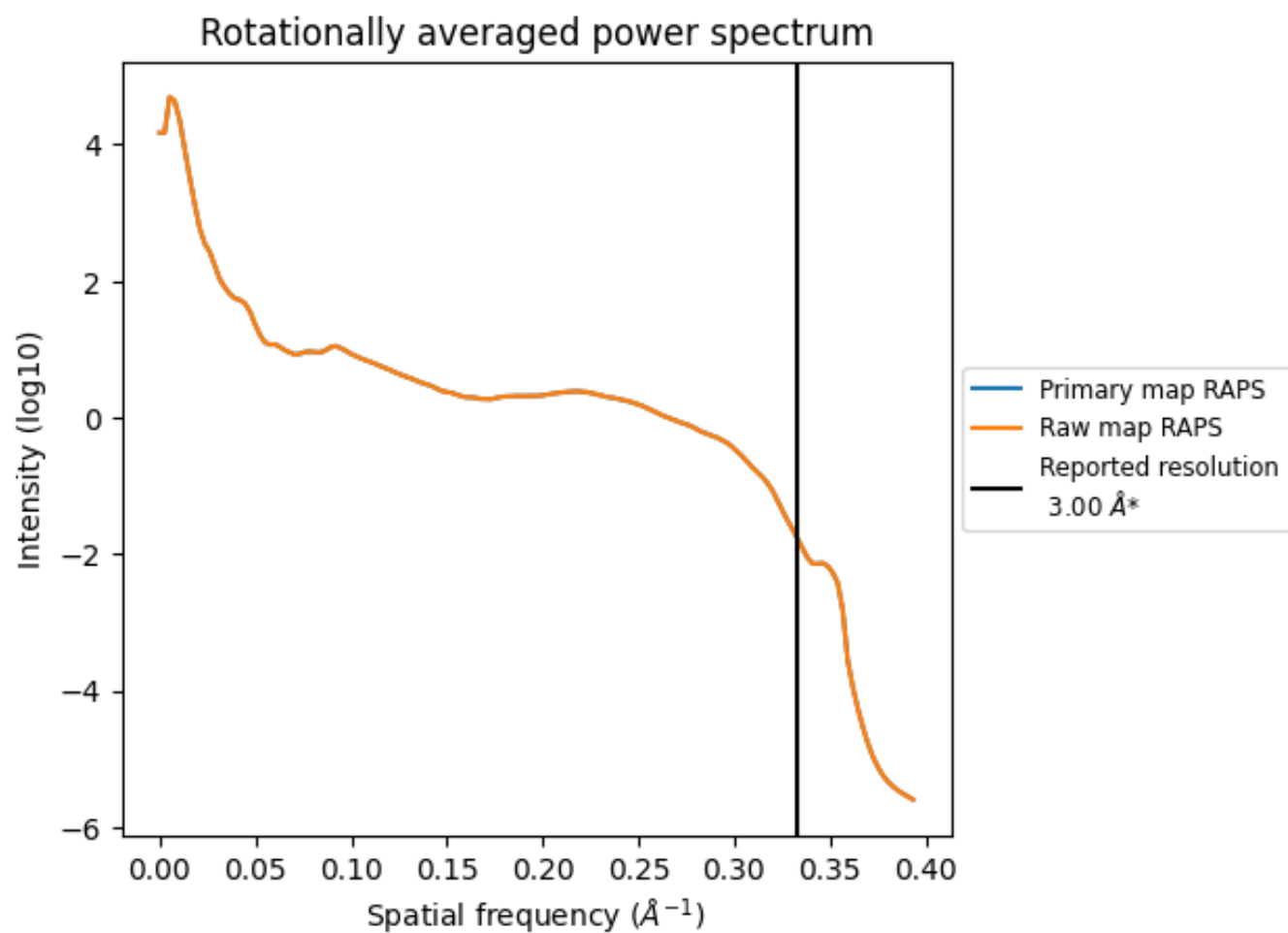
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

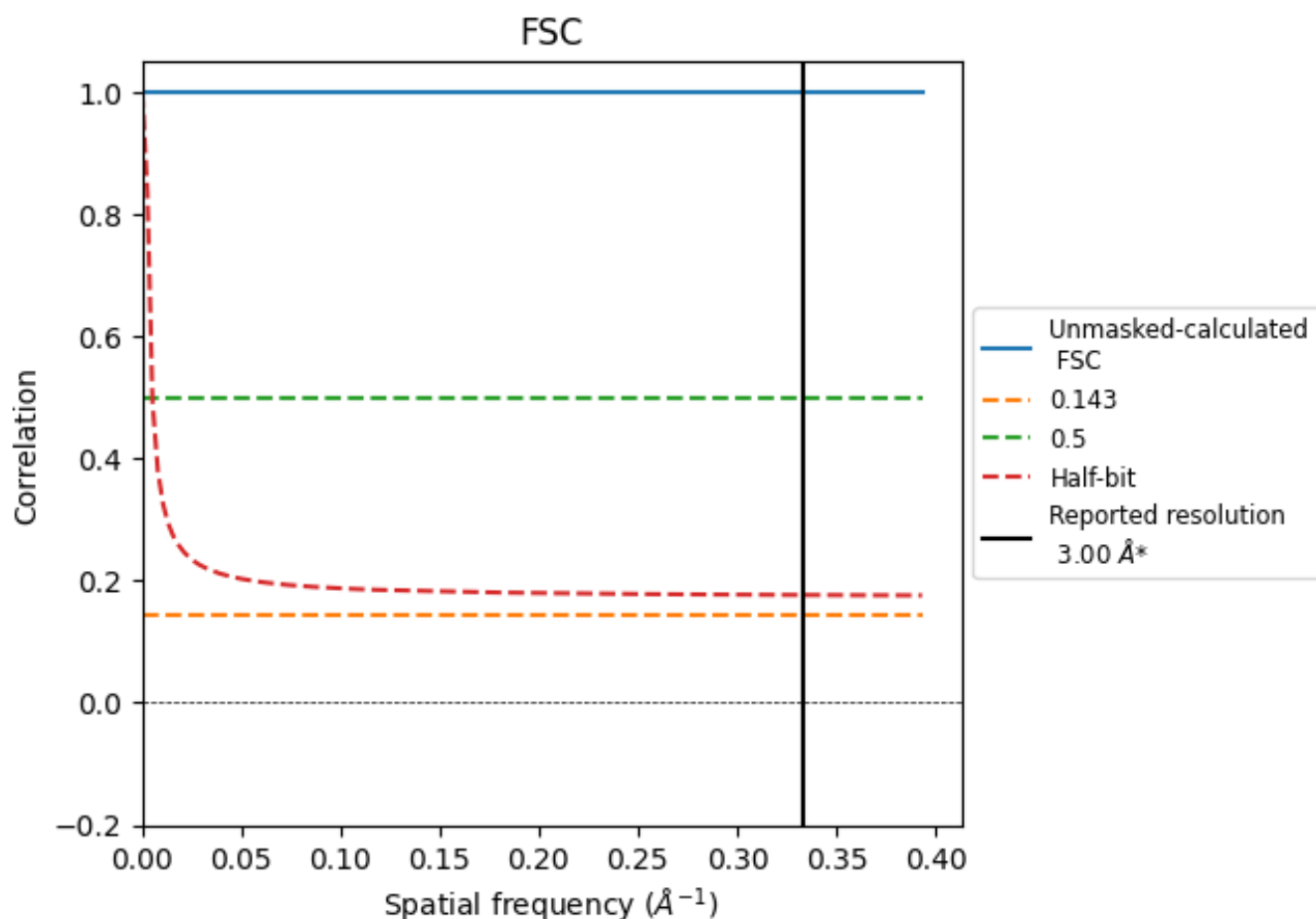


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

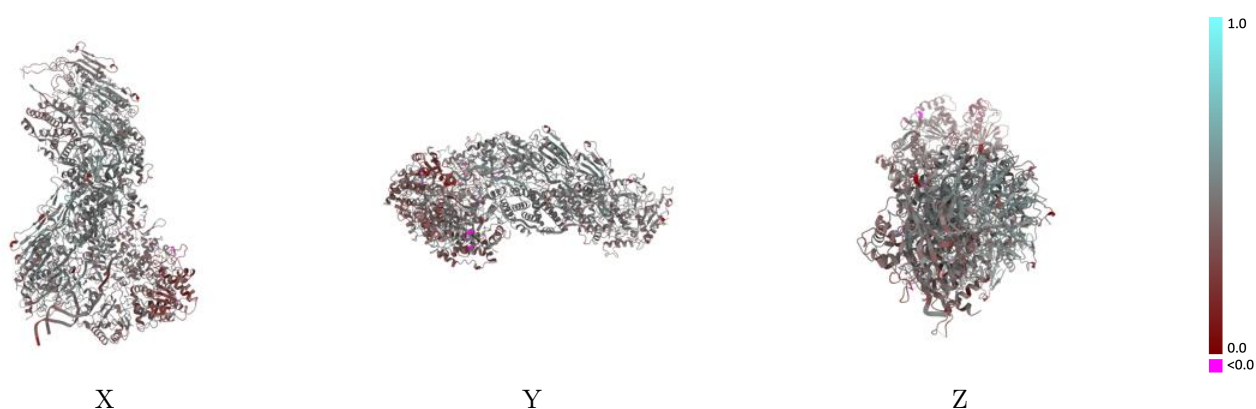
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29879 and PDB model 8G9U. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

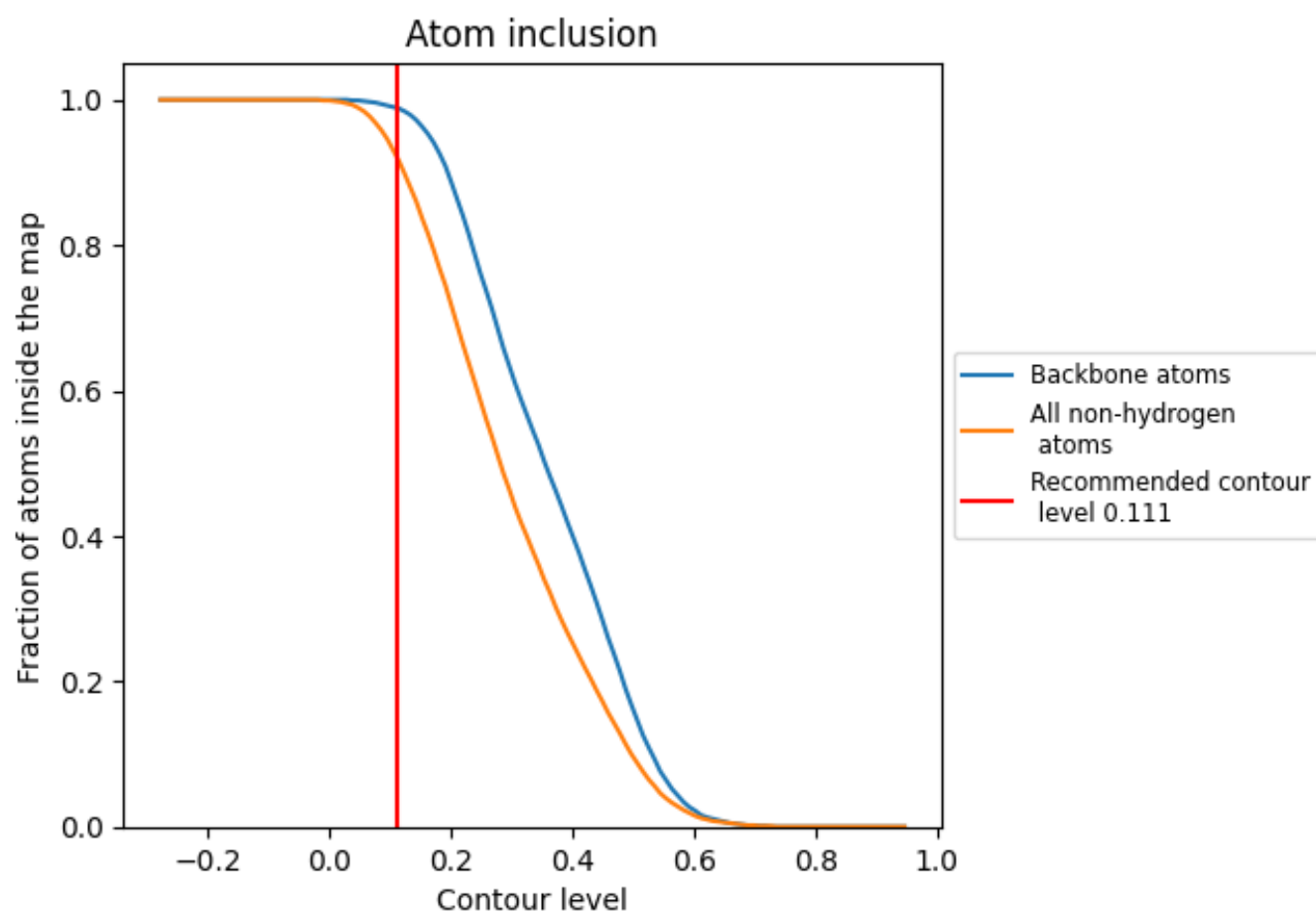


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.4400
A	 0.9470	 0.4750
B	 0.9280	 0.4660
C	 0.9490	 0.4800
D	 0.9320	 0.4710
E	 0.9180	 0.4500
F	 0.9050	 0.4000
G	 0.8340	 0.4130
H	 0.9250	 0.4580
I	 0.9340	 0.4510
J	 0.9500	 0.4620
K	 0.9960	 0.4920
L	 0.9950	 0.4760
M	 0.9210	 0.4580
N	 0.9220	 0.4530
O	 0.9760	 0.3930
P	 0.8840	 0.3630
Q	 0.9400	 0.4630

