



Full wwPDB EM Validation Report ⓘ

Jun 2, 2024 – 04:52 PM EDT

PDB ID : 8DFO
EMDB ID : EMD-27409
Title : type I-C Cascade bound to AcrIC4
Authors : O'Brien, R.E.; Bravo, J.P.K.; Ramos, D.; Hibshman, G.N.; Wright, J.T.; Taylor, D.W.
Deposited on : 2022-06-22
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

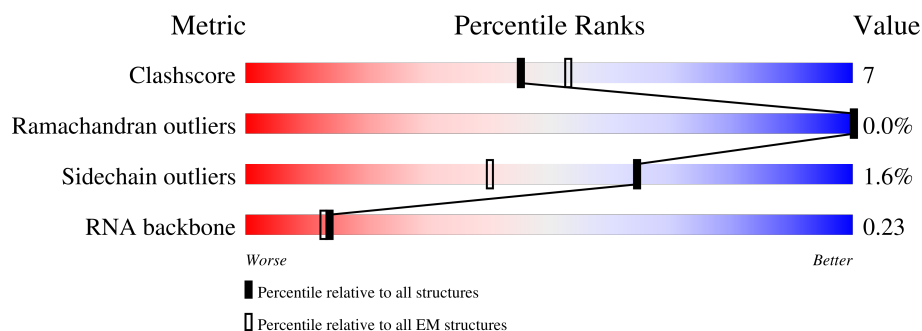
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 3.10 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	<div> <div>47%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
2	B	290	<div> <div>60%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
2	C	290	<div> <div>79%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	D	290	<div> <div>72%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	E	290	<div> <div>78%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
2	F	290	<div> <div>77%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
2	G	290	<div> <div>83%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	290	<div><div></div><div>90%</div><div>78%</div><div>19%</div><div>..</div></div>
3	I	612	<div><div></div><div>55%</div><div>57%</div><div>10%</div><div>•</div><div>32%</div></div>
4	J	124	<div><div></div><div>77%</div><div>75%</div><div>19%</div><div>•</div><div>6%</div></div>
4	K	124	<div><div></div><div>85%</div><div>87%</div><div>7%</div><div>6%</div></div>
5	L	45	<div><div></div><div>78%</div><div>20%</div><div>13%</div><div>64%</div></div>
6	M	57	<div><div></div><div>93%</div><div>74%</div><div>21%</div><div>5%</div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23861 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 pre-crRNA processing endonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	220	Total	C	N	O	S	0	0
			1774	1123	323	318	10		

- Molecule 2 is a protein called CRISPR-associated protein, TM1801 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	270	Total	C	N	O	S	0	0
			2112	1324	378	397	13		
2	C	286	Total	C	N	O	S	0	0
			2238	1406	399	419	14		
2	D	286	Total	C	N	O	S	0	0
			2238	1406	399	419	14		
2	E	286	Total	C	N	O	S	0	0
			2238	1406	399	419	14		
2	F	286	Total	C	N	O	S	0	0
			2238	1406	399	419	14		
2	G	286	Total	C	N	O	S	0	0
			2238	1406	399	419	14		
2	H	286	Total	C	N	O	S	0	0
			2238	1406	399	419	14		

- Molecule 3 is a protein called CRISPR-associated protein, CT1133 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	415	Total	C	N	O	S	0	0
			3261	2061	586	599	15		

- Molecule 4 is a protein called CRISPR-associated protein, CT1133 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	117	Total	C	N	O	S	0	0
			930	589	164	172	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	117	Total	C	N	O	S	0	0
			930	589	164	172	5		

- Molecule 5 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	45	Total	C	N	O	P	0	0
			960	428	173	314	45		

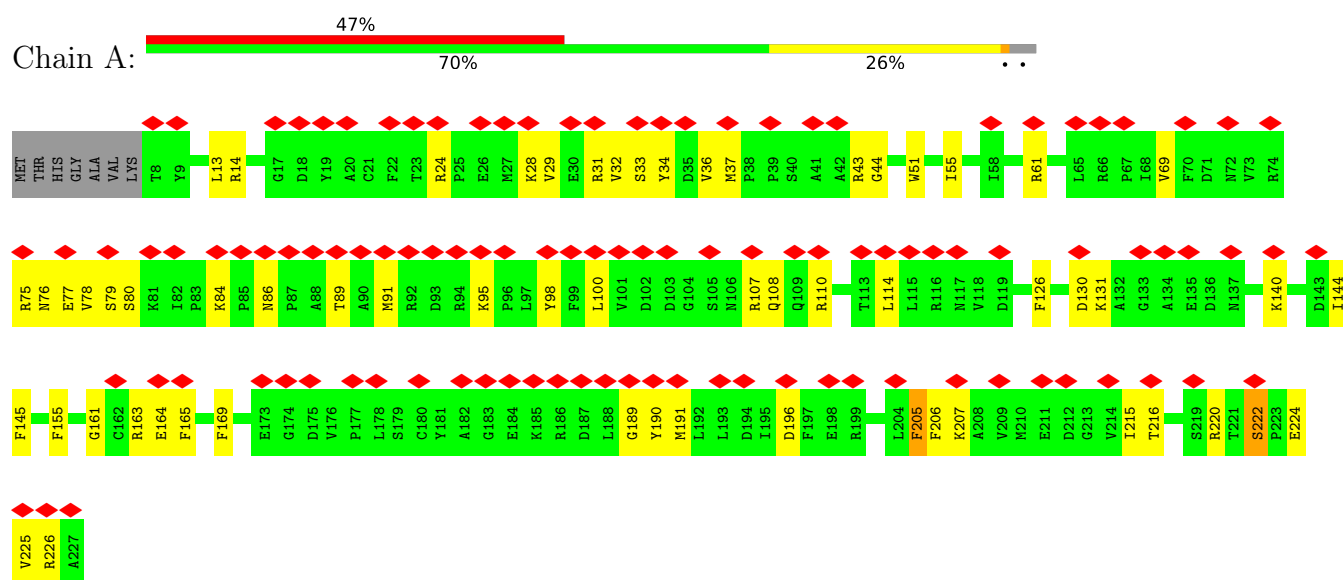
- Molecule 6 is a protein called AcrIC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	57	Total	C	N	O	S	0	0
			466	289	77	97	3		

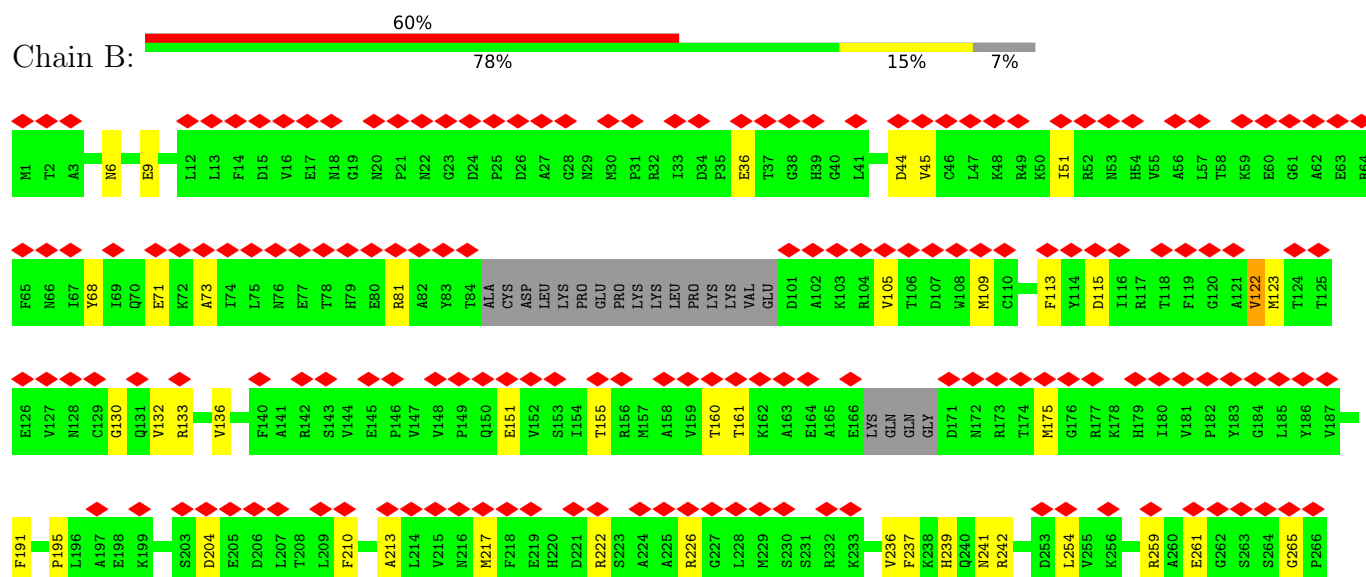
3 Residue-property plots

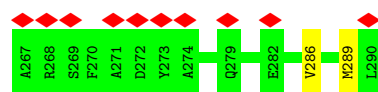
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: pre-crRNA processing endonuclease

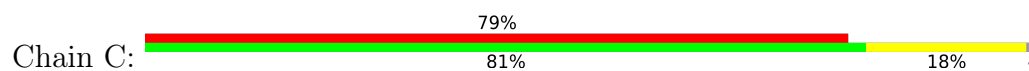


- Molecule 2: CRISPR-associated protein, TM1801 family

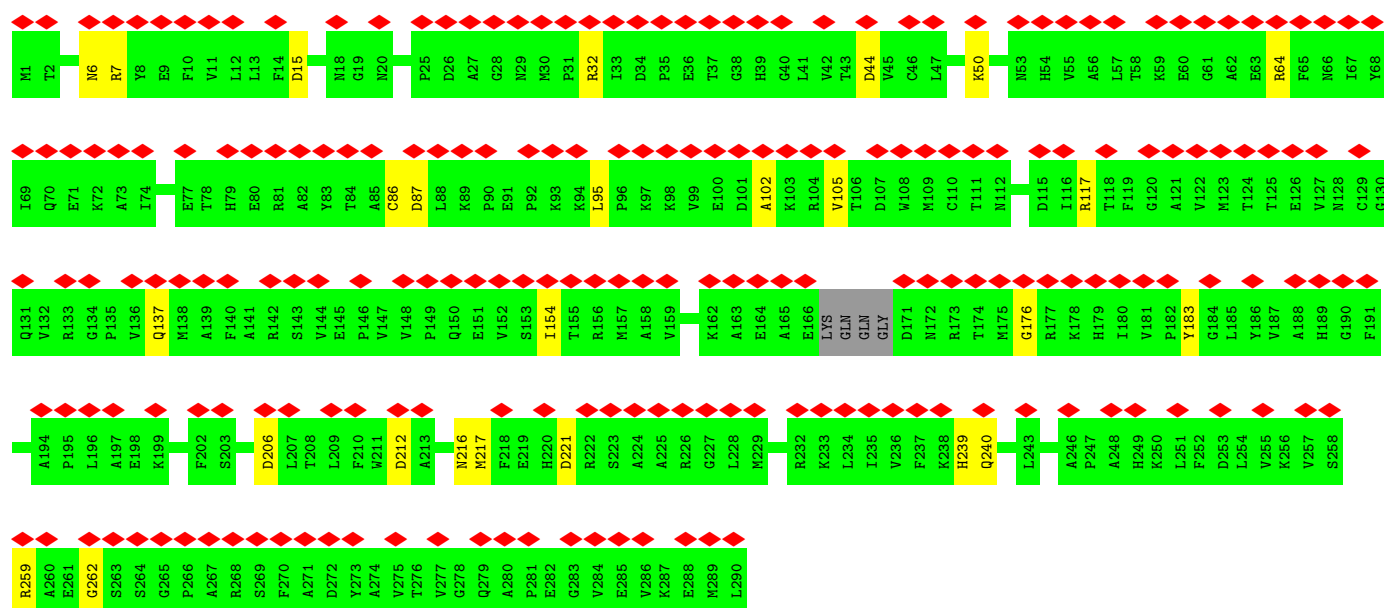
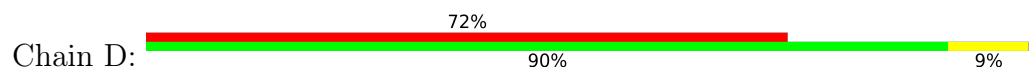




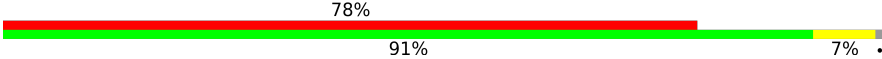
- Molecule 2: CRISPR-associated protein, TM1801 family

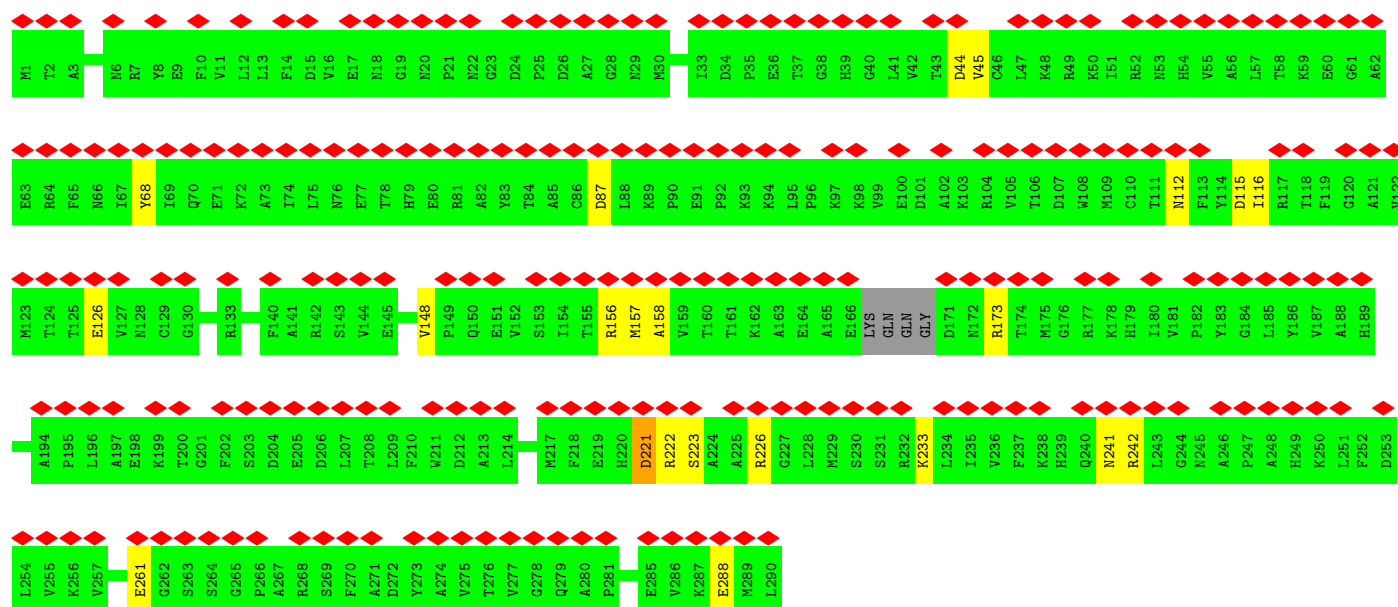


- Molecule 2: CRISPR-associated protein, TM1801 family

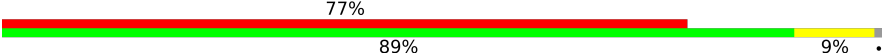


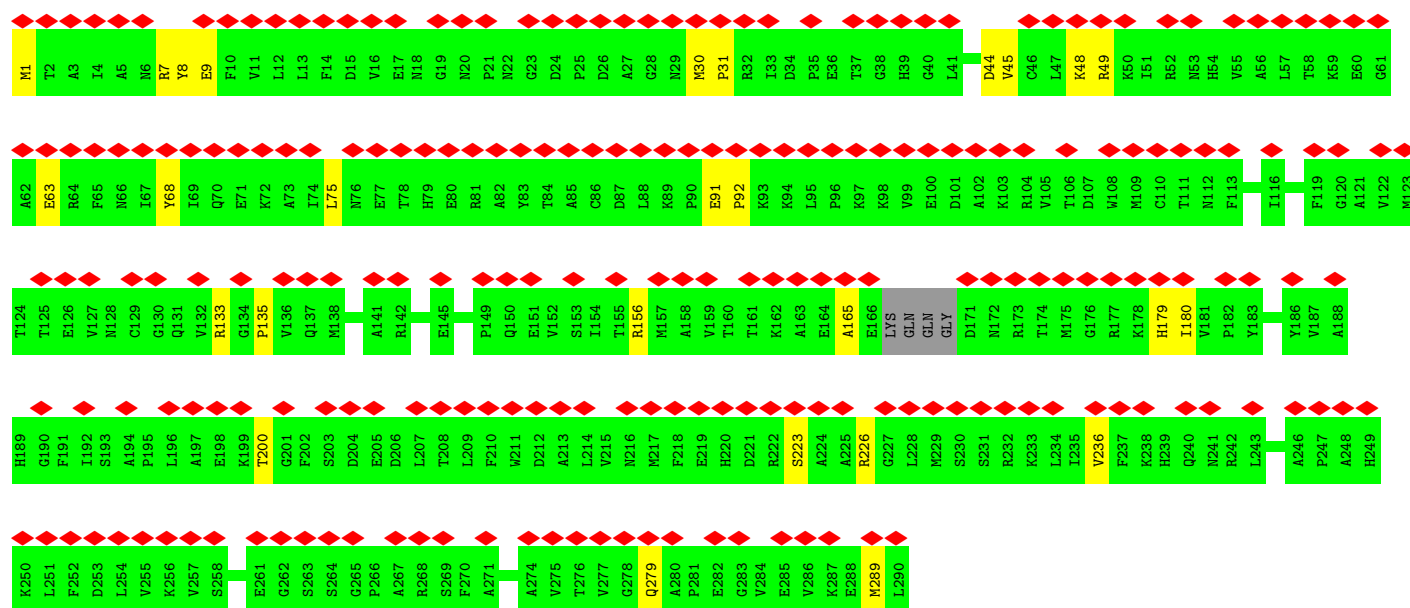
- Molecule 2: CRISPR-associated protein, TM1801 family

Chain E: 




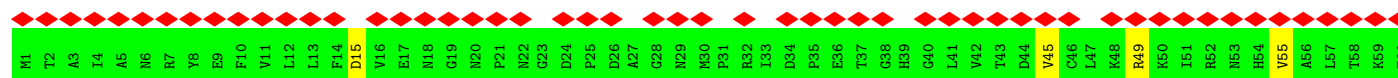
- Molecule 2: CRISPR-associated protein, TM1801 family

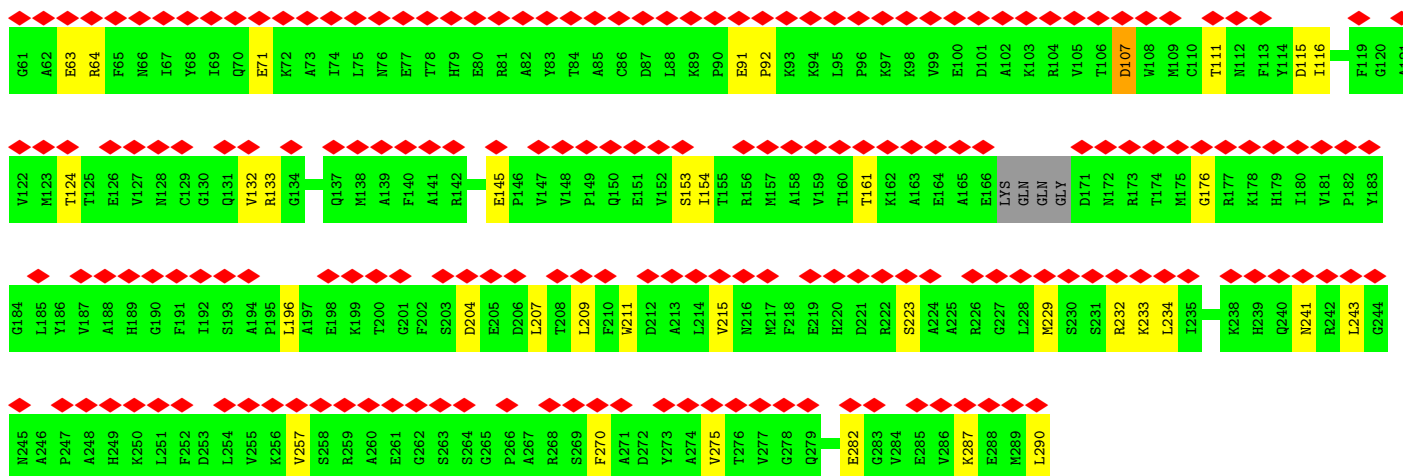
Chain F: 



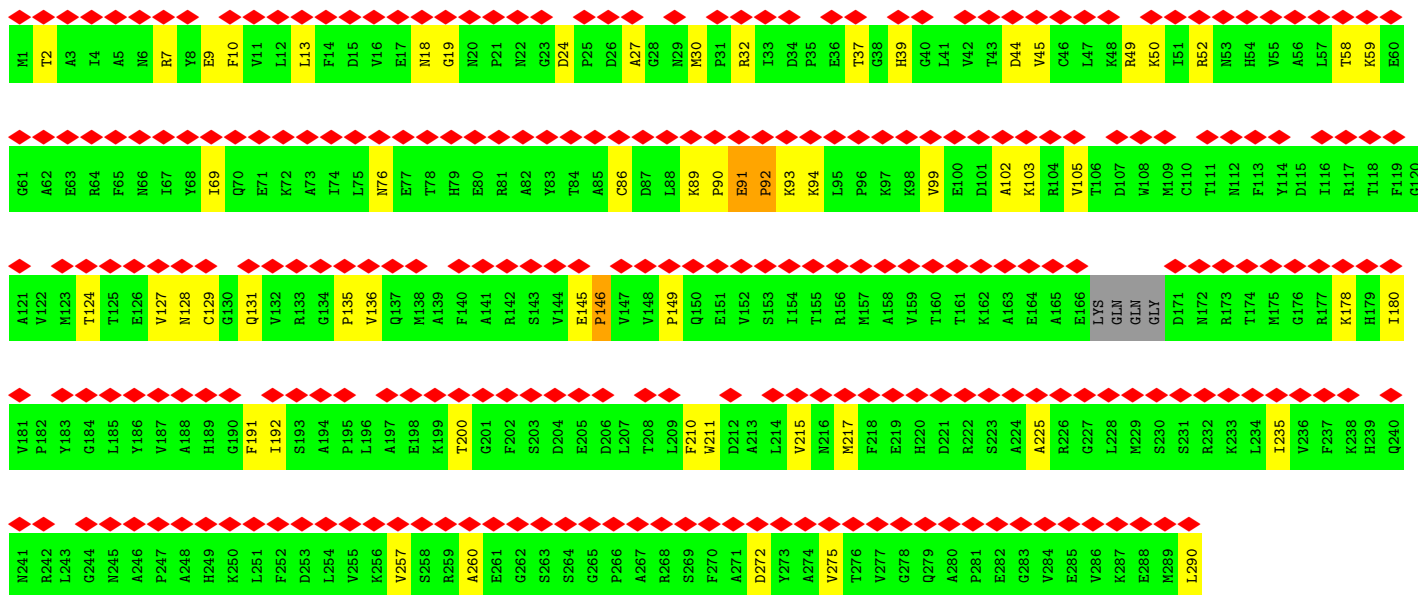
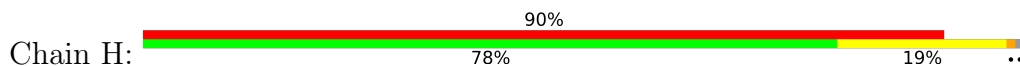
- Molecule 2: CRISPR-associated protein, TM1801 family

Chain G: 

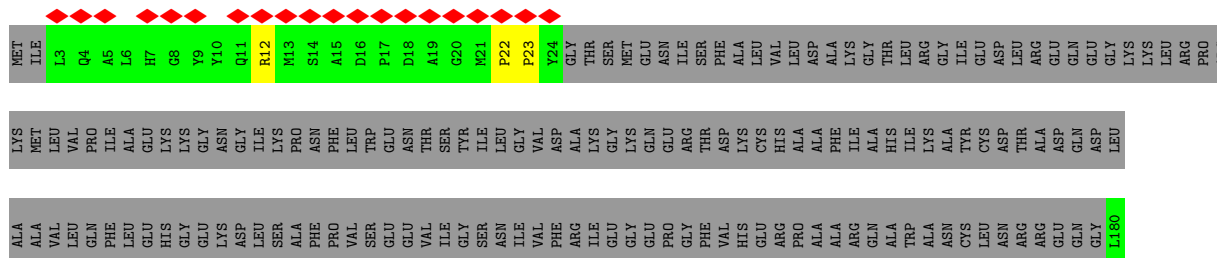


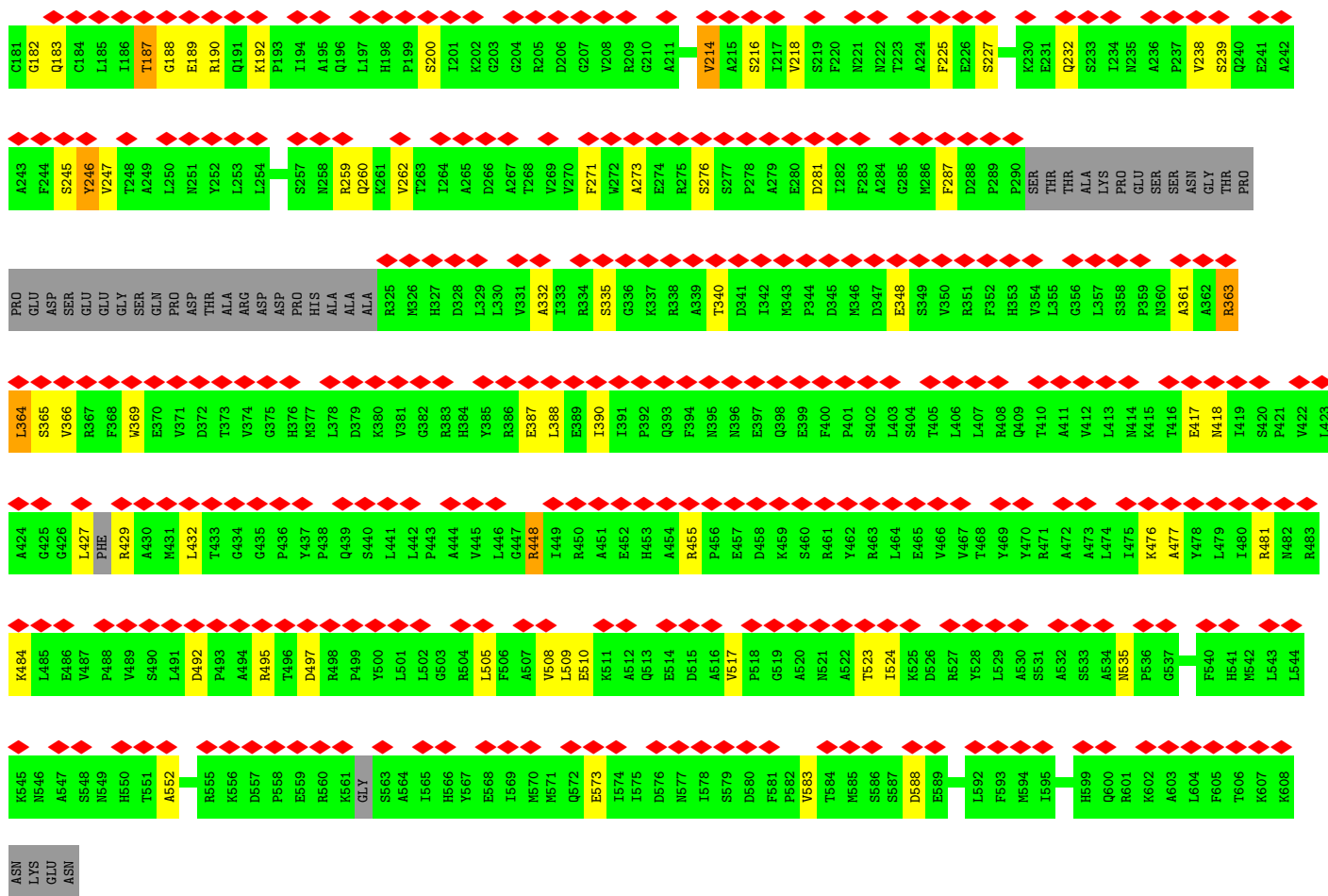


• Molecule 2: CRISPR-associated protein, TM1801 family

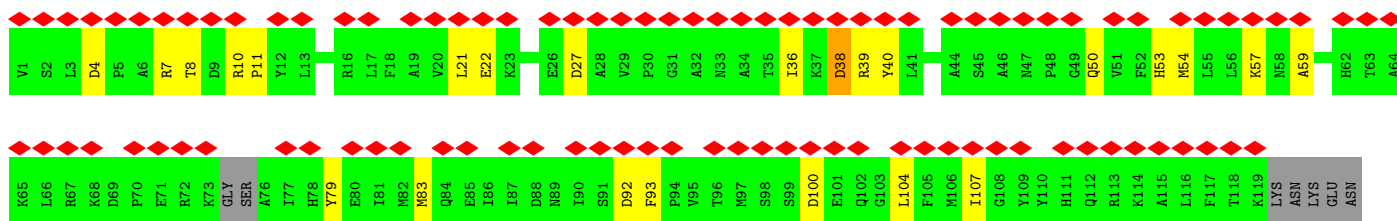
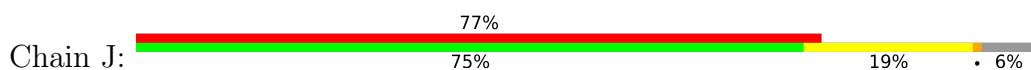


• Molecule 3: CRISPR-associated protein, CT1133 family

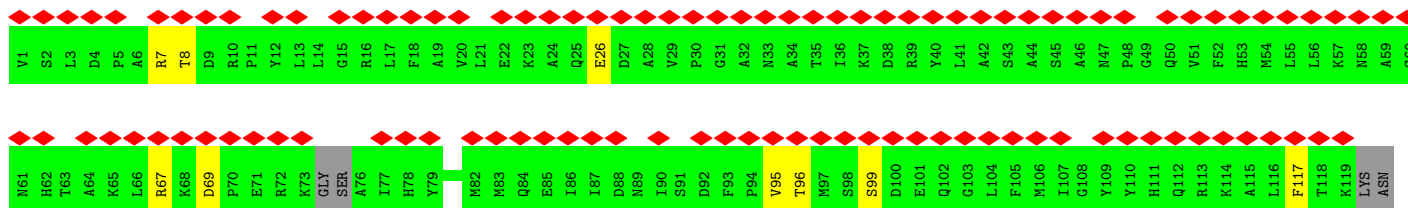
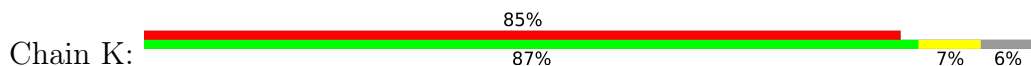




- Molecule 4: CRISPR-associated protein, CT1133 family

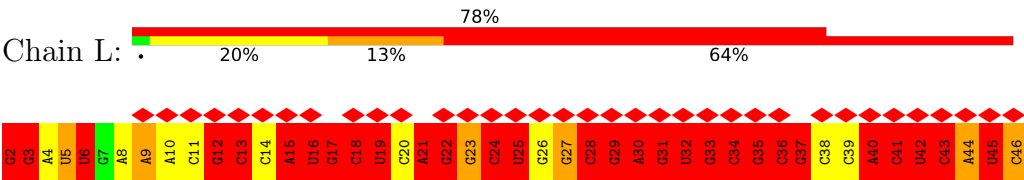


- Molecule 4: CRISPR-associated protein, CT1133 family

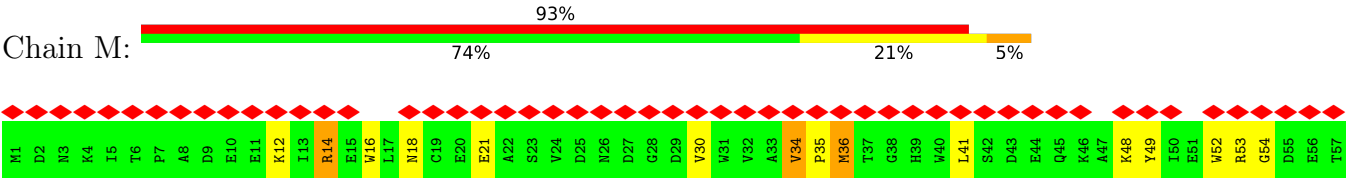


LYS
GLU
ASN

● Molecule 5: RNA (45-MER)



● Molecule 6: AcrIC4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.674	Depositor
Minimum map value	-0.942	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.253	Depositor
Map size (\AA)	394.8, 394.8, 394.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.94, 0.94, 0.94	Depositor

5 Model quality

5.1 Standard geometry

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	1.60	36/1817 (2.0%)	1.29	14/2460 (0.6%)
2	B	0.81	11/2153 (0.5%)	0.76	4/2909 (0.1%)
2	C	1.43	31/2283 (1.4%)	1.21	8/3085 (0.3%)
2	D	0.48	2/2283 (0.1%)	0.59	2/3085 (0.1%)
2	E	0.30	0/2283	0.54	0/3085
2	F	0.29	0/2283	0.52	0/3085
2	G	0.27	0/2283	0.52	0/3085
2	H	0.67	3/2283 (0.1%)	0.84	6/3085 (0.2%)
3	I	0.92	20/3329 (0.6%)	0.85	3/4503 (0.1%)
4	J	0.29	0/948	0.53	0/1277
4	K	0.28	0/948	0.48	0/1277
5	L	1.46	22/1072 (2.1%)	2.23	97/1669 (5.8%)
6	M	1.63	11/477 (2.3%)	1.32	2/648 (0.3%)
All	All	0.89	136/24442 (0.6%)	0.94	136/33253 (0.4%)

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
5	L	0	1

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	92	PRO	CB-CG	23.55	2.67	1.50
2	H	92	PRO	CG-CD	-14.05	1.04	1.50
5	L	10	A	C6-N6	-12.47	1.24	1.33
5	L	9	A	C6-N6	-12.40	1.24	1.33
5	L	4	A	C6-N6	-11.99	1.24	1.33
5	L	8	A	C6-N6	-11.81	1.24	1.33
5	L	3	G	C2-N2	-9.93	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	5	U	C5-C6	-8.71	1.26	1.34
2	D	7	ARG	CZ-NH2	-7.93	1.22	1.33
2	C	242	ARG	CZ-NH2	-7.93	1.22	1.33
1	A	163	ARG	CZ-NH2	-7.92	1.22	1.33
2	C	7	ARG	CZ-NH2	-7.91	1.22	1.33
6	M	14	ARG	CZ-NH2	-7.89	1.22	1.33
3	I	363	ARG	CZ-NH2	-7.86	1.22	1.33
2	B	133	ARG	CZ-NH2	-7.85	1.22	1.33
2	B	222	ARG	CZ-NH2	-7.82	1.22	1.33
2	C	232	ARG	CZ-NH2	-7.77	1.23	1.33
1	A	107	ARG	CZ-NH2	-7.71	1.23	1.33
3	I	190	ARG	CZ-NH2	-7.69	1.23	1.33
6	M	53	ARG	CZ-NH2	-7.64	1.23	1.33
1	A	226	ARG	CZ-NH2	-7.62	1.23	1.33
1	A	110	ARG	CZ-NH2	-7.62	1.23	1.33
1	A	24	ARG	CZ-NH2	-7.60	1.23	1.33
1	A	31	ARG	CZ-NH2	-7.57	1.23	1.33
1	A	220	ARG	CZ-NH2	-7.55	1.23	1.33
1	A	43	ARG	CZ-NH2	-7.52	1.23	1.33
6	M	14	ARG	CZ-NH1	-7.41	1.23	1.33
2	B	133	ARG	CZ-NH1	-7.38	1.23	1.33
1	A	107	ARG	CZ-NH1	-7.36	1.23	1.33
2	C	232	ARG	CZ-NH1	-7.34	1.23	1.33
2	D	7	ARG	CZ-NH1	-7.32	1.23	1.33
2	C	7	ARG	CZ-NH1	-7.32	1.23	1.33
2	B	222	ARG	CZ-NH1	-7.30	1.23	1.33
1	A	163	ARG	CZ-NH1	-7.30	1.23	1.33
5	L	3	G	C8-N7	-7.29	1.26	1.30
2	C	242	ARG	CZ-NH1	-7.26	1.23	1.33
3	I	363	ARG	CZ-NH1	-7.19	1.23	1.33
1	A	220	ARG	CZ-NH1	-7.17	1.23	1.33
1	A	24	ARG	CZ-NH1	-7.10	1.23	1.33
1	A	43	ARG	CZ-NH1	-7.09	1.23	1.33
1	A	110	ARG	CZ-NH1	-7.06	1.23	1.33
6	M	53	ARG	CZ-NH1	-7.05	1.23	1.33
1	A	226	ARG	CZ-NH1	-7.02	1.24	1.33
3	I	190	ARG	CZ-NH1	-7.00	1.24	1.33
1	A	31	ARG	CZ-NH1	-6.99	1.24	1.33
2	H	92	PRO	N-CD	6.87	1.57	1.47
5	L	8	A	C5'-C4'	-6.67	1.43	1.51
2	B	122	VAL	CB-CG2	-6.65	1.38	1.52
2	C	186	TYR	CD2-CE2	-6.27	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	186	TYR	CD1-CE1	-6.25	1.29	1.39
5	L	9	A	C8-N7	-6.24	1.27	1.31
2	C	273	TYR	CD1-CE1	-6.16	1.30	1.39
1	A	34	TYR	CD1-CE1	-6.16	1.30	1.39
1	A	34	TYR	CD2-CE2	-6.13	1.30	1.39
5	L	3	G	N9-C8	-6.06	1.33	1.37
2	C	273	TYR	CD2-CE2	-6.05	1.30	1.39
5	L	5	U	C2-N3	-5.99	1.33	1.37
1	A	190	TYR	CD2-CE2	-5.92	1.30	1.39
5	L	10	A	C5'-C4'	-5.92	1.44	1.51
6	M	49	TYR	CD1-CE1	-5.92	1.30	1.39
6	M	49	TYR	CD2-CE2	-5.91	1.30	1.39
5	L	8	A	C8-N7	-5.88	1.27	1.31
5	L	10	A	C8-N7	-5.86	1.27	1.31
1	A	190	TYR	CD1-CE1	-5.81	1.30	1.39
5	L	9	A	C5'-C4'	-5.78	1.44	1.51
2	B	68	TYR	CD1-CE1	-5.77	1.30	1.39
1	A	189	GLY	N-CA	-5.75	1.37	1.46
2	C	136	VAL	CB-CG2	-5.75	1.40	1.52
2	C	114	TYR	CD1-CE1	-5.74	1.30	1.39
2	B	68	TYR	CD2-CE2	-5.74	1.30	1.39
3	I	246	TYR	CD2-CE2	-5.73	1.30	1.39
3	I	246	TYR	CD1-CE1	-5.71	1.30	1.39
5	L	9	A	N9-C8	-5.70	1.33	1.37
2	C	244	GLY	N-CA	-5.66	1.37	1.46
2	B	122	VAL	CB-CG1	-5.63	1.41	1.52
2	C	114	TYR	CD2-CE2	-5.63	1.30	1.39
1	A	29	VAL	CB-CG2	-5.62	1.41	1.52
5	L	4	A	C5'-C4'	-5.61	1.44	1.51
2	C	230	SER	CB-OG	-5.58	1.34	1.42
5	L	5	U	C5'-C4'	-5.58	1.44	1.51
2	C	231	SER	CB-OG	-5.56	1.35	1.42
5	L	4	A	N9-C8	-5.54	1.33	1.37
1	A	78	VAL	CB-CG1	-5.53	1.41	1.52
2	C	187	VAL	CB-CG2	-5.53	1.41	1.52
3	I	188	GLY	N-CA	-5.51	1.37	1.46
5	L	4	A	C8-N7	-5.49	1.27	1.31
2	C	136	VAL	CB-CG1	-5.47	1.41	1.52
3	I	239	SER	CB-OG	-5.47	1.35	1.42
2	C	187	VAL	CB-CG1	-5.45	1.41	1.52
2	C	193	SER	CB-OG	-5.45	1.35	1.42
2	C	11	VAL	CB-CG2	-5.42	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	256	LYS	CE-NZ	-5.41	1.35	1.49
3	I	247	VAL	CB-CG2	-5.40	1.41	1.52
1	A	161	GLY	N-CA	-5.38	1.38	1.46
1	A	32	VAL	CB-CG2	-5.38	1.41	1.52
2	C	275	VAL	CB-CG1	-5.37	1.41	1.52
3	I	247	VAL	CB-CG1	-5.36	1.41	1.52
2	C	275	VAL	CB-CG2	-5.35	1.41	1.52
3	I	182	GLY	N-CA	-5.35	1.38	1.46
1	A	33	SER	CB-OG	-5.35	1.35	1.42
1	A	80	SER	CB-OG	-5.34	1.35	1.42
2	B	132	VAL	CB-CG1	-5.34	1.41	1.52
1	A	84	LYS	CE-NZ	-5.33	1.35	1.49
2	C	257	VAL	CB-CG1	-5.33	1.41	1.52
1	A	225	VAL	CB-CG2	-5.32	1.41	1.52
3	I	216	SER	CB-OG	-5.31	1.35	1.42
2	C	255	VAL	CB-CG1	-5.30	1.41	1.52
6	M	52	TRP	CD1-NE1	-5.29	1.28	1.38
6	M	16	TRP	CD1-NE1	-5.28	1.28	1.38
2	C	257	VAL	CB-CG2	-5.28	1.41	1.52
3	I	366	VAL	CB-CG1	-5.28	1.41	1.52
1	A	44	GLY	N-CA	-5.28	1.38	1.46
3	I	214	VAL	CB-CG2	-5.27	1.41	1.52
3	I	366	VAL	CB-CG2	-5.27	1.41	1.52
2	C	250	LYS	CE-NZ	-5.26	1.35	1.49
3	I	369	TRP	CD1-NE1	-5.26	1.29	1.38
5	L	8	A	N9-C8	-5.26	1.33	1.37
1	A	32	VAL	CB-CG1	-5.26	1.41	1.52
2	C	255	VAL	CB-CG2	-5.24	1.41	1.52
3	I	200	SER	CB-OG	-5.24	1.35	1.42
2	C	190	GLY	N-CA	-5.24	1.38	1.46
1	A	222	SER	CB-OG	-5.23	1.35	1.42
2	C	11	VAL	CB-CG1	-5.22	1.41	1.52
6	M	54	GLY	N-CA	-5.22	1.38	1.46
1	A	79	SER	CB-OG	-5.21	1.35	1.42
2	B	132	VAL	CB-CG2	-5.20	1.42	1.52
5	L	3	G	C6-N1	-5.19	1.35	1.39
1	A	225	VAL	CB-CG1	-5.14	1.42	1.52
2	B	130	GLY	N-CA	-5.12	1.38	1.46
3	I	365	SER	CB-OG	-5.06	1.35	1.42
6	M	48	LYS	CE-NZ	-5.06	1.36	1.49
1	A	78	VAL	CB-CG2	-5.04	1.42	1.52
3	I	192	LYS	CE-NZ	-5.01	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	12	LYS	CE-NZ	-5.01	1.36	1.49
3	I	245	SER	CB-OG	-5.01	1.35	1.42
1	A	207	LYS	CE-NZ	-5.01	1.36	1.49

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	92	PRO	CB-CG-CD	-27.29	0.05	106.50
2	H	92	PRO	CA-N-CD	-15.70	89.53	111.50
5	L	3	G	N7-C8-N9	12.82	119.51	113.10
5	L	13	C	O4'-C1'-N1	12.51	118.21	108.20
5	L	10	A	N7-C8-N9	12.27	119.93	113.80
5	L	8	A	N1-C2-N3	11.87	135.24	129.30
5	L	9	A	N1-C2-N3	11.84	135.22	129.30
5	L	10	A	N1-C2-N3	11.79	135.20	129.30
5	L	8	A	N7-C8-N9	11.34	119.47	113.80
5	L	4	A	N1-C2-N3	11.15	134.87	129.30
5	L	18	C	O4'-C1'-N1	11.04	117.04	108.20
5	L	9	A	N7-C8-N9	11.02	119.31	113.80
2	H	92	PRO	CA-CB-CG	-10.37	84.29	104.00
5	L	4	A	N7-C8-N9	10.37	118.99	113.80
5	L	25	U	O4'-C1'-N1	-9.85	100.32	108.20
2	H	91	GLU	C-N-CD	9.38	148.09	128.40
2	H	92	PRO	N-CA-CB	-9.16	92.31	103.30
5	L	5	U	C2-N3-C4	9.11	132.47	127.00
5	L	3	G	C6-N1-C2	8.99	130.49	125.10
5	L	5	U	N3-C4-C5	-8.69	109.39	114.60
5	L	3	G	C8-N9-C4	-8.69	102.93	106.40
5	L	13	C	OP1-P-OP2	-8.44	106.94	119.60
5	L	36	C	OP1-P-OP2	-8.41	106.99	119.60
5	L	10	A	C8-N9-C4	-8.38	102.45	105.80
5	L	43	C	OP1-P-OP2	-8.30	107.15	119.60
5	L	34	C	O4'-C1'-N1	8.29	114.83	108.20
5	L	29	G	OP1-P-OP2	-8.04	107.55	119.60
5	L	21	A	OP1-P-OP2	-7.87	107.79	119.60
5	L	42	U	OP1-P-O3'	7.87	122.50	105.20
5	L	5	U	O4'-C1'-N1	7.69	114.35	108.20
5	L	25	U	N1-C1'-C2'	7.66	123.96	114.00
5	L	33	G	OP1-P-OP2	-7.62	108.17	119.60
5	L	22	G	OP1-P-OP2	-7.55	108.28	119.60
5	L	28	C	OP1-P-O3'	7.53	121.77	105.20
5	L	34	C	OP1-P-OP2	-7.51	108.33	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	35	G	OP1-P-OP2	-7.49	108.36	119.60
5	L	45	U	O4'-C1'-N1	7.38	114.10	108.20
5	L	33	G	OP1-P-O3'	7.37	121.41	105.20
5	L	12	G	OP1-P-O3'	7.34	121.36	105.20
5	L	18	C	OP1-P-OP2	-7.30	108.65	119.60
5	L	19	U	OP1-P-OP2	-7.21	108.78	119.60
5	L	35	G	OP1-P-O3'	7.21	121.07	105.20
5	L	39	C	N1-C1'-C2'	7.18	123.34	114.00
5	L	41	C	OP1-P-OP2	-7.15	108.88	119.60
5	L	25	U	OP1-P-OP2	-7.13	108.90	119.60
1	A	34	TYR	CB-CG-CD2	7.08	125.25	121.00
5	L	12	G	OP1-P-OP2	-7.01	109.08	119.60
5	L	24	C	OP1-P-OP2	-6.98	109.13	119.60
5	L	2	G	OP1-P-OP2	-6.89	109.26	119.60
3	I	190	ARG	CD-NE-CZ	6.89	133.24	123.60
5	L	44	A	OP1-P-OP2	-6.89	109.27	119.60
5	L	4	A	OP1-P-OP2	-6.87	109.30	119.60
5	L	32	U	OP1-P-OP2	-6.86	109.30	119.60
5	L	9	A	C8-N9-C4	-6.86	103.06	105.80
5	L	8	A	C8-N9-C4	-6.84	103.06	105.80
2	D	7	ARG	CD-NE-CZ	6.80	133.12	123.60
5	L	17	G	OP1-P-OP2	-6.77	109.44	119.60
2	C	7	ARG	CD-NE-CZ	6.73	133.02	123.60
2	C	252	PHE	CB-CG-CD2	6.71	125.50	120.80
5	L	15	A	OP1-P-OP2	-6.69	109.56	119.60
5	L	4	A	C8-N9-C4	-6.69	103.12	105.80
5	L	45	U	OP1-P-OP2	-6.67	109.60	119.60
3	I	363	ARG	CD-NE-CZ	6.66	132.92	123.60
1	A	31	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	43	ARG	CD-NE-CZ	6.64	132.90	123.60
6	M	53	ARG	CD-NE-CZ	6.64	132.90	123.60
5	L	5	U	OP1-P-OP2	-6.64	109.64	119.60
1	A	226	ARG	CD-NE-CZ	6.63	132.89	123.60
5	L	39	C	OP1-P-OP2	-6.63	109.66	119.60
1	A	107	ARG	CD-NE-CZ	6.61	132.86	123.60
5	L	28	C	OP1-P-OP2	-6.60	109.69	119.60
5	L	40	A	OP1-P-OP2	-6.60	109.69	119.60
5	L	19	U	N1-C1'-C2'	6.53	122.49	114.00
5	L	10	A	C5-N7-C8	-6.53	100.63	103.90
1	A	163	ARG	CD-NE-CZ	6.48	132.67	123.60
5	L	8	A	OP1-P-OP2	-6.45	109.92	119.60
2	C	232	ARG	CD-NE-CZ	6.43	132.60	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	37	G	OP1-P-OP2	-6.42	109.97	119.60
1	A	165	PHE	CB-CG-CD2	6.39	125.27	120.80
5	L	8	A	C5-N7-C8	-6.37	100.72	103.90
5	L	31	G	OP1-P-OP2	-6.36	110.06	119.60
5	L	6	U	N1-C1'-C2'	6.36	122.27	114.00
1	A	110	ARG	CD-NE-CZ	6.32	132.45	123.60
2	B	222	ARG	CD-NE-CZ	6.31	132.43	123.60
2	C	217	MET	CA-CB-CG	6.29	123.99	113.30
5	L	20	C	OP1-P-OP2	-6.25	110.22	119.60
5	L	11	C	OP1-P-OP2	-6.20	110.31	119.60
5	L	20	C	OP1-P-O3'	6.19	118.82	105.20
5	L	3	G	C5-N7-C8	-6.17	101.22	104.30
5	L	43	C	OP2-P-O3'	6.13	118.69	105.20
5	L	42	U	OP1-P-OP2	-6.08	110.48	119.60
5	L	6	U	N3-C2-O2	-6.03	117.98	122.20
5	L	21	A	OP1-P-O3'	5.94	118.26	105.20
1	A	205	PHE	CB-CG-CD2	5.88	124.92	120.80
5	L	8	A	C2-N3-C4	-5.87	107.66	110.60
5	L	9	A	C2-N3-C4	-5.81	107.69	110.60
5	L	5	U	N1-C1'-C2'	5.77	121.50	114.00
5	L	24	C	N1-C1'-C2'	5.75	121.47	114.00
5	L	24	C	C2-N1-C1'	5.72	125.09	118.80
5	L	30	A	OP1-P-OP2	-5.69	111.07	119.60
2	H	146	PRO	CA-N-CD	-5.67	103.56	111.50
5	L	5	U	C5-C6-N1	5.66	125.53	122.70
5	L	32	U	OP1-P-O3'	5.62	117.57	105.20
5	L	4	A	OP2-P-O3'	5.62	117.55	105.20
5	L	26	G	OP1-P-OP2	-5.61	111.19	119.60
5	L	9	A	C5-N7-C8	-5.60	101.10	103.90
5	L	42	U	O4'-C1'-N1	5.59	112.67	108.20
2	B	222	ARG	CG-CD-NE	5.58	123.53	111.80
2	C	270	PHE	CB-CG-CD2	5.57	124.70	120.80
5	L	16	U	OP1-P-OP2	-5.57	111.25	119.60
5	L	12	G	O4'-C1'-N9	5.51	112.61	108.20
5	L	4	A	C2-N3-C4	-5.46	107.87	110.60
5	L	16	U	O4'-C1'-N1	5.46	112.56	108.20
2	C	242	ARG	CD-NE-CZ	5.43	131.20	123.60
5	L	10	A	C6-N1-C2	-5.41	115.36	118.60
2	C	186	TYR	CB-CG-CD2	5.38	124.23	121.00
1	A	37	MET	CA-CB-CG	5.37	122.43	113.30
5	L	27	G	OP1-P-O3'	5.37	117.00	105.20
6	M	36	MET	CA-CB-CG	5.33	122.36	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	10	A	C2-N3-C4	-5.30	107.95	110.60
2	B	123	MET	CA-CB-CG	5.29	122.30	113.30
5	L	9	A	C6-N1-C2	-5.27	115.44	118.60
5	L	3	G	C5-C6-N1	-5.24	108.88	111.50
1	A	191	MET	CA-CB-CG	5.17	122.08	113.30
3	I	363	ARG	CA-CB-CG	5.13	124.68	113.40
2	D	7	ARG	CG-CD-NE	5.11	122.53	111.80
1	A	24	ARG	CD-NE-CZ	5.10	130.74	123.60
2	B	68	TYR	CB-CG-CD2	5.08	124.05	121.00
1	A	206	PHE	CB-CG-CD2	5.07	124.35	120.80
5	L	3	G	OP1-P-O3'	5.06	116.34	105.20
5	L	31	G	OP1-P-O3'	5.06	116.34	105.20
5	L	32	U	O4'-C1'-N1	5.06	112.25	108.20
5	L	8	A	C6-N1-C2	-5.05	115.57	118.60
5	L	43	C	N1-C1'-C2'	5.04	120.55	114.00
2	C	114	TYR	CD1-CG-CD2	-5.02	112.38	117.90
1	A	31	ARG	CG-CD-NE	5.01	122.33	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	6	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1774	0	1762	28	0
2	B	2112	0	2079	26	0
2	C	2238	0	2223	18	0
2	D	2238	0	2223	14	0
2	E	2238	0	2223	18	0
2	F	2238	0	2223	23	0
2	G	2238	0	2223	29	0
2	H	2238	0	2223	41	0
3	I	3261	0	3256	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	930	0	932	22	0
4	K	930	0	932	5	0
5	L	960	0	476	77	0
6	M	466	0	426	7	0
All	All	23861	0	23201	309	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 7.

All (309) 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)
5:L:12:G:O2'	5:L:13:C:O5'	1.72	1.03
5:L:15:A:O2'	5:L:16:U:O5'	1.74	1.03
5:L:33:G:O2'	5:L:34:C:O5'	1.80	0.99
5:L:42:U:O2'	5:L:43:C:O5'	1.80	0.98
5:L:34:C:O2'	5:L:35:G:OP1	1.84	0.94
5:L:28:C:O2'	5:L:29:G:OP1	1.88	0.90
2:F:7:ARG:NH2	2:F:9:GLU:OE2	2.06	0.87
2:F:9:GLU:OE1	2:F:9:GLU:N	2.09	0.85
5:L:35:G:O2'	5:L:36:C:OP1	1.93	0.85
2:F:8:TYR:C	2:F:9:GLU:OE1	2.17	0.83
3:I:427:LEU:O	3:I:429:ARG:N	2.11	0.83
5:L:24:C:O2'	5:L:25:U:O5'	1.97	0.82
5:L:16:U:O2'	5:L:17:G:OP1	1.98	0.81
2:F:236:VAL:HG21	2:F:289:MET:CE	2.11	0.81
1:A:55:ILE:HD12	1:A:126:PHE:CE1	2.17	0.80
1:A:98:TYR:CD1	1:A:100:LEU:CD1	2.65	0.79
2:G:71:GLU:N	2:G:71:GLU:OE1	2.17	0.78
5:L:36:C:O2'	5:L:37:G:O4'	2.03	0.76
5:L:36:C:O2'	5:L:37:G:O5'	2.03	0.76
3:I:510:GLU:OE2	3:I:523:THR:HG21	1.85	0.75
5:L:40:A:O2'	5:L:41:C:OP1	2.03	0.75
2:E:126:GLU:N	2:E:126:GLU:OE1	2.19	0.75
1:A:98:TYR:CD1	1:A:100:LEU:HD13	2.22	0.74
5:L:22:G:O2'	5:L:23:G:OP1	2.04	0.74
2:F:236:VAL:HG21	2:F:289:MET:HE3	1.69	0.74
5:L:12:G:HO2'	5:L:13:C:P	2.10	0.74
2:D:117:ARG:NH2	2:D:206:ASP:OD2	2.21	0.73
2:E:241:ASN:OD1	2:E:242:ARG:N	2.21	0.73
2:D:212:ASP:OD1	2:D:216:ASN:ND2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:30:A:O2'	5:L:31:G:O5'	2.05	0.72
5:L:2:G:O2'	5:L:3:G:O5'	2.06	0.72
2:C:151:GLU:OE2	2:C:177:ARG:NE	2.23	0.71
2:C:93:LYS:NZ	6:M:21:GLU:OE1	2.25	0.69
3:I:361:ALA:HB3	6:M:18:ASN:OD1	1.92	0.69
1:A:98:TYR:CD1	1:A:100:LEU:HD11	2.28	0.68
2:H:91:GLU:HG2	2:H:92:PRO:HG3	1.75	0.68
3:I:390:ILE:HD11	3:I:476:LYS:HD2	1.76	0.68
2:B:241:ASN:OD1	2:B:242:ARG:N	2.26	0.68
4:J:8:THR:HG23	4:J:8:THR:O	1.95	0.67
3:I:390:ILE:HD11	3:I:476:LYS:CD	2.25	0.67
5:L:18:C:O2'	5:L:19:U:O5'	2.13	0.67
1:A:86:ASN:OD1	1:A:89:THR:OG1	2.05	0.66
1:A:75:ARG:NH2	1:A:164:GLU:OE2	2.29	0.66
2:G:133:ARG:NH2	2:G:196:LEU:HD21	2.11	0.66
2:G:211:TRP:O	2:G:215:VAL:HG13	1.97	0.65
3:I:517:VAL:HG23	3:I:517:VAL:O	1.96	0.65
1:A:98:TYR:HD1	1:A:100:LEU:HD13	1.58	0.64
5:L:45:U:O2'	5:L:46:C:O5'	2.04	0.64
3:I:535:ASN:ND2	3:I:583:VAL:O	2.30	0.64
5:L:18:C:O2'	5:L:19:U:O4'	2.16	0.64
2:G:257:VAL:O	2:G:257:VAL:HG13	1.97	0.64
4:J:4:ASP:OD1	4:J:7:ARG:N	2.31	0.64
2:E:233:LYS:NZ	2:E:288:GLU:OE1	2.22	0.63
2:F:236:VAL:HG21	2:F:289:MET:HE2	1.79	0.63
4:J:27:ASP:OD2	4:J:79:TYR:OH	2.08	0.63
3:I:387:GLU:OE1	3:I:481:ARG:NE	2.26	0.63
2:C:241:ASN:ND2	2:C:243:LEU:O	2.33	0.62
2:F:45:VAL:HG13	5:L:34:C:O3'	1.99	0.62
2:H:89:LYS:HE2	2:H:90:PRO:O	1.99	0.62
2:E:226:ARG:NH2	5:L:32:U:OP2	2.32	0.62
1:A:205:PHE:HB2	3:I:183:GLN:OE1	1.99	0.62
1:A:55:ILE:HD12	1:A:126:PHE:CZ	2.34	0.62
3:I:332:ALA:O	3:I:335:SER:OG	2.17	0.61
4:J:22:GLU:HA	4:J:36:ILE:HD11	1.83	0.61
2:B:44:ASP:OD1	2:B:45:VAL:N	2.33	0.61
2:C:221:ASP:OD2	2:C:226:ARG:NH2	2.34	0.61
3:I:552:ALA:HB2	4:J:38:ASP:OD2	2.02	0.59
2:D:259:ARG:NH1	2:D:262:GLY:O	2.34	0.59
2:G:241:ASN:ND2	2:G:243:LEU:O	2.35	0.59
2:B:226:ARG:NH1	5:L:14:C:OP1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:ASP:OD2	2:H:27:ALA:N	2.36	0.59
5:L:34:C:HO2'	5:L:35:G:P	2.21	0.58
2:G:287:LYS:HE3	2:G:290:LEU:HD11	1.84	0.58
2:E:223:SER:OG	5:L:32:U:OP2	2.19	0.58
5:L:21:A:O2'	5:L:22:G:P	2.62	0.58
5:L:30:A:HO2'	5:L:31:G:P	2.27	0.58
2:E:148:VAL:O	2:E:148:VAL:HG23	2.03	0.57
2:B:44:ASP:OD1	2:B:45:VAL:HG13	2.05	0.56
2:F:135:PRO:HG3	2:F:200:THR:HG21	1.87	0.56
3:I:12:ARG:NH2	3:I:273:ALA:O	2.39	0.56
2:B:259:ARG:NH2	2:B:265:GLY:O	2.30	0.56
2:F:179:HIS:O	2:F:180:ILE:HD13	2.05	0.56
4:J:39:ARG:NH1	4:J:40:TYR:OH	2.38	0.56
5:L:24:C:O2'	5:L:25:U:C5'	2.54	0.56
2:C:207:LEU:HD12	2:C:207:LEU:O	2.05	0.56
2:F:49:ARG:HB2	5:L:35:G:H5''	1.88	0.56
5:L:18:C:O2'	5:L:19:U:C5'	2.55	0.55
2:B:213:ALA:O	2:B:217:MET:N	2.39	0.55
3:I:22:PRO:N	3:I:23:PRO:CD	2.70	0.55
5:L:35:G:O2'	5:L:36:C:P	2.65	0.55
3:I:22:PRO:N	3:I:23:PRO:HD3	2.22	0.54
2:H:18:ASN:CA	2:H:180:ILE:HD11	2.37	0.54
6:M:34:VAL:HB	6:M:35:PRO:HD3	1.88	0.54
2:E:223:SER:OG	2:E:226:ARG:NH2	2.40	0.54
2:H:124:THR:HG23	2:H:124:THR:O	2.08	0.54
2:G:233:LYS:HD3	2:G:275:VAL:HG11	1.88	0.54
5:L:28:C:O2'	5:L:29:G:P	2.66	0.54
1:A:216:THR:HG23	1:A:216:THR:O	2.08	0.54
2:G:223:SER:OG	5:L:44:A:OP1	2.21	0.54
1:A:95:LYS:O	2:B:81:ARG:NH1	2.41	0.54
4:J:8:THR:O	4:J:8:THR:CG2	2.54	0.54
2:G:45:VAL:HG13	5:L:40:A:O3'	2.08	0.53
2:B:136:VAL:HG11	2:B:210:PHE:CZ	2.42	0.53
3:I:432:LEU:H	3:I:432:LEU:HD23	1.72	0.53
2:H:18:ASN:HA	2:H:180:ILE:HD11	1.89	0.53
3:I:510:GLU:C	3:I:510:GLU:OE1	2.46	0.53
2:G:132:VAL:O	5:L:38:C:O2'	2.26	0.53
2:G:107:ASP:O	2:G:111:THR:HG23	2.09	0.53
3:I:363:ARG:HE	6:M:18:ASN:ND2	2.07	0.53
2:B:261:GLU:N	2:B:261:GLU:OE1	2.41	0.53
2:G:124:THR:O	2:G:124:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:31:G:O2'	5:L:32:U:P	2.67	0.52
3:I:364:LEU:C	3:I:364:LEU:HD12	2.30	0.52
3:I:481:ARG:O	3:I:484:LYS:HE2	2.09	0.52
2:E:261:GLU:OE1	2:E:261:GLU:N	2.34	0.52
2:E:45:VAL:HG13	5:L:28:C:O3'	2.10	0.52
3:I:388:LEU:HD12	3:I:477:ALA:HB2	1.92	0.52
2:D:50:LYS:NZ	2:D:221:ASP:OD2	2.32	0.51
5:L:2:G:HO2'	5:L:3:G:P	2.33	0.51
5:L:21:A:HO2'	5:L:22:G:P	2.33	0.51
2:G:234:LEU:O	2:G:290:LEU:HD13	2.11	0.51
5:L:16:U:HO2'	5:L:17:G:P	2.29	0.51
5:L:33:G:O2'	5:L:34:C:C5'	2.59	0.51
5:L:15:A:HO2'	5:L:16:U:P	2.33	0.51
3:I:260:GLN:NE2	3:I:271:PHE:O	2.38	0.51
6:M:30:VAL:HG13	6:M:41:LEU:HB2	1.93	0.51
2:H:191:PHE:C	2:H:192:ILE:HD13	2.31	0.51
5:L:35:G:HO2'	5:L:36:C:P	2.32	0.50
2:H:2:THR:O	2:H:2:THR:HG23	2.11	0.50
5:L:33:G:O2'	5:L:34:C:P	2.68	0.50
2:F:165:ALA:O	2:H:94:LYS:NZ	2.29	0.50
1:A:13:LEU:HD12	1:A:145:PHE:HZ	1.77	0.50
4:J:10:ARG:HB3	4:J:11:PRO:HD3	1.94	0.50
4:J:50:GLN:HG3	4:K:99:SER:OG	2.12	0.50
5:L:24:C:O2'	5:L:25:U:O4'	2.28	0.50
4:J:92:ASP:OD1	4:J:93:PHE:N	2.44	0.50
5:L:45:U:HO2'	5:L:46:C:P	2.31	0.50
2:H:131:GLN:OE1	2:H:131:GLN:N	2.45	0.49
5:L:16:U:O2'	5:L:17:G:P	2.70	0.49
1:A:13:LEU:HD21	1:A:169:PHE:HB2	1.93	0.49
2:E:221:ASP:OD1	2:E:221:ASP:C	2.50	0.49
3:I:214:VAL:HG13	3:I:214:VAL:O	2.13	0.49
2:F:30:MET:HG2	2:F:31:PRO:HD2	1.92	0.49
3:I:523:THR:HG22	3:I:524:ILE:N	2.26	0.49
5:L:33:G:HO2'	5:L:34:C:P	2.31	0.49
2:D:64:ARG:O	2:D:117:ARG:NH1	2.38	0.49
2:H:136:VAL:HG11	2:H:210:PHE:CE2	2.48	0.49
3:I:340:THR:HG23	3:I:348:GLU:OE2	2.13	0.49
2:C:42:VAL:HB	2:C:141:ALA:HB3	1.94	0.49
2:H:211:TRP:O	2:H:215:VAL:HG23	2.12	0.48
4:J:104:LEU:HD12	4:J:107:ILE:HD11	1.93	0.48
2:G:154:ILE:O	2:G:176:GLY:N	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:VAL:HG12	5:L:46:C:H5''	1.95	0.48
3:I:364:LEU:HD12	3:I:364:LEU:O	2.12	0.48
2:C:125:THR:OG1	2:C:126:GLU:OE1	2.29	0.48
5:L:42:U:O2'	5:L:43:C:O2	2.17	0.48
5:L:21:A:O2'	5:L:22:G:O5'	2.31	0.48
2:B:151:GLU:OE1	3:I:448:ARG:NH1	2.35	0.48
2:B:236:VAL:HG21	2:B:289:MET:HE3	1.96	0.48
2:H:30:MET:HE1	2:H:149:PRO:HB2	1.96	0.48
2:H:146:PRO:HD2	2:H:146:PRO:O	2.13	0.48
2:H:91:GLU:O	2:H:93:LYS:N	2.47	0.47
3:I:552:ALA:CB	4:J:38:ASP:OD2	2.61	0.47
1:A:140:LYS:O	1:A:144:ILE:HG12	2.13	0.47
2:H:257:VAL:HG22	2:H:275:VAL:HG22	1.97	0.47
4:J:22:GLU:CA	4:J:36:ILE:HD11	2.44	0.47
2:H:127:VAL:HG13	2:H:127:VAL:O	2.14	0.47
1:A:155:PHE:CE1	2:B:195:PRO:HB3	2.50	0.47
2:C:101:ASP:OD1	2:C:104:ARG:NH2	2.44	0.47
2:D:137:GLN:NE2	5:L:21:A:OP1	2.48	0.47
2:H:44:ASP:N	2:H:44:ASP:OD1	2.46	0.47
1:A:13:LEU:HD23	1:A:14:ARG:N	2.30	0.46
2:C:45:VAL:HG13	5:L:16:U:O3'	2.14	0.46
2:C:15:ASP:OD1	2:C:183:TYR:OH	2.23	0.46
2:C:156:ARG:HA	5:L:22:G:O2'	2.15	0.46
3:I:390:ILE:HD11	3:I:476:LYS:HD3	1.95	0.46
3:I:573:GLU:HA	3:I:573:GLU:OE1	2.16	0.46
2:B:160:THR:HG23	2:B:161:THR:HG23	1.98	0.46
2:E:44:ASP:OD1	2:E:44:ASP:N	2.49	0.46
2:C:87:ASP:OD1	2:C:87:ASP:C	2.53	0.46
2:B:122:VAL:HG21	5:L:9:A:C5	2.50	0.46
2:C:141:ALA:HB2	2:C:188:ALA:HB2	1.97	0.46
2:D:154:ILE:O	2:D:176:GLY:N	2.49	0.46
2:H:10:PHE:HE1	2:H:192:ILE:HD11	1.81	0.46
2:H:19:GLY:N	2:H:180:ILE:HG13	2.31	0.46
2:F:91:GLU:HG3	2:F:92:PRO:HD2	1.98	0.46
2:H:145:GLU:HB2	2:H:146:PRO:CD	2.46	0.46
1:A:51:TRP:CZ2	5:L:3:G:C6	3.04	0.46
2:D:15:ASP:OD2	2:D:183:TYR:OH	2.25	0.46
2:E:87:ASP:OD1	2:E:87:ASP:O	2.34	0.46
5:L:27:G:O2'	5:L:28:C:OP2	2.33	0.46
2:C:155:THR:O	5:L:22:G:O2'	2.34	0.45
5:L:31:G:O2'	5:L:32:U:OP1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:OD1	2:B:115:ASP:N	2.50	0.45
2:G:145:GLU:OE1	2:G:145:GLU:HA	2.16	0.45
2:G:55:VAL:HG23	2:G:209:LEU:HD21	1.98	0.45
2:E:68:TYR:N	2:E:115:ASP:OD2	2.47	0.45
2:F:156:ARG:HA	5:L:40:A:O2'	2.17	0.45
2:G:133:ARG:HH21	2:G:196:LEU:HD21	1.80	0.45
5:L:2:G:H4'	5:L:3:G:OP1	2.17	0.45
1:A:77:GLU:N	1:A:108:GLN:O	2.47	0.45
2:F:236:VAL:CG2	2:F:289:MET:HE2	2.46	0.45
2:H:136:VAL:HG11	2:H:210:PHE:CZ	2.51	0.45
5:L:44:A:H5'	5:L:45:U:OP2	2.17	0.45
1:A:205:PHE:HD2	3:I:183:GLN:OE1	2.00	0.45
2:B:155:THR:HG1	5:L:17:G:H8	1.63	0.45
1:A:36:VAL:HG21	1:A:215:ILE:HD13	1.97	0.45
2:E:156:ARG:NH2	2:E:158:ALA:O	2.50	0.45
3:I:387:GLU:OE1	3:I:481:ARG:HG3	2.16	0.45
4:K:26:GLU:C	4:K:26:GLU:OE1	2.56	0.45
2:B:9:GLU:OE1	2:B:239:HIS:NE2	2.49	0.44
2:H:18:ASN:C	2:H:180:ILE:HD11	2.37	0.44
5:L:30:A:O2'	5:L:31:G:C5'	2.64	0.44
2:E:222:ARG:O	2:F:133:ARG:NH1	2.50	0.44
4:J:53:HIS:O	4:J:57:LYS:HG2	2.17	0.44
1:A:28:LYS:HE3	3:I:227:SER:HB2	1.99	0.44
2:B:105:VAL:O	2:B:109:MET:HG2	2.17	0.44
2:H:102:ALA:O	2:H:105:VAL:HG22	2.18	0.44
2:H:260:ALA:N	2:H:272:ASP:O	2.44	0.44
3:I:510:GLU:OE1	3:I:510:GLU:O	2.35	0.44
2:F:68:TYR:CE1	2:F:75:LEU:HD12	2.53	0.44
2:F:63:GLU:N	2:F:63:GLU:OE1	2.50	0.44
2:F:226:ARG:NH1	5:L:38:C:OP1	2.51	0.44
2:H:128:ASN:OD1	2:H:129:CYS:N	2.51	0.44
5:L:34:C:O2'	5:L:35:G:P	2.70	0.44
2:H:135:PRO:HD3	2:H:200:THR:HG21	1.99	0.44
3:I:390:ILE:CD1	3:I:476:LYS:HD3	2.47	0.44
4:J:4:ASP:OD1	4:J:4:ASP:C	2.55	0.44
2:C:173:ARG:NH1	5:L:23:G:O6	2.49	0.44
2:G:282:GLU:OE1	2:G:282:GLU:N	2.49	0.44
4:K:95:VAL:HG23	4:K:96:THR:HG23	2.00	0.44
4:K:7:ARG:O	4:K:8:THR:HB	2.17	0.43
2:G:63:GLU:OE1	2:G:64:ARG:N	2.45	0.43
2:H:58:THR:HG23	2:H:59:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:LEU:HD21	2:H:257:VAL:HG21	2.01	0.43
2:H:215:VAL:HG13	2:H:290:LEU:HD11	2.00	0.43
4:J:4:ASP:CG	4:J:7:ARG:HB2	2.38	0.43
5:L:35:G:O2'	5:L:36:C:H4'	2.19	0.43
2:D:6:ASN:ND2	2:D:239:HIS:O	2.47	0.43
2:G:133:ARG:NH2	2:G:196:LEU:HD11	2.34	0.43
2:G:257:VAL:O	2:G:257:VAL:CG1	2.66	0.43
5:L:15:A:O2'	5:L:16:U:P	2.74	0.43
5:L:17:G:H2'	5:L:18:C:H4'	2.01	0.43
2:F:223:SER:CB	5:L:38:C:OP1	2.66	0.43
2:D:32:ARG:NH1	5:L:24:C:OP1	2.48	0.43
1:A:55:ILE:HB	1:A:126:PHE:CD1	2.54	0.42
2:G:207:LEU:HD11	2:G:211:TRP:CZ2	2.54	0.42
3:I:588:ASP:OD1	3:I:588:ASP:N	2.51	0.42
2:B:51:ILE:HG13	2:B:217:MET:SD	2.60	0.42
2:B:71:GLU:O	2:B:73:ALA:N	2.47	0.42
2:C:63:GLU:O	2:C:64:ARG:HB2	2.19	0.42
2:C:93:LYS:O	2:C:93:LYS:HG2	2.20	0.42
2:D:102:ALA:O	2:D:105:VAL:HG22	2.19	0.42
1:A:69:VAL:HG11	2:B:36:GLU:OE1	2.19	0.42
2:B:109:MET:HE3	2:B:113:PHE:CE2	2.54	0.42
2:H:178:LYS:HD2	2:H:225:ALA:HB2	2.02	0.42
4:J:10:ARG:NH2	4:J:92:ASP:O	2.52	0.42
4:J:21:LEU:HG	4:J:59:ALA:HB2	2.02	0.42
3:I:417:GLU:OE1	3:I:418:ASN:N	2.40	0.42
2:C:63:GLU:N	2:C:63:GLU:OE1	2.52	0.42
3:I:505:LEU:O	3:I:508:VAL:HG22	2.20	0.42
6:M:14:ARG:O	6:M:18:ASN:N	2.53	0.42
2:E:156:ARG:HG3	2:E:157:MET:N	2.34	0.42
2:F:44:ASP:OD1	2:F:44:ASP:N	2.53	0.42
3:I:262:VAL:HG11	3:I:287:PHE:CE1	2.55	0.42
2:H:99:VAL:O	2:H:103:LYS:HG2	2.20	0.42
1:A:130:ASP:OD1	1:A:131:LYS:N	2.52	0.42
2:D:44:ASP:OD1	2:D:44:ASP:N	2.53	0.42
4:K:8:THR:O	4:K:8:THR:CG2	2.67	0.42
2:G:49:ARG:O	2:G:49:ARG:HD3	2.20	0.41
2:G:15:ASP:O	2:G:229:MET:HG2	2.20	0.41
3:I:259:ARG:NE	3:I:281:ASP:OD1	2.50	0.41
3:I:505:LEU:O	3:I:509:LEU:HG	2.19	0.41
3:I:492:ASP:N	3:I:492:ASP:OD1	2.54	0.41
5:L:33:G:HO2'	5:L:34:C:C5'	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:115:ASP:OD1	2:E:116:ILE:N	2.53	0.41
2:H:69:ILE:HD13	2:H:69:ILE:HA	1.96	0.41
4:J:79:TYR:O	4:J:83:MET:HG3	2.21	0.41
4:J:104:LEU:CD1	4:J:107:ILE:HD11	2.50	0.41
3:I:495:ARG:NE	3:I:497:ASP:OD2	2.36	0.41
5:L:45:U:O2'	5:L:46:C:O4'	2.38	0.41
2:G:91:GLU:HB3	2:G:92:PRO:HD3	2.03	0.41
2:B:237:PHE:CD1	2:B:286:VAL:HG22	2.56	0.41
2:G:115:ASP:OD1	2:G:116:ILE:N	2.54	0.41
2:G:153:SER:O	2:H:32:ARG:NH1	2.46	0.41
2:G:161:THR:HG22	2:H:76:ASN:HD21	1.86	0.41
2:H:37:THR:HG23	2:H:39:HIS:H	1.84	0.41
3:I:187:THR:OG1	3:I:189:GLU:HG3	2.20	0.41
5:L:21:A:C2'	5:L:22:G:O5'	2.69	0.41
2:H:235:ILE:N	2:H:235:ILE:HD12	2.35	0.41
4:J:53:HIS:CG	4:J:54:MET:N	2.89	0.41
2:B:254:LEU:HD12	2:B:254:LEU:N	2.36	0.40
2:D:95:LEU:HD23	2:D:102:ALA:HB1	2.03	0.40
2:H:50:LYS:HB3	2:H:217:MET:HG3	2.03	0.40
4:J:22:GLU:N	4:J:36:ILE:HD11	2.36	0.40
2:F:49:ARG:O	2:F:49:ARG:HD3	2.21	0.40
6:M:34:VAL:CB	6:M:35:PRO:HD3	2.49	0.40
1:A:196:ASP:OD1	1:A:196:ASP:O	2.38	0.40
1:A:222:SER:OG	1:A:224:GLU:OE2	2.29	0.40
2:H:49:ARG:O	2:H:52:ARG:HG2	2.22	0.40
1:A:155:PHE:CE1	2:B:195:PRO:CB	3.04	0.40
2:E:112:ASN:OD1	2:E:112:ASN:C	2.59	0.40
2:H:7:ARG:NH2	2:H:9:GLU:OE2	2.54	0.40
1:A:155:PHE:CD1	5:L:2:G:C6	3.09	0.40
2:B:160:THR:HG23	2:B:161:THR:N	2.37	0.40
2:D:86:CYS:O	2:D:87:ASP:CG	2.60	0.40
2:F:48:LYS:HD3	5:L:34:C:OP2	2.22	0.40
2:G:232:ARG:HE	2:G:270:PHE:HB2	1.87	0.40
5:L:18:C:H4'	5:L:19:U:OP1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/227 (96%)	208 (95%)	10 (5%)	0	100	100
2	B	264/290 (91%)	251 (95%)	13 (5%)	0	100	100
2	C	282/290 (97%)	266 (94%)	16 (6%)	0	100	100
2	D	282/290 (97%)	275 (98%)	7 (2%)	0	100	100
2	E	282/290 (97%)	267 (95%)	15 (5%)	0	100	100
2	F	282/290 (97%)	268 (95%)	14 (5%)	0	100	100
2	G	282/290 (97%)	267 (95%)	15 (5%)	0	100	100
2	H	282/290 (97%)	266 (94%)	16 (6%)	0	100	100
3	I	405/612 (66%)	384 (95%)	21 (5%)	0	100	100
4	J	113/124 (91%)	109 (96%)	4 (4%)	0	100	100
4	K	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
6	M	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	8	34
All	All	2860/3174 (90%)	2723 (95%)	136 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	34	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/194 (97%)	185 (98%)	4 (2%)	53	79
2	B	224/242 (93%)	220 (98%)	4 (2%)	59	82
2	C	239/242 (99%)	234 (98%)	5 (2%)	53	79
2	D	239/242 (99%)	237 (99%)	2 (1%)	81	92
2	E	239/242 (99%)	237 (99%)	2 (1%)	81	92
2	F	239/242 (99%)	237 (99%)	2 (1%)	81	92
2	G	239/242 (99%)	237 (99%)	2 (1%)	81	92
2	H	239/242 (99%)	238 (100%)	1 (0%)	91	96
3	I	346/508 (68%)	336 (97%)	10 (3%)	42	72
4	J	99/105 (94%)	97 (98%)	2 (2%)	55	80
4	K	99/105 (94%)	96 (97%)	3 (3%)	41	71
6	M	50/50 (100%)	49 (98%)	1 (2%)	55	80
All	All	2441/2656 (92%)	2403 (98%)	38 (2%)	64	84

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	76	ASN
1	A	91	MET
1	A	114	LEU
2	B	6	ASN
2	B	175	MET
2	B	191	PHE
2	B	204	ASP
2	C	72	LYS
2	C	88	LEU
2	C	191	PHE
2	C	206	ASP
2	C	229	MET
2	D	217	MET
2	D	240	GLN
2	E	173	ARG
2	E	221	ASP
2	F	1	MET
2	F	279	GLN
2	G	107	ASP
2	G	204	ASP
2	H	86	CYS

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Mol	Chain	Res	Type
3	I	187	THR
3	I	218	VAL
3	I	225	PHE
3	I	232	GLN
3	I	238	VAL
3	I	246	TYR
3	I	276	SER
3	I	364	LEU
3	I	448	ARG
3	I	455	ARG
4	J	38	ASP
4	J	100	ASP
4	K	67	ARG
4	K	69	ASP
4	K	117	PHE
6	M	36	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	150	GLN
2	D	179	HIS
2	H	76	ASN
6	M	18	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L	45/45 (100%)	28 (62%)	20 (44%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L	3	G
5	L	5	U
5	L	6	U
5	L	12	G
5	L	13	C
5	L	16	U
5	L	17	G

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Mol	Chain	Res	Type
5	L	18	C
5	L	19	U
5	L	22	G
5	L	23	G
5	L	24	C
5	L	25	U
5	L	28	C
5	L	29	G
5	L	30	A
5	L	31	G
5	L	32	U
5	L	33	G
5	L	34	C
5	L	35	G
5	L	36	C
5	L	37	G
5	L	40	A
5	L	41	C
5	L	42	U
5	L	43	C
5	L	46	C

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L	2	G
5	L	5	U
5	L	6	U
5	L	12	G
5	L	15	A
5	L	16	U
5	L	18	C
5	L	21	A
5	L	22	G
5	L	24	C
5	L	28	C
5	L	30	A
5	L	31	G
5	L	33	G
5	L	34	C
5	L	35	G
5	L	36	C

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Mol	Chain	Res	Type
5	L	40	A
5	L	42	U
5	L	45	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.

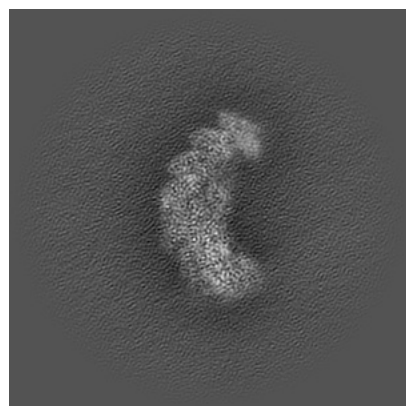
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27409. These allow visual inspection of the internal detail of the map and identification of artifacts.

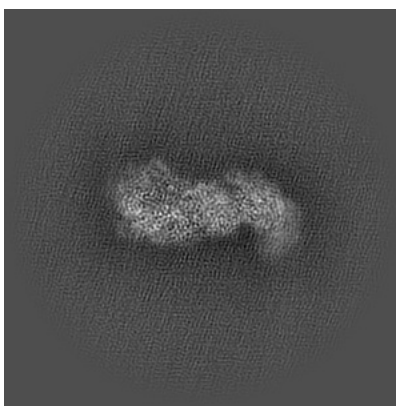
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

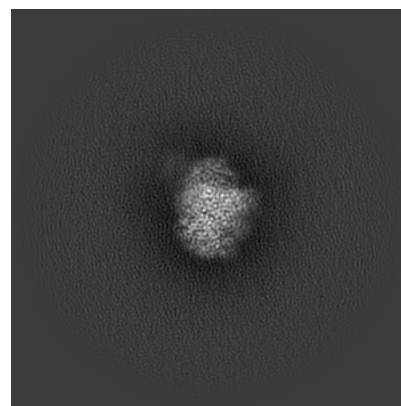
6.1.1 Primary map



X

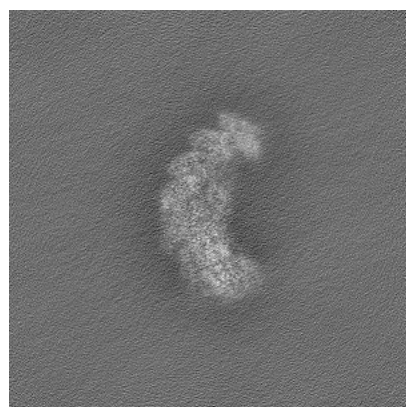


Y

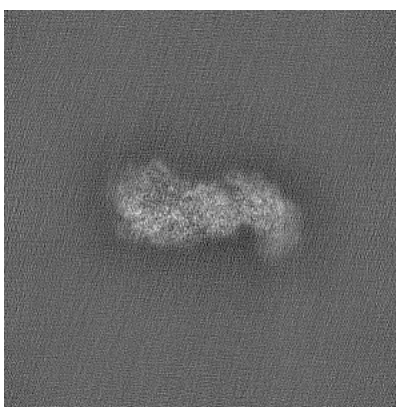


Z

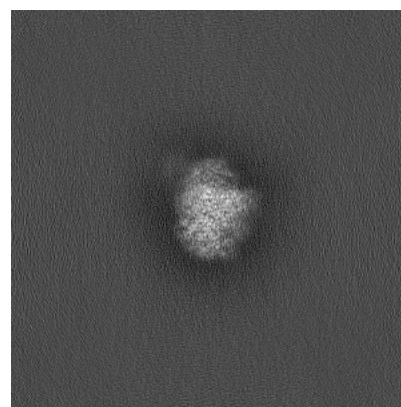
6.1.2 Raw map



X



Y

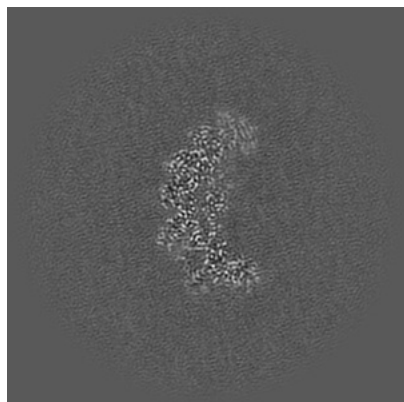


Z

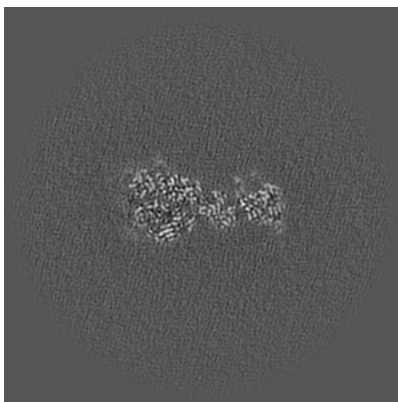
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

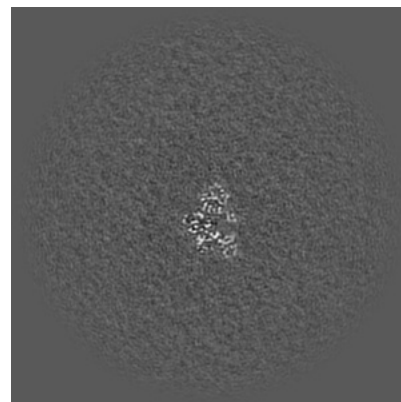
6.2.1 Primary map



X Index: 210

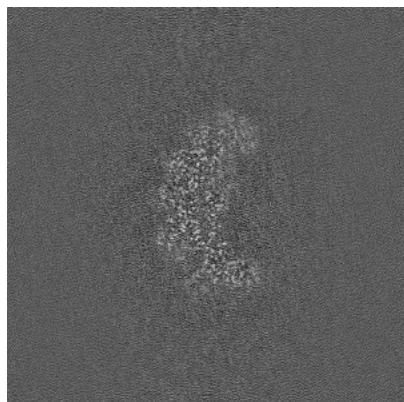


Y Index: 210

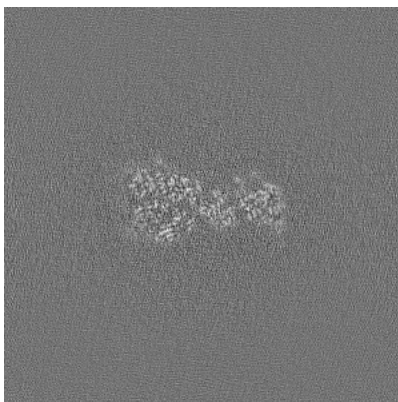


Z Index: 210

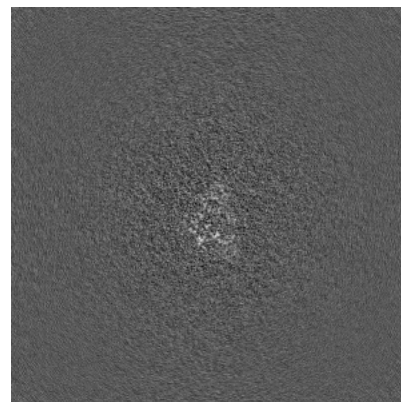
6.2.2 Raw map



X Index: 210



Y Index: 210

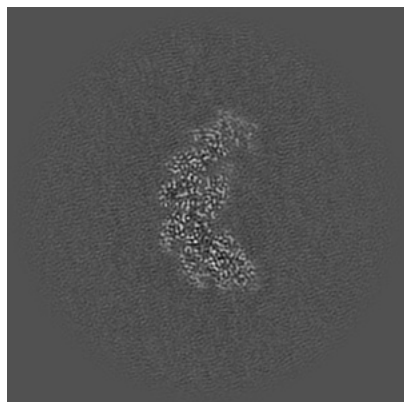


Z Index: 210

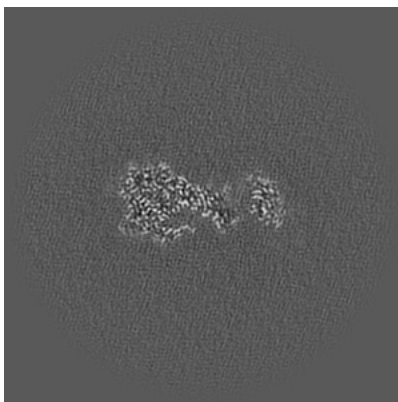
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

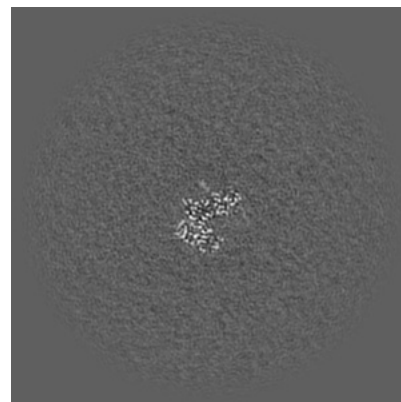
6.3.1 Primary map



X Index: 204

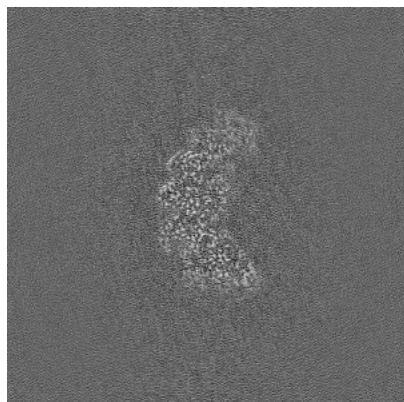


Y Index: 218

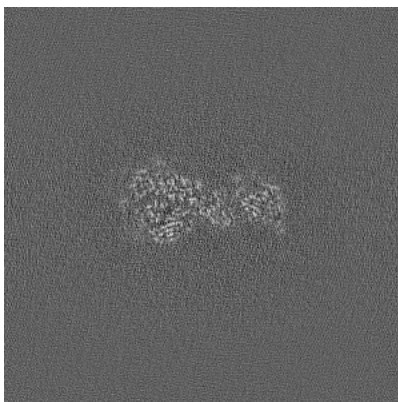


Z Index: 185

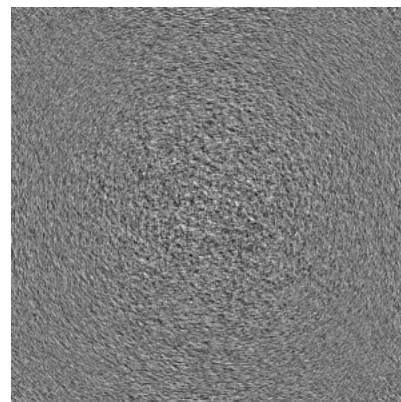
6.3.2 Raw map



X Index: 206



Y Index: 209

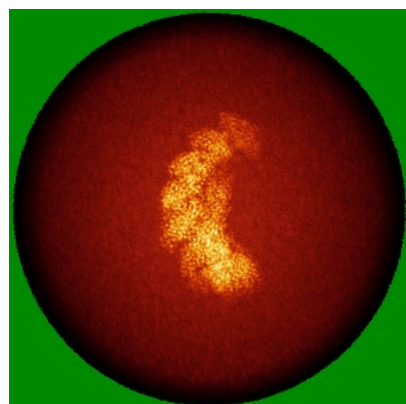


Z Index: 419

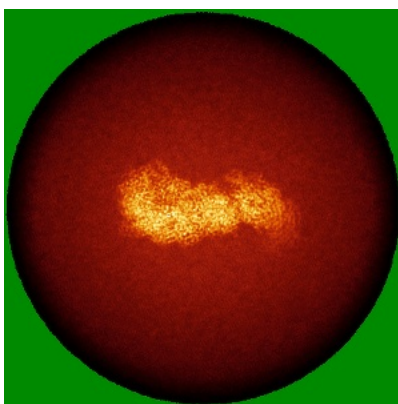
The images above show the largest variance slices of the map in three orthogonal directions.

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

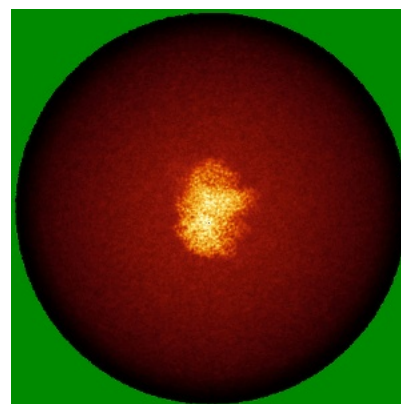
6.4.1 Primary map



X

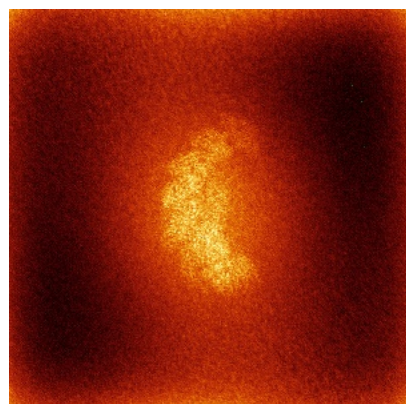


Y

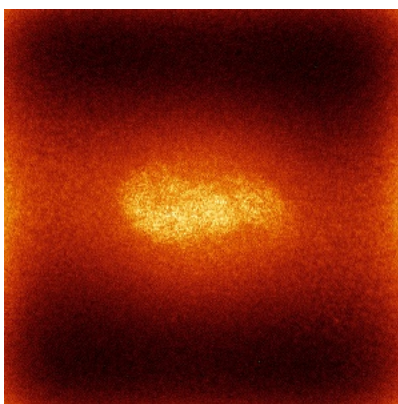


Z

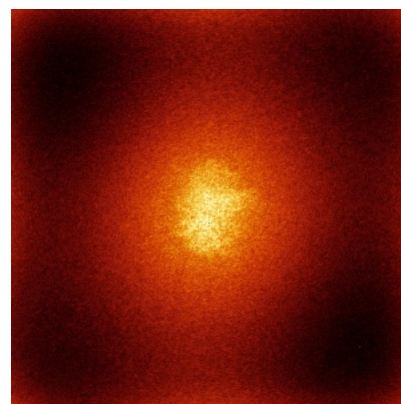
6.4.2 Raw map



X



Y

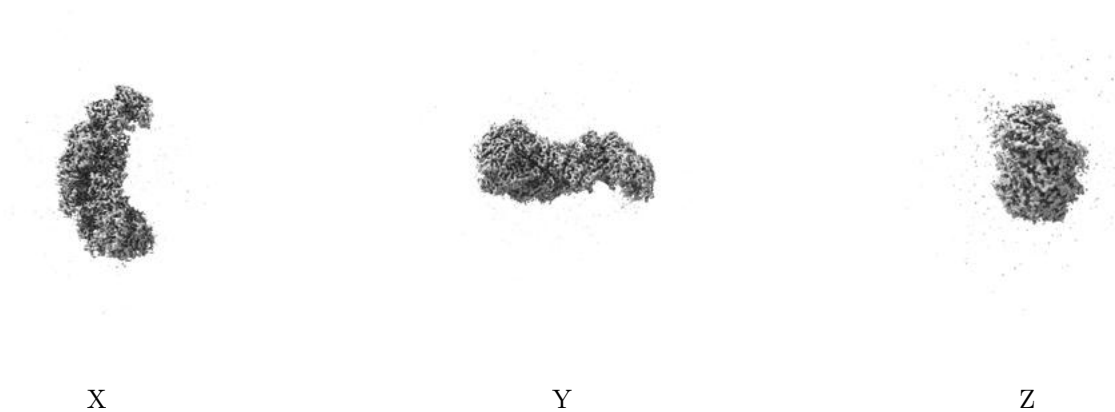


Z

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

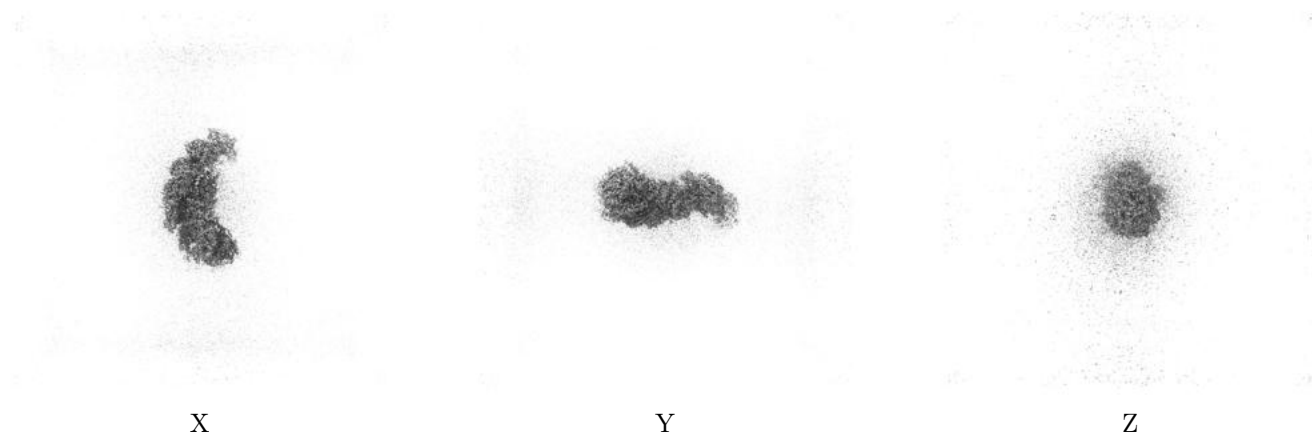
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.253. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

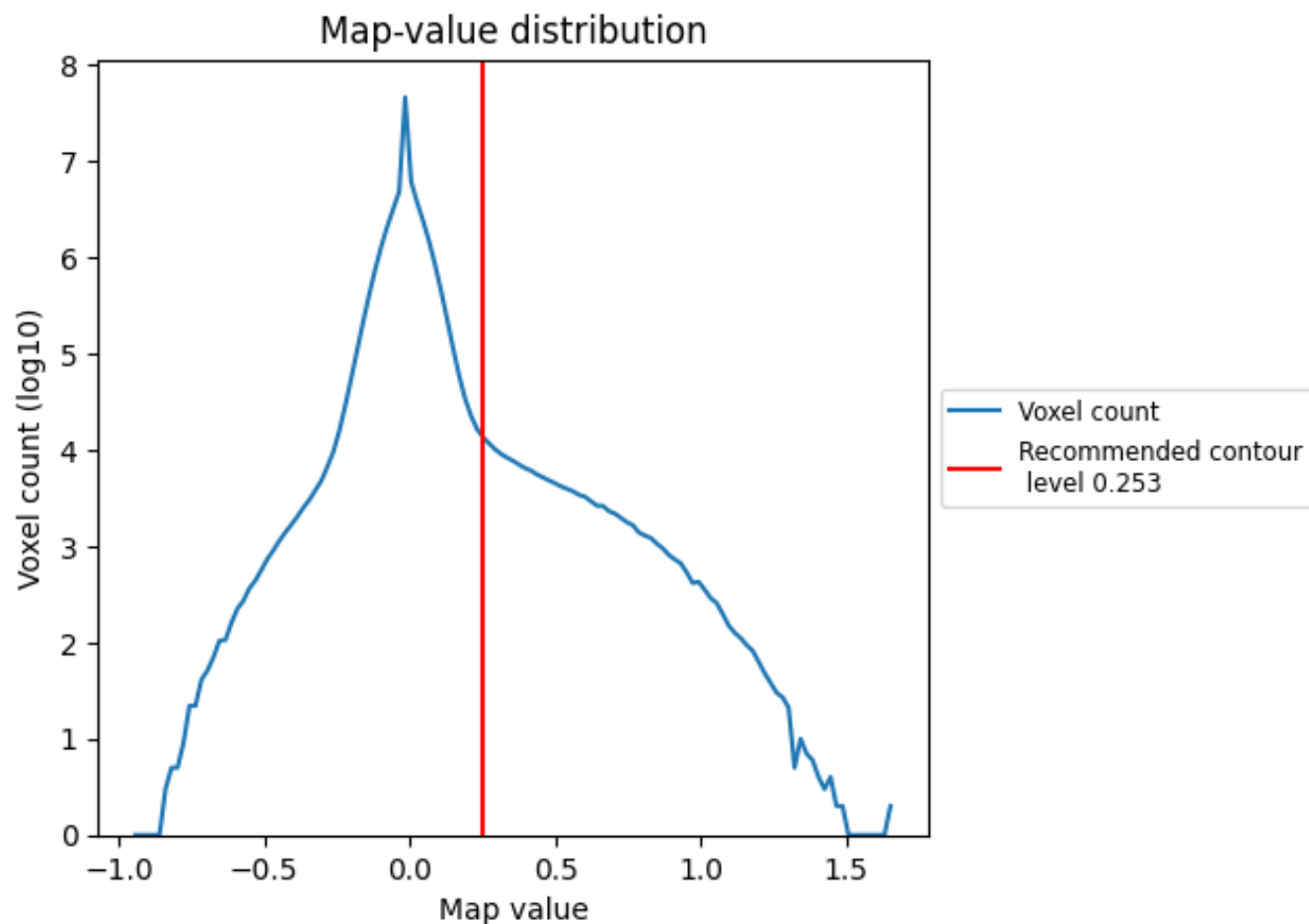
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

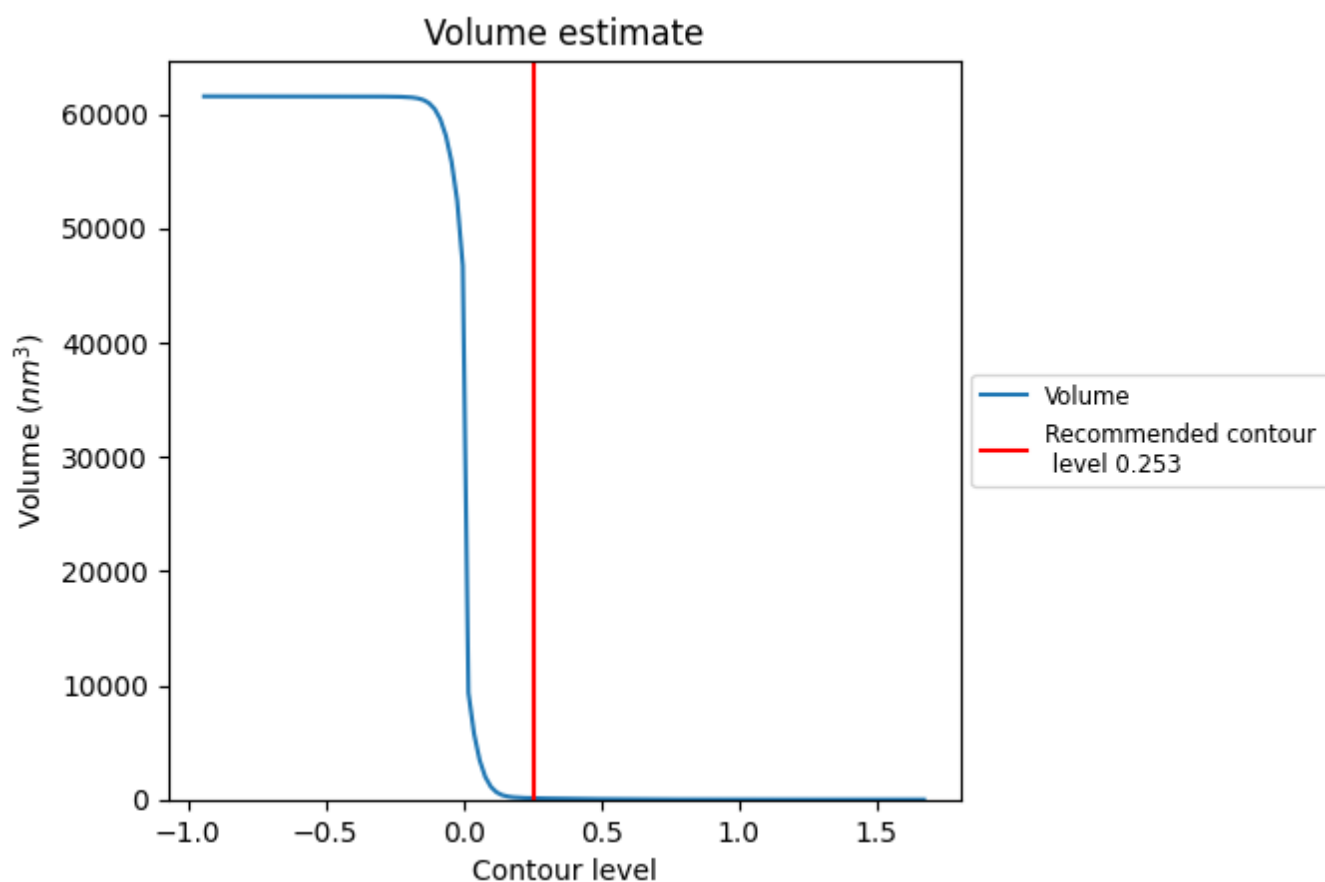
This section contains the results of statistical analysis of the map.

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.

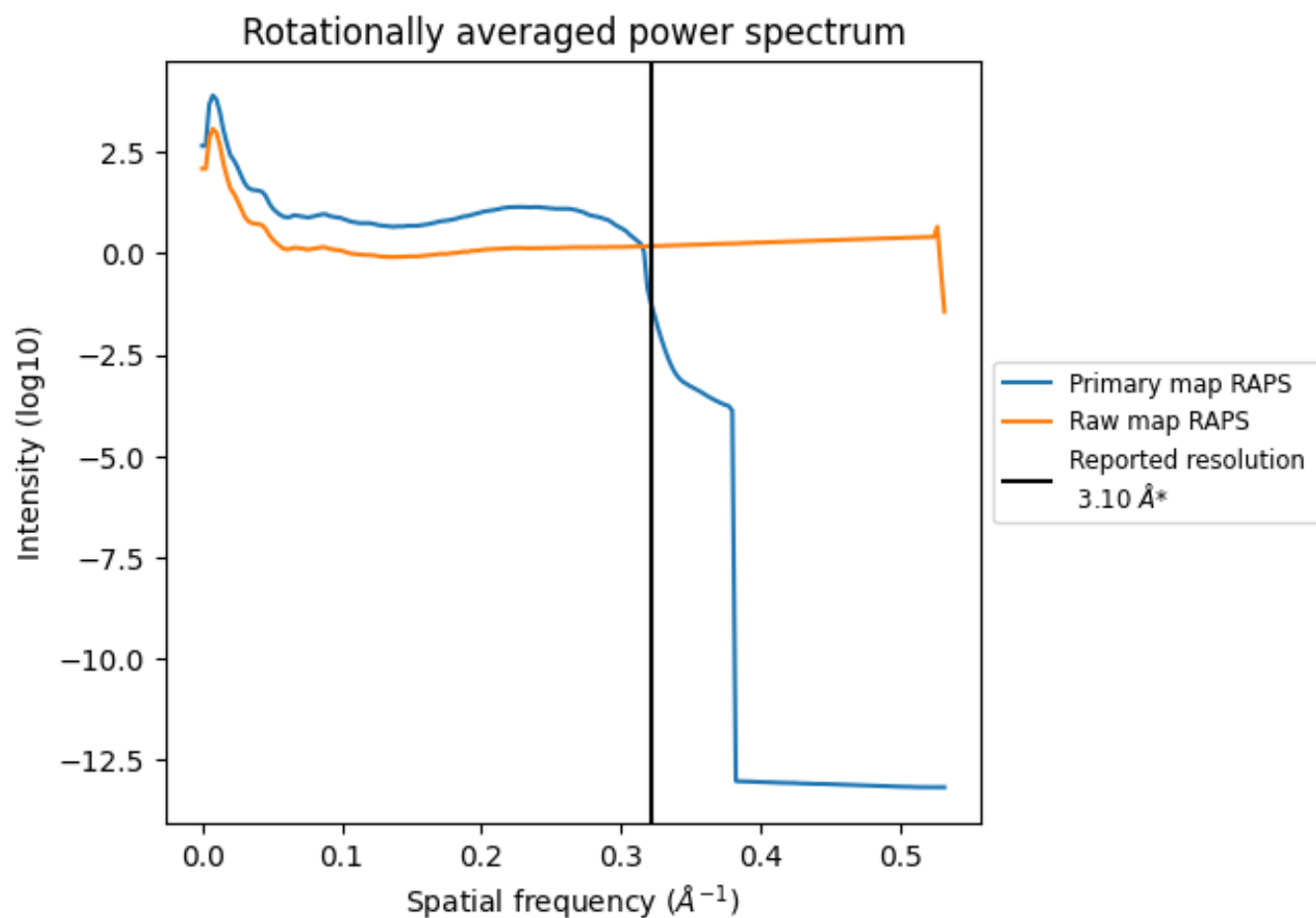
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 123 nm³; this corresponds to an approximate mass of 111 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 ⓘ

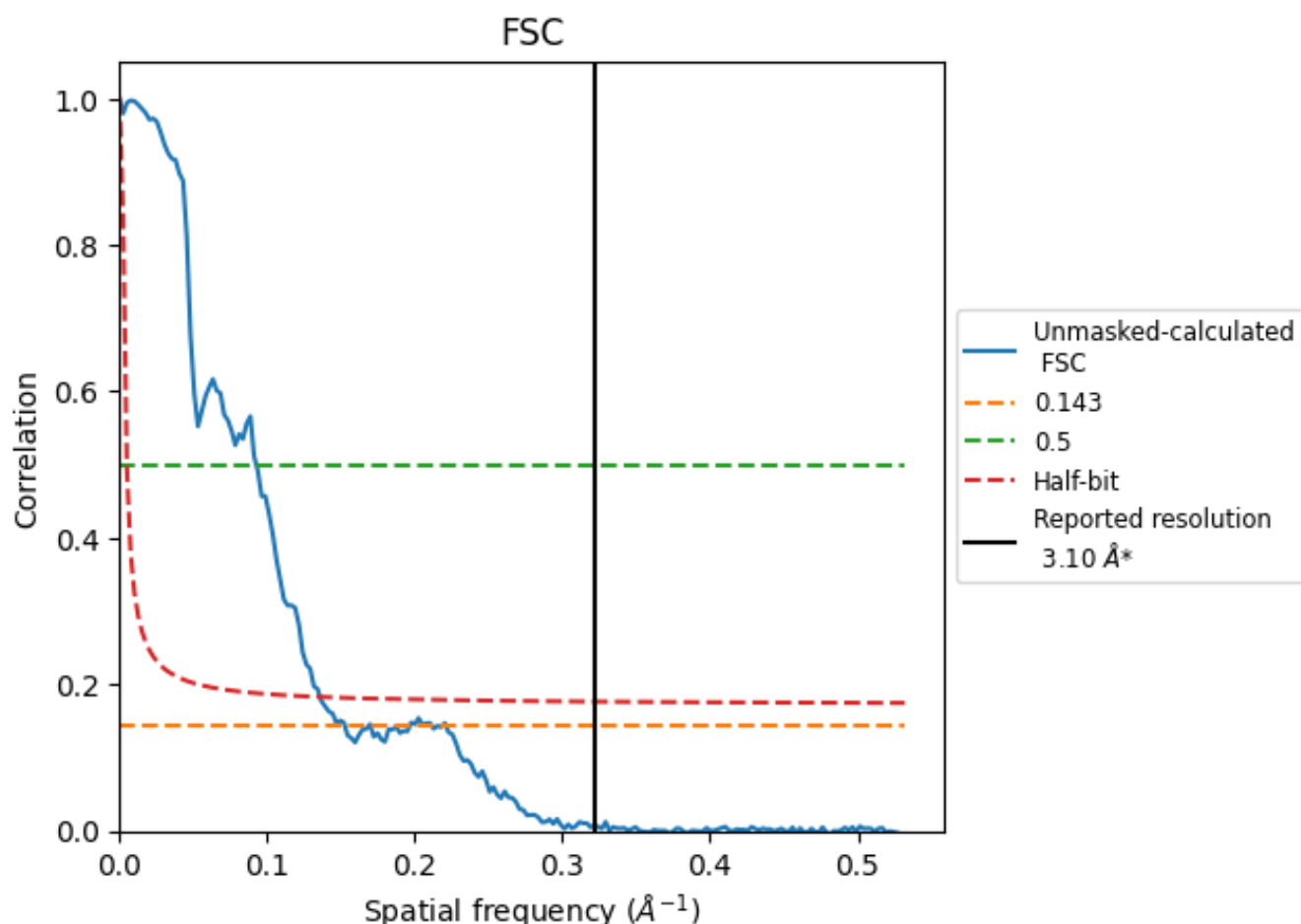


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

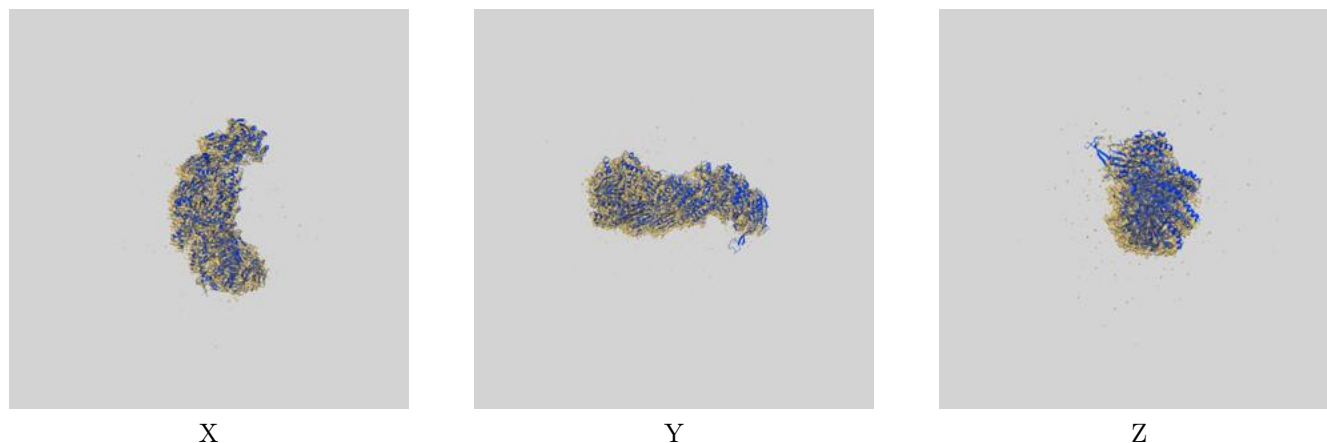
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.55	10.80	7.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.55 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

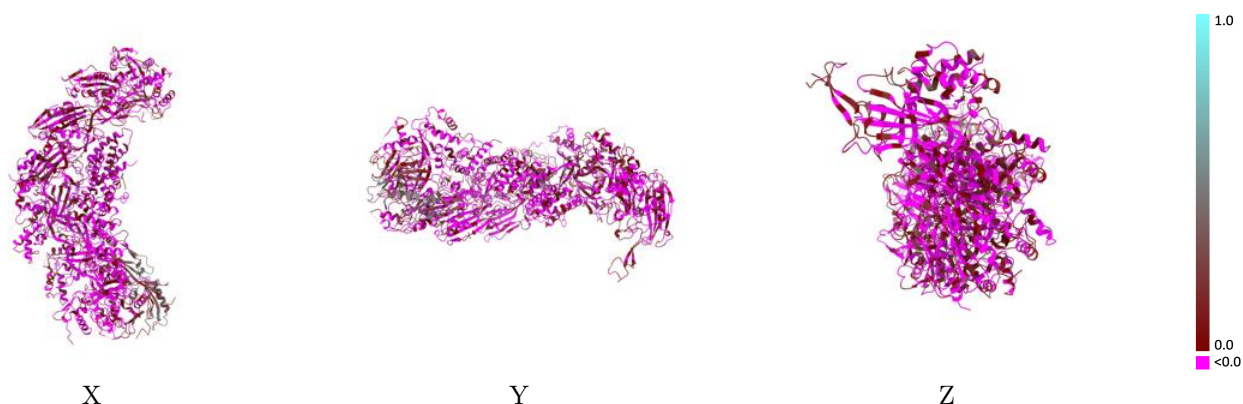
This section contains information regarding the fit between EMDB map EMD-27409 and PDB model 8DFO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



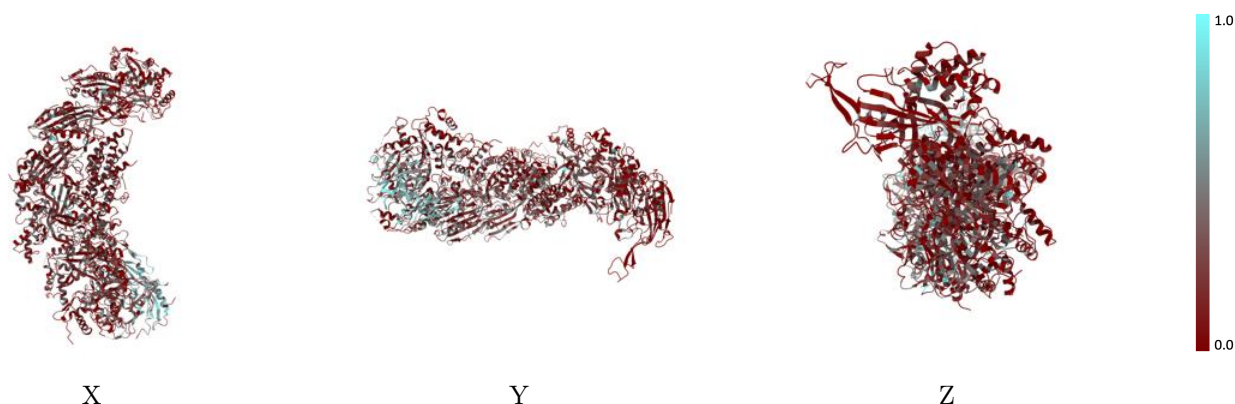
The images above show the 3D surface view of the map at the recommended contour level 0.253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



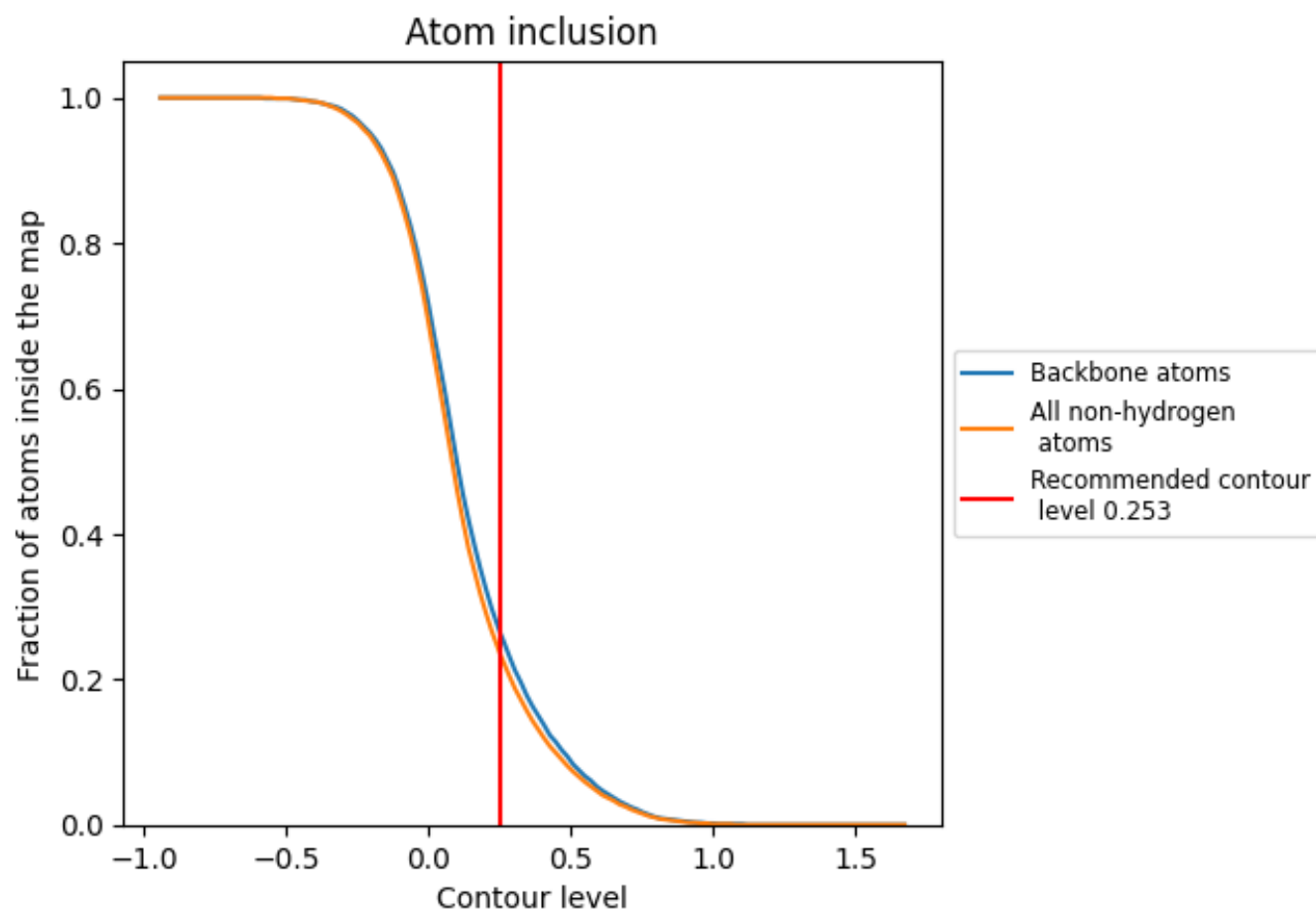
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.253).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 26% of all backbone atoms, 23% 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 (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2340	 -0.0080
A	 0.4280	 0.1490
B	 0.3310	 0.0470
C	 0.2270	 -0.0740
D	 0.2430	 -0.0220
E	 0.2360	 -0.0010
F	 0.2140	 -0.0020
G	 0.1810	 -0.0070
H	 0.1200	 0.0020
I	 0.2110	 -0.0510
J	 0.2240	 -0.0280
K	 0.1770	 -0.0750
L	 0.2980	 -0.0130
M	 0.1180	 -0.1050

