



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:36 AM UTC

PDB ID : 8ZKK / pdb_00008zkk
EMDB ID : EMD-60197
Title : Portal-tail of Vibrio cholerae typing phage mature VP1
Authors : Liu, H.R.; Pang, H.
Deposited on : 2024-05-16
Resolution : 3.60 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:

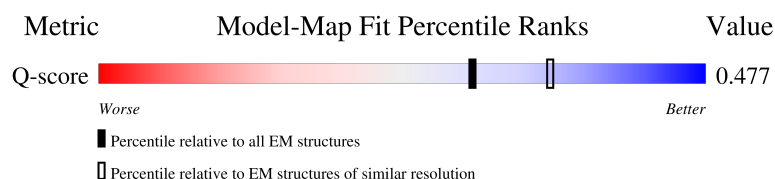
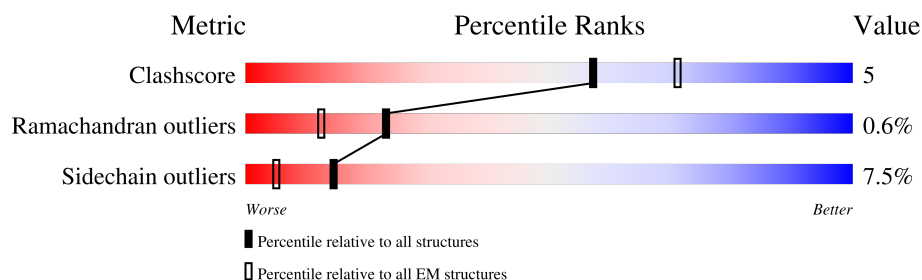
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.60 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	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	O	521	 78% 17% . .
2	A	652	 70% 17% . 10%
2	U	652	 68% 19% . 10%
3	B	202	 83% 15% .

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Mol	Chain	Length	Quality of chain
3	D	202	83% 16% .
4	m	239	92% . .
5	p	93	38% 15% . 46%
5	u	93	37% 12% . 47%
5	z	93	34% 16% .. 47%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18220 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 nozzle gp16.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	521	Total	C	N	O	S	0	0
			4173	2679	692	790	12		

- Molecule 2 is a protein called portal gp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	589	Total	C	N	O	S	0	0
			4697	3000	791	877	29		
2	U	589	Total	C	N	O	S	0	0
			4697	3000	791	877	29		

- Molecule 3 is a protein called adaptor gp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	202	Total	C	N	O	S	0	0
			1660	1061	281	310	8		
3	D	202	Total	C	N	O	S	0	0
			1660	1061	281	310	8		

- Molecule 4 is a protein called ring protein gp10.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	m	19	Total	C	N	O	0	0
			153	98	25	30		

- Molecule 5 is a protein called gp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	p	50	Total	C	N	O	S	0	0
			396	253	66	76	1		
5	u	49	Total	C	N	O	S	0	0
			392	251	65	75	1		

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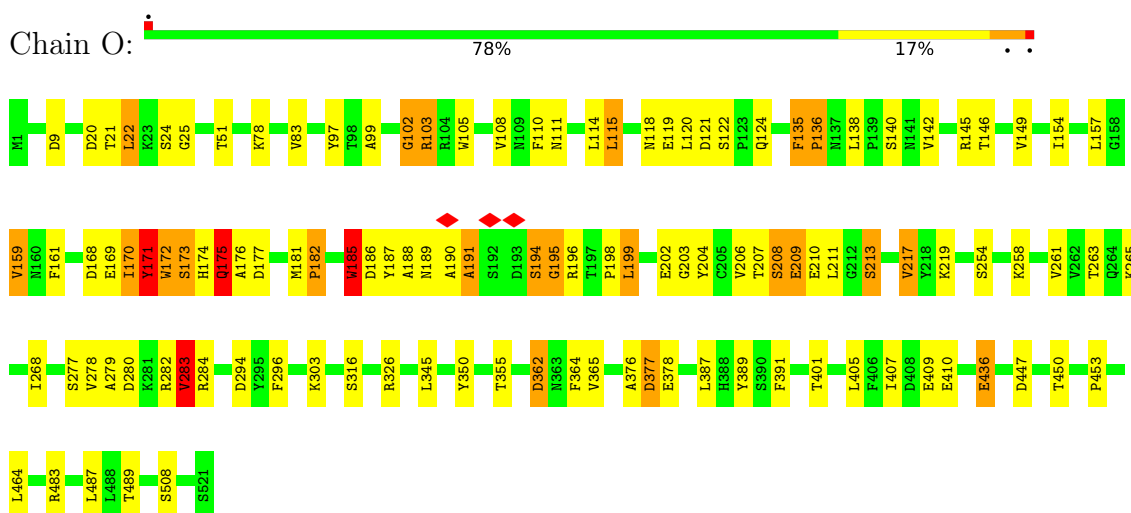
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	z	49	Total	C	N	O	S	0	0
			392	251	65	75	1		

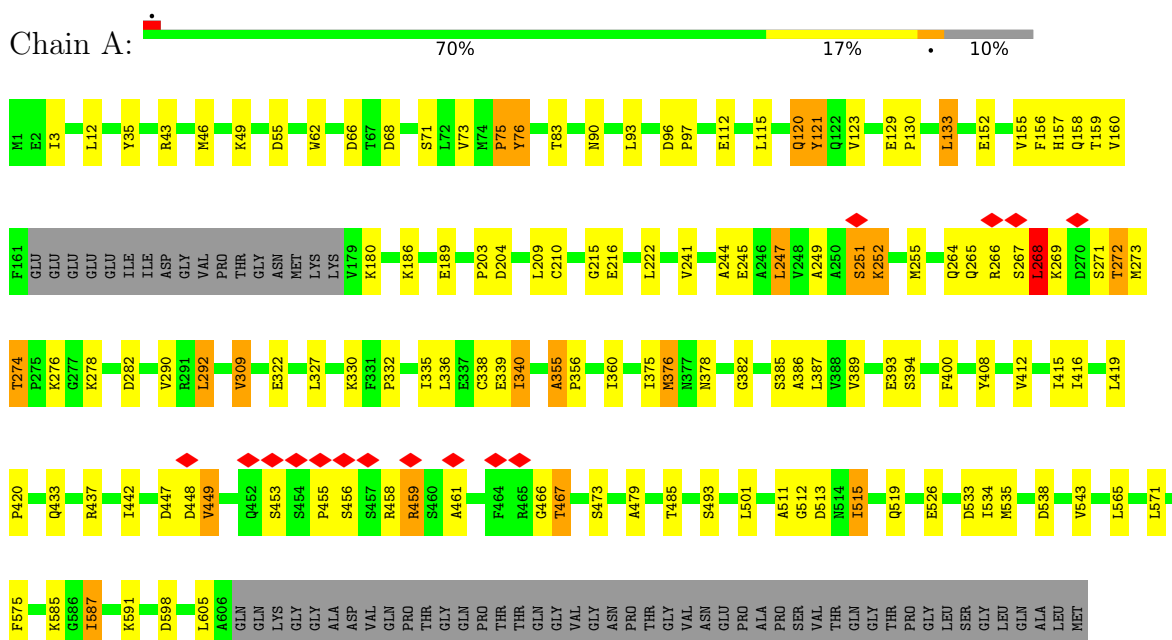
3 Residue-property plots

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.

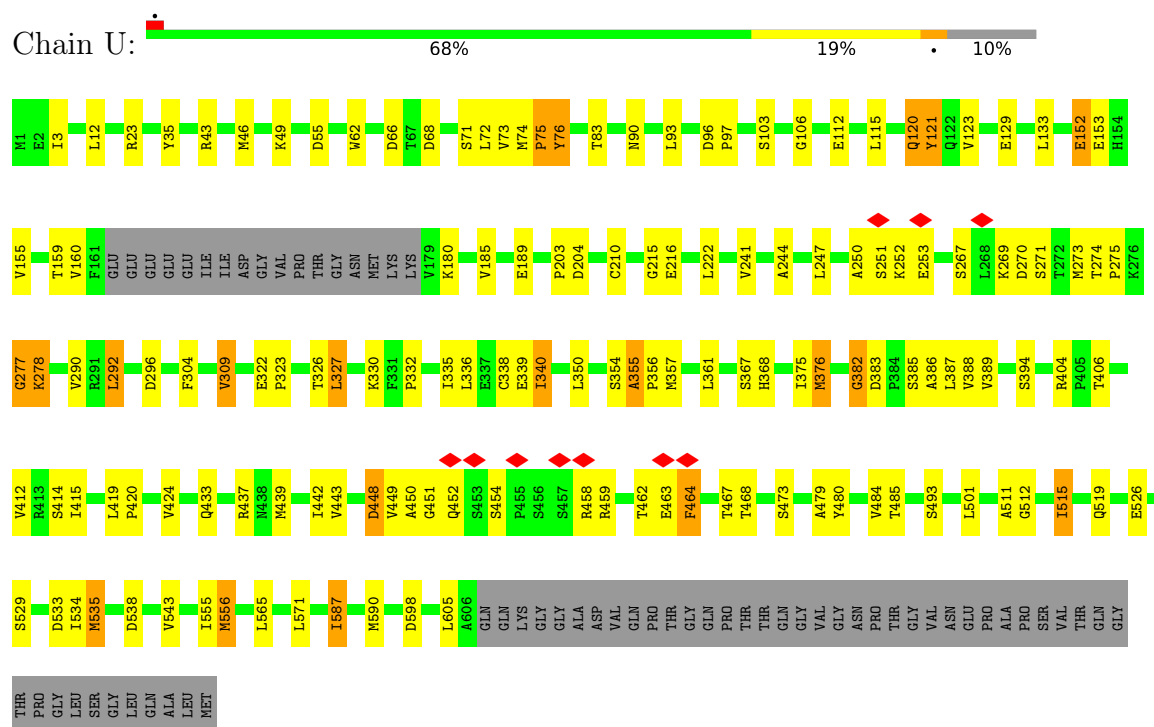
• Molecule 1: nozzle gp16



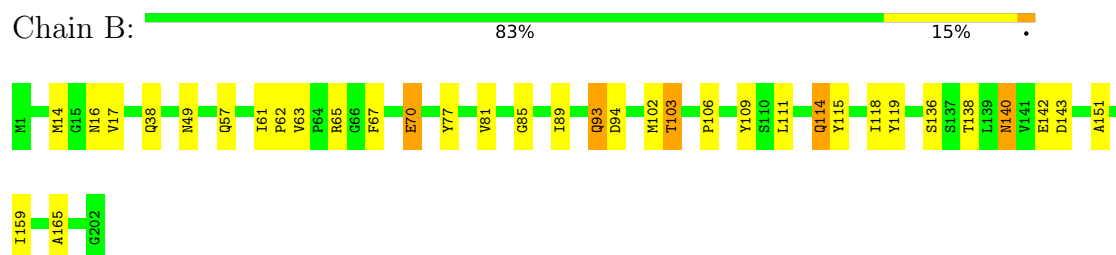
• Molecule 2: portal gp5



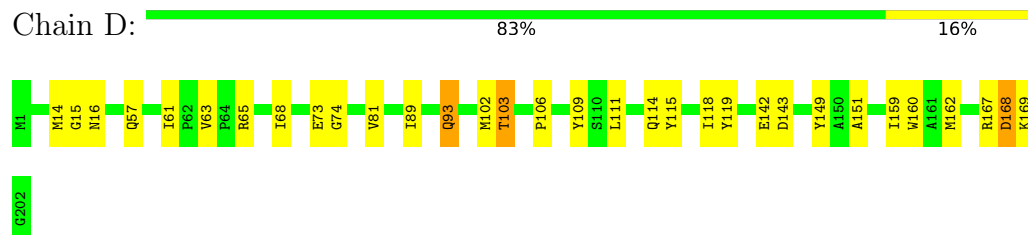
- Molecule 2: portal gp5



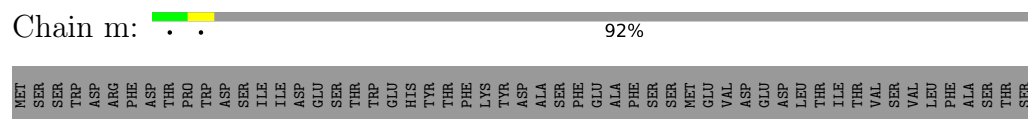
- Molecule 3: adaptor gp12



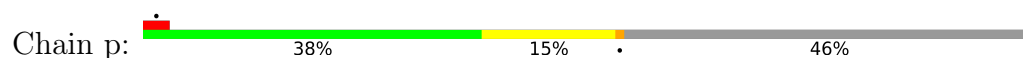
- Molecule 3: adaptor gp12



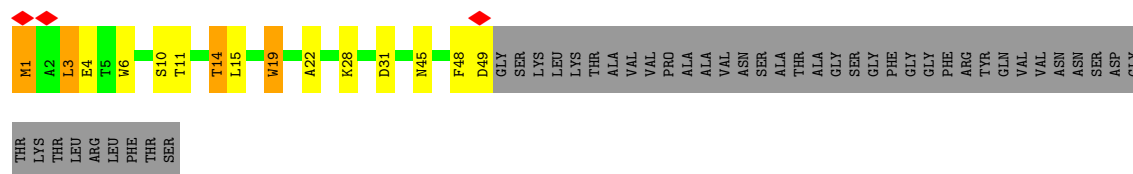
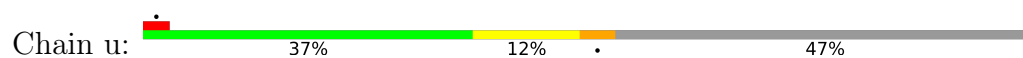
- Molecule 4: ring protein gp10



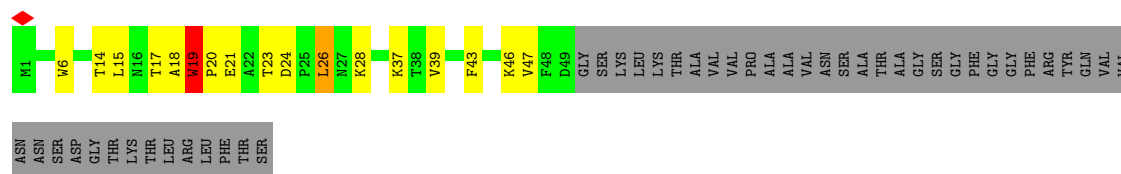
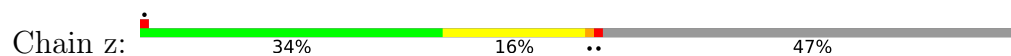
- Molecule 5: gp13



- Molecule 5: gp13



- Molecule 5: gp13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47456	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	15.619	Depositor
Minimum map value	-7.104	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.840	Depositor
Recommended contour level	1.7	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	O	0.71	3/4292 (0.1%)	1.03	44/5834 (0.8%)
2	A	1.40	12/4793 (0.3%)	1.25	58/6472 (0.9%)
2	U	1.41	11/4793 (0.2%)	1.30	62/6472 (1.0%)
3	B	1.09	2/1696 (0.1%)	1.01	13/2289 (0.6%)
3	D	1.13	2/1696 (0.1%)	0.99	14/2289 (0.6%)
4	m	1.08	0/160	1.65	6/221 (2.7%)
5	p	0.94	0/407	1.23	5/559 (0.9%)
5	u	0.88	0/403	1.18	7/554 (1.3%)
5	z	0.84	0/403	1.26	6/554 (1.1%)
All	All	1.19	30/18643 (0.2%)	1.18	215/25244 (0.9%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	338	CYS	C-N	7.96	1.44	1.33
2	U	338	CYS	C-N	7.94	1.44	1.33
2	A	115	LEU	CA-C	-6.49	1.44	1.52
2	U	115	LEU	CA-C	-6.46	1.44	1.52
1	O	171	TYR	CA-C	-6.42	1.46	1.53
2	A	336	LEU	C-N	6.28	1.43	1.33
2	U	336	LEU	C-N	6.26	1.43	1.33
3	B	165	ALA	C-O	-6.00	1.17	1.24
2	U	451	GLY	CA-C	-5.77	1.46	1.51
2	A	479	ALA	CA-C	-5.75	1.45	1.52
2	U	121	TYR	CA-C	-5.75	1.45	1.52
3	D	61	ILE	CA-C	-5.71	1.47	1.52
2	A	121	TYR	CA-C	-5.70	1.45	1.52
3	B	61	ILE	CA-C	-5.70	1.47	1.52
2	A	433	GLN	CA-C	-5.68	1.45	1.52
2	U	450	ALA	CA-C	-5.67	1.45	1.52
2	U	479	ALA	CA-C	-5.65	1.45	1.52
1	O	24	SER	CA-C	-5.59	1.45	1.52
2	U	433	GLN	CA-C	-5.57	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	160	TRP	CA-C	-5.49	1.45	1.52
2	A	271	SER	CA-C	-5.39	1.47	1.53
2	A	394	SER	CA-C	-5.30	1.46	1.52
2	U	394	SER	CA-C	-5.26	1.46	1.52
2	A	269	LYS	CA-C	-5.16	1.46	1.52
2	U	535	MET	CA-C	-5.14	1.48	1.52
2	A	437	ARG	CA-C	-5.13	1.46	1.52
2	U	437	ARG	CA-C	-5.12	1.46	1.52
2	A	274	THR	CA-CB	-5.11	1.47	1.54
1	O	199	LEU	N-CA	5.06	1.50	1.46
2	A	535	MET	CA-C	-5.05	1.48	1.52

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	VAL	N-CA-C	13.52	124.37	110.72
2	U	389	VAL	N-CA-C	13.50	124.36	110.72
1	O	294	ASP	N-CA-C	-12.56	97.67	111.36
2	U	415	ILE	N-CA-C	11.70	122.55	110.62
2	U	93	LEU	N-CA-C	11.50	123.89	111.36
2	A	93	LEU	N-CA-C	11.44	123.83	111.36
2	U	270	ASP	N-CA-C	10.79	123.12	111.36
1	O	103	ARG	N-CA-C	-10.64	100.41	113.50
2	U	376	MET	N-CA-C	9.90	122.16	111.36
2	U	277	GLY	CA-C-O	-9.78	115.48	122.23
4	m	214	ASP	N-CA-C	9.23	123.95	108.90
2	U	251	SER	N-CA-C	9.13	124.15	112.92
5	z	14	THR	N-CA-C	9.01	121.10	111.28
3	D	68	ILE	N-CA-C	-8.89	103.92	111.56
2	U	71	SER	N-CA-C	8.89	122.26	110.53
2	U	375	ILE	N-CA-C	8.87	121.42	112.90
2	U	485	THR	N-CA-C	8.83	120.67	111.14
3	D	102	MET	N-CA-C	-8.76	98.14	110.50
2	A	485	THR	N-CA-C	8.76	120.60	111.14
3	B	102	MET	N-CA-C	-8.74	98.17	110.50
1	O	22	LEU	N-CA-C	8.73	123.98	113.16
3	D	65	ARG	N-CA-C	8.71	120.39	111.07
3	B	65	ARG	N-CA-C	8.68	120.36	111.07
2	U	414	SER	N-CA-C	8.68	120.74	111.28
2	A	71	SER	N-CA-C	8.54	121.81	110.53
1	O	280	ASP	N-CA-C	8.53	120.36	111.14
2	U	252	LYS	N-CA-C	8.34	122.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	335	ILE	N-CA-C	8.28	119.70	108.11
2	U	335	ILE	N-CA-C	8.27	119.69	108.11
2	A	340	ILE	N-CA-C	8.19	119.99	112.29
2	A	241	VAL	N-CA-C	8.15	118.93	110.62
2	U	340	ILE	N-CA-C	8.14	119.94	112.29
1	O	136	PRO	N-CA-C	8.12	124.81	113.53
2	U	241	VAL	N-CA-C	8.06	118.84	110.62
2	U	121	TYR	N-CA-C	-7.94	102.57	111.07
2	A	204	ASP	CA-C-N	-7.93	112.75	120.83
2	A	204	ASP	C-N-CA	-7.93	112.75	120.83
2	U	204	ASP	CA-C-N	-7.93	112.75	120.83
2	U	204	ASP	C-N-CA	-7.93	112.75	120.83
2	A	121	TYR	N-CA-C	-7.90	102.61	111.07
4	m	211	VAL	N-CA-C	7.89	117.95	110.53
2	U	216	GLU	N-CA-C	7.80	119.79	111.28
1	O	194	SER	N-CA-C	-7.76	103.80	112.57
1	O	140	SER	N-CA-C	7.75	119.73	111.28
2	A	216	GLU	N-CA-C	7.75	119.72	111.28
1	O	189	ASN	N-CA-C	7.74	121.25	108.48
2	U	250	ALA	N-CA-C	7.66	122.34	112.92
1	O	209	GLU	N-CA-C	7.60	119.56	111.28
3	D	142	GLU	N-CA-C	7.53	119.28	111.14
5	p	17	THR	N-CA-C	7.47	119.50	111.36
3	B	142	GLU	N-CA-C	7.43	119.16	111.14
5	u	10	SER	N-CA-C	7.39	119.42	111.36
2	A	442	ILE	CB-CA-C	-7.39	102.33	112.02
2	U	442	ILE	CB-CA-C	-7.39	102.34	112.02
2	A	355	ALA	CA-C-N	-7.37	110.87	119.05
2	A	355	ALA	C-N-CA	-7.37	110.87	119.05
1	O	278	VAL	N-CA-C	-7.36	102.03	110.05
1	O	410	GLU	N-CA-C	7.34	121.99	110.32
2	A	501	LEU	N-CA-C	7.32	119.34	111.36
2	U	55	ASP	N-CA-C	7.30	119.24	111.28
2	A	55	ASP	N-CA-C	7.30	119.23	111.28
1	O	159	VAL	N-CA-C	7.29	119.08	108.58
2	U	501	LEU	N-CA-C	7.29	119.31	111.36
1	O	204	TYR	N-CA-C	7.24	121.82	112.26
1	O	391	PHE	N-CA-C	7.21	121.38	112.59
1	O	169	GLU	N-CA-C	7.17	120.64	109.52
1	O	198	PRO	N-CA-C	7.17	123.01	113.40
1	O	203	GLY	N-CA-C	7.17	123.16	112.41
3	B	115	TYR	N-CA-C	7.11	121.14	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	268	LEU	N-CA-C	-7.08	101.91	111.54
5	z	20	PRO	N-CA-C	-7.08	99.39	110.50
2	A	112	GLU	N-CA-C	6.99	118.89	111.28
1	O	283	VAL	N-CA-C	6.97	123.83	109.34
2	A	375	ILE	N-CA-C	6.97	121.02	113.43
2	A	447	ASP	N-CA-C	6.93	120.75	109.59
2	A	338	CYS	O-C-N	6.93	130.05	122.15
2	U	112	GLU	N-CA-C	6.92	118.83	111.28
2	U	338	CYS	O-C-N	6.91	130.02	122.15
2	A	512	GLY	N-CA-C	6.89	123.83	111.02
2	U	512	GLY	N-CA-C	6.87	123.79	111.02
1	O	365	VAL	N-CA-C	6.83	119.59	112.83
2	U	386	ALA	N-CA-C	6.72	121.08	113.01
2	A	386	ALA	N-CA-C	6.69	121.04	113.01
1	O	190	ALA	N-CA-C	6.69	118.57	111.28
1	O	195	GLY	N-CA-C	6.66	118.99	110.20
2	U	385	SER	N-CA-C	6.64	118.52	111.28
1	O	376	ALA	N-CA-C	-6.64	100.45	110.28
2	A	385	SER	N-CA-C	6.63	118.50	111.28
2	A	461	ALA	N-CA-C	6.60	118.13	111.07
2	U	271	SER	N-CA-C	6.56	120.73	110.17
2	A	332	PRO	CB-CA-C	-6.52	104.22	113.09
2	A	180	LYS	N-CA-C	6.52	120.54	111.74
2	U	355	ALA	CA-C-N	-6.51	111.83	119.05
2	U	355	ALA	C-N-CA	-6.51	111.83	119.05
2	A	511	ALA	N-CA-C	6.50	121.49	113.50
2	A	322	GLU	N-CA-C	6.49	114.06	108.22
2	U	332	PRO	CB-CA-C	-6.49	104.26	113.09
2	A	449	VAL	N-CA-C	6.45	119.11	111.05
2	A	249	ALA	N-CA-C	6.44	117.97	111.07
5	z	19	TRP	CA-C-N	-6.44	112.31	120.23
5	z	19	TRP	C-N-CA	-6.44	112.31	120.23
2	U	511	ALA	N-CA-C	6.44	121.42	113.50
2	U	153	GLU	N-CA-C	-6.43	98.91	109.40
2	A	269	LYS	N-CA-C	6.43	119.68	110.10
5	u	6	TRP	N-CA-C	6.41	118.81	109.07
2	U	322	GLU	N-CA-C	6.39	113.97	108.22
4	m	209	LYS	N-CA-C	6.34	119.33	110.20
2	U	180	LYS	N-CA-C	6.32	120.37	111.52
1	O	208	SER	N-CA-C	-6.30	104.90	112.59
2	U	412	VAL	N-CA-C	6.29	117.03	110.62
2	U	277	GLY	N-CA-C	-6.25	105.28	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	296	PHE	N-CA-C	-6.25	105.33	114.39
1	O	213	SER	N-CA-C	-6.22	97.55	110.80
1	O	21	THR	CB-CA-C	-6.21	101.46	111.28
2	U	330	LYS	N-CA-C	6.21	119.25	110.50
2	U	244	ALA	N-CA-C	6.20	118.04	111.28
2	A	244	ALA	N-CA-C	6.20	118.03	111.28
2	A	330	LYS	N-CA-C	6.17	119.20	110.50
3	D	115	TYR	N-CA-C	6.17	119.60	108.69
1	O	407	ILE	N-CA-C	-6.15	104.75	110.53
4	m	203	ASP	N-CA-C	6.15	119.26	108.56
4	m	217	THR	N-CA-C	6.11	118.47	109.24
2	U	75	PRO	N-CA-C	6.10	121.58	113.40
1	O	185	TRP	N-CA-C	-6.09	98.59	108.52
5	u	19	TRP	CA-C-N	-6.09	112.23	119.84
5	u	19	TRP	C-N-CA	-6.09	112.23	119.84
2	U	464	PHE	N-CA-C	-6.08	104.65	111.28
3	D	151	ALA	N-CA-C	6.04	117.87	111.28
5	u	22	ALA	N-CA-C	6.04	117.86	111.28
2	U	35	TYR	N-CA-C	6.04	117.94	111.36
2	U	74	MET	N-CA-C	6.03	117.30	109.64
2	A	75	PRO	N-CA-C	6.03	121.48	113.40
3	D	149	TYR	N-CA-C	6.03	120.91	113.50
2	A	35	TYR	N-CA-C	6.00	117.89	111.36
5	u	19	TRP	N-CA-C	5.95	121.61	113.16
3	B	61	ILE	CA-C-N	-5.88	114.21	120.03
3	B	61	ILE	C-N-CA	-5.88	114.21	120.03
3	D	61	ILE	CA-C-N	-5.88	114.21	120.03
3	D	61	ILE	C-N-CA	-5.88	114.21	120.03
3	D	109	TYR	N-CA-C	5.86	117.97	109.07
3	B	109	TYR	N-CA-C	5.86	117.97	109.07
1	O	171	TYR	CB-CA-C	-5.85	103.02	111.91
1	O	191	ALA	N-CA-C	-5.84	105.74	112.92
2	A	255	MET	N-CA-C	5.83	117.43	111.14
2	U	129	GLU	CA-C-N	-5.82	112.59	119.05
2	U	129	GLU	C-N-CA	-5.82	112.59	119.05
2	A	515	ILE	CB-CA-C	-5.80	106.07	112.68
2	U	515	ILE	CB-CA-C	-5.79	106.08	112.68
3	B	165	ALA	CA-C-N	5.79	129.86	120.60
3	B	165	ALA	C-N-CA	5.79	129.86	120.60
3	B	103	THR	N-CA-C	5.74	118.76	109.40
5	p	18	ALA	N-CA-C	5.73	120.39	113.17
2	A	360	ILE	N-CA-C	-5.72	103.90	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	175	GLN	N-CA-C	5.70	119.11	111.24
3	D	103	THR	N-CA-C	5.70	118.69	109.40
2	A	129	GLU	CA-C-N	-5.68	112.74	119.05
2	A	129	GLU	C-N-CA	-5.68	112.74	119.05
2	A	215	GLY	N-CA-C	5.68	121.20	112.51
5	u	14	THR	CB-CA-C	-5.68	103.87	111.88
1	O	21	THR	N-CA-C	5.67	119.86	111.87
2	U	215	GLY	N-CA-C	5.67	121.18	112.51
1	O	135	PHE	N-CA-C	5.66	116.83	109.64
2	U	96	ASP	N-CA-C	5.60	119.86	112.35
2	A	96	ASP	N-CA-C	5.59	119.84	112.35
2	A	309	VAL	CB-CA-C	-5.58	102.30	110.62
5	p	48	PHE	N-CA-C	5.58	117.04	111.07
2	U	309	VAL	CB-CA-C	-5.56	102.34	110.62
2	A	466	GLY	N-CA-C	5.54	118.93	112.50
5	z	6	TRP	N-CA-C	5.53	117.80	109.23
5	z	43	PHE	N-CA-C	5.53	117.39	111.36
1	O	122	SER	N-CA-C	5.53	116.66	109.64
1	O	182	PRO	N-CA-C	5.52	117.43	110.70
1	O	210	GLU	N-CA-C	5.52	118.64	110.48
2	U	533	ASP	N-CA-C	5.49	122.50	110.80
2	A	533	ASP	N-CA-C	5.47	122.46	110.80
2	A	415	ILE	N-CA-C	5.45	115.65	110.53
3	B	89	ILE	N-CA-C	5.44	115.78	108.17
2	A	376	MET	N-CA-C	5.42	117.75	109.62
3	D	89	ILE	N-CA-C	5.40	115.73	108.17
2	U	123	VAL	CB-CA-C	-5.38	104.97	112.02
2	U	3	ILE	N-CA-C	-5.37	100.01	107.80
2	U	267	SER	N-CA-C	-5.34	105.37	111.14
1	O	362	ASP	N-CA-C	5.34	117.10	111.28
2	A	3	ILE	N-CA-C	-5.34	100.06	107.80
1	O	453	PRO	N-CA-C	5.33	119.85	111.38
2	A	123	VAL	CB-CA-C	-5.32	105.05	112.02
2	U	452	GLN	N-CA-C	-5.30	105.51	111.28
2	A	382	GLY	N-CA-C	5.29	120.94	110.83
1	O	405	LEU	N-CA-C	5.29	119.37	113.02
1	O	198	PRO	CA-C-O	-5.29	112.08	119.74
2	A	292	LEU	N-CA-C	5.27	117.19	109.24
2	U	382	GLY	N-CA-C	5.26	120.88	110.83
2	U	292	LEU	N-CA-C	5.24	117.15	109.24
3	B	93	GLN	N-CA-C	5.23	116.98	111.28
1	O	102	GLY	N-CA-C	-5.22	108.14	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	151	ALA	N-CA-C	5.21	116.96	111.28
2	U	357	MET	N-CA-C	5.21	117.04	111.36
3	D	93	GLN	N-CA-C	5.20	116.95	111.28
2	A	473	SER	N-CA-C	5.18	117.67	111.71
3	D	167	ARG	N-CA-C	5.18	118.73	111.74
1	O	409	GLU	N-CA-C	5.17	117.35	110.53
4	m	213	SER	N-CA-C	5.14	121.85	114.39
2	U	339	GLU	N-CA-C	5.12	118.06	110.48
2	A	339	GLU	N-CA-C	5.11	118.04	110.48
2	A	416	ILE	CB-CA-C	-5.11	102.21	110.28
2	A	251	SER	N-CA-C	5.10	116.84	111.28
2	U	538	ASP	N-CA-C	5.09	115.01	108.34
2	A	272	THR	N-CA-C	-5.09	100.88	109.07
2	U	473	SER	N-CA-C	5.09	117.56	111.71
2	A	538	ASP	N-CA-C	5.08	115.00	108.34
2	U	361	LEU	N-CA-C	5.08	116.81	111.28
1	O	436	GLU	N-CA-C	5.05	120.07	113.30
5	p	10	SER	N-CA-C	5.04	117.74	110.28
5	p	22	ALA	N-CA-C	5.02	116.75	111.28
1	O	377	ASP	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

There are no planarity outliers.

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	O	4173	0	3980	51	0
2	A	4697	0	4695	50	0
2	U	4697	0	4695	50	0
3	B	1660	0	1637	18	0
3	D	1660	0	1637	18	0
4	m	153	0	135	6	0
5	p	396	0	381	4	0
5	u	392	0	378	9	0
5	z	392	0	378	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18220	0	17916	172	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (172) 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)
2:A:400:PHE:CZ	2:U:382:GLY:HA3	1.95	1.01
2:A:120:GLN:HE22	2:U:535:MET:HE1	1.23	1.01
1:O:355:THR:HA	1:O:378:GLU:HG2	1.42	1.00
2:U:459:ARG:HB3	2:U:463:GLU:HB3	1.56	0.88
5:u:4:GLU:HA	5:u:19:TRP:HZ3	1.39	0.86
1:O:173:SER:HB2	1:O:182:PRO:HB3	1.58	0.83
3:B:106:PRO:HB3	3:B:118:ILE:CG2	2.11	0.81
2:A:456:SER:HB3	2:A:459:ARG:HH11	1.46	0.80
3:D:106:PRO:HB3	3:D:118:ILE:CG2	2.11	0.78
3:B:93:GLN:HG3	3:B:119:TYR:OH	1.84	0.78
2:A:120:GLN:NE2	2:U:535:MET:HE1	1.99	0.77
4:m:203:ASP:N	4:m:203:ASP:OD1	2.13	0.77
3:D:93:GLN:HG3	3:D:119:TYR:OH	1.84	0.77
1:O:170:ILE:HD12	1:O:195:GLY:HA3	1.68	0.75
5:u:1:MET:HA	5:u:19:TRP:CD1	2.21	0.74
5:z:21:GLU:HG3	5:z:24:ASP:HB2	1.71	0.72
2:A:400:PHE:CZ	2:U:382:GLY:CA	2.74	0.71
3:B:49:ASN:O	4:m:207:PRO:HD3	1.91	0.70
3:B:106:PRO:HB3	3:B:118:ILE:HG21	1.74	0.68
5:p:15:LEU:HD11	5:p:39:VAL:HG21	1.75	0.68
3:D:106:PRO:HB3	3:D:118:ILE:HG21	1.74	0.68
2:A:408:TYR:CE1	2:U:383:ASP:OD1	2.47	0.68
1:O:364:PHE:CE2	5:z:26:LEU:HD13	2.30	0.67
1:O:489:THR:CG2	3:D:15:GLY:O	2.45	0.64
2:A:393:GLU:HG2	3:D:200:PHE:O	1.98	0.64
1:O:489:THR:HG23	3:D:15:GLY:O	1.96	0.64
2:A:448:ASP:OD1	2:A:455:PRO:HD2	1.98	0.63
2:A:400:PHE:CE1	2:U:382:GLY:C	2.77	0.62
2:A:400:PHE:CE1	2:U:382:GLY:CA	2.82	0.62
2:U:388:VAL:HG22	2:U:404:ARG:HG2	1.82	0.61
2:U:459:ARG:HB3	2:U:463:GLU:CB	2.29	0.61
5:u:3:LEU:HD11	5:u:31:ASP:CB	2.31	0.60
2:A:133:LEU:HD11	2:U:480:TYR:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:172:TRP:CE3	1:O:185:TRP:HB2	2.37	0.59
1:O:118:ASN:HD21	1:O:121:ASP:HB2	1.66	0.59
1:O:279:ALA:O	1:O:284:ARG:HB2	2.03	0.58
1:O:483:ARG:HH22	3:B:16:ASN:HB3	1.68	0.57
1:O:170:ILE:CD1	1:O:195:GLY:HA3	2.34	0.57
2:U:448:ASP:HA	2:U:454:SER:CB	2.35	0.56
5:z:19:TRP:CE3	5:z:19:TRP:HA	2.40	0.56
1:O:110:PHE:HB2	1:O:149:VAL:HG11	1.87	0.56
1:O:447:ASP:OD2	1:O:508:SER:OG	2.23	0.56
3:B:67:PHE:HZ	3:B:70:GLU:HG2	1.71	0.55
1:O:208:SER:HA	1:O:217:VAL:HA	1.88	0.55
1:O:78:LYS:HE2	1:O:99:ALA:HB2	1.88	0.55
1:O:254:SER:O	1:O:303:LYS:NZ	2.36	0.55
5:u:4:GLU:HA	5:u:19:TRP:CZ3	2.30	0.55
2:A:453:SER:HB2	2:A:467:THR:HB	1.89	0.54
2:A:252:LYS:HE2	2:A:282:ASP:HB2	1.89	0.54
4:m:202:TYR:HB3	4:m:203:ASP:OD1	2.08	0.53
2:A:400:PHE:HE1	2:U:382:GLY:C	2.16	0.53
5:u:3:LEU:HD11	5:u:31:ASP:HB2	1.90	0.53
1:O:171:TYR:H	1:O:195:GLY:HA2	1.74	0.52
2:U:448:ASP:HA	2:U:454:SER:HB2	1.92	0.52
1:O:350:TYR:HB3	1:O:387:LEU:HD23	1.91	0.52
3:D:93:GLN:NE2	3:D:119:TYR:OH	2.43	0.52
3:B:38:GLN:OE1	3:D:184:ARG:NH1	2.43	0.51
5:u:1:MET:HA	5:u:19:TRP:NE1	2.26	0.51
3:B:93:GLN:NE2	3:B:119:TYR:OH	2.43	0.51
1:O:119:GLU:HG3	1:O:145:ARG:HA	1.93	0.51
1:O:174:HIS:HD2	1:O:191:ALA:HB2	1.76	0.51
1:O:97:TYR:HE1	1:O:124:GLN:NE2	2.09	0.51
1:O:108:VAL:HG13	1:O:115:LEU:HD12	1.92	0.51
2:A:133:LEU:HD11	2:U:480:TYR:HE2	1.75	0.51
5:u:4:GLU:CA	5:u:19:TRP:HZ3	2.18	0.51
1:O:102:GLY:HA2	1:O:105:TRP:HD1	1.77	0.50
1:O:316:SER:HB3	1:O:326:ARG:HD2	1.92	0.50
2:A:247:LEU:O	2:A:251:SER:HB2	2.12	0.50
3:B:94:ASP:OD1	3:D:73:GLU:C	2.55	0.50
2:U:152:GLU:O	2:U:189:GLU:HA	2.12	0.50
1:O:487:LEU:HG	3:D:16:ASN:HB2	1.93	0.50
3:D:93:GLN:CG	3:D:119:TYR:OH	2.57	0.50
1:O:9:ASP:OD1	1:O:25:GLY:HA3	2.11	0.50
3:D:14:MET:HG3	3:D:159:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:176:ALA:HB2	1:O:182:PRO:HA	1.93	0.50
2:A:156:PHE:HZ	2:U:327:LEU:O	1.94	0.49
5:u:45:ASN:O	5:u:49:ASP:HB3	2.12	0.49
2:A:272:THR:HB	2:U:23:ARG:NH1	2.28	0.48
2:A:400:PHE:HE1	2:U:382:GLY:O	1.96	0.48
3:B:93:GLN:CG	3:B:119:TYR:OH	2.57	0.48
1:O:173:SER:HB2	1:O:182:PRO:CB	2.37	0.48
2:U:464:PHE:O	2:U:468:THR:HG22	2.14	0.48
4:m:202:TYR:CB	4:m:203:ASP:OD1	2.61	0.48
1:O:268:ILE:HG22	1:O:277:SER:HA	1.96	0.48
1:O:172:TRP:HE3	1:O:185:TRP:HB2	1.76	0.47
1:O:489:THR:HG21	3:D:15:GLY:O	2.14	0.47
3:B:62:PRO:HG2	4:m:202:TYR:CD2	2.50	0.47
2:A:156:PHE:CZ	2:U:327:LEU:O	2.66	0.47
2:A:130:PRO:HD3	2:U:484:VAL:CG1	2.45	0.47
2:A:448:ASP:OD1	2:A:455:PRO:CD	2.63	0.47
2:A:575:PHE:HZ	2:U:555:ILE:HG23	1.79	0.47
3:B:94:ASP:OD1	3:D:74:GLY:N	2.47	0.46
1:O:355:THR:CA	1:O:378:GLU:HG2	2.30	0.46
5:p:28:LYS:HD3	5:p:28:LYS:HA	1.71	0.46
1:O:157:LEU:HD21	1:O:208:SER:OG	2.15	0.46
2:A:49:LYS:HB2	2:A:73:VAL:HG23	1.98	0.46
2:A:152:GLU:O	2:A:189:GLU:HA	2.15	0.46
2:U:556:MET:HE3	2:U:556:MET:HB2	1.71	0.46
2:A:159:THR:HG23	2:U:323:PRO:HB3	1.97	0.45
2:U:587:ILE:H	2:U:587:ILE:HG13	1.26	0.45
1:O:142:VAL:HG12	1:O:161:PHE:HA	1.98	0.45
3:B:14:MET:HG3	3:B:159:ILE:HG23	1.97	0.45
1:O:219:LYS:HB3	1:O:219:LYS:HE3	1.38	0.45
2:U:277:GLY:O	2:U:278:LYS:HB2	2.16	0.45
3:B:77:TYR:CE1	3:B:85:GLY:HA3	2.52	0.45
1:O:51:THR:HG23	1:O:83:VAL:HG11	1.98	0.44
1:O:110:PHE:O	1:O:111:ASN:C	2.60	0.44
1:O:345:LEU:HD11	1:O:389:TYR:HD2	1.81	0.44
5:u:28:LYS:HA	5:u:28:LYS:HD3	1.77	0.44
2:U:419:LEU:HA	2:U:420:PRO:HD3	1.83	0.44
2:U:459:ARG:HE	2:U:464:PHE:HE1	1.64	0.44
2:U:350:LEU:HD22	2:U:443:VAL:HG13	2.00	0.44
1:O:135:PHE:HA	1:O:136:PRO:HD3	1.82	0.44
2:U:75:PRO:O	2:U:76:TYR:C	2.60	0.44
3:D:168:ASP:N	3:D:168:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:273:MET:HE3	2:A:273:MET:HB3	1.83	0.44
2:A:267:SER:O	2:A:268:LEU:C	2.61	0.44
2:U:354:SER:HB2	2:U:439:MET:HE3	2.00	0.44
1:O:187:TYR:HA	1:O:194:SER:H	1.82	0.43
2:A:419:LEU:HA	2:A:420:PRO:HD3	1.83	0.43
1:O:146:THR:HG23	1:O:157:LEU:HD23	2.00	0.43
2:A:157:HIS:CD2	2:U:304:PHE:HB3	2.53	0.43
2:U:448:ASP:HA	2:U:454:SER:HB3	1.99	0.43
3:B:114:GLN:H	3:B:114:GLN:HG2	1.35	0.43
2:U:49:LYS:HB2	2:U:73:VAL:HG23	2.00	0.43
5:p:25:PRO:HB2	5:p:27:ASN:OD1	2.18	0.43
5:z:19:TRP:HA	5:z:19:TRP:HE3	1.83	0.43
2:A:513:ASP:OD2	2:U:106:GLY:HA3	2.19	0.43
2:U:367:SER:O	2:U:368:HIS:C	2.59	0.43
2:A:130:PRO:HG3	2:U:484:VAL:HG12	1.99	0.43
2:A:378:ASN:OD1	2:U:424:VAL:HG22	2.18	0.43
1:O:487:LEU:O	3:D:16:ASN:ND2	2.52	0.42
1:O:175:GLN:HE21	1:O:175:GLN:HB3	1.57	0.42
2:A:585:LYS:HE3	2:U:103:SER:O	2.19	0.42
5:z:17:THR:O	5:z:18:ALA:HB3	2.19	0.42
5:z:28:LYS:HA	5:z:28:LYS:HD3	1.83	0.42
2:A:62:TRP:NE1	2:A:68:ASP:H	2.17	0.42
2:U:12:LEU:HD12	2:U:12:LEU:HA	1.89	0.42
2:A:458:ARG:HA	2:A:458:ARG:HD3	1.71	0.42
2:A:46:MET:HE3	2:A:46:MET:HB3	1.92	0.42
2:U:458:ARG:HD3	2:U:458:ARG:HA	1.55	0.42
1:O:186:ASP:C	1:O:188:ALA:H	2.28	0.42
3:B:140:ASN:HB3	4:m:206:ARG:HH11	1.84	0.42
2:U:273:MET:HE2	2:U:273:MET:HB3	1.90	0.42
2:A:456:SER:HB3	2:A:459:ARG:NH1	2.26	0.42
2:U:62:TRP:NE1	2:U:68:ASP:H	2.17	0.42
1:O:170:ILE:HD12	1:O:196:ARG:H	1.85	0.41
1:O:362:ASP:OD1	5:p:22:ALA:HB1	2.20	0.41
2:A:591:LYS:HE2	2:A:591:LYS:HB3	1.89	0.41
2:U:355:ALA:O	2:U:356:PRO:C	2.59	0.41
1:O:159:VAL:HG12	1:O:168:ASP:O	2.20	0.41
1:O:181:MET:HE3	1:O:182:PRO:HD2	2.02	0.41
1:O:464:LEU:HD23	1:O:464:LEU:HA	1.86	0.41
2:A:245:GLU:H	2:A:245:GLU:HG3	1.74	0.41
3:D:162:MET:HE3	3:D:162:MET:HB3	1.84	0.41
2:A:75:PRO:O	2:A:76:TYR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:120:GLN:O	2:A:121:TYR:C	2.58	0.41
2:A:587:ILE:H	2:A:587:ILE:HG13	1.31	0.41
2:U:46:MET:HE3	2:U:46:MET:HB3	1.92	0.41
2:A:276:LYS:HB2	2:U:296:ASP:O	2.20	0.41
2:A:355:ALA:HB3	2:A:356:PRO:HD3	2.03	0.41
3:B:136:SER:C	3:B:138:THR:N	2.78	0.41
2:A:186:LYS:O	2:U:529:SER:OG	2.32	0.40
2:A:209:LEU:HD12	2:A:209:LEU:HA	1.89	0.40
1:O:258:LYS:HE2	1:O:258:LYS:HB2	1.90	0.40
2:A:158:GLN:NE2	2:U:326:THR:O	2.54	0.40
1:O:263:THR:HG22	1:O:265:LYS:H	1.87	0.40
2:A:12:LEU:HD12	2:A:12:LEU:HA	1.89	0.40
2:A:265:GLN:O	2:A:266:ARG:HB2	2.21	0.40
2:U:120:GLN:O	2:U:121:TYR:C	2.58	0.40
3:B:14:MET:HE2	3:B:17:VAL:HG21	2.04	0.40
3:D:201:MET:HE3	3:D:201:MET:HB3	1.88	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	O	492/521 (94%)	452 (92%)	37 (8%)	3 (1%)	21	54
2	A	505/652 (78%)	491 (97%)	10 (2%)	4 (1%)	16	49
2	U	585/652 (90%)	567 (97%)	14 (2%)	4 (1%)	18	51
3	B	200/202 (99%)	193 (96%)	7 (4%)	0	100	100
3	D	200/202 (99%)	190 (95%)	10 (5%)	0	100	100
4	m	17/239 (7%)	16 (94%)	1 (6%)	0	100	100
5	p	48/93 (52%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	u	47/93 (50%)	44 (94%)	2 (4%)	1 (2%)	5	31
5	z	47/93 (50%)	45 (96%)	2 (4%)	0	100	100
All	All	2141/2747 (78%)	2043 (95%)	86 (4%)	12 (1%)	23	54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	283	VAL
2	U	278	LYS
1	O	206	VAL
1	O	213	SER
2	A	76	TYR
2	U	76	TYR
2	A	203	PRO
2	U	203	PRO
2	A	278	LYS
2	A	97	PRO
2	U	97	PRO
5	u	11	THR

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	O	449/450 (100%)	421 (94%)	28 (6%)	16	44
2	A	511/560 (91%)	474 (93%)	37 (7%)	13	40
2	U	511/560 (91%)	467 (91%)	44 (9%)	10	34
3	B	175/175 (100%)	166 (95%)	9 (5%)	21	49
3	D	175/175 (100%)	166 (95%)	9 (5%)	21	49
4	m	17/208 (8%)	14 (82%)	3 (18%)	2	12
5	p	43/76 (57%)	38 (88%)	5 (12%)	5	25
5	u	43/76 (57%)	38 (88%)	5 (12%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	z	43/76 (57%)	35 (81%)	8 (19%)	1	10
All	All	1967/2356 (84%)	1819 (92%)	148 (8%)	14	39

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	20	ASP
1	O	22	LEU
1	O	103	ARG
1	O	114	LEU
1	O	115	LEU
1	O	120	LEU
1	O	138	LEU
1	O	154	ILE
1	O	170	ILE
1	O	171	TYR
1	O	172	TRP
1	O	173	SER
1	O	175	GLN
1	O	177	ASP
1	O	185	TRP
1	O	199	LEU
1	O	202	GLU
1	O	207	THR
1	O	209	GLU
1	O	211	LEU
1	O	217	VAL
1	O	261	VAL
1	O	282	ARG
1	O	283	VAL
1	O	377	ASP
1	O	401	THR
1	O	436	GLU
1	O	450	THR
2	A	43	ARG
2	A	66	ASP
2	A	83	THR
2	A	90	ASN
2	A	120	GLN
2	A	133	LEU
2	A	155	VAL
2	A	160	VAL

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Mol	Chain	Res	Type
2	A	210	CYS
2	A	222	LEU
2	A	247	LEU
2	A	252	LYS
2	A	264	GLN
2	A	268	LEU
2	A	274	THR
2	A	290	VAL
2	A	292	LEU
2	A	309	VAL
2	A	327	LEU
2	A	340	ILE
2	A	376	MET
2	A	387	LEU
2	A	412	VAL
2	A	449	VAL
2	A	459	ARG
2	A	467	THR
2	A	493	SER
2	A	515	ILE
2	A	519	GLN
2	A	526	GLU
2	A	534	ILE
2	A	543	VAL
2	A	565	LEU
2	A	571	LEU
2	A	587	ILE
2	A	598	ASP
2	A	605	LEU
3	B	57	GLN
3	B	63	VAL
3	B	70	GLU
3	B	81	VAL
3	B	103	THR
3	B	111	LEU
3	B	114	GLN
3	B	140	ASN
3	B	143	ASP
2	U	43	ARG
2	U	66	ASP
2	U	72	LEU
2	U	83	THR

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Mol	Chain	Res	Type
2	U	90	ASN
2	U	120	GLN
2	U	133	LEU
2	U	152	GLU
2	U	155	VAL
2	U	159	THR
2	U	160	VAL
2	U	185	VAL
2	U	210	CYS
2	U	222	LEU
2	U	247	LEU
2	U	253	GLU
2	U	269	LYS
2	U	274	THR
2	U	275	PRO
2	U	290	VAL
2	U	292	LEU
2	U	309	VAL
2	U	327	LEU
2	U	340	ILE
2	U	376	MET
2	U	387	LEU
2	U	406	THR
2	U	448	ASP
2	U	449	VAL
2	U	462	THR
2	U	467	THR
2	U	493	SER
2	U	515	ILE
2	U	519	GLN
2	U	526	GLU
2	U	534	ILE
2	U	543	VAL
2	U	556	MET
2	U	565	LEU
2	U	571	LEU
2	U	587	ILE
2	U	590	MET
2	U	598	ASP
2	U	605	LEU
3	D	57	GLN
3	D	63	VAL

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Mol	Chain	Res	Type
3	D	81	VAL
3	D	103	THR
3	D	111	LEU
3	D	114	GLN
3	D	143	ASP
3	D	168	ASP
3	D	169	LYS
4	m	203	ASP
4	m	208	VAL
4	m	209	LYS
5	p	7	ASP
5	p	19	TRP
5	p	30	ASP
5	p	35	LEU
5	p	47	VAL
5	u	1	MET
5	u	3	LEU
5	u	14	THR
5	u	15	LEU
5	u	48	PHE
5	z	15	LEU
5	z	19	TRP
5	z	23	THR
5	z	26	LEU
5	z	37	LYS
5	z	39	VAL
5	z	46	LYS
5	z	47	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	82	GLN
1	O	117	ASN
1	O	174	HIS
1	O	175	GLN
1	O	375	GLN
2	A	120	GLN
2	A	195	ASN
2	A	243	HIS
2	A	440	GLN
3	B	108	HIS

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Mol	Chain	Res	Type
3	B	114	GLN
3	B	140	ASN
2	U	120	GLN
2	U	195	ASN
2	U	243	HIS
2	U	264	GLN
3	D	20	GLN
3	D	108	HIS
5	u	32	HIS
5	u	42	ASN
5	u	45	ASN
5	z	42	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

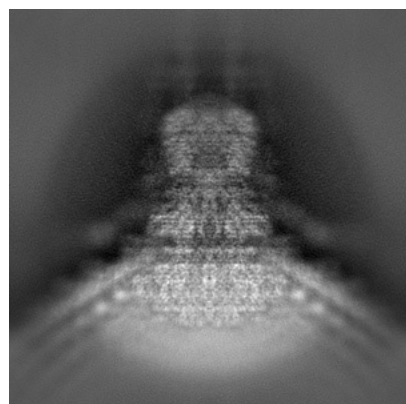
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60197. These allow visual inspection of the internal detail of the map and identification of artifacts.

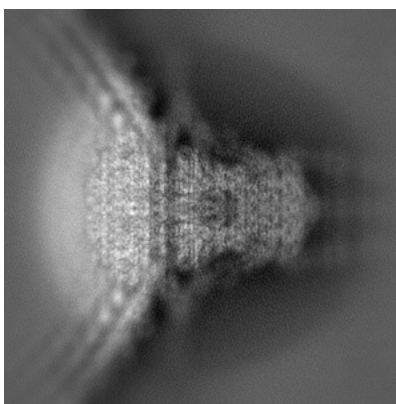
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

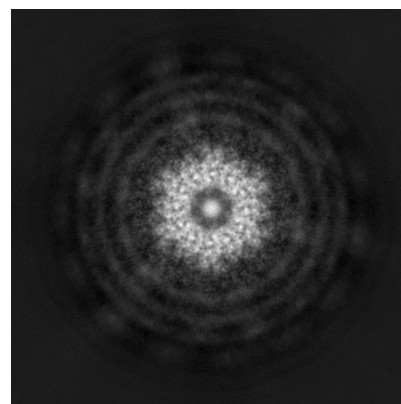
6.1.1 Primary map



X

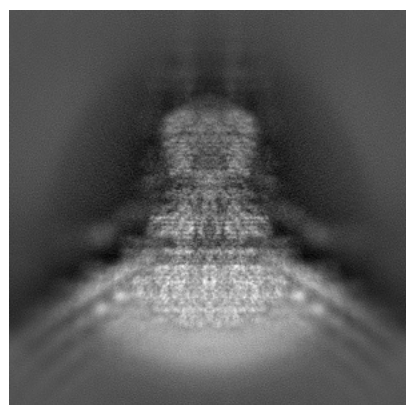


Y

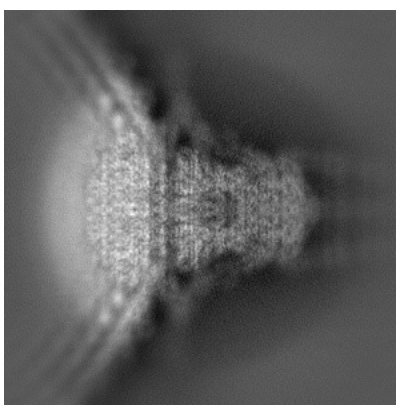


Z

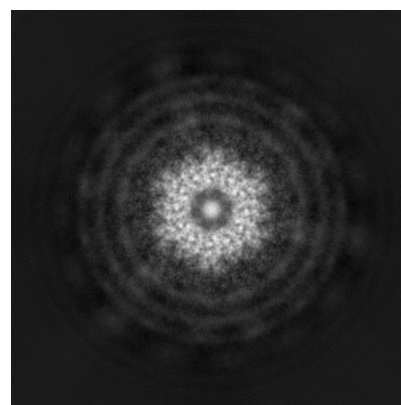
6.1.2 Raw map



X



Y

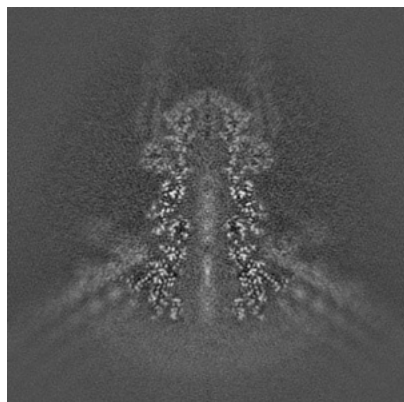


Z

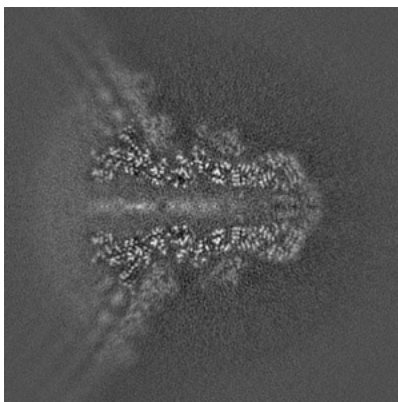
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

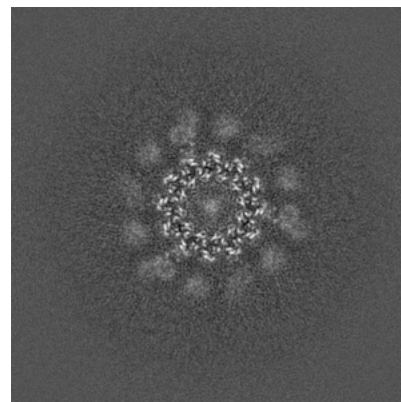
6.2.1 Primary map



X Index: 200

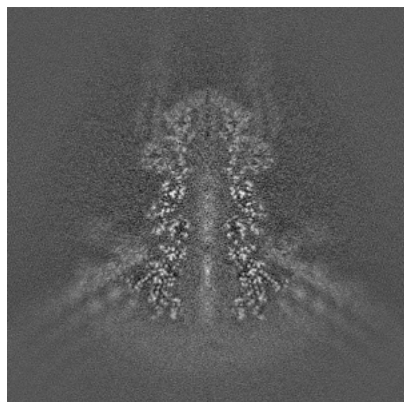


Y Index: 200

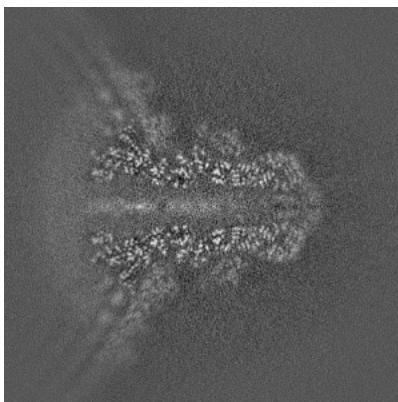


Z Index: 200

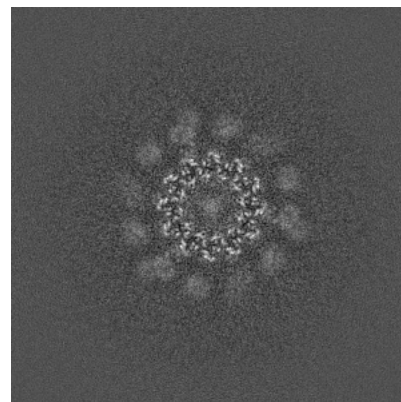
6.2.2 Raw map



X Index: 200



Y Index: 200

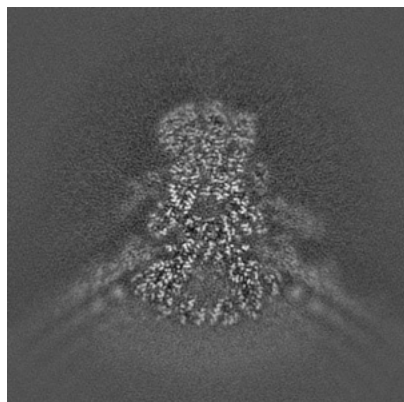


Z Index: 200

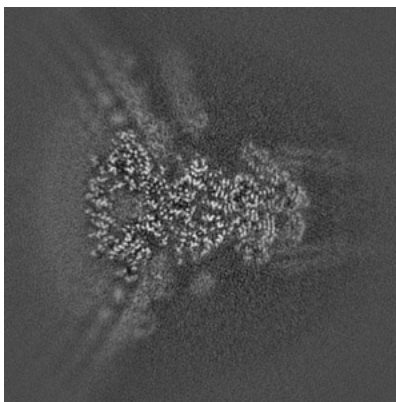
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

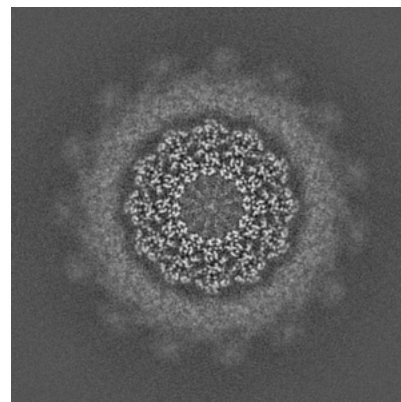
6.3.1 Primary map



X Index: 176

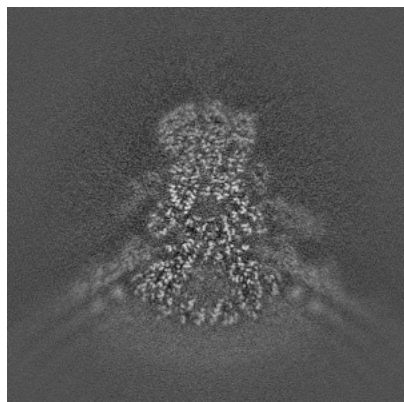


Y Index: 173

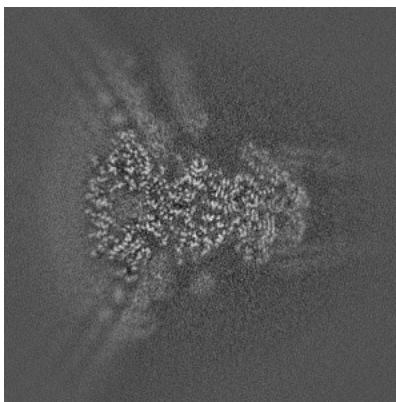


Z Index: 127

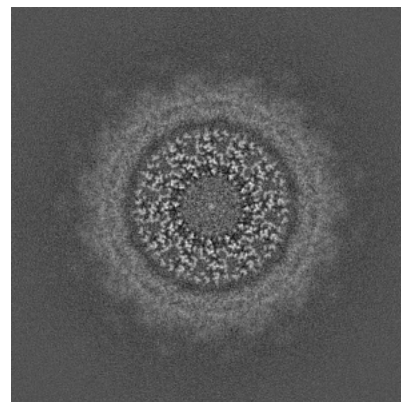
6.3.2 Raw map



X Index: 176



Y Index: 173

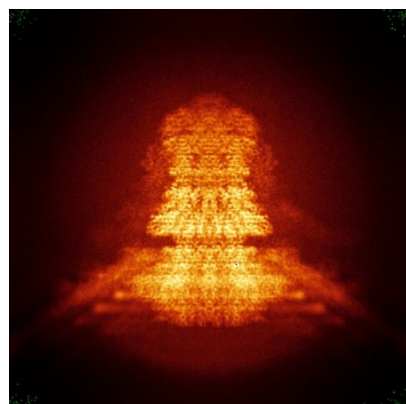


Z Index: 132

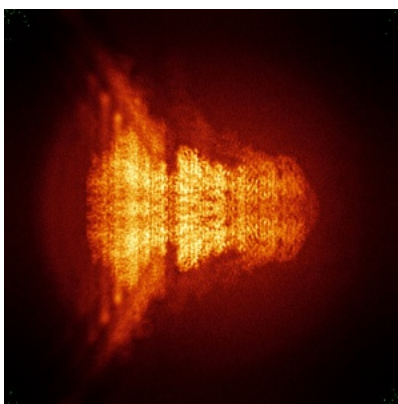
The images above show the largest variance slices of the map in three orthogonal directions.

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

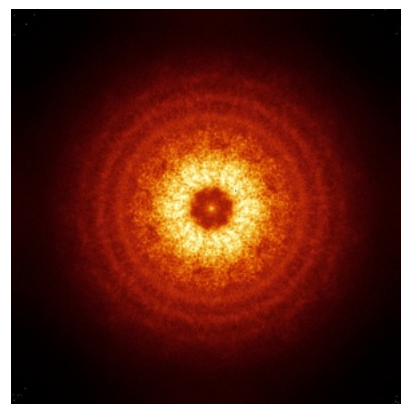
6.4.1 Primary map



X

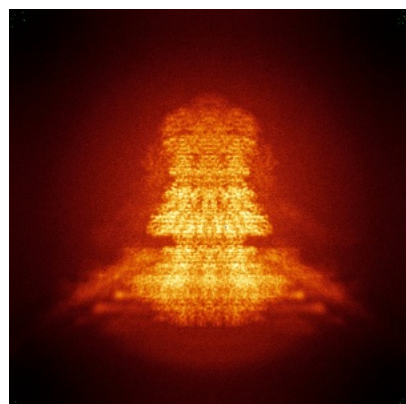


Y

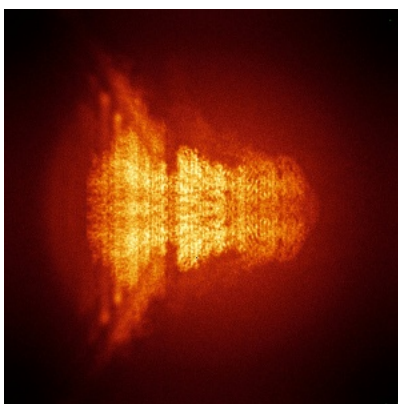


Z

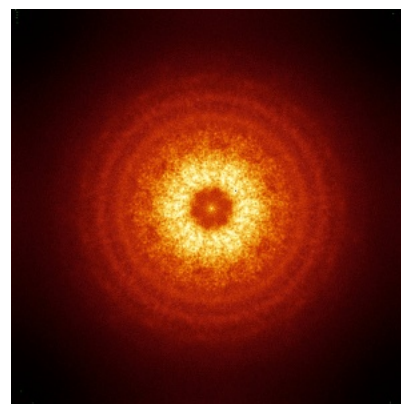
6.4.2 Raw map



X



Y

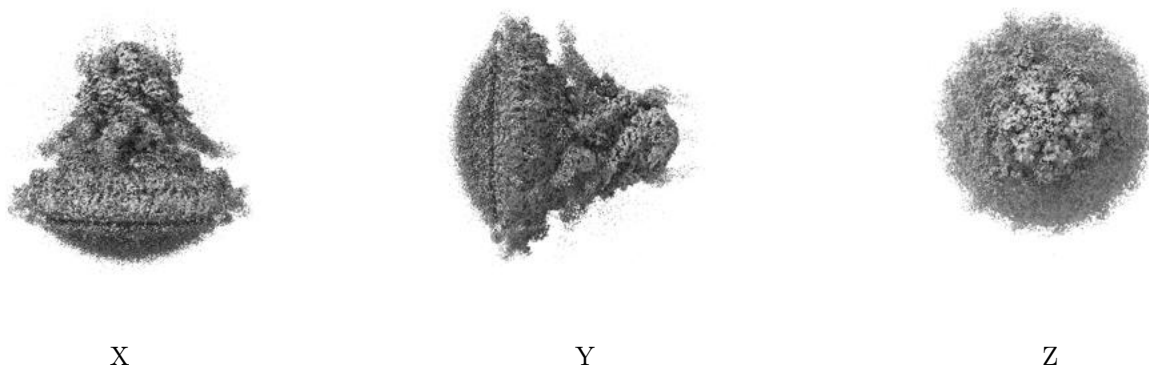


Z

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 1.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

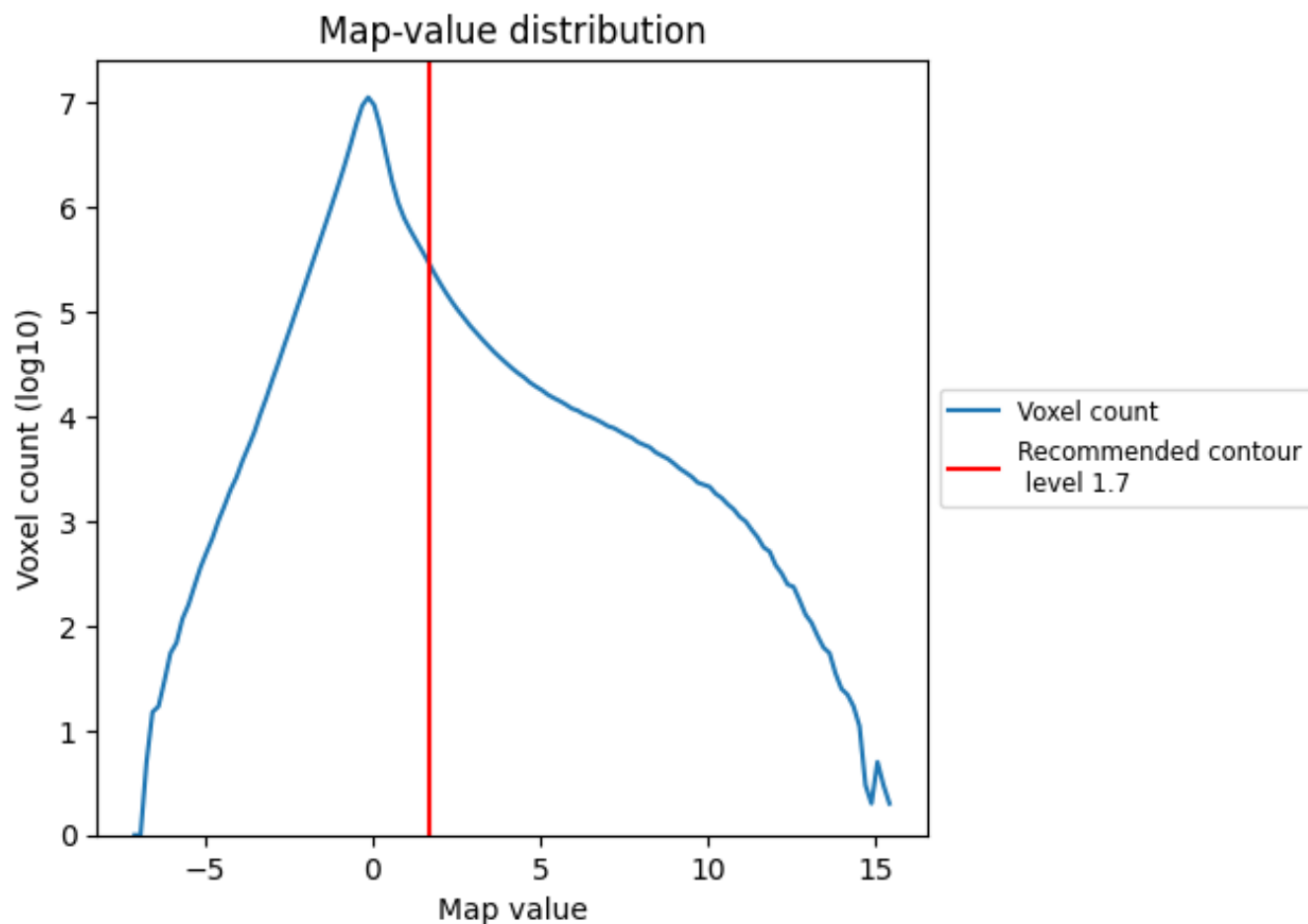
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

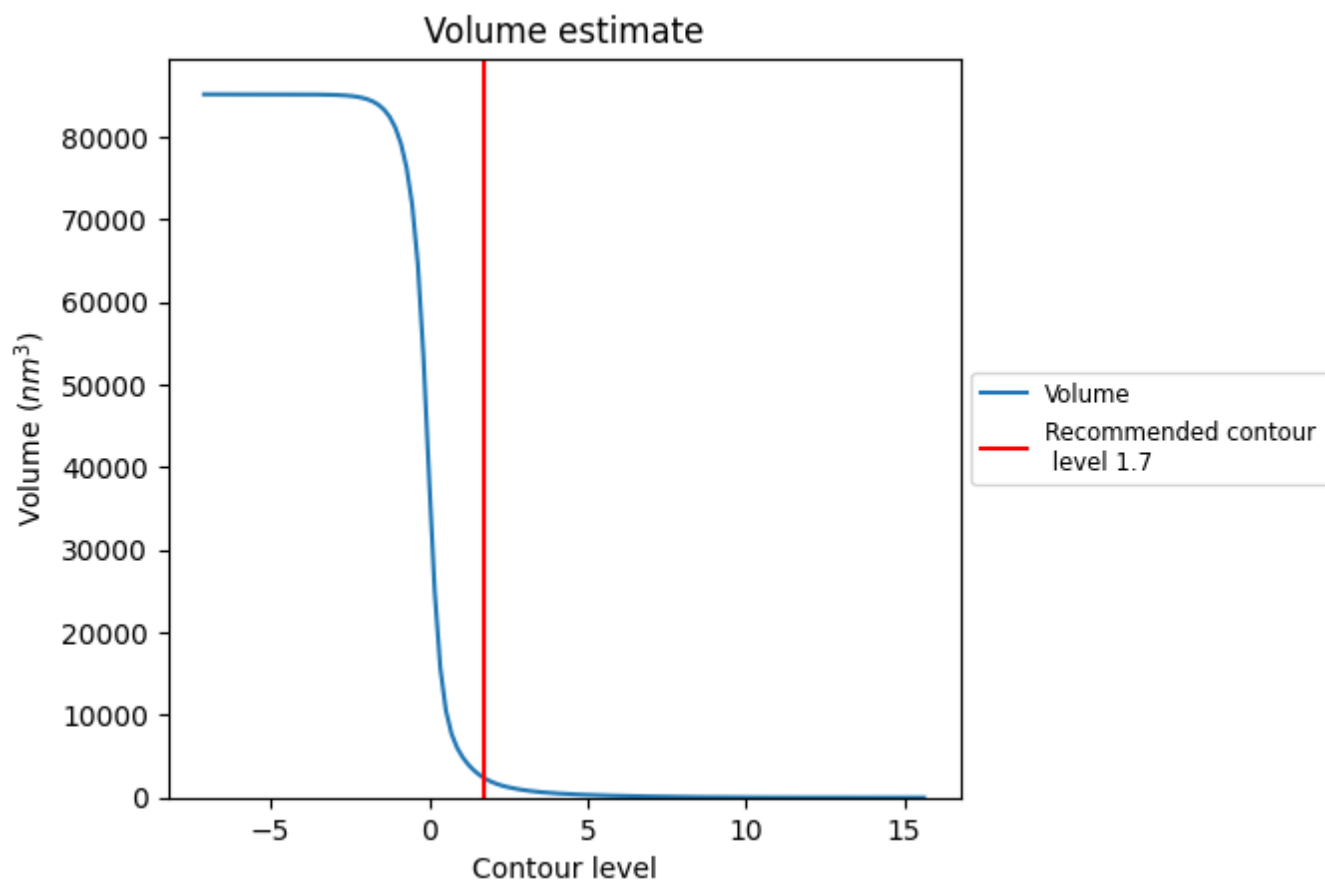
This section contains the results of statistical analysis of the map.

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.

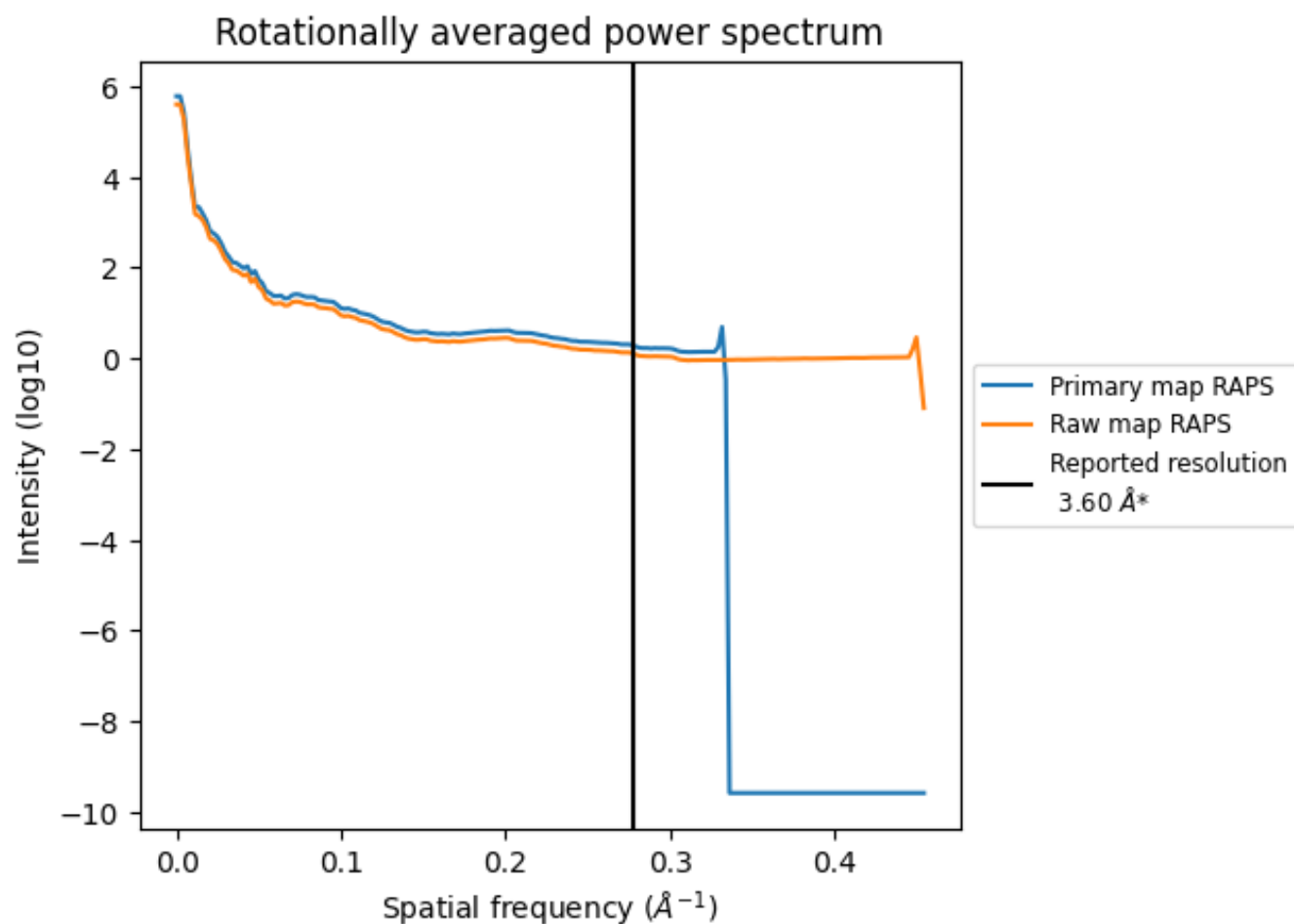
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2461 nm^3 ; this corresponds to an approximate mass of 2224 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 ⓘ

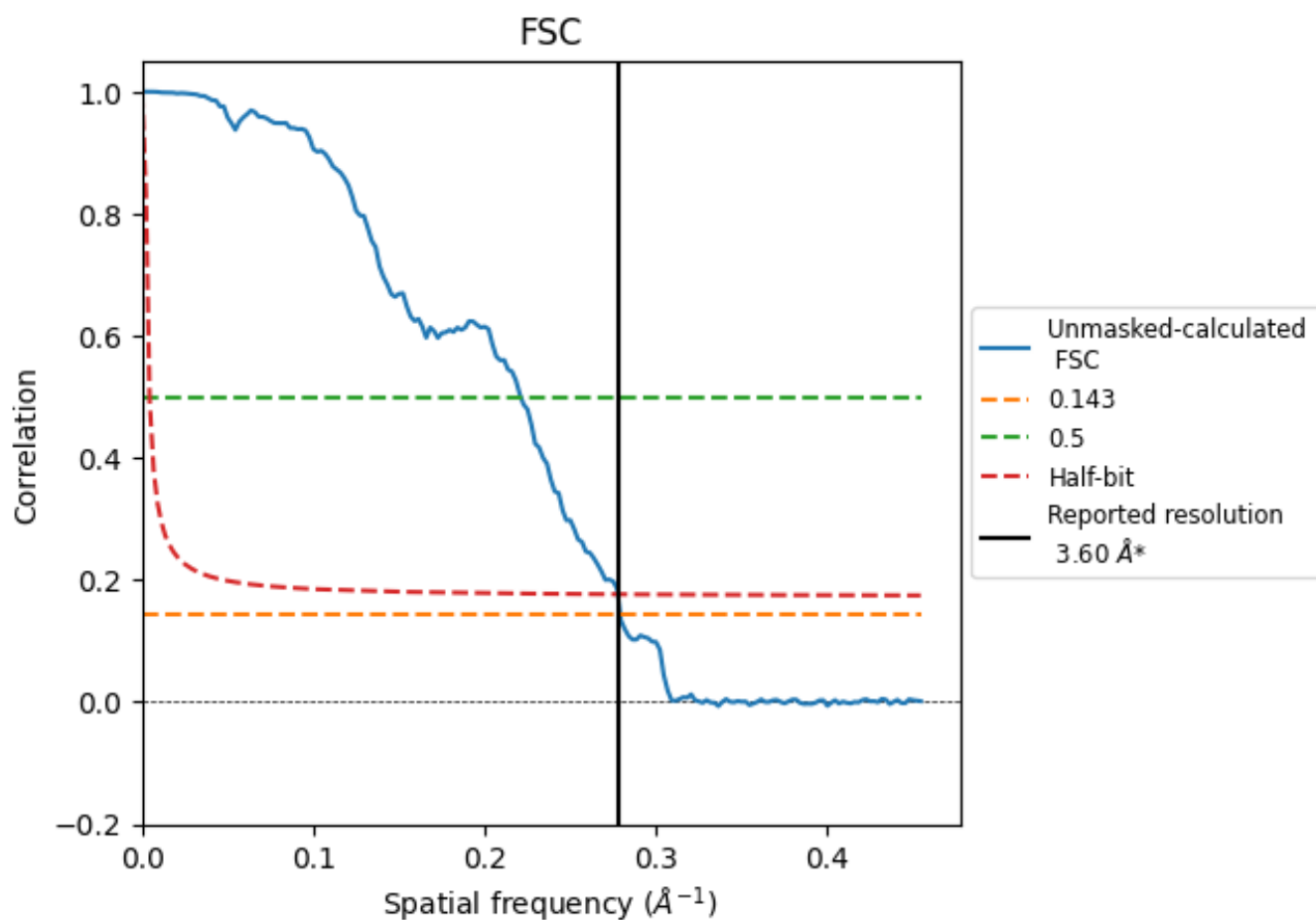


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.52	3.60

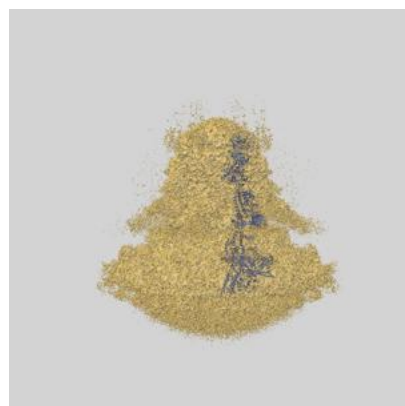
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60197 and PDB model 8ZKK. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

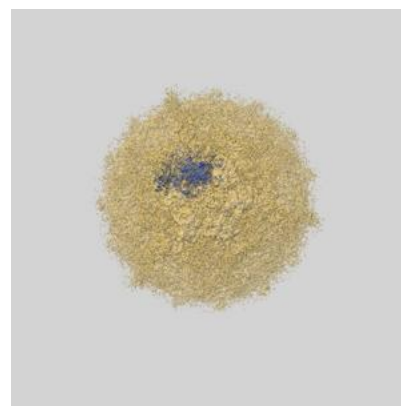
9.1.1 Map-model overlay [i](#)



X

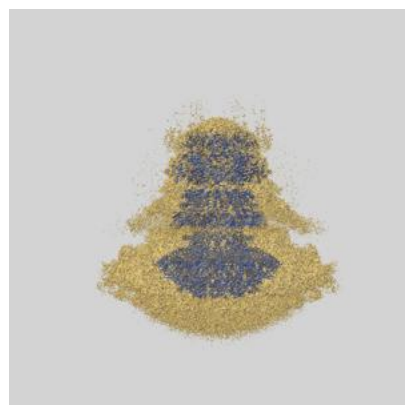


Y

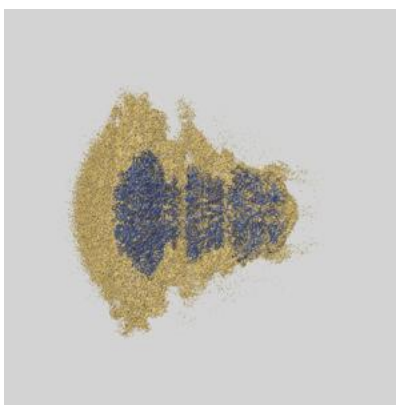


Z

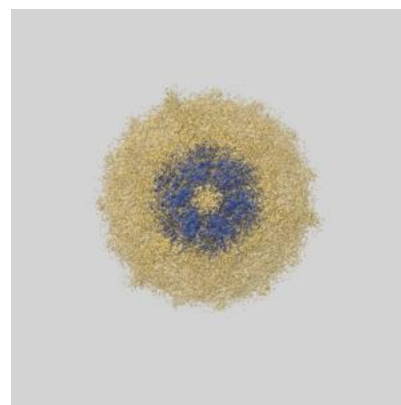
9.1.2 Map-model assembly overlay [i](#)



X



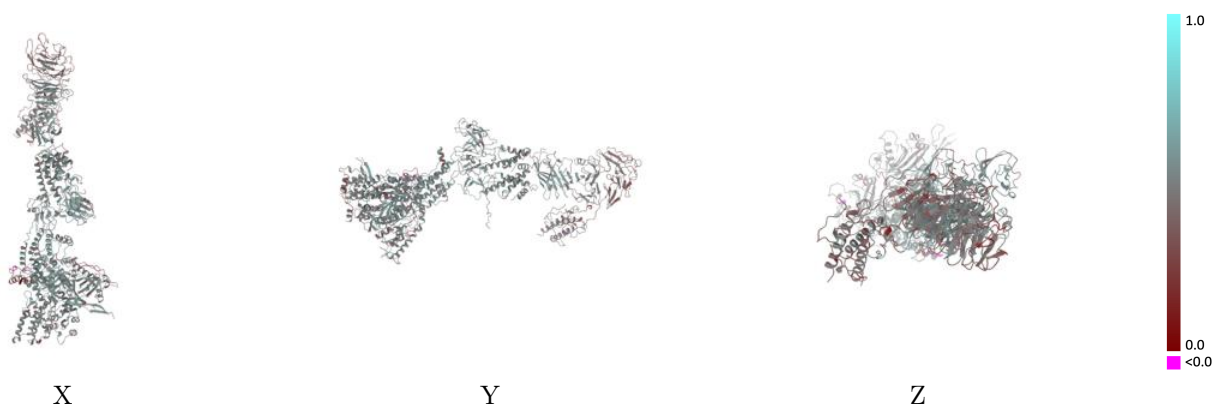
Y



Z

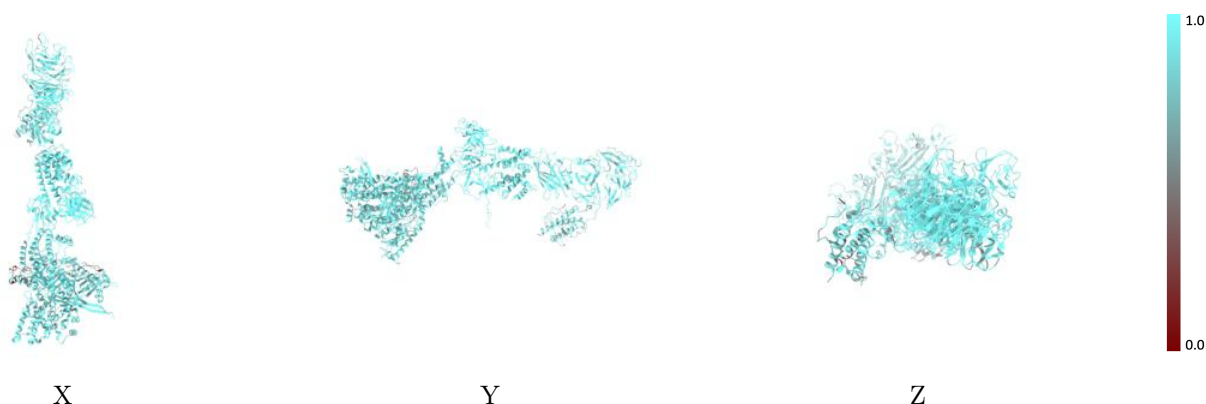
The images above show the 3D surface view of the map at the recommended contour level 1.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



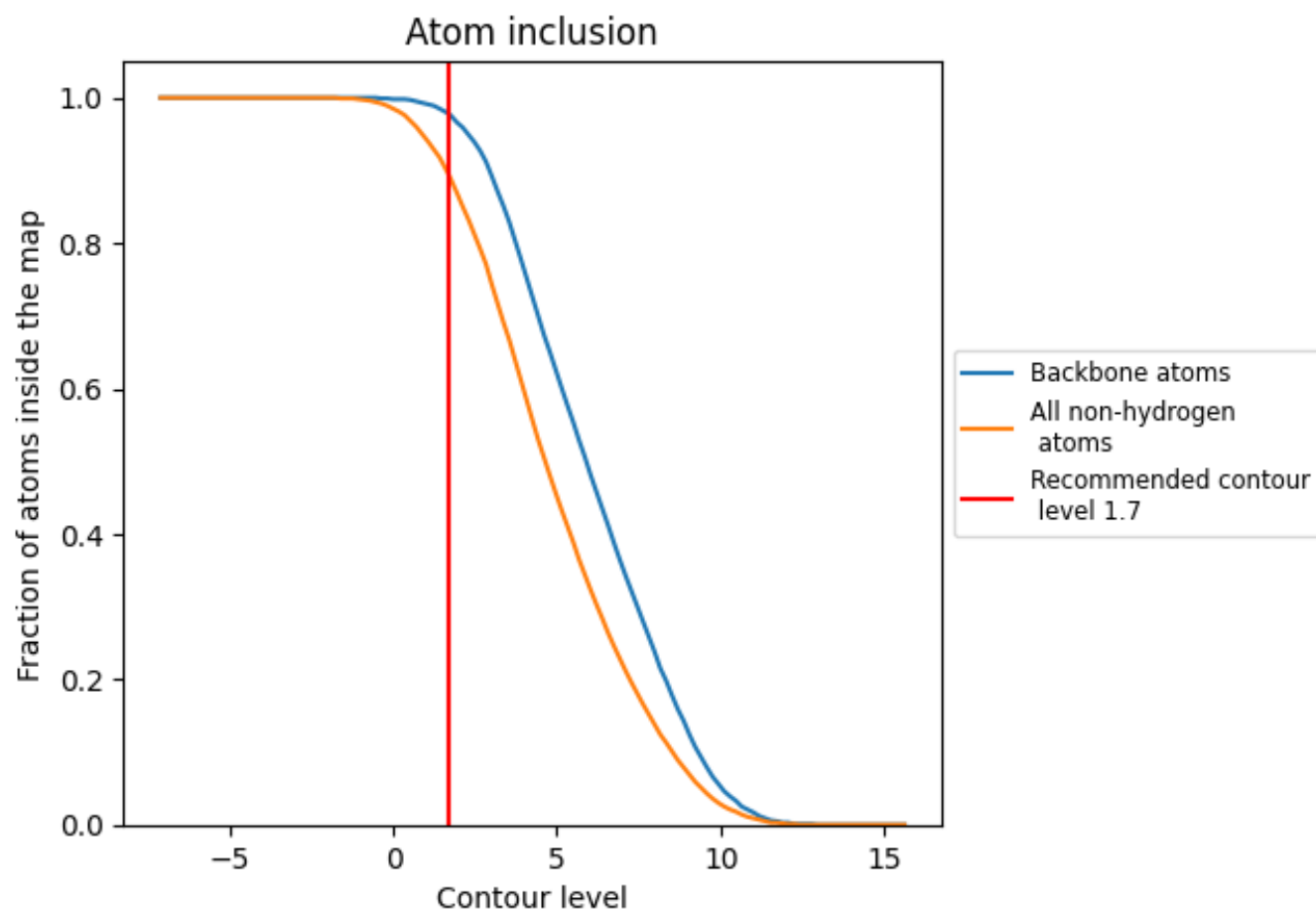
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 89% 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 (1.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.4770
A	0.8810	0.4900
B	0.9510	0.5120
D	0.9450	0.5060
O	0.9110	0.4440
U	0.8820	0.4890
m	0.8990	0.4520
p	0.7670	0.4050
u	0.7960	0.4230
z	0.7830	0.4020

1.0

0.0

<0.0