



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:01 PM UTC

PDB ID : 7TQU / pdb_00007tqu
EMDB ID : EMD-26072
Title : Coxsackievirus A21 capsid subdomain in complex with mouse polyclonal antibody pAbC-1
Authors : Antanasijevic, A.; Ward, A.B.
Deposited on : 2022-01-27
Resolution : 3.80 Å(reported)
Based on initial model : 1Z7S

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:

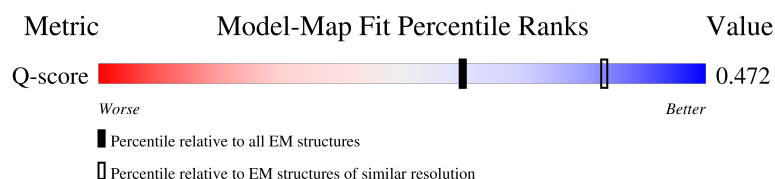
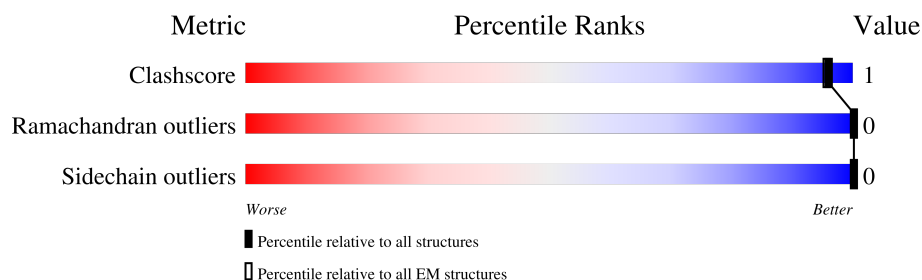
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.80 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.



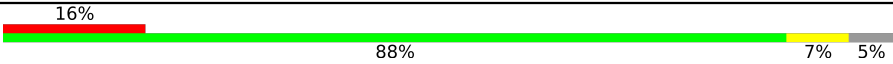
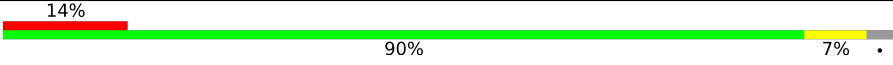
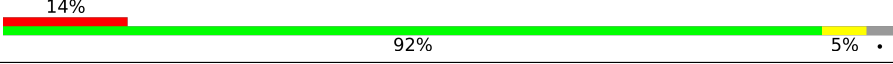
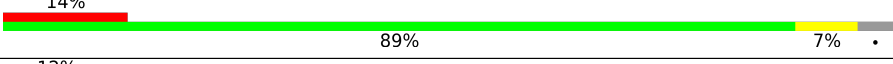
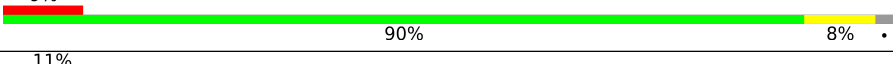
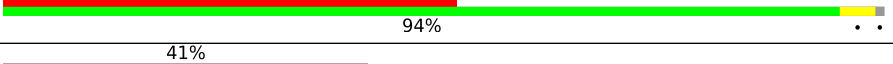
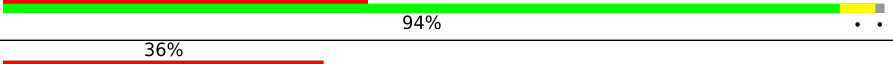
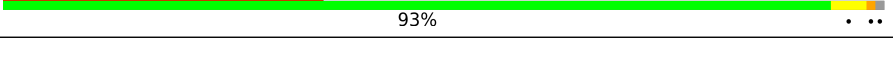
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	H	112	
2	L	102	
3	a	298	
3	e	298	

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Mol	Chain	Length	Quality of chain
3	i	298	
4	b	272	
4	f	272	
4	j	272	
5	c	240	
5	g	240	
5	k	240	
6	d	69	
6	h	69	
6	l	69	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 20891 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 pAbC-1 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	H	112	Total	C	N	O	0	0
			560	336	112	112		

- Molecule 2 is a protein called pAbC-1 light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	102	Total	C	N	O	0	0
			510	306	102	102		

- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	283	Total	C	N	O	S	0	0
			2226	1410	380	426	10		
3	e	282	Total	C	N	O	S	0	0
			2219	1405	379	425	10		
3	i	283	Total	C	N	O	S	0	0
			2226	1410	380	426	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	290	ALA	THR	conflict	UNP Q7T7N6
e	290	ALA	THR	conflict	UNP Q7T7N6
i	290	ALA	THR	conflict	UNP Q7T7N6

- Molecule 4 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	263	Total	C	N	O	S	0	0
			2043	1300	345	386	12		
4	f	265	Total	C	N	O	S	0	0
			2057	1308	347	391	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	j	261	Total	C	N	O	S	0	0
			2029	1293	342	383	11		

- Molecule 5 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	233	Total	C	N	O	S	0	0
			1801	1148	297	336	20		
5	g	234	Total	C	N	O	S	0	0
			1810	1154	299	337	20		
5	k	236	Total	C	N	O	S	0	0
			1826	1166	301	339	20		

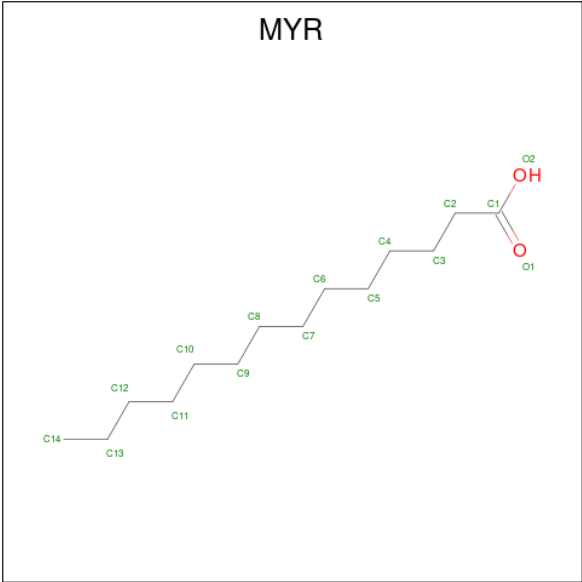
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	225	ARG	LYS	conflict	UNP Q7T7N6
g	225	ARG	LYS	conflict	UNP Q7T7N6
k	225	ARG	LYS	conflict	UNP Q7T7N6

- Molecule 6 is a protein called VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	h	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	l	68	Total	C	N	O	S	0	0
			512	311	90	110	1		

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).

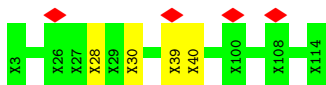


Mol	Chain	Residues	Atoms			AltConf
7	a	1	Total	C	O	0
			16	14	2	
7	e	1	Total	C	O	0
			16	14	2	
7	i	1	Total	C	O	0
			16	14	2	

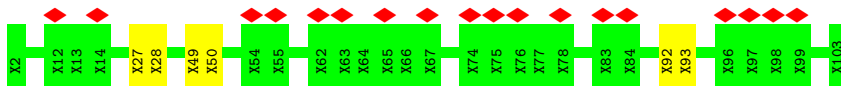
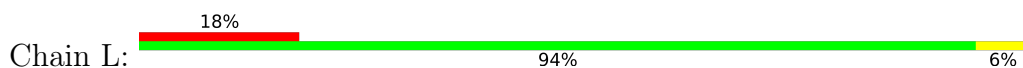
3 Residue-property plots [i](#)

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

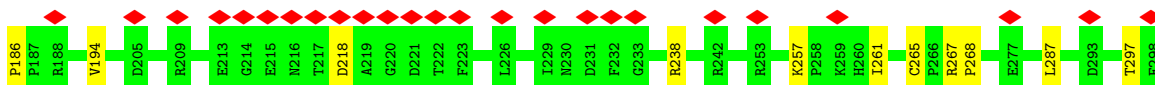
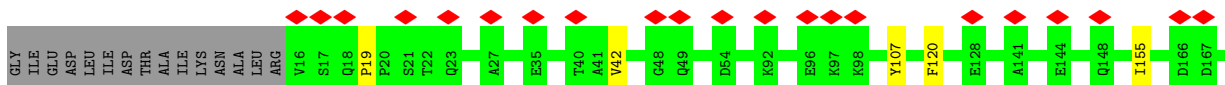
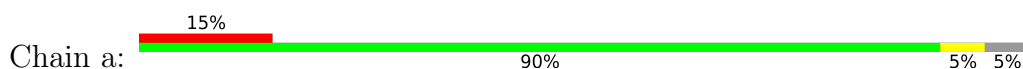
- Molecule 1: pAbC-1 heavy chain



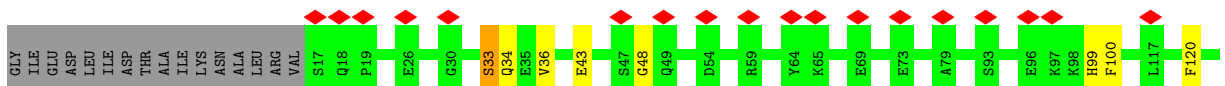
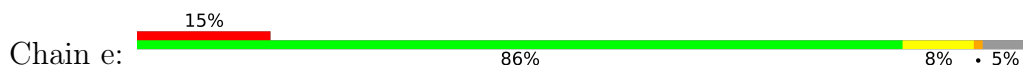
- Molecule 2: pAbC-1 light chain

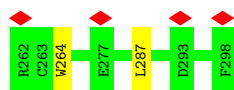


- Molecule 3: VP1

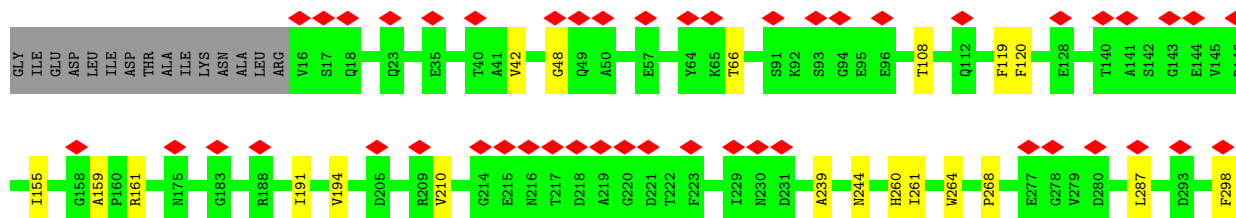
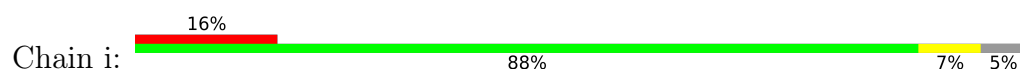


- Molecule 3: VP1

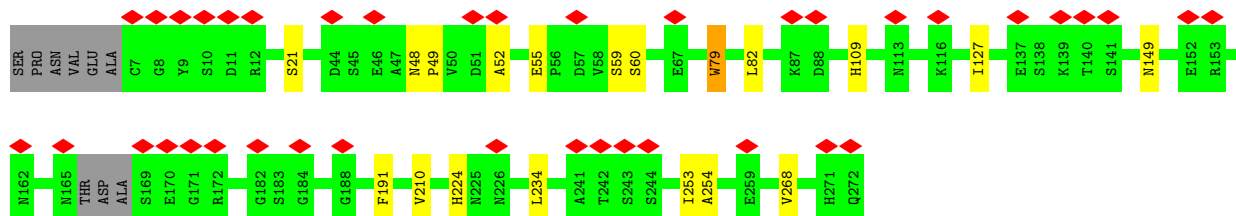
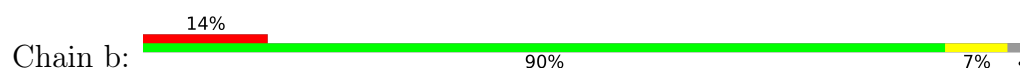




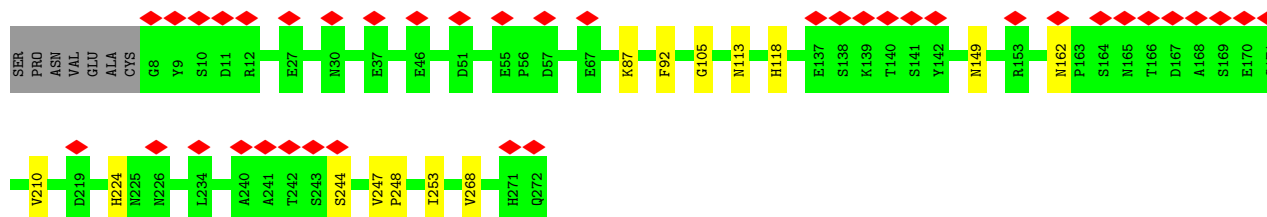
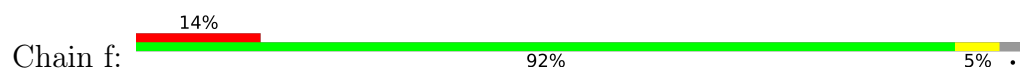
• Molecule 3: VP1



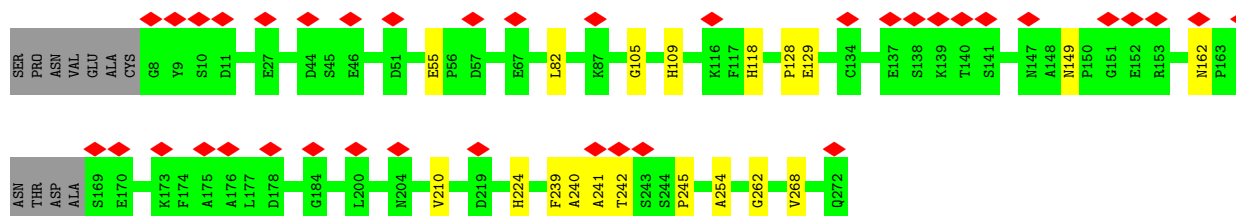
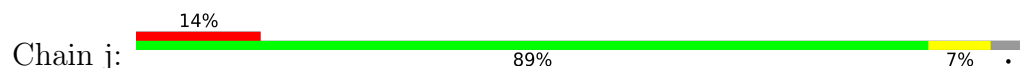
• Molecule 4: VP2



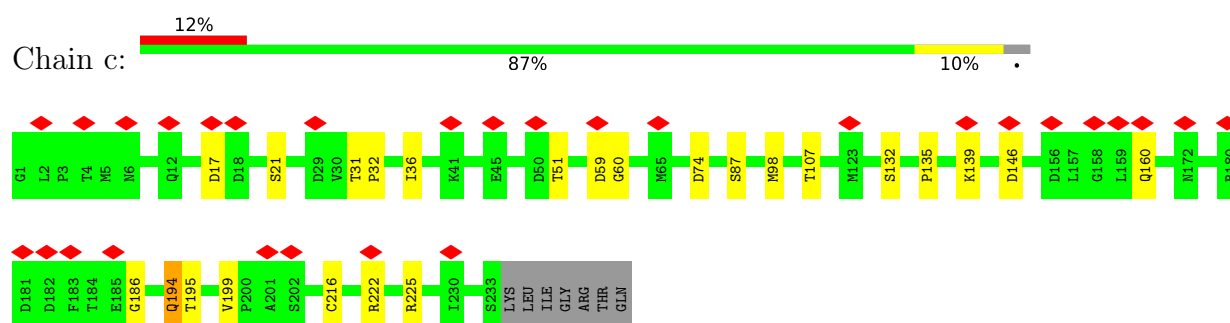
• Molecule 4: VP2



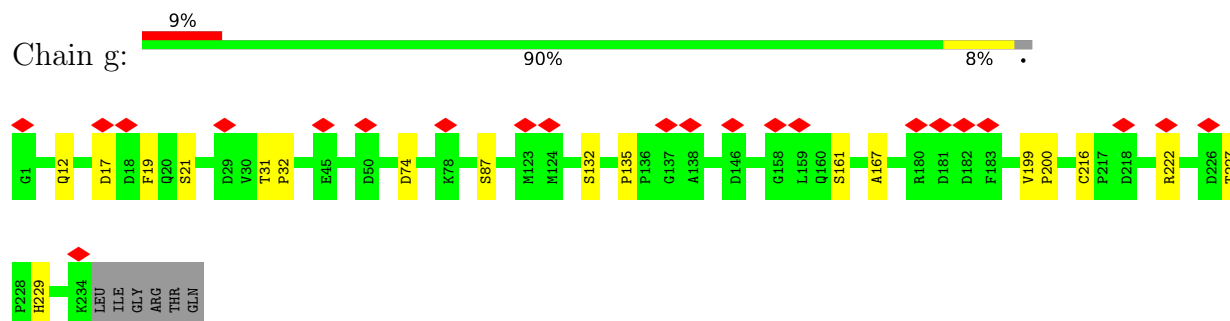
• Molecule 4: VP2



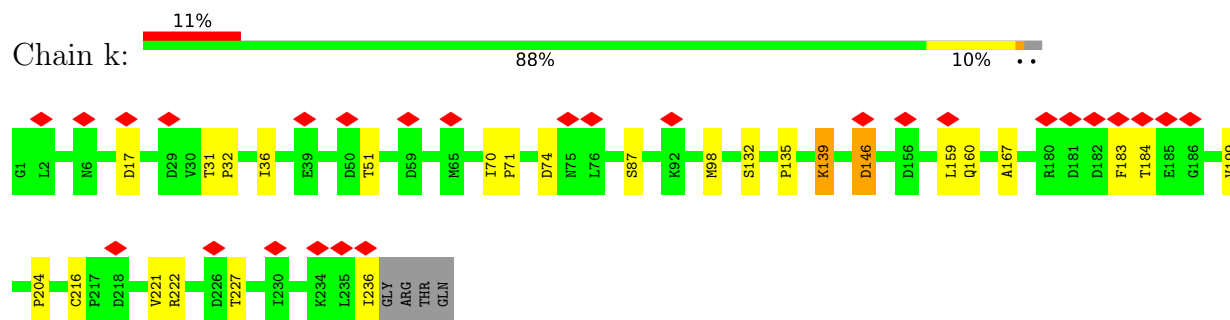
• Molecule 5: VP3



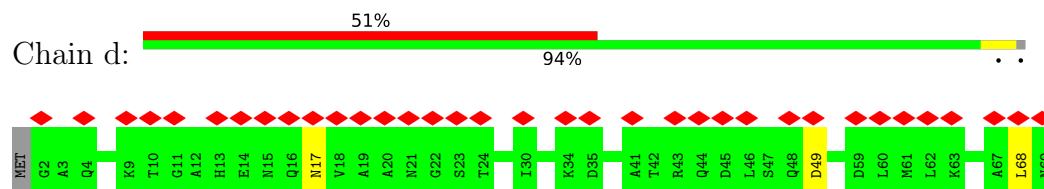
- Molecule 5: VP3



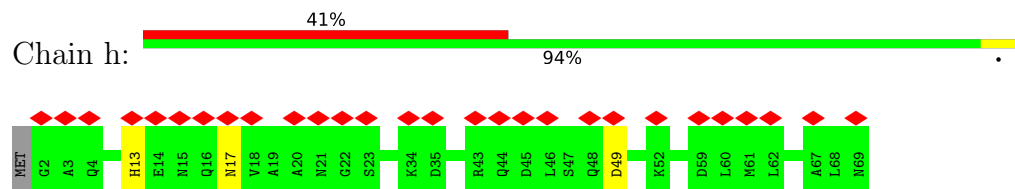
- Molecule 5: VP3



- Molecule 6: VP4

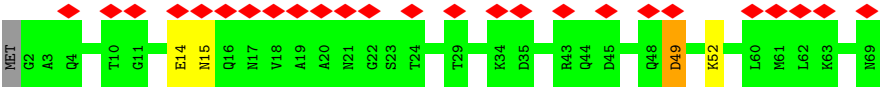


- Molecule 6: VP4



- Molecule 6: VP4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19748	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size ($\text{\AA}$)	292.59998, 292.59998, 292.59998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	$\# Z > 5$
3	a	1.13	1/2288 (0.0%)	1.34	22/3121 (0.7%)
3	e	1.12	3/2281 (0.1%)	1.34	28/3111 (0.9%)
3	i	1.13	3/2288 (0.1%)	1.32	26/3121 (0.8%)
4	b	1.18	2/2099 (0.1%)	1.34	20/2870 (0.7%)
4	f	1.16	3/2114 (0.1%)	1.31	17/2893 (0.6%)
4	j	1.23	3/2085 (0.1%)	1.31	19/2851 (0.7%)
5	c	1.08	0/1850	1.32	20/2520 (0.8%)
5	g	1.08	0/1859	1.38	24/2531 (0.9%)
5	k	1.16	2/1875 (0.1%)	1.45	27/2553 (1.1%)
6	d	1.01	0/519	1.15	4/705 (0.6%)
6	h	1.02	0/519	1.16	4/705 (0.6%)
6	l	1.00	0/519	1.23	4/705 (0.6%)
All	All	1.13	17/20296 (0.1%)	1.33	215/27686 (0.8%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	k	236	ILE	CB-CG1	7.32	1.68	1.53
3	i	268	PRO	CA-CB	-6.10	1.48	1.54
4	f	224	HIS	CB-CG	-5.98	1.41	1.50
5	k	221	VAL	CA-C	5.96	1.58	1.52
4	b	224	HIS	CB-CG	-5.72	1.42	1.50
4	f	248	PRO	N-CD	-5.55	1.40	1.47
4	b	109	HIS	CB-CG	-5.54	1.42	1.50
4	f	113	ASN	CB-CG	-5.46	1.38	1.52
4	j	224	HIS	CB-CG	-5.42	1.42	1.50
3	e	100	PHE	CB-CG	-5.36	1.38	1.50
3	e	170	TRP	NE1-CE2	-5.33	1.31	1.37
4	j	109	HIS	CB-CG	-5.16	1.43	1.50
3	i	298	PHE	CG-CD2	5.14	1.49	1.38
3	a	268	PRO	CA-CB	-5.14	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	43	GLU	CG-CD	-5.11	1.39	1.52
4	j	129	GLU	CG-CD	-5.10	1.39	1.52
3	i	264	TRP	NE1-CE2	-5.06	1.31	1.37

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	k	221	VAL	N-CA-C	11.79	124.52	113.20
5	k	135	PRO	CA-C-N	9.44	129.27	120.21
5	k	135	PRO	C-N-CA	9.44	129.27	120.21
3	e	264	TRP	N-CA-C	8.82	123.35	112.59
5	k	222	ARG	CB-CA-C	-8.67	106.57	116.54
4	b	234	LEU	N-CA-C	-8.56	103.35	113.88
3	i	42	VAL	N-CA-C	-8.42	104.97	113.47
4	j	268	VAL	CA-C-N	8.26	128.14	120.21
4	j	268	VAL	C-N-CA	8.26	128.14	120.21
5	k	222	ARG	N-CA-C	8.25	120.85	108.31
4	f	268	VAL	CA-C-N	8.22	128.72	119.92
4	f	268	VAL	C-N-CA	8.22	128.72	119.92
5	k	159	LEU	N-CA-C	-8.04	103.61	113.41
5	g	135	PRO	CA-C-N	7.83	129.63	119.84
5	g	135	PRO	C-N-CA	7.83	129.63	119.84
3	a	42	VAL	N-CA-C	-7.60	105.73	113.10
3	i	155	ILE	CA-C-N	7.60	125.21	119.66
3	i	155	ILE	C-N-CA	7.60	125.21	119.66
4	b	268	VAL	CA-C-N	7.60	127.50	120.21
4	b	268	VAL	C-N-CA	7.60	127.50	120.21
4	j	162	ASN	CA-C-N	7.57	127.58	119.78
4	j	162	ASN	C-N-CA	7.57	127.58	119.78
5	k	227	THR	CA-C-N	7.57	127.74	119.87
5	k	227	THR	C-N-CA	7.57	127.74	119.87
5	g	87	SER	CA-C-N	7.48	128.15	119.47
5	g	87	SER	C-N-CA	7.48	128.15	119.47
5	k	31	THR	CA-C-N	7.45	125.02	119.66
5	k	31	THR	C-N-CA	7.45	125.02	119.66
5	c	31	THR	CA-C-N	7.41	125.07	119.66
5	c	31	THR	C-N-CA	7.41	125.07	119.66
5	c	199	VAL	CA-C-N	7.39	127.31	120.21
5	c	199	VAL	C-N-CA	7.39	127.31	120.21
4	b	149	ASN	CA-C-N	7.39	127.02	119.56
4	b	149	ASN	C-N-CA	7.39	127.02	119.56
4	f	149	ASN	CA-C-N	7.29	127.45	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	149	ASN	C-N-CA	7.29	127.45	119.87
5	c	135	PRO	CA-C-N	7.21	127.17	120.03
5	c	135	PRO	C-N-CA	7.21	127.17	120.03
3	e	261	ILE	N-CA-C	7.13	118.56	108.36
5	k	199	VAL	CA-C-N	7.04	126.97	120.21
5	k	199	VAL	C-N-CA	7.04	126.97	120.21
5	k	167	ALA	CA-C-N	6.93	126.86	120.21
5	k	167	ALA	C-N-CA	6.93	126.86	120.21
3	a	186	PRO	CA-C-N	6.84	126.76	119.85
3	a	186	PRO	C-N-CA	6.84	126.76	119.85
5	g	31	THR	CA-C-N	6.81	124.56	119.66
5	g	31	THR	C-N-CA	6.81	124.56	119.66
5	k	32	PRO	CA-C-N	6.74	126.91	120.31
5	k	32	PRO	C-N-CA	6.74	126.91	120.31
6	d	17	ASN	CA-C-N	6.60	129.80	120.42
6	d	17	ASN	C-N-CA	6.60	129.80	120.42
5	c	194	GLN	N-CA-C	-6.60	99.54	110.17
3	a	268	PRO	CA-C-N	6.56	126.52	120.03
3	a	268	PRO	C-N-CA	6.56	126.52	120.03
5	k	160	GLN	N-CA-C	-6.55	97.86	108.41
5	k	216	CYS	CA-C-N	6.54	126.23	119.82
5	k	216	CYS	C-N-CA	6.54	126.23	119.82
5	k	132	SER	N-CA-C	6.54	120.18	109.06
3	a	297	THR	N-CA-C	6.52	118.39	111.28
3	i	287	LEU	CA-C-N	6.48	126.11	119.56
3	i	287	LEU	C-N-CA	6.48	126.11	119.56
3	i	264	TRP	N-CA-C	6.41	121.26	113.38
5	c	87	SER	CA-C-N	6.37	126.85	119.47
5	c	87	SER	C-N-CA	6.37	126.85	119.47
5	g	229	HIS	CA-C-N	-6.36	115.31	123.19
5	g	229	HIS	C-N-CA	-6.36	115.31	123.19
3	e	33	SER	N-CA-C	6.34	116.94	108.38
5	g	199	VAL	CA-C-N	6.34	126.79	120.52
5	g	199	VAL	C-N-CA	6.34	126.79	120.52
3	i	120	PHE	CA-CB-CG	-6.33	107.47	113.80
4	j	242	THR	N-CA-C	-6.32	104.39	111.28
5	g	216	CYS	CA-C-N	6.28	125.97	119.56
5	g	216	CYS	C-N-CA	6.28	125.97	119.56
5	k	87	SER	CA-C-N	6.22	125.91	119.56
5	k	87	SER	C-N-CA	6.22	125.91	119.56
3	i	261	ILE	N-CA-C	6.21	116.87	108.17
3	a	120	PHE	CA-CB-CG	-6.20	107.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	188	ARG	CB-CG-CD	-6.20	97.05	111.30
3	a	261	ILE	N-CA-C	6.15	117.16	108.36
5	c	186	GLY	N-CA-C	6.15	120.64	112.77
5	c	132	SER	N-CA-C	6.12	119.47	109.06
4	b	55	GLU	CA-C-N	6.09	125.77	119.56
4	b	55	GLU	C-N-CA	6.09	125.77	119.56
4	f	247	VAL	CA-C-N	6.08	126.27	120.31
4	f	247	VAL	C-N-CA	6.08	126.27	120.31
3	e	161	ARG	CA-C-N	6.07	125.98	119.85
3	e	161	ARG	C-N-CA	6.07	125.98	119.85
5	g	32	PRO	CA-C-N	6.04	126.55	120.14
5	g	32	PRO	C-N-CA	6.04	126.55	120.14
3	e	287	LEU	CA-C-N	6.03	125.65	119.56
3	e	287	LEU	C-N-CA	6.03	125.65	119.56
4	j	55	GLU	CA-C-N	6.02	125.64	119.56
4	j	55	GLU	C-N-CA	6.02	125.64	119.56
5	g	222	ARG	N-CA-C	6.02	120.45	111.96
4	j	149	ASN	CA-C-N	6.02	126.13	119.87
4	j	149	ASN	C-N-CA	6.02	126.13	119.87
3	a	287	LEU	CA-C-N	6.00	125.62	119.56
3	a	287	LEU	C-N-CA	6.00	125.62	119.56
5	g	161	SER	N-CA-C	5.96	120.28	112.89
6	l	14	GLU	N-CA-C	5.96	118.90	110.50
4	b	127	ILE	N-CA-C	5.93	114.49	107.73
5	c	21	SER	CA-C-N	5.92	125.86	119.76
5	c	21	SER	C-N-CA	5.92	125.86	119.76
5	g	12	GLN	CB-CG-CD	-5.88	102.60	112.60
4	b	254	ALA	CA-C-N	5.88	125.79	119.85
4	b	254	ALA	C-N-CA	5.88	125.79	119.85
4	j	82	LEU	N-CA-C	5.88	120.49	112.55
3	a	238	ARG	N-CA-C	5.85	119.01	109.24
6	h	49	ASP	CA-C-N	5.83	125.44	119.56
6	h	49	ASP	C-N-CA	5.83	125.44	119.56
4	j	128	PRO	N-CA-C	-5.82	102.05	111.19
6	l	49	ASP	CA-C-N	5.79	125.47	119.56
6	l	49	ASP	C-N-CA	5.79	125.47	119.56
3	e	120	PHE	CA-CB-CG	-5.78	108.02	113.80
3	e	127	LEU	N-CA-C	5.77	118.31	108.90
4	f	118	HIS	CA-CB-CG	5.76	119.56	113.80
6	l	15	ASN	N-CA-C	5.76	121.57	113.56
3	i	161	ARG	CA-C-N	5.76	125.67	119.85
3	i	161	ARG	C-N-CA	5.76	125.67	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	194	VAL	CB-CA-C	-5.72	104.67	111.65
5	g	167	ALA	CA-C-N	5.71	126.02	119.92
5	g	167	ALA	C-N-CA	5.71	126.02	119.92
5	k	36	ILE	CA-C-N	5.71	125.66	119.78
5	k	36	ILE	C-N-CA	5.71	125.66	119.78
3	e	223	PHE	CA-CB-CG	5.69	119.49	113.80
5	k	146	ASP	N-CA-C	-5.68	106.02	113.12
3	a	265	CYS	CA-C-N	5.67	125.57	119.85
3	a	265	CYS	C-N-CA	5.67	125.57	119.85
4	b	253	ILE	N-CA-C	5.64	116.87	108.46
4	j	105	GLY	N-CA-C	-5.61	103.72	112.58
6	h	17	ASN	CA-C-N	5.59	128.36	120.42
6	h	17	ASN	C-N-CA	5.59	128.36	120.42
4	b	79	TRP	N-CA-C	5.57	117.98	108.90
4	f	92	PHE	N-CA-C	-5.56	105.30	111.36
3	e	229	ILE	N-CA-C	5.47	116.52	111.81
3	e	36	VAL	CA-C-N	5.47	125.14	119.56
3	e	36	VAL	C-N-CA	5.47	125.14	119.56
4	f	253	ILE	N-CA-C	5.44	116.57	108.46
4	b	52	ALA	CA-C-N	5.44	125.35	119.85
4	b	52	ALA	C-N-CA	5.44	125.35	119.85
3	i	244	ASN	CA-C-N	5.44	125.11	119.56
3	i	244	ASN	C-N-CA	5.44	125.11	119.56
3	e	190	SER	N-CA-C	5.43	117.75	108.90
4	j	254	ALA	CA-C-N	5.39	125.33	119.78
4	j	254	ALA	C-N-CA	5.39	125.33	119.78
4	f	105	GLY	N-CA-C	-5.38	104.09	112.58
4	f	244	SER	CA-C-N	5.37	125.34	120.03
4	f	244	SER	C-N-CA	5.37	125.34	120.03
5	k	139	LYS	CA-C-N	5.35	123.56	119.66
5	k	139	LYS	C-N-CA	5.35	123.56	119.66
3	a	107	TYR	CA-C-N	5.35	127.44	120.28
3	a	107	TYR	C-N-CA	5.35	127.44	120.28
4	f	210	VAL	CA-C-N	5.33	125.31	120.03
4	f	210	VAL	C-N-CA	5.33	125.31	120.03
3	a	155	ILE	CA-C-N	5.30	125.83	120.38
3	a	155	ILE	C-N-CA	5.30	125.83	120.38
5	c	222	ARG	N-CA-C	5.29	120.39	113.88
3	e	239	ALA	N-CA-C	-5.27	103.07	110.50
4	b	21	SER	N-CA-C	5.26	116.99	108.41
4	j	210	VAL	CA-C-N	5.26	125.24	120.03
4	j	210	VAL	C-N-CA	5.26	125.24	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	b	224	HIS	N-CA-C	5.25	116.97	108.41
4	b	210	VAL	CA-C-N	5.25	125.45	120.31
4	b	210	VAL	C-N-CA	5.25	125.45	120.31
3	i	66	THR	N-CA-C	5.23	119.81	113.38
5	c	216	CYS	CA-C-N	5.22	125.53	119.47
5	c	216	CYS	C-N-CA	5.22	125.53	119.47
3	e	137	TYR	CA-C-N	5.22	125.68	120.04
3	e	137	TYR	C-N-CA	5.22	125.68	120.04
3	i	119	PHE	CA-CB-CG	5.22	119.02	113.80
3	i	239	ALA	N-CA-C	-5.21	103.16	110.50
5	c	32	PRO	CA-C-N	5.20	125.65	120.14
5	c	32	PRO	C-N-CA	5.20	125.65	120.14
5	g	227	THR	CA-C-N	5.20	125.65	120.04
5	g	227	THR	C-N-CA	5.20	125.65	120.04
5	c	36	ILE	CA-C-N	5.19	125.13	119.78
5	c	36	ILE	C-N-CA	5.19	125.13	119.78
3	i	194	VAL	CB-CA-C	-5.19	105.25	112.36
4	f	162	ASN	CA-C-N	5.18	125.16	120.03
4	f	162	ASN	C-N-CA	5.18	125.16	120.03
5	g	21	SER	CA-C-N	5.17	125.07	119.85
5	g	21	SER	C-N-CA	5.17	125.07	119.85
3	e	155	ILE	CA-C-N	5.17	125.70	120.38
3	e	155	ILE	C-N-CA	5.17	125.70	120.38
3	i	191	ILE	CA-C-N	5.16	125.14	120.03
3	i	191	ILE	C-N-CA	5.16	125.14	120.03
3	i	260	HIS	N-CA-C	-5.16	104.30	111.52
3	a	267	ARG	CA-C-N	5.15	123.36	119.66
3	a	267	ARG	C-N-CA	5.15	123.36	119.66
3	a	19	PRO	CA-C-N	5.14	125.38	119.83
3	a	19	PRO	C-N-CA	5.14	125.38	119.83
5	g	132	SER	N-CA-C	5.13	116.87	109.07
3	i	268	PRO	CA-C-N	5.12	125.10	120.03
3	i	268	PRO	C-N-CA	5.12	125.10	120.03
3	i	48	GLY	N-CA-C	-5.12	105.54	112.14
3	i	159	ALA	CA-C-N	5.10	125.01	119.76
3	i	159	ALA	C-N-CA	5.10	125.01	119.76
6	d	49	ASP	CA-C-N	5.10	124.89	119.28
6	d	49	ASP	C-N-CA	5.10	124.89	119.28
4	j	118	HIS	CA-CB-CG	5.10	118.90	113.80
4	b	191	PHE	CA-CB-CG	-5.09	108.71	113.80
4	j	262	GLY	N-CA-C	-5.07	105.30	112.81
3	i	210	VAL	CB-CA-C	-5.07	105.06	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	244	ASN	CA-C-N	5.07	125.35	119.47
3	e	244	ASN	C-N-CA	5.07	125.35	119.47
3	e	159	ALA	CA-C-N	5.06	124.97	119.76
3	e	159	ALA	C-N-CA	5.06	124.97	119.76
3	e	48	GLY	N-CA-C	-5.05	105.62	112.14
4	j	210	VAL	N-CA-C	5.05	115.69	107.71
4	b	82	LEU	N-CA-C	5.03	119.00	112.17
3	i	108	THR	N-CA-C	5.02	119.38	113.16
3	e	191	ILE	CA-C-N	5.01	124.99	120.03
3	e	191	ILE	C-N-CA	5.01	124.99	120.03
3	e	99	HIS	CA-CB-CG	5.00	118.81	113.80
4	f	87	LYS	N-CA-C	5.00	117.46	111.71

There are no chirality outliers.

There are no planarity outliers.

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	H	560	0	144	2	0
2	L	510	0	123	3	0
3	a	2226	0	2146	2	0
3	e	2219	0	2137	5	0
3	i	2226	0	2146	0	0
4	b	2043	0	1966	3	0
4	f	2057	0	1978	0	0
4	j	2029	0	1955	4	0
5	c	1801	0	1778	8	0
5	g	1810	0	1791	5	0
5	k	1826	0	1813	10	0
6	d	512	0	493	1	0
6	h	512	0	493	1	0
6	l	512	0	493	1	0
7	a	16	0	27	0	0
7	e	16	0	27	0	0
7	i	16	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20891	0	19537	38	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 1.

All (38) 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:k:70:ILE:HG22	5:k:71:PRO:HD2	1.76	0.65
5:c:194:GLN:O	5:c:195:THR:C	2.45	0.59
3:e:188:ARG:HH22	5:g:19:PHE:HB2	1.70	0.56
1:H:28:UNK:C	1:H:30:UNK:N	2.70	0.54
5:c:160:GLN:HE22	6:d:68:LEU:H	1.55	0.54
2:L:27:UNK:O	2:L:28:UNK:C	2.56	0.53
5:c:139:LYS:NZ	5:c:146:ASP:OD2	2.42	0.53
5:k:183:PHE:HD2	5:k:184:THR:HG23	1.73	0.52
5:k:70:ILE:CG2	5:k:71:PRO:HD2	2.42	0.50
5:k:139:LYS:NZ	5:k:146:ASP:OD1	2.46	0.49
5:k:183:PHE:CD2	5:k:184:THR:HG23	2.48	0.47
5:c:51:THR:HG21	5:c:98:MET:H	1.80	0.47
4:j:239:PHE:C	4:j:241:ALA:H	2.23	0.47
5:g:74:ASP:OD1	5:g:74:ASP:N	2.46	0.46
4:b:79:TRP:CD1	4:b:79:TRP:C	2.94	0.45
3:e:257:LYS:NZ	5:g:17:ASP:O	2.50	0.45
3:a:257:LYS:NZ	5:c:17:ASP:O	2.49	0.45
5:g:200:PRO:HA	4:j:239:PHE:HZ	1.82	0.45
3:e:188:ARG:HH22	5:g:19:PHE:CB	2.29	0.44
6:h:13:HIS:CG	6:h:13:HIS:O	2.71	0.44
5:k:51:THR:HG21	5:k:98:MET:H	1.83	0.43
5:k:74:ASP:N	5:k:74:ASP:OD1	2.48	0.43
5:c:107:THR:HG22	5:c:225:ARG:HD3	2.01	0.43
4:j:239:PHE:HB3	4:j:245:PRO:HB3	2.01	0.43
6:l:49:ASP:OD2	6:l:52:LYS:NZ	2.52	0.43
5:c:59:ASP:OD1	5:c:60:GLY:N	2.51	0.43
2:L:49:UNK:O	2:L:50:UNK:C	2.63	0.42
5:k:17:ASP:OD1	5:k:17:ASP:C	2.62	0.42
1:H:39:UNK:O	1:H:40:UNK:C	2.63	0.42
3:a:218:ASP:OD1	3:a:218:ASP:N	2.53	0.42
5:k:70:ILE:H	5:k:70:ILE:HG13	1.68	0.42
5:c:74:ASP:N	5:c:74:ASP:OD1	2.48	0.42
2:L:92:UNK:O	2:L:93:UNK:C	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:33:SER:OG	3:e:34:GLN:N	2.52	0.41
4:b:59:SER:OG	4:b:60:SER:N	2.54	0.41
3:e:174:SER:OG	3:e:175:ASN:N	2.54	0.41
4:j:240:ALA:H	5:k:204:PRO:HG3	1.86	0.41
4:b:48:ASN:N	4:b:49:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	281/298 (94%)	275 (98%)	6 (2%)	0	100	100
3	e	280/298 (94%)	276 (99%)	4 (1%)	0	100	100
3	i	281/298 (94%)	276 (98%)	5 (2%)	0	100	100
4	b	259/272 (95%)	252 (97%)	7 (3%)	0	100	100
4	f	263/272 (97%)	256 (97%)	7 (3%)	0	100	100
4	j	257/272 (94%)	247 (96%)	10 (4%)	0	100	100
5	c	231/240 (96%)	227 (98%)	4 (2%)	0	100	100
5	g	232/240 (97%)	228 (98%)	4 (2%)	0	100	100
5	k	234/240 (98%)	231 (99%)	3 (1%)	0	100	100
6	d	66/69 (96%)	65 (98%)	1 (2%)	0	100	100
6	h	66/69 (96%)	65 (98%)	1 (2%)	0	100	100
6	l	66/69 (96%)	66 (100%)	0	0	100	100
All	All	2516/2637 (95%)	2464 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	a	248/260 (95%)	248 (100%)	0	100	100
3	e	247/260 (95%)	247 (100%)	0	100	100
3	i	248/260 (95%)	248 (100%)	0	100	100
4	b	223/230 (97%)	223 (100%)	0	100	100
4	f	224/230 (97%)	224 (100%)	0	100	100
4	j	221/230 (96%)	221 (100%)	0	100	100
5	c	207/213 (97%)	207 (100%)	0	100	100
5	g	208/213 (98%)	208 (100%)	0	100	100
5	k	210/213 (99%)	210 (100%)	0	100	100
6	d	57/58 (98%)	57 (100%)	0	100	100
6	h	57/58 (98%)	57 (100%)	0	100	100
6	l	57/58 (98%)	57 (100%)	0	100	100
All	All	2207/2283 (97%)	2207 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	a	198	ASN
4	f	61	ASN
4	f	94	GLN
4	f	111	GLN
4	f	149	ASN
4	f	203	ASN
4	f	225	ASN
6	h	26	ASN
3	i	198	ASN
4	j	61	ASN
6	l	69	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	MYR	i	300	-	15,15,15	1.47	2 (13%)	15,15,15	1.19	2 (13%)
7	MYR	e	300	-	15,15,15	1.47	2 (13%)	15,15,15	1.30	2 (13%)
7	MYR	a	300	-	15,15,15	1.42	2 (13%)	15,15,15	1.12	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MYR	i	300	-	-	4/13/13/13	-
7	MYR	e	300	-	-	6/13/13/13	-
7	MYR	a	300	-	-	5/13/13/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	300	MYR	O2-C1	-3.31	1.19	1.30
7	i	300	MYR	O2-C1	-3.21	1.20	1.30
7	e	300	MYR	O2-C1	-3.18	1.20	1.30
7	a	300	MYR	O1-C1	3.00	1.31	1.22
7	e	300	MYR	O1-C1	2.98	1.31	1.22
7	i	300	MYR	O1-C1	2.93	1.31	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	300	MYR	O2-C1-O1	-3.77	113.63	123.33
7	e	300	MYR	O2-C1-C2	3.20	124.12	114.00
7	i	300	MYR	O2-C1-O1	-3.17	115.18	123.33
7	i	300	MYR	O2-C1-C2	3.09	123.76	114.00
7	a	300	MYR	O2-C1-O1	-3.00	115.61	123.33
7	a	300	MYR	O2-C1-C2	2.64	122.33	114.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	e	300	MYR	C1-C2-C3-C4
7	i	300	MYR	C7-C8-C9-C10
7	i	300	MYR	C6-C7-C8-C9
7	i	300	MYR	C2-C3-C4-C5
7	i	300	MYR	C1-C2-C3-C4
7	a	300	MYR	C3-C4-C5-C6
7	e	300	MYR	C2-C3-C4-C5
7	a	300	MYR	C7-C8-C9-C10
7	e	300	MYR	C5-C6-C7-C8
7	a	300	MYR	O2-C1-C2-C3
7	a	300	MYR	C5-C6-C7-C8
7	e	300	MYR	O2-C1-C2-C3
7	e	300	MYR	O1-C1-C2-C3
7	a	300	MYR	O1-C1-C2-C3
7	e	300	MYR	C11-C12-C13-C14

There are no ring outliers.

No monomer is involved in short contacts.

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.

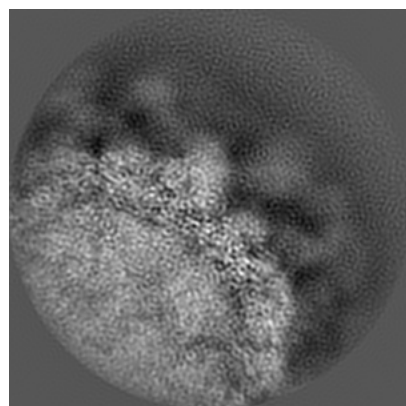
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26072. These allow visual inspection of the internal detail of the map and identification of artifacts.

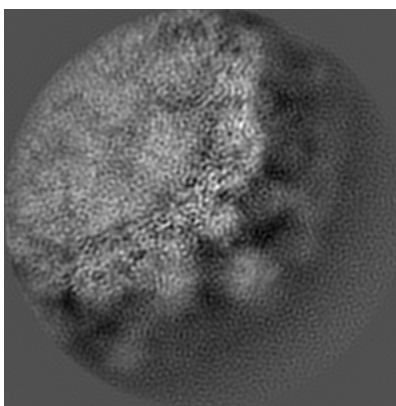
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

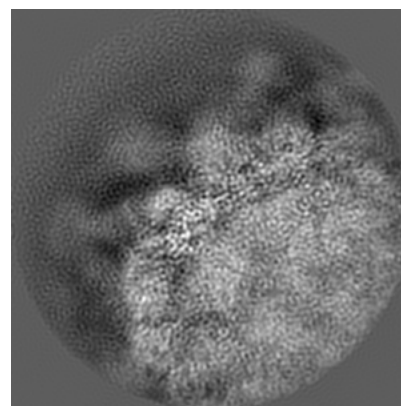
6.1.1 Primary map



X

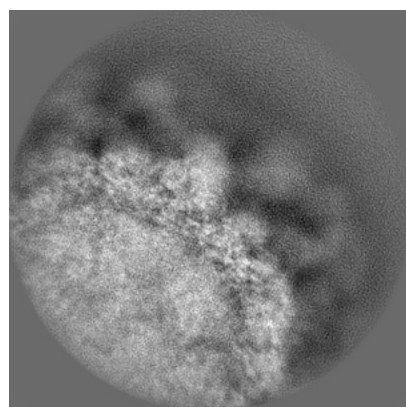


Y

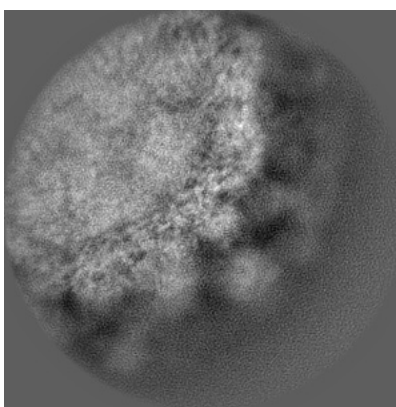


Z

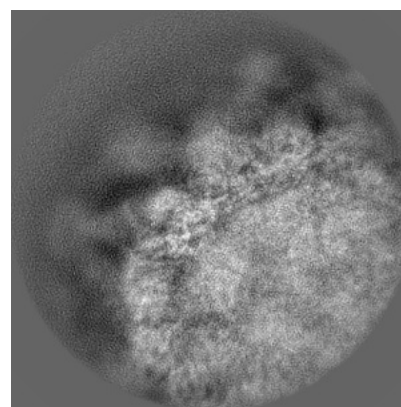
6.1.2 Raw map



X



Y

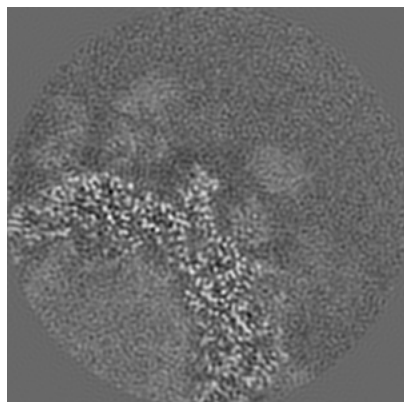


Z

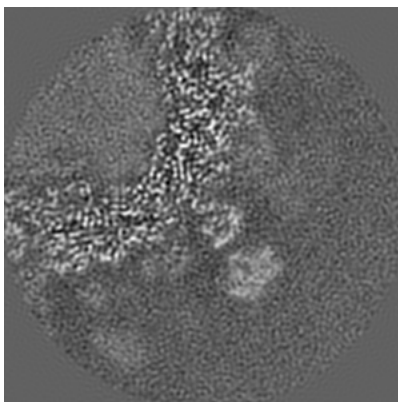
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

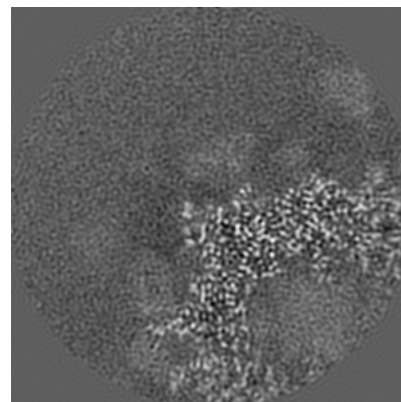
6.2.1 Primary map



X Index: 140

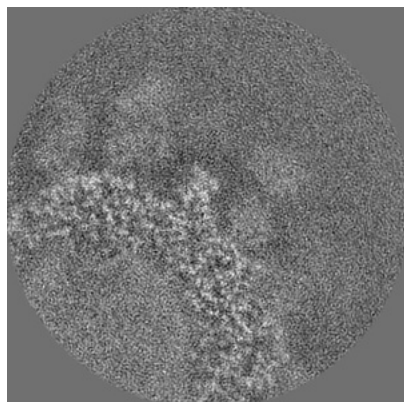


Y Index: 140

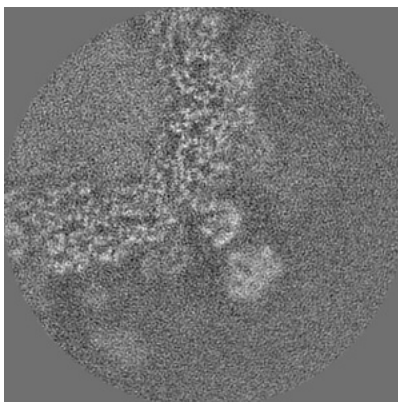


Z Index: 140

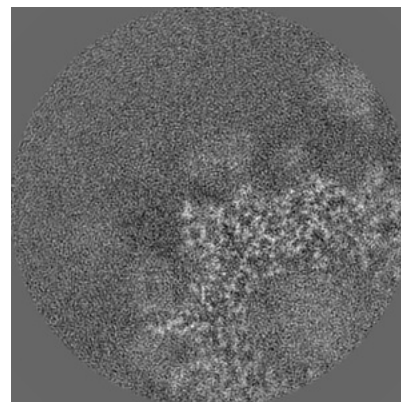
6.2.2 Raw map



X Index: 140



Y Index: 140

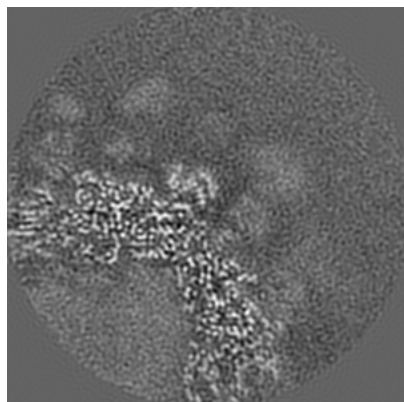


Z Index: 140

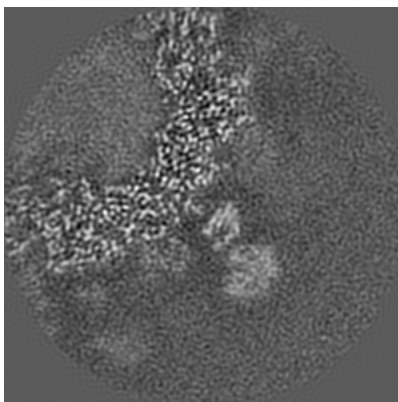
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

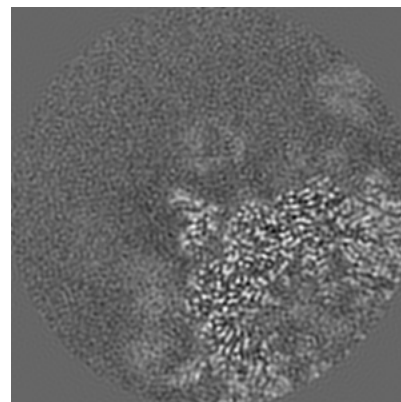
6.3.1 Primary map



X Index: 134

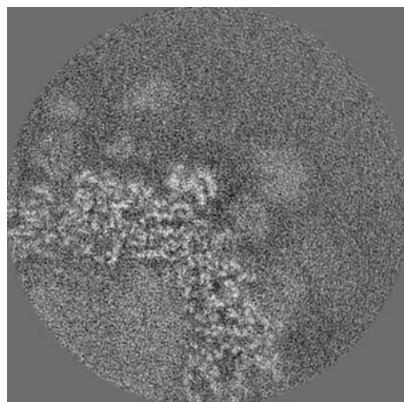


Y Index: 142

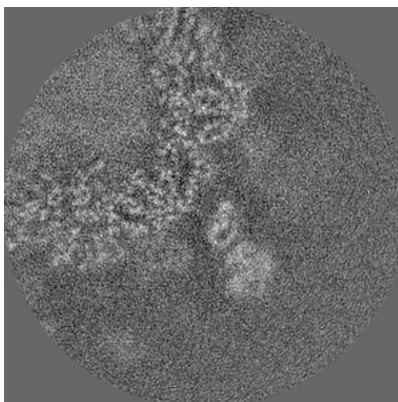


Z Index: 146

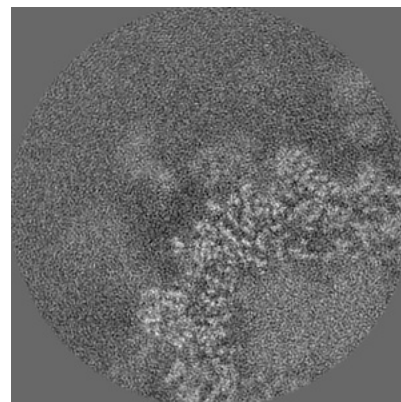
6.3.2 Raw map



X Index: 134



Y Index: 145

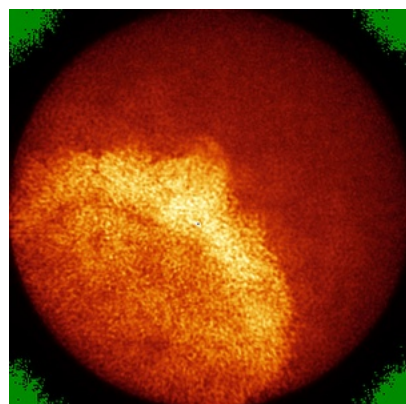


Z Index: 133

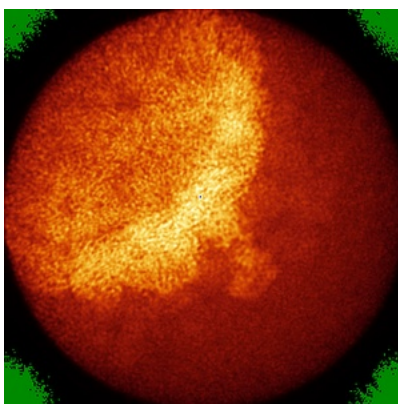
The images above show the largest variance slices of the map in three orthogonal directions.

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

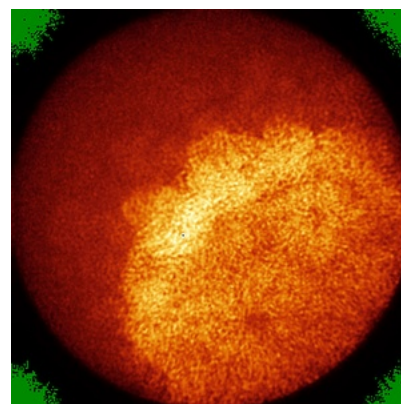
6.4.1 Primary map



X

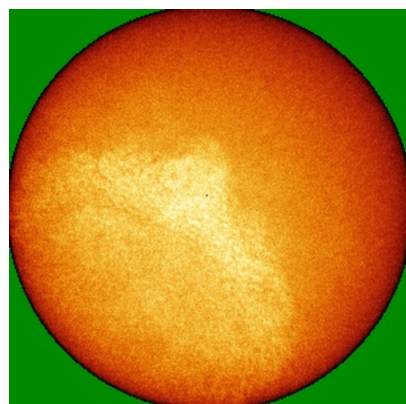


Y

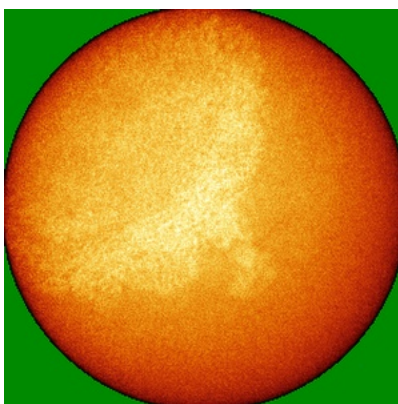


Z

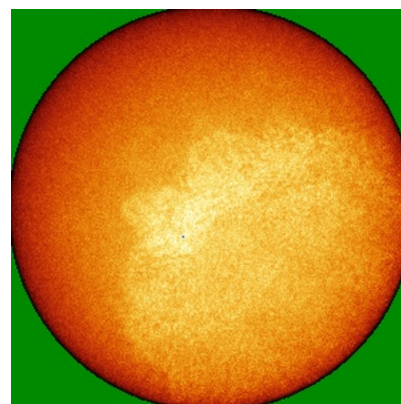
6.4.2 Raw map



X



Y

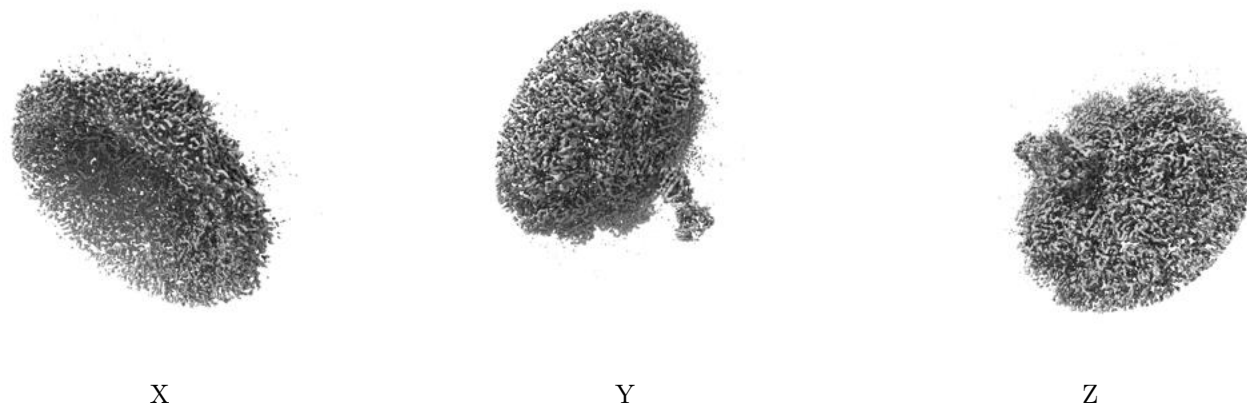


Z

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.

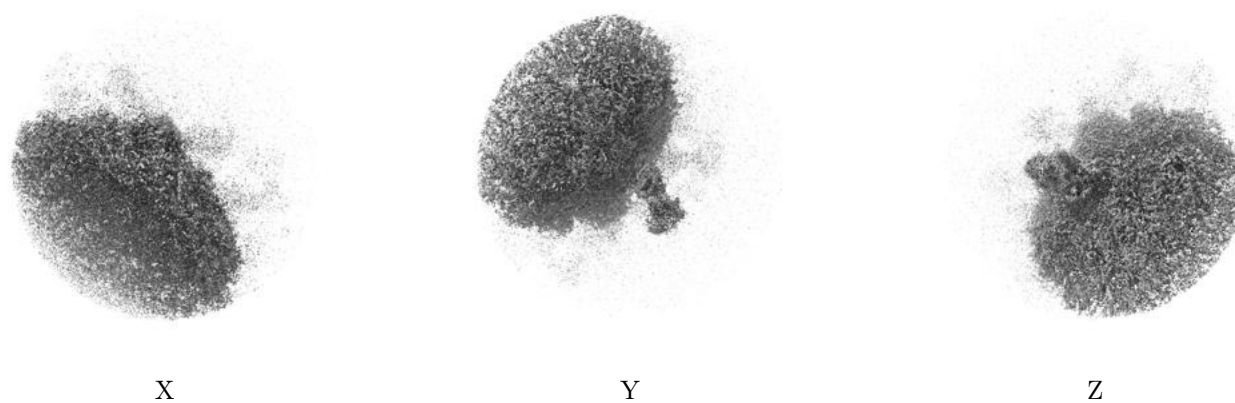
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

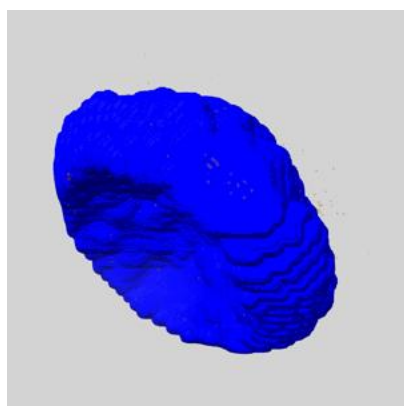
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

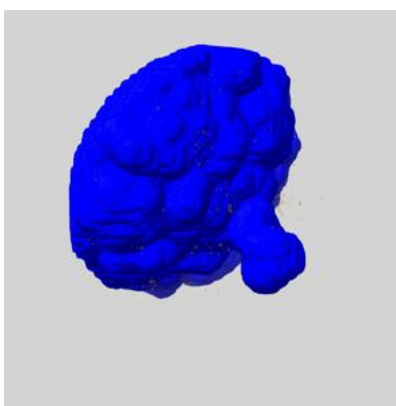
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

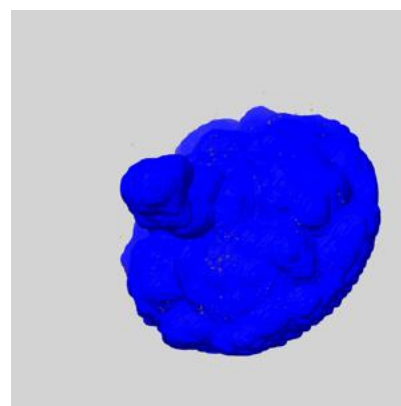
6.6.1 emd_26072_msk_1.map [i](#)



X



Y

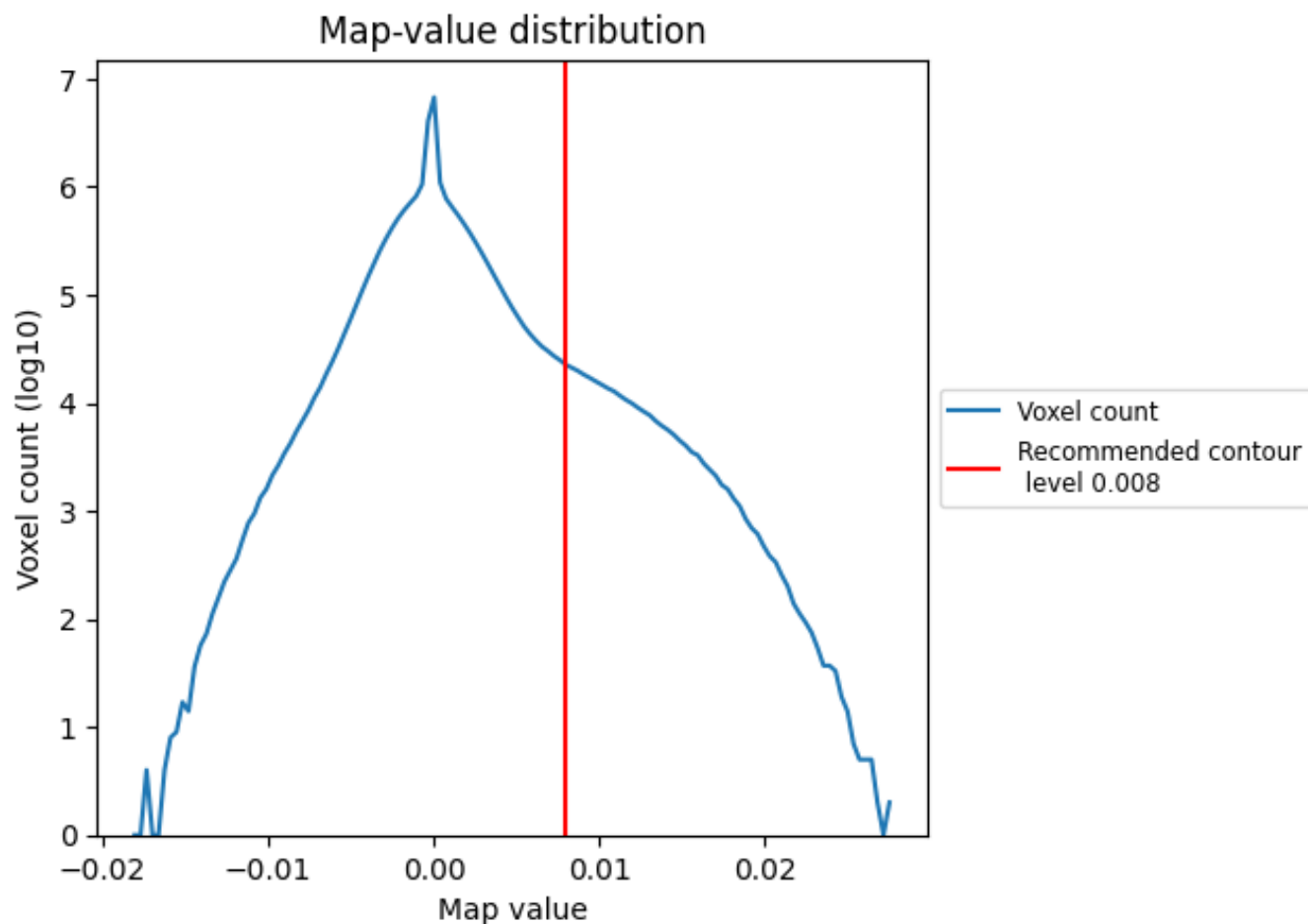


Z

7 Map analysis [i](#)

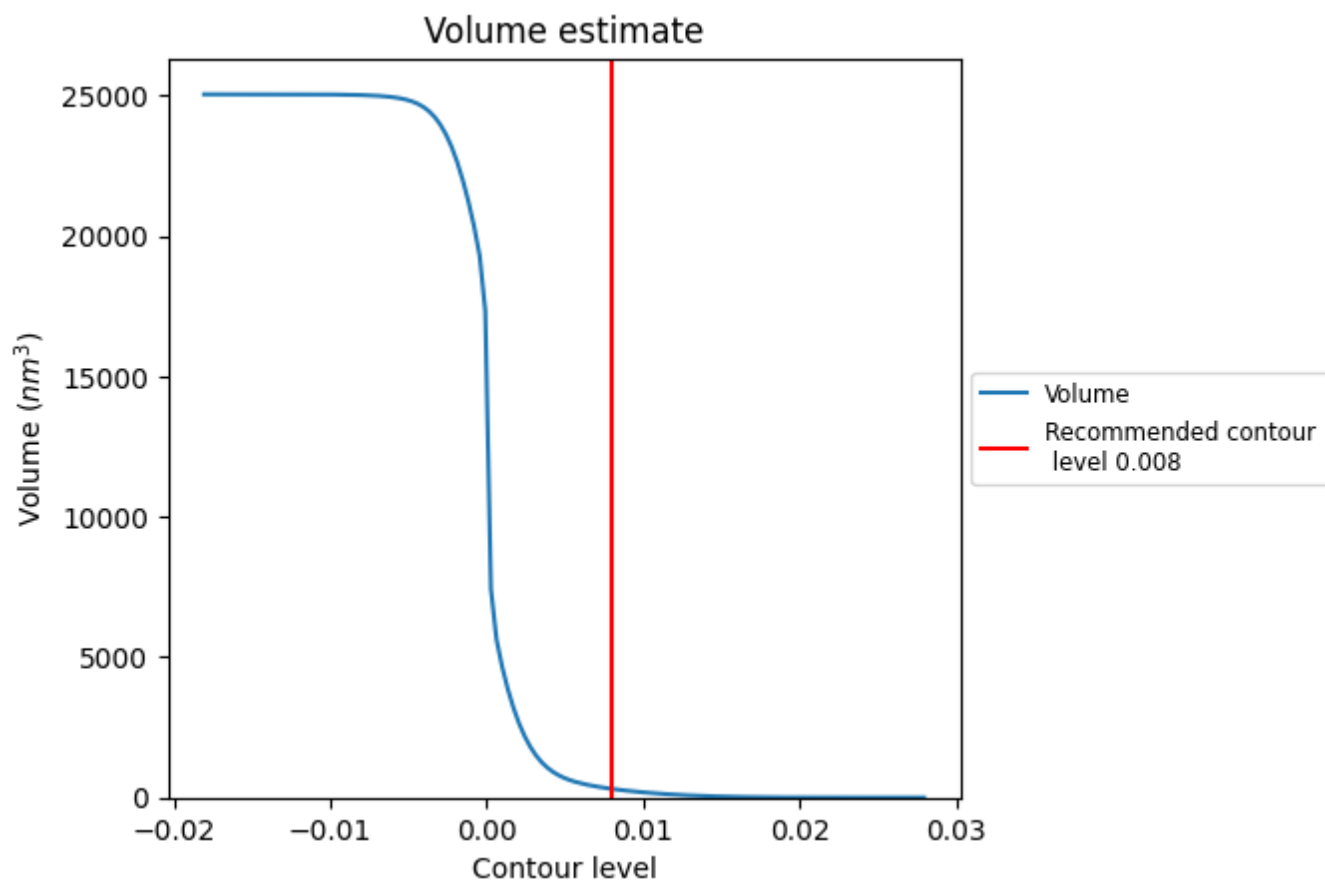
This section contains the results of statistical analysis of the map.

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.

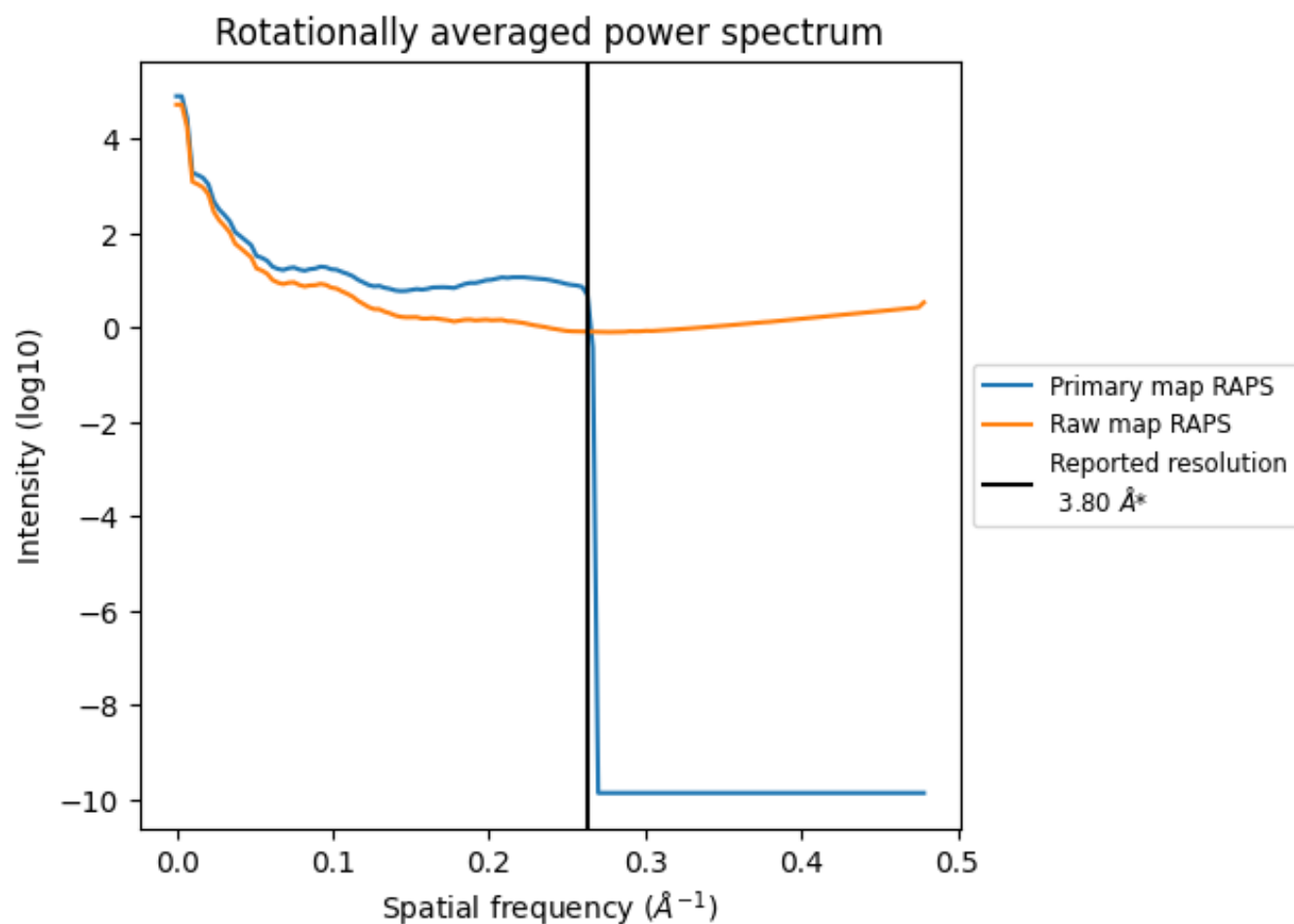
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm³; this corresponds to an approximate mass of 279 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 ⓘ

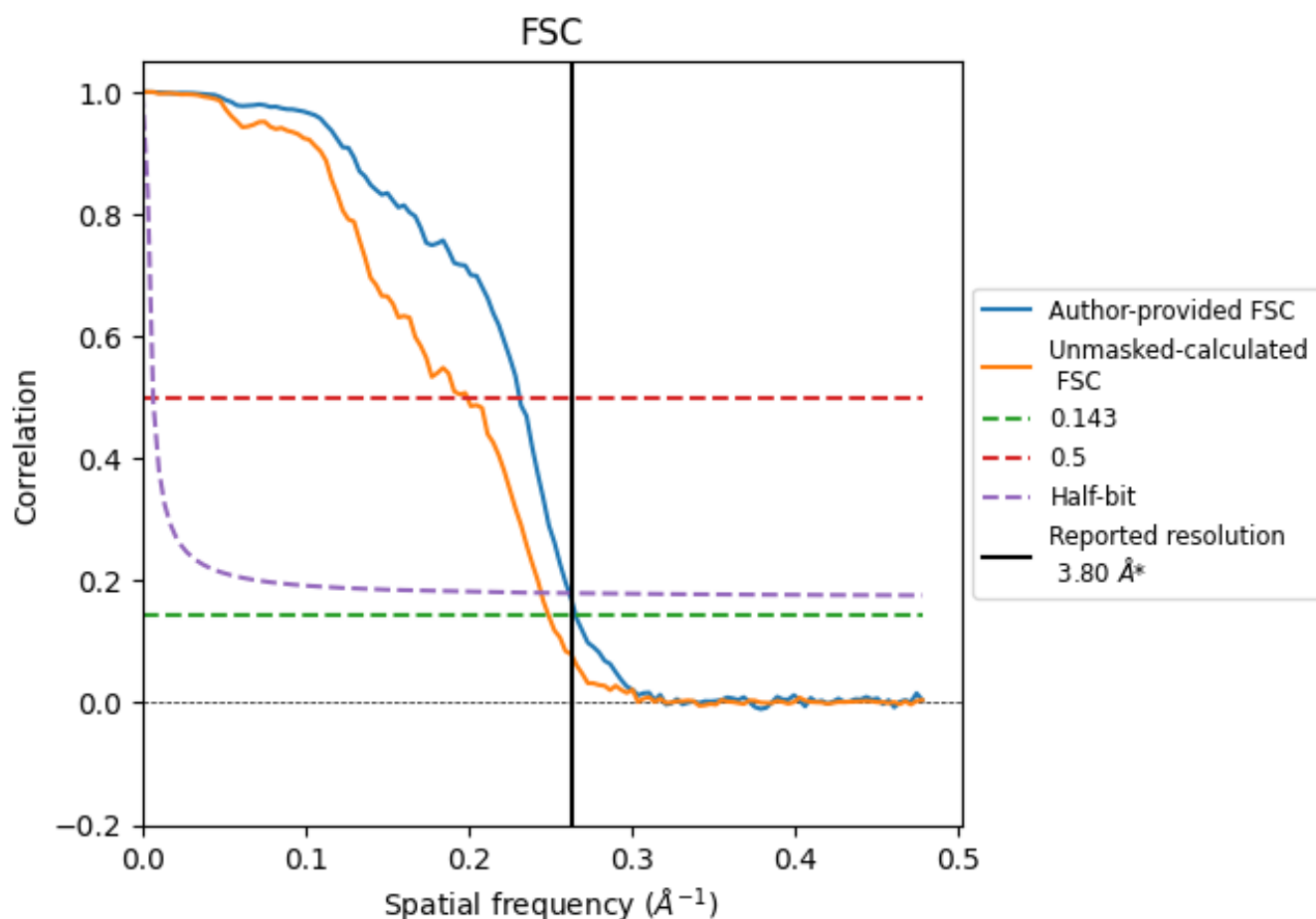


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

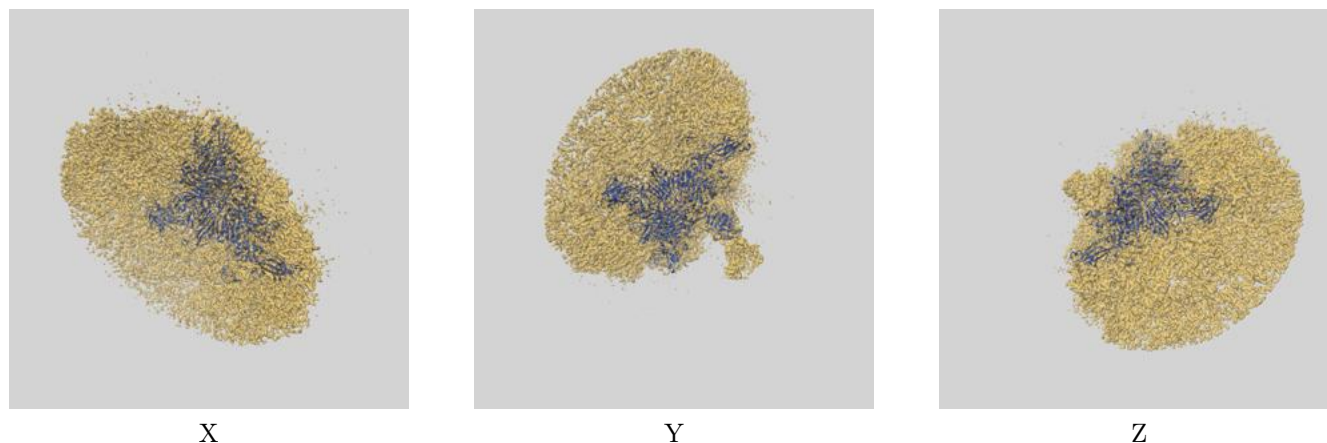
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.32	3.82
Unmasked-calculated*	4.01	5.02	4.09

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

9 Map-model fit [i](#)

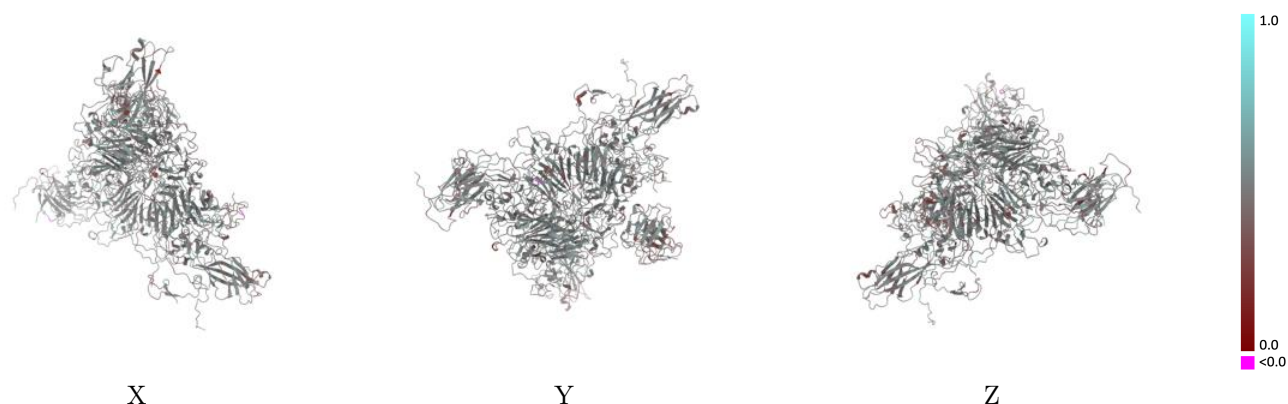
This section contains information regarding the fit between EMDB map EMD-26072 and PDB model 7TQU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



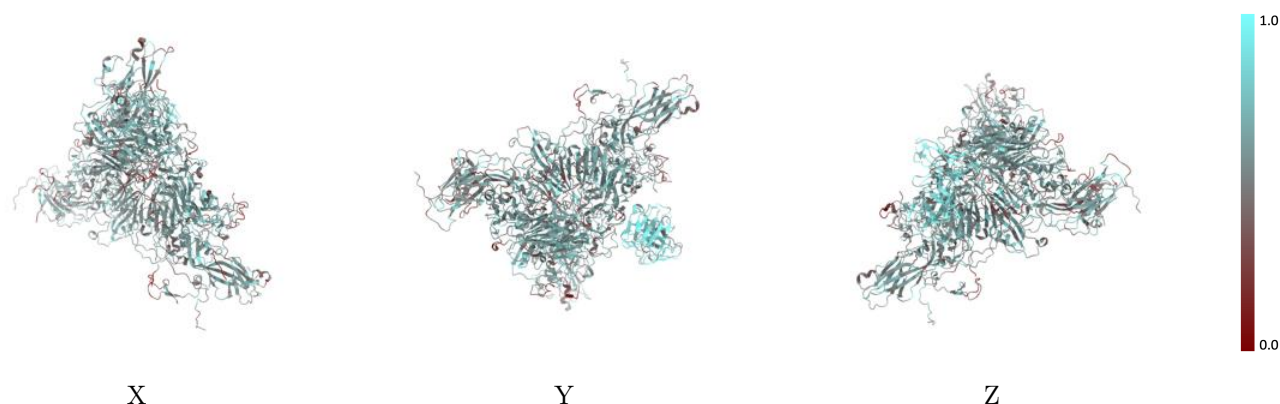
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



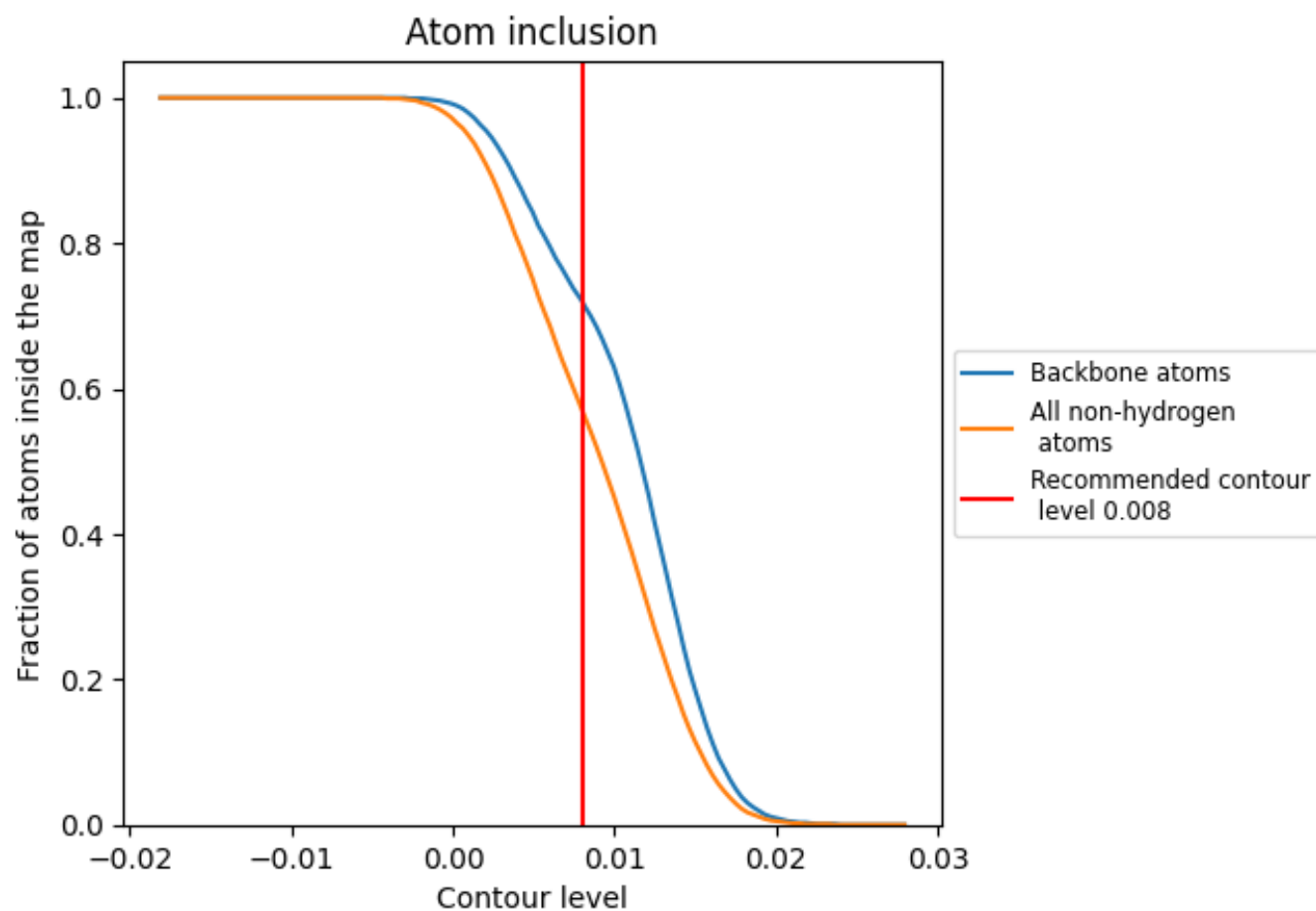
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 57% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5700	0.4720
H	0.7840	0.4460
L	0.7200	0.4210
a	0.5450	0.4670
b	0.5750	0.4770
c	0.5750	0.4820
d	0.4100	0.4430
e	0.5610	0.4780
f	0.5810	0.4770
g	0.5970	0.4800
h	0.4460	0.4420
i	0.5470	0.4730
j	0.5810	0.4840
k	0.5810	0.4760
l	0.4420	0.4550

1.0

0.0

<0.0