



## Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 07:49 pm BST

PDB ID : 9TIS / pdb\_00009tis  
EMDB ID : EMD-55968  
Title : Baseplate arm of phage 812 in the post-contraction state  
Authors : Binovsky, J.; Plevka, P.  
Deposited on : 2025-12-05  
Resolution : 4.10 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](mailto: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>.

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

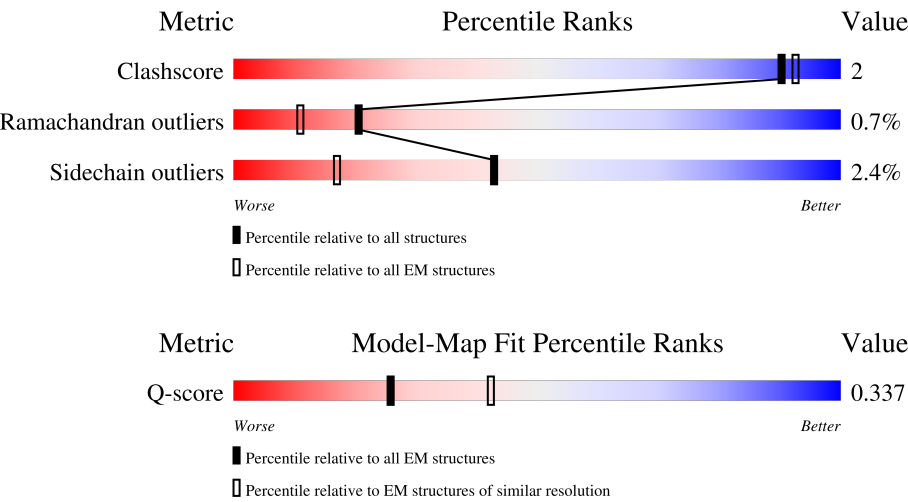
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 ( 3.60 - 4.60 )

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  $\geq 3$ , 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	1019	<div><div>9%</div><div>28%</div><div>6%</div><div>64%</div></div>
2	B	173	<div><div>13%</div><div>87%</div><div>10%</div><div>..</div></div>
2	C	173	<div><div>16%</div><div>86%</div><div>10%</div><div>...</div></div>
2	D	173	<div><div>12%</div><div>90%</div><div>6%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
2	E	173	
2	F	173	
2	G	173	
3	H	1152	
3	I	1152	
3	J	1152	
3	K	1152	
3	L	1152	
3	N	1152	
4	O	458	
4	P	458	
4	Q	458	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 64702 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 ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	364	Total	C	N	O	S	0	0
			2994	1924	472	590	8		

- Molecule 2 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	170	Total	C	N	O	S	0	0
			1336	849	219	267	1		
2	C	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	D	170	Total	C	N	O	S	0	0
			1336	849	219	267	1		
2	E	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	F	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	G	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		

- Molecule 3 is a protein called ORF65.

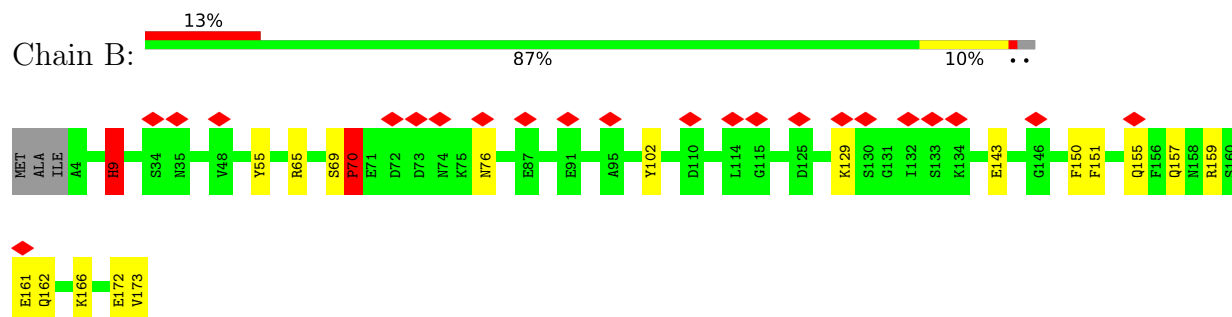
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
3	I	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
3	J	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
3	K	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
3	L	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
3	N	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		

- Molecule 4 is a protein called ORF68.

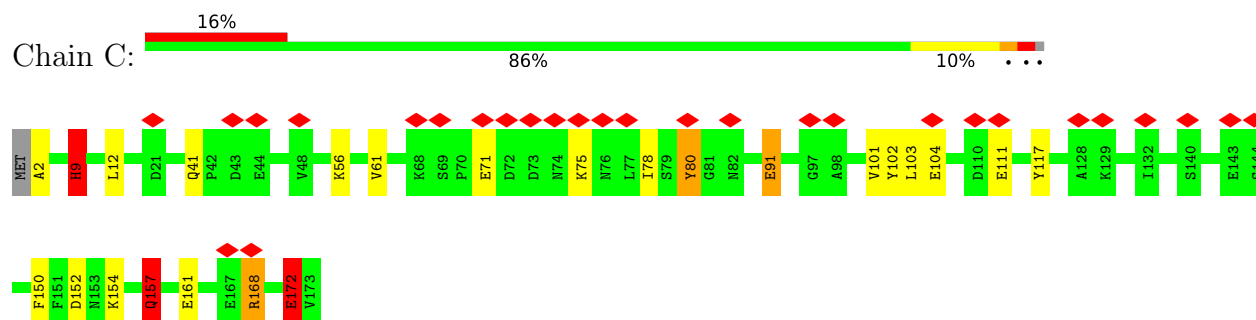
Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
4	P	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
4	Q	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		



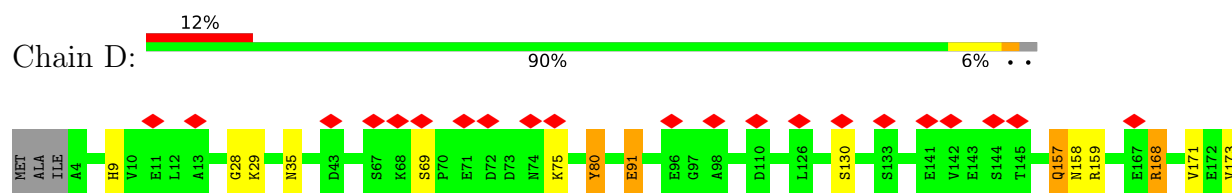
- Molecule 2: ORF64



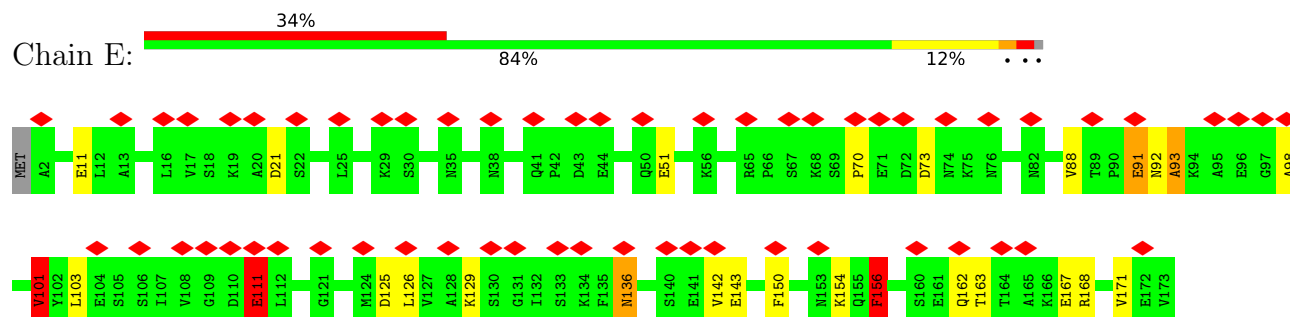
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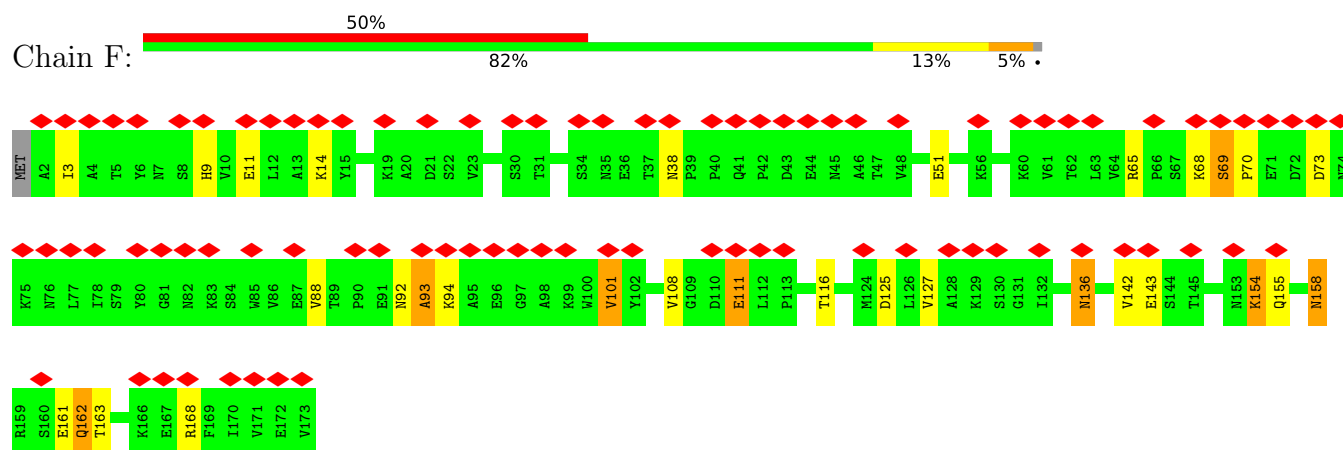
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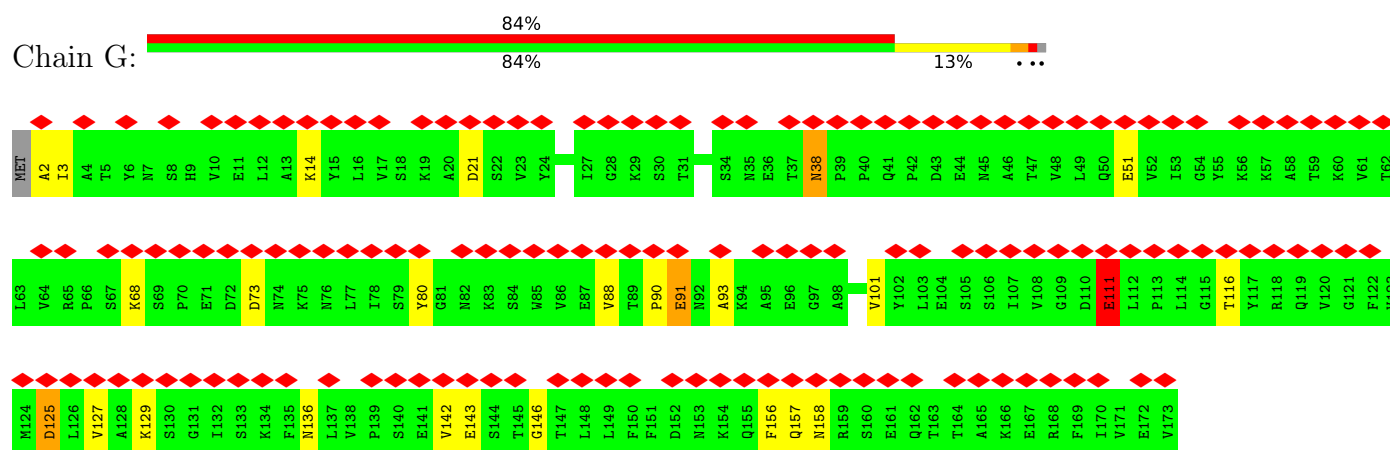
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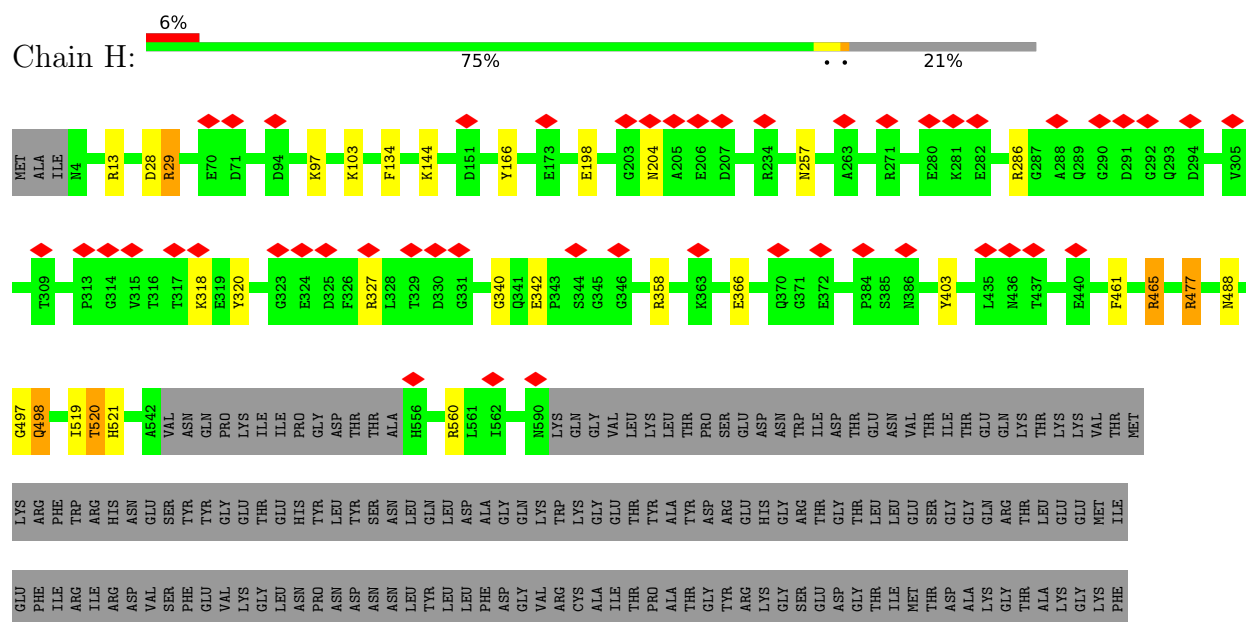
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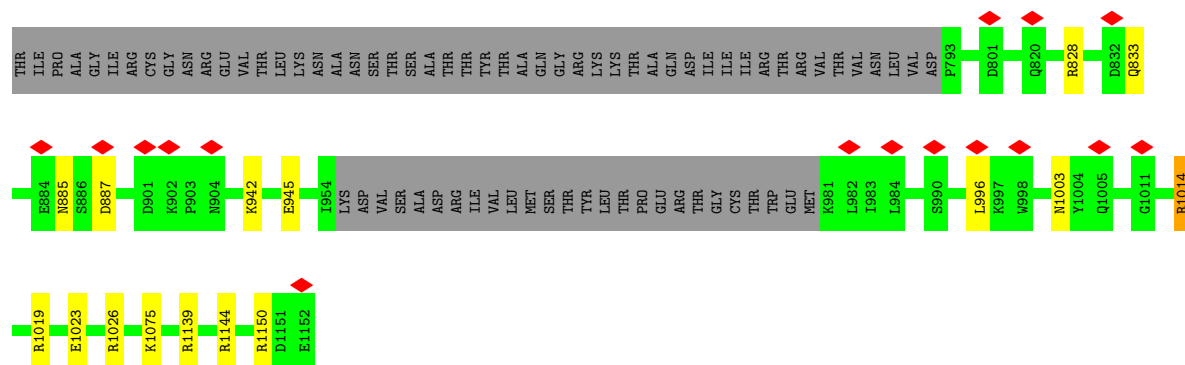
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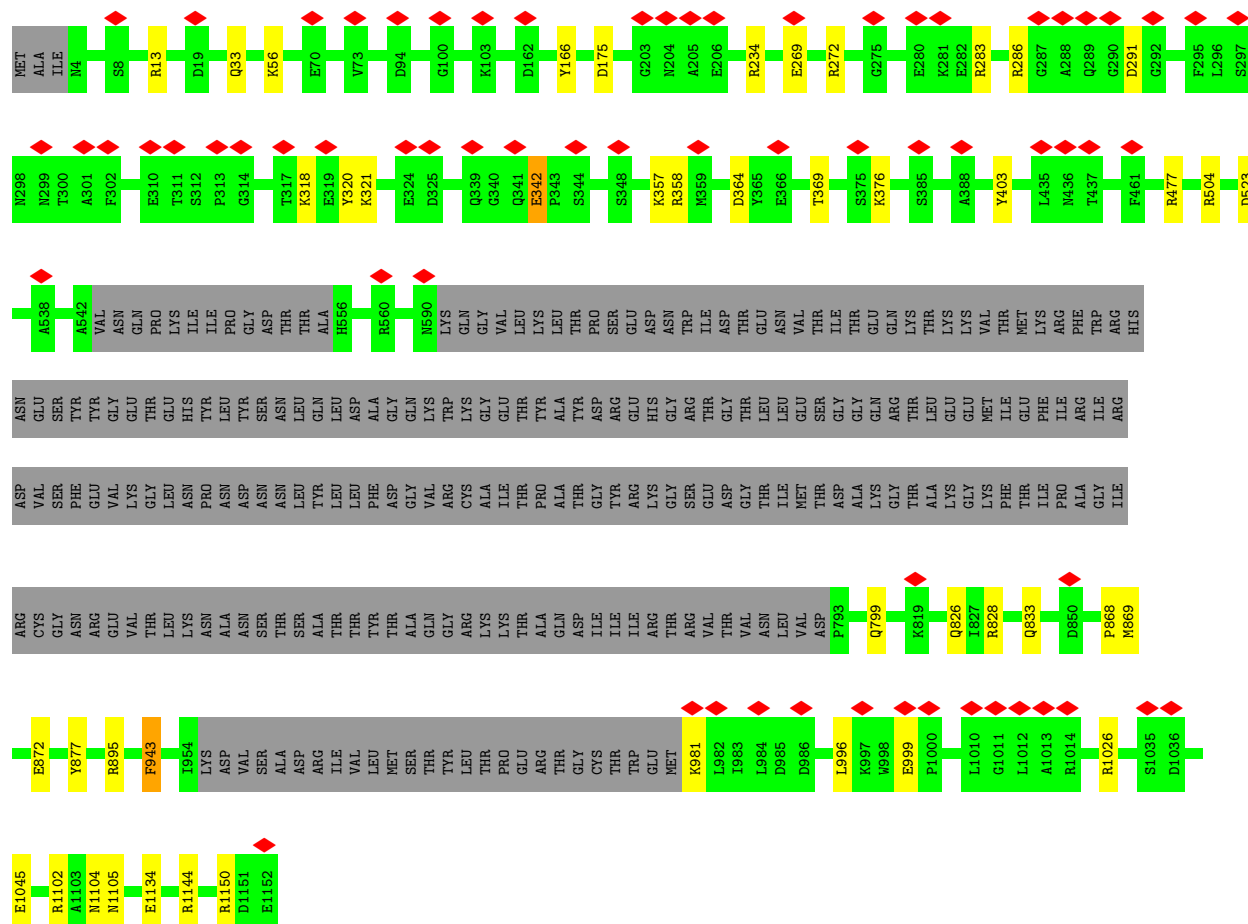
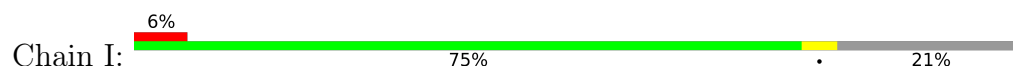
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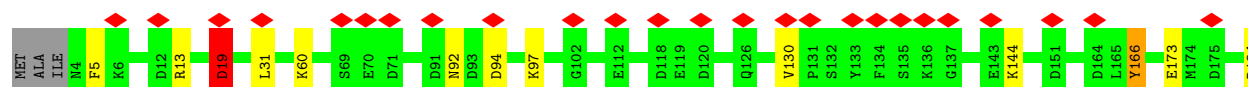
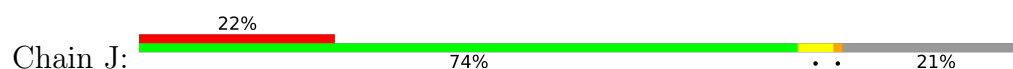




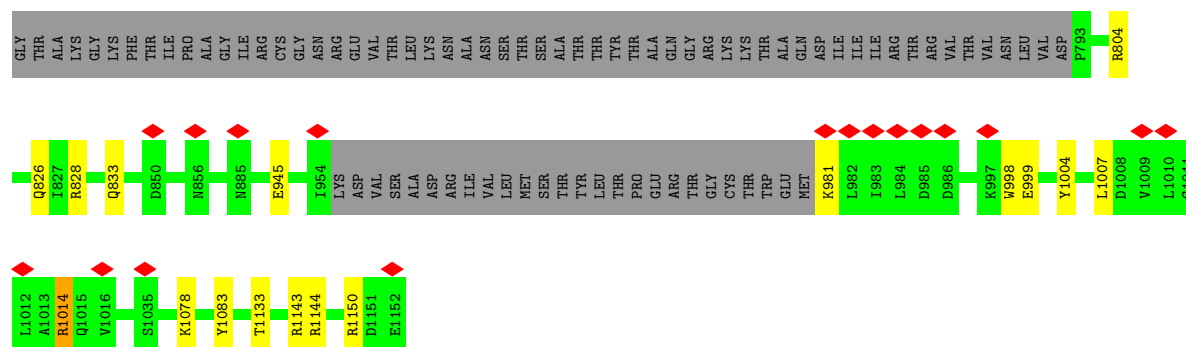
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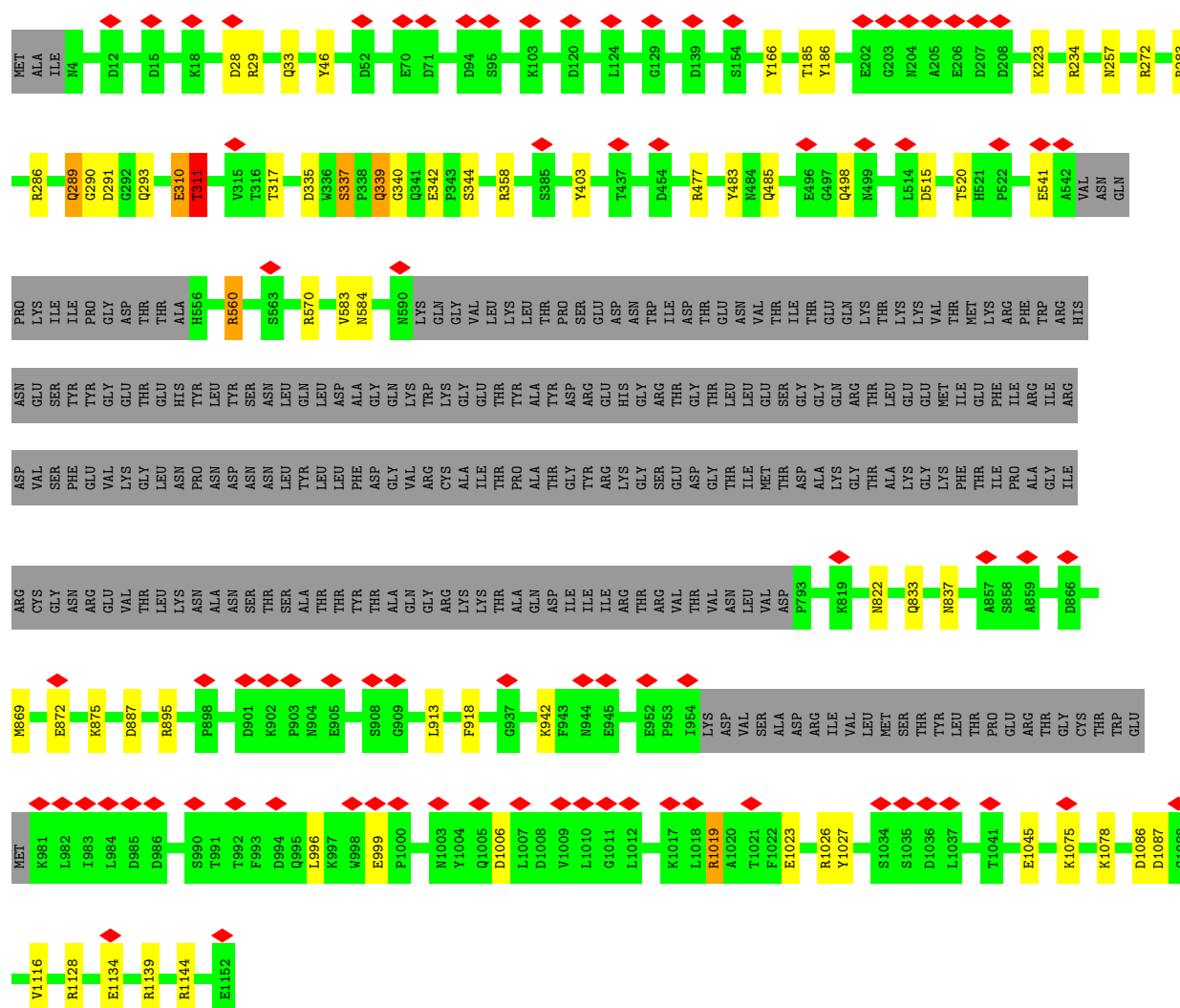
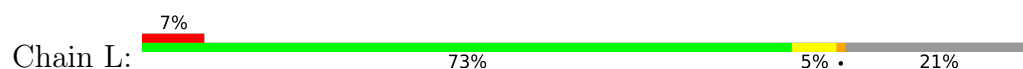
- Molecule 3: ORF65



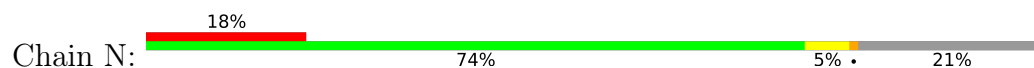




### • Molecule 3: ORF65

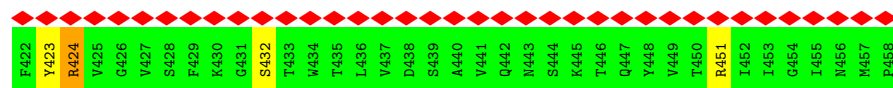


### • Molecule 3: ORF65

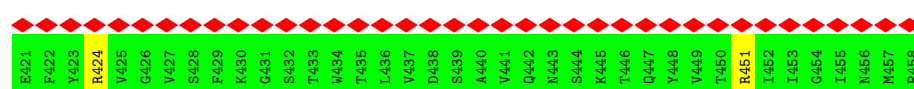
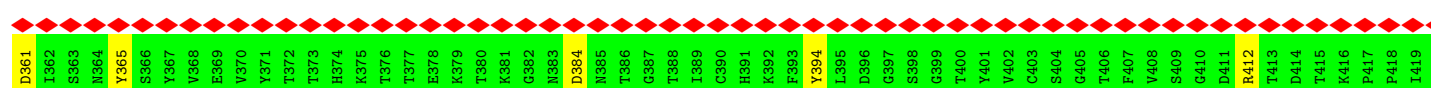
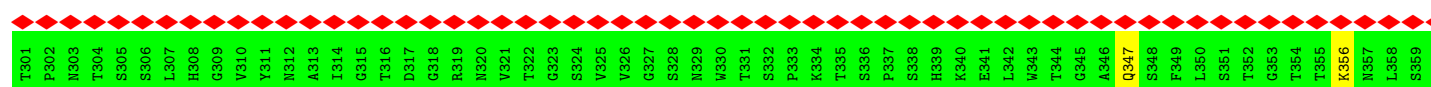
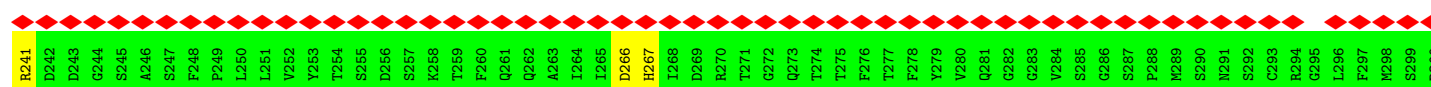
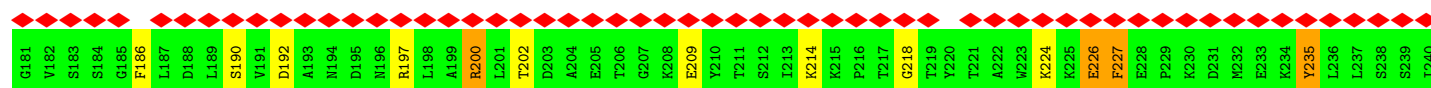
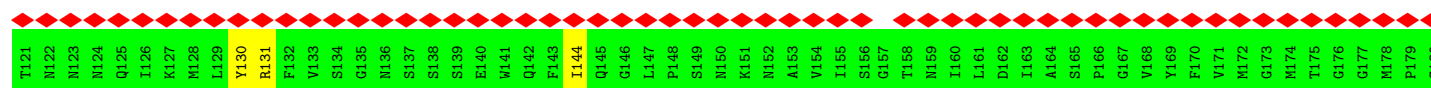
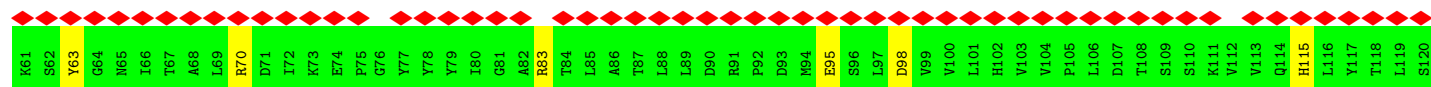
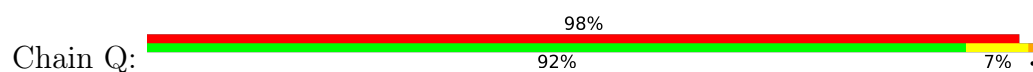








• Molecule 4: ORF68



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	507.36002, 507.36002, 507.36002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	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	0.77	0/3064	1.42	26/4160 (0.6%)
2	B	0.72	0/1364	1.40	7/1854 (0.4%)
2	C	0.78	0/1377	1.44	5/1872 (0.3%)
2	D	0.72	0/1364	1.36	5/1854 (0.3%)
2	E	0.72	0/1377	1.39	8/1872 (0.4%)
2	F	0.73	0/1377	1.41	11/1872 (0.6%)
2	G	0.74	0/1377	1.41	6/1872 (0.3%)
3	H	0.71	0/7308	1.27	18/9911 (0.2%)
3	I	0.71	0/7308	1.25	16/9911 (0.2%)
3	J	0.72	0/7308	1.29	22/9911 (0.2%)
3	K	0.71	0/7308	1.25	17/9911 (0.2%)
3	L	0.71	0/7308	1.28	27/9911 (0.3%)
3	N	0.74	0/7308	1.31	27/9911 (0.3%)
4	O	0.76	0/3619	1.29	13/4913 (0.3%)
4	P	0.77	0/3619	1.34	17/4913 (0.3%)
4	Q	0.78	0/3619	1.32	15/4913 (0.3%)
All	All	0.73	0/66005	1.31	240/89561 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	B	0	2
2	C	0	3
2	D	0	2
2	E	0	1
2	F	0	1
2	G	0	1
3	H	0	6
3	I	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	5
3	K	0	10
3	L	0	8
3	N	0	13
4	O	0	6
4	P	0	7
4	Q	0	7
All	All	0	86

There are no bond length outliers.

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	227	PHE	N-CA-C	11.19	126.68	108.55
1	A	462	ASP	CA-CB-CG	11.13	123.73	112.60
1	A	191	LEU	N-CA-C	10.80	125.83	112.87
3	L	311	THR	CA-CB-CG2	9.85	127.25	110.50
1	A	280	ALA	CB-CA-C	9.55	131.00	110.19
4	P	231	ASP	CA-CB-CG	9.26	121.86	112.60
2	B	69	SER	CA-C-N	9.19	131.33	119.84
2	B	69	SER	C-N-CA	9.19	131.33	119.84
2	B	70	PRO	CA-N-CD	-8.91	99.53	112.00
3	H	1144	ARG	NE-CZ-NH2	8.66	127.00	119.20
3	L	1144	ARG	NE-CZ-NH2	8.62	126.96	119.20
4	P	266	ASP	CA-CB-CG	8.12	120.72	112.60
3	K	1144	ARG	NE-CZ-NH2	8.04	126.43	119.20
3	N	477	ARG	NE-CZ-NH2	7.93	126.34	119.20
3	N	1144	ARG	NE-CZ-NH2	7.88	126.30	119.20
3	I	1144	ARG	NE-CZ-NH2	7.67	126.11	119.20
3	J	1144	ARG	NE-CZ-NH2	7.48	125.93	119.20
4	P	136	ASN	N-CA-C	7.41	122.35	113.16
3	H	520	THR	OG1-CB-CG2	-7.41	94.49	109.30
2	F	136	ASN	CA-CB-CG	7.38	119.98	112.60
3	J	477	ARG	NE-CZ-NH2	7.32	125.79	119.20
2	E	21	ASP	CA-CB-CG	-7.29	105.31	112.60
4	Q	200	ARG	NE-CZ-NH2	7.17	125.65	119.20
1	A	292	ASP	CA-CB-CG	7.17	119.77	112.60
4	O	266	ASP	CA-CB-CG	7.16	119.76	112.60
3	H	29	ARG	NE-CZ-NH2	7.07	125.56	119.20
3	L	310	GLU	CB-CA-C	7.05	123.22	114.40
2	F	111	GLU	CB-CG-CD	7.02	124.54	112.60
4	Q	267	HIS	CB-CG-CD2	-7.00	122.09	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	200	ARG	NE-CZ-NH2	6.97	125.47	119.20
2	C	157	GLN	OE1-CD-NE2	-6.96	115.64	122.60
3	N	399	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	321	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	A	181	THR	CA-CB-OG1	6.85	119.88	109.60
3	I	477	ARG	NE-CZ-NH2	6.79	125.31	119.20
3	J	528	PHE	CA-CB-CG	6.76	120.56	113.80
3	L	311	THR	OG1-CB-CG2	-6.76	95.79	109.30
2	E	136	ASN	CA-CB-CG	6.75	119.35	112.60
3	H	286	ARG	NE-CZ-NH2	6.69	125.22	119.20
3	H	477	ARG	NE-CZ-NH2	6.69	125.22	119.20
1	A	192	ASP	CB-CA-C	6.68	121.55	111.80
3	I	504	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	A	194	LEU	CA-C-N	6.56	126.69	119.87
1	A	194	LEU	C-N-CA	6.56	126.69	119.87
1	A	297	THR	CA-C-N	6.54	131.80	120.68
1	A	297	THR	C-N-CA	6.54	131.80	120.68
2	B	9	HIS	CB-CG-CD2	-6.53	122.70	131.20
3	N	32	GLN	N-CA-C	6.48	119.61	109.96
3	H	1026	ARG	NE-CZ-NH2	6.47	125.03	119.20
3	N	210	HIS	CB-CG-CD2	-6.46	122.81	131.20
3	I	272	ARG	NE-CZ-NH2	6.45	125.00	119.20
3	I	286	ARG	NE-CZ-NH2	6.44	124.99	119.20
3	J	321	LYS	CB-CG-CD	-6.39	96.60	111.30
3	N	804	ARG	NE-CZ-NH2	6.34	124.91	119.20
3	N	1023	GLU	CB-CG-CD	-6.32	101.86	112.60
4	Q	451	ARG	NE-CZ-NH2	6.29	124.86	119.20
3	H	1023	GLU	CB-CG-CD	-6.28	101.93	112.60
1	A	108	ARG	NE-CZ-NH2	6.27	124.84	119.20
3	L	477	ARG	NE-CZ-NH2	6.24	124.82	119.20
4	Q	23	ASN	CA-CB-CG	6.23	118.83	112.60
3	L	29	ARG	NE-CZ-NH2	6.21	124.79	119.20
2	D	130	SER	N-CA-C	6.21	118.84	111.33
4	Q	384	ASP	CA-CB-CG	6.20	118.80	112.60
3	J	996	LEU	CA-C-N	6.18	131.26	121.44
3	J	996	LEU	C-N-CA	6.18	131.26	121.44
3	J	321	LYS	CG-CD-CE	6.16	125.47	111.30
3	J	1019	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	A	190	TRP	CA-CB-CG	6.15	125.28	113.60
3	J	184	ARG	NE-CZ-NH2	6.14	124.72	119.20
4	P	424	ARG	NE-CZ-NH2	6.12	124.70	119.20
2	F	158	ASN	OD1-CG-ND2	-6.10	116.50	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	895	ARG	NE-CZ-NH2	6.08	124.67	119.20
4	P	273	GLN	OE1-CD-NE2	-6.04	116.56	122.60
3	J	286	ARG	NE-CZ-NH2	6.03	124.63	119.20
2	C	168	ARG	NE-CZ-NH2	6.01	124.61	119.20
3	L	1026	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	A	336	ASP	CA-CB-CG	-5.99	106.61	112.60
2	B	70	PRO	N-CA-C	5.99	124.80	112.47
4	Q	424	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	129	HIS	CB-CG-CD2	-5.98	123.42	131.20
3	L	272	ARG	NE-CZ-NH2	5.97	124.58	119.20
3	H	1150	ARG	NE-CZ-NH2	5.97	124.57	119.20
2	E	101	VAL	CA-CB-CG1	5.96	120.53	110.40
3	K	286	ARG	NE-CZ-NH2	5.95	124.56	119.20
4	P	319	ARG	NE-CZ-NH2	5.93	124.54	119.20
3	J	1019	ARG	NE-CZ-NH1	-5.91	115.59	121.50
2	D	157	GLN	OE1-CD-NE2	-5.91	116.69	122.60
2	F	9	HIS	CA-CB-CG	5.91	119.71	113.80
4	O	424	ARG	NE-CZ-NH2	5.90	124.51	119.20
3	H	465	ARG	CD-NE-CZ	5.87	132.62	124.40
3	K	504	ARG	NE-CZ-NH2	5.87	124.48	119.20
3	N	32	GLN	OE1-CD-NE2	-5.86	116.74	122.60
2	C	9	HIS	CA-CB-CG	5.84	119.64	113.80
3	J	504	ARG	NE-CZ-NH2	5.83	124.45	119.20
4	P	267	HIS	CB-CG-CD2	-5.82	123.63	131.20
3	L	570	ARG	NE-CZ-NH2	5.81	124.43	119.20
4	O	361	ASP	CA-CB-CG	-5.81	106.79	112.60
4	Q	266	ASP	CA-CB-CG	5.81	118.41	112.60
3	K	826	GLN	OE1-CD-NE2	-5.80	116.80	122.60
3	K	1143	ARG	NE-CZ-NH2	5.80	124.42	119.20
3	L	286	ARG	NE-CZ-NH2	5.79	124.42	119.20
3	K	804	ARG	NE-CZ-NH2	5.78	124.41	119.20
3	I	321	LYS	CG-CD-CE	5.78	124.60	111.30
3	K	477	ARG	NE-CZ-NH2	5.76	124.39	119.20
3	H	1019	ARG	NE-CZ-NH1	-5.74	115.76	121.50
3	N	914	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	183	ARG	NE-CZ-NH2	5.73	124.35	119.20
2	G	21	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	374	GLN	OE1-CD-NE2	-5.72	116.88	122.60
2	E	111	GLU	CB-CG-CD	5.71	122.31	112.60
4	Q	361	ASP	CA-CB-CG	-5.71	106.89	112.60
4	P	414	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	192	ASP	CA-CB-CG	-5.67	106.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	131	ARG	NE-CZ-NH2	5.67	124.30	119.20
4	P	227	PHE	CA-CB-CG	-5.66	108.14	113.80
3	I	826	GLN	OE1-CD-NE2	-5.66	116.94	122.60
3	I	868	PRO	N-CA-CB	5.64	106.08	102.92
1	A	142	ARG	NE-CZ-NH2	5.63	124.27	119.20
3	N	828	ARG	NE-CZ-NH1	-5.61	115.89	121.50
3	N	826	GLN	OE1-CD-NE2	-5.61	116.99	122.60
2	B	65	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	G	38	ASN	CA-CB-CG	5.61	118.21	112.60
3	J	204	ASN	CA-CB-CG	5.60	118.20	112.60
4	P	74	GLU	CB-CG-CD	-5.59	103.10	112.60
1	A	401	ASN	CA-CB-CG	-5.58	107.02	112.60
3	I	895	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	343	ARG	NE-CZ-NH2	5.58	124.22	119.20
3	I	321	LYS	CB-CG-CD	-5.56	98.51	111.30
3	L	1023	GLU	CB-CG-CD	-5.56	103.15	112.60
4	O	424	ARG	CD-NE-CZ	5.55	132.17	124.40
3	L	1019	ARG	NE-CZ-NH2	5.54	124.19	119.20
4	O	417	PRO	N-CA-CB	5.53	106.10	103.22
3	L	918	PHE	CA-CB-CG	5.53	119.33	113.80
3	K	1150	ARG	NE-CZ-NH2	5.53	124.17	119.20
3	L	887	ASP	CA-CB-CG	-5.52	107.08	112.60
3	I	1026	ARG	NE-CZ-NH2	5.51	124.16	119.20
3	N	13	ARG	NE-CZ-NH2	5.50	124.15	119.20
3	N	140	ARG	NE-CZ-NH2	5.50	124.15	119.20
3	H	833	GLN	OE1-CD-NE2	-5.49	117.11	122.60
4	Q	131	ARG	NE-CZ-NH2	5.49	124.14	119.20
3	K	13	ARG	NE-CZ-NH2	5.47	124.13	119.20
3	I	342	GLU	O-C-N	-5.45	118.22	121.71
3	L	485	GLN	OE1-CD-NE2	-5.45	117.15	122.60
3	N	564	ALA	CA-C-N	5.45	125.07	119.56
3	N	564	ALA	C-N-CA	5.45	125.07	119.56
4	O	320	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	181	THR	OG1-CB-CG2	5.45	120.20	109.30
4	Q	197	ARG	NE-CZ-NH2	5.44	124.10	119.20
3	K	184	ARG	NE-CZ-NH2	5.43	124.09	119.20
3	I	828	ARG	NE-CZ-NH1	-5.42	116.08	121.50
2	D	35	ASN	OD1-CG-ND2	-5.42	117.18	122.60
4	P	162	ASP	CA-CB-CG	5.42	118.02	112.60
3	J	1109	ARG	NE-CZ-NH2	5.40	124.06	119.20
3	H	461	PHE	CA-CB-CG	5.38	119.19	113.80
3	K	828	ARG	NE-CZ-NH1	-5.38	116.12	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	822	ASN	OD1-CG-ND2	-5.36	117.24	122.60
3	I	1150	ARG	NE-CZ-NH2	5.36	124.02	119.20
3	N	1150	ARG	NE-CZ-NH2	5.36	124.02	119.20
3	K	560	ARG	NE-CZ-NH2	5.35	124.01	119.20
3	I	799	GLN	OE1-CD-NE2	-5.35	117.25	122.60
4	P	248	PHE	CA-CB-CG	5.34	119.14	113.80
2	E	93	ALA	CA-C-N	5.33	127.69	120.38
2	E	93	ALA	C-N-CA	5.33	127.69	120.38
3	L	358	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	190	TRP	CB-CG-CD1	-5.33	118.90	126.90
3	N	358	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	L	289	GLN	CA-C-N	5.32	125.16	120.10
3	L	289	GLN	C-N-CA	5.32	125.16	120.10
4	O	35	PHE	CA-CB-CG	5.32	119.12	113.80
2	D	28	GLY	CA-C-N	5.32	131.69	121.54
2	D	28	GLY	C-N-CA	5.32	131.69	121.54
2	G	21	ASP	N-CA-C	5.30	119.00	112.54
3	K	488	ASN	OD1-CG-ND2	-5.27	117.33	122.60
3	K	399	ASP	CA-CB-CG	5.27	117.87	112.60
4	O	384	ASP	CA-CB-CG	5.27	117.87	112.60
3	K	92	ASN	OD1-CG-ND2	-5.25	117.34	122.60
3	J	19	ASP	CA-CB-CG	5.25	117.85	112.60
3	H	488	ASN	OD1-CG-ND2	-5.25	117.35	122.60
3	H	498	GLN	OE1-CD-NE2	-5.24	117.36	122.60
4	Q	241	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	F	65	ARG	NE-CZ-NH1	-5.23	116.27	121.50
4	O	32	ARG	NE-CZ-NH2	5.22	123.90	119.20
2	G	111	GLU	CB-CG-CD	5.21	121.46	112.60
4	Q	32	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	K	1014	ARG	CD-NE-CZ	5.19	131.66	124.40
2	F	111	GLU	CA-C-N	5.19	134.45	121.80
2	F	111	GLU	C-N-CA	5.19	134.45	121.80
3	H	204	ASN	CA-CB-CG	5.19	117.79	112.60
3	L	310	GLU	CA-C-N	5.18	131.43	121.54
3	L	310	GLU	C-N-CA	5.18	131.43	121.54
2	B	162	GLN	OE1-CD-NE2	-5.17	117.43	122.60
3	J	272	ARG	CD-NE-CZ	5.17	131.63	124.40
1	A	367	GLU	CB-CG-CD	-5.16	103.82	112.60
4	Q	98	ASP	CA-CB-CG	5.16	117.76	112.60
3	H	1014	ARG	NE-CZ-NH2	5.16	123.85	119.20
2	C	168	ARG	CD-NE-CZ	5.16	131.62	124.40
4	P	451	ARG	NE-CZ-NH2	5.16	123.84	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	158	ASN	N-CA-C	5.16	117.69	111.40
4	P	384	ASP	CA-CB-CG	5.16	117.75	112.60
3	L	293	GLN	OE1-CD-NE2	-5.15	117.45	122.60
3	L	335	ASP	CA-CB-CG	5.13	117.73	112.60
4	O	131	ARG	NE-CZ-NH2	5.13	123.82	119.20
3	J	804	ARG	NE-CZ-NH2	5.13	123.81	119.20
3	J	1015	GLN	OE1-CD-NE2	-5.12	117.47	122.60
3	I	234	ARG	NE-CZ-NH2	5.12	123.81	119.20
4	O	40	ASP	CA-CB-CG	5.12	117.72	112.60
2	C	172	GLU	CB-CG-CD	5.11	121.28	112.60
3	N	312	SER	CA-C-N	5.10	126.22	119.84
3	N	312	SER	C-N-CA	5.10	126.22	119.84
1	A	341	GLU	CB-CG-CD	-5.10	103.94	112.60
3	H	828	ARG	NE-CZ-NH1	-5.09	116.41	121.50
3	H	521	HIS	CB-CG-CD2	-5.08	124.60	131.20
3	N	833	GLN	OE1-CD-NE2	-5.08	117.52	122.60
3	N	289	GLN	CA-C-N	5.08	125.16	120.34
3	N	289	GLN	C-N-CA	5.08	125.16	120.34
3	N	862	ARG	NE-CZ-NH2	5.07	123.76	119.20
3	L	1006	ASP	CA-CB-CG	5.07	117.67	112.60
3	L	234	ARG	NE-CZ-NH2	5.07	123.76	119.20
4	O	339	HIS	CB-CG-CD2	-5.06	124.62	131.20
4	P	11	ASN	OD1-CG-ND2	-5.06	117.54	122.60
3	L	837	ASN	CA-CB-CG	5.05	117.66	112.60
3	J	822	ASN	CA-CB-CG	5.05	117.65	112.60
2	E	156	PHE	CA-CB-CG	5.05	118.85	113.80
3	N	521	HIS	CB-CG-CD2	-5.05	124.63	131.20
2	F	101	VAL	CA-CB-CG1	5.05	118.98	110.40
2	E	103	LEU	N-CA-CB	-5.04	103.10	110.86
3	L	498	GLN	OE1-CD-NE2	-5.04	117.56	122.60
3	L	895	ARG	NE-CZ-NH2	5.04	123.73	119.20
4	Q	347	GLN	OE1-CD-NE2	-5.03	117.57	122.60
3	N	38	GLU	CA-C-N	5.03	127.33	120.54
3	N	38	GLU	C-N-CA	5.03	127.33	120.54
2	G	156	PHE	CA-CB-CG	5.03	118.83	113.80
4	O	23	ASN	CA-CB-CG	5.02	117.62	112.60
3	J	166	TYR	N-CA-C	5.02	116.83	111.36
2	G	136	ASN	CA-CB-CG	5.02	117.62	112.60
2	F	136	ASN	OD1-CG-ND2	-5.01	117.58	122.60
3	K	833	GLN	OE1-CD-NE2	-5.01	117.59	122.60
3	N	178	ASN	CA-CB-CG	-5.01	107.59	112.60
1	A	348	ASP	CA-CB-CG	5.01	117.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	69	SER	N-CA-C	5.00	120.86	109.81

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	TYR	Sidechain
1	A	203	PHE	Sidechain
1	A	216	HIS	Sidechain
1	A	418	ARG	Sidechain
1	A	426	ARG	Sidechain
1	A	448	TYR	Sidechain
1	A	460	TYR	Sidechain
2	B	102	TYR	Sidechain
2	B	55	TYR	Sidechain
2	C	102	TYR	Sidechain
2	C	117	TYR	Sidechain
2	C	80	TYR	Sidechain
2	D	168	ARG	Sidechain
2	D	80	TYR	Sidechain
2	E	168	ARG	Sidechain
2	F	168	ARG	Sidechain
2	G	80	TYR	Sidechain
3	H	1139	ARG	Sidechain
3	H	13	ARG	Sidechain
3	H	166	TYR	Sidechain
3	H	327	ARG	Sidechain
3	H	403	TYR	Sidechain
3	H	477	ARG	Sidechain
3	I	13	ARG	Sidechain
3	I	166	TYR	Sidechain
3	I	283	ARG	Sidechain
3	I	403	TYR	Sidechain
3	I	523	ASP	Sidechain
3	I	872	GLU	Sidechain
3	I	943	PHE	Sidechain
3	J	1019	ARG	Sidechain
3	J	13	ARG	Sidechain
3	J	166	TYR	Sidechain
3	J	403	TYR	Sidechain
3	J	5	PHE	Sidechain
3	K	1004	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	K	1014	ARG	Sidechain
3	K	1083	TYR	Sidechain
3	K	166	TYR	Sidechain
3	K	192	TYR	Sidechain
3	K	286	ARG	Sidechain
3	K	350	TYR	Sidechain
3	K	46	TYR	Sidechain
3	K	477	ARG	Sidechain
3	K	570	ARG	Sidechain
3	L	1019	ARG	Sidechain
3	L	1027	TYR	Sidechain
3	L	1128	ARG	Sidechain
3	L	1139	ARG	Sidechain
3	L	166	TYR	Sidechain
3	L	403	TYR	Sidechain
3	L	46	TYR	Sidechain
3	L	560	ARG	Sidechain
3	N	1004	TYR	Sidechain
3	N	1026	ARG	Sidechain
3	N	1041	THR	Peptide
3	N	133	TYR	Sidechain
3	N	166	TYR	Sidechain
3	N	210	HIS	Sidechain
3	N	286	ARG	Sidechain
3	N	29	ARG	Sidechain
3	N	350	TYR	Sidechain
3	N	465	ARG	Sidechain
3	N	477	ARG	Sidechain
3	N	523	ASP	Sidechain
3	N	560	ARG	Sidechain
4	O	220	TYR	Sidechain
4	O	365	TYR	Sidechain
4	O	367	TYR	Sidechain
4	O	401	TYR	Sidechain
4	O	423	TYR	Sidechain
4	O	79	TYR	Sidechain
4	P	117	TYR	Sidechain
4	P	220	TYR	Sidechain
4	P	365	TYR	Sidechain
4	P	367	TYR	Sidechain
4	P	401	TYR	Sidechain
4	P	423	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	P	78	TYR	Sidechain
4	Q	115	HIS	Sidechain
4	Q	200	ARG	Sidechain
4	Q	235	TYR	Sidechain
4	Q	365	TYR	Sidechain
4	Q	394	TYR	Sidechain
4	Q	412	ARG	Sidechain
4	Q	63	TYR	Sidechain

## 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	A	2994	0	2862	117	0
2	B	1336	0	1323	17	0
2	C	1349	0	1339	31	0
2	D	1336	0	1323	12	0
2	E	1349	0	1339	11	0
2	F	1349	0	1339	9	0
2	G	1349	0	1339	18	0
3	H	7166	0	6971	20	0
3	I	7166	0	6971	16	0
3	J	7166	0	6971	23	0
3	K	7166	0	6971	9	0
3	L	7166	0	6971	29	0
3	N	7166	0	6971	18	0
4	O	3548	0	3468	3	0
4	P	3548	0	3468	9	0
4	Q	3548	0	3468	9	0
All	All	64702	0	63094	216	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 2.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ALA:HB3	3:J:130:VAL:HG21	1.22	1.09
1:A:280:ALA:HB3	3:J:130:VAL:CG2	1.86	1.06
1:A:192:ASP:HA	2:B:173:VAL:CB	1.96	0.94
1:A:460:TYR:CE2	2:F:162:GLN:HA	2.04	0.92
1:A:459:ASN:OD1	2:E:154:LYS:NZ	2.01	0.92
1:A:192:ASP:HA	2:B:173:VAL:HB	1.54	0.88
1:A:192:ASP:HA	2:B:173:VAL:CG1	2.03	0.87
1:A:469:VAL:HG22	2:G:2:ALA:CB	2.06	0.86
1:A:245:VAL:HB	3:N:28:ASP:HA	1.56	0.86
1:A:192:ASP:CA	2:B:173:VAL:HB	2.08	0.84
1:A:469:VAL:HG22	2:G:2:ALA:HB1	1.60	0.84
1:A:280:ALA:C	3:J:130:VAL:HG11	2.02	0.83
1:A:245:VAL:CB	3:N:28:ASP:HA	2.09	0.82
1:A:281:SER:HB2	3:J:130:VAL:HG12	1.61	0.80
1:A:196:LYS:HB2	2:C:172:GLU:CB	2.13	0.79
1:A:192:ASP:HA	2:B:173:VAL:HG11	1.64	0.78
1:A:280:ALA:CB	3:J:130:VAL:CG2	2.60	0.77
1:A:196:LYS:HB2	2:C:172:GLU:CG	2.15	0.77
3:I:1105:ASN:HB2	3:L:291:ASP:CG	2.10	0.76
1:A:197:ILE:HG21	2:C:150:PHE:CD1	2.22	0.74
1:A:464:SER:O	2:E:163:THR:HA	1.86	0.74
1:A:192:ASP:H	2:B:173:VAL:CG2	2.00	0.73
1:A:469:VAL:HG13	2:G:3:ILE:CA	2.18	0.73
1:A:191:LEU:HD22	1:A:195:PRO:HD3	1.72	0.71
3:H:520:THR:HA	3:L:311:THR:HA	1.73	0.71
1:A:196:LYS:HG3	2:C:172:GLU:HG3	1.74	0.69
1:A:281:SER:CB	3:J:130:VAL:HG12	2.21	0.69
1:A:196:LYS:HB2	2:C:172:GLU:HG2	1.75	0.66
2:D:91:GLU:CD	2:D:91:GLU:H	2.04	0.66
1:A:192:ASP:CA	2:B:173:VAL:CB	2.68	0.66
1:A:280:ALA:C	3:J:130:VAL:CG1	2.69	0.65
1:A:469:VAL:HG13	2:G:3:ILE:HA	1.76	0.65
1:A:469:VAL:HG11	2:G:3:ILE:C	2.22	0.64
1:A:188:ILE:HG12	2:C:2:ALA:HB3	1.78	0.64
3:I:1105:ASN:CB	3:L:291:ASP:CG	2.71	0.64
2:C:157:GLN:HG2	2:D:158:ASN:HB3	1.81	0.63
3:H:318:LYS:HE3	3:H:320:TYR:CE2	2.34	0.63
1:A:241:ASN:OD1	3:N:33:GLN:HG3	1.99	0.62
3:I:943:PHE:CE2	3:L:339:GLN:HG3	2.35	0.62
1:A:245:VAL:HB	3:N:28:ASP:CA	2.26	0.62
1:A:280:ALA:HB1	3:J:130:VAL:HB	1.82	0.61
1:A:280:ALA:CB	3:J:130:VAL:HG21	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LYS:HB2	2:C:172:GLU:HB2	1.80	0.61
1:A:467:THR:OG1	2:F:154:LYS:NZ	2.34	0.61
1:A:280:ALA:CB	3:J:130:VAL:CB	2.80	0.60
1:A:127:LYS:HB3	3:K:131:PRO:HG2	1.83	0.60
1:A:196:LYS:CA	2:C:172:GLU:HB3	2.32	0.60
1:A:245:VAL:CG1	3:N:28:ASP:C	2.74	0.60
1:A:461:LEU:HD13	2:E:167:GLU:OE2	2.01	0.60
3:I:1104:ASN:HA	3:L:290:GLY:HA3	1.83	0.59
1:A:469:VAL:CG2	2:G:2:ALA:HB1	2.32	0.59
1:A:191:LEU:HD22	1:A:195:PRO:CD	2.32	0.58
3:I:1104:ASN:HA	3:L:290:GLY:CA	2.34	0.58
1:A:191:LEU:CD2	1:A:195:PRO:HD3	2.32	0.58
1:A:191:LEU:CD2	1:A:195:PRO:CD	2.82	0.58
3:I:318:LYS:HE3	3:I:320:TYR:CE2	2.39	0.57
1:A:280:ALA:O	3:J:130:VAL:HG11	2.06	0.56
1:A:280:ALA:CB	3:J:130:VAL:HB	2.35	0.56
3:I:1105:ASN:HB2	3:L:291:ASP:OD1	2.06	0.56
1:A:245:VAL:HA	3:N:29:ARG:O	2.05	0.56
1:A:469:VAL:CG1	2:G:3:ILE:C	2.79	0.55
2:C:157:GLN:NE2	2:D:157:GLN:HE21	2.04	0.55
3:H:519:ILE:HG13	3:L:311:THR:HG22	1.88	0.55
1:A:192:ASP:N	2:B:173:VAL:HB	2.20	0.55
3:I:1102:ARG:HH21	3:L:289:GLN:NE2	2.06	0.54
1:A:245:VAL:HG12	3:N:28:ASP:C	2.32	0.53
1:A:193:GLY:C	1:A:194:LEU:HG	2.34	0.53
3:I:1105:ASN:HB2	3:L:291:ASP:CB	2.39	0.53
1:A:126:ASN:O	3:K:132:SER:HB3	2.09	0.53
2:C:91:GLU:H	2:C:91:GLU:CD	2.17	0.53
3:J:504:ARG:HD3	3:L:483:TYR:CE1	2.44	0.53
1:A:197:ILE:CG2	2:C:150:PHE:CD1	2.92	0.52
1:A:131:ASN:HB2	3:H:28:ASP:OD1	2.10	0.52
1:A:196:LYS:CB	2:C:172:GLU:CG	2.84	0.52
1:A:196:LYS:CB	2:C:172:GLU:CB	2.86	0.52
1:A:126:ASN:ND2	3:K:130:VAL:HG21	2.25	0.52
1:A:137:MET:SD	3:H:134:PHE:HB3	2.49	0.52
1:A:452:PRO:HG2	2:D:173:VAL:C	2.35	0.51
3:I:357:LYS:HZ3	3:I:364:ASP:CG	2.18	0.51
1:A:196:LYS:C	2:C:172:GLU:HB3	2.35	0.51
3:N:309:THR:HG23	3:N:320:TYR:CE1	2.46	0.51
1:A:188:ILE:CG1	2:C:2:ALA:HB3	2.41	0.51
3:H:498:GLN:HA	3:L:344:SER:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:N	2:B:173:VAL:CG2	2.73	0.50
1:A:469:VAL:HG13	2:G:3:ILE:N	2.25	0.50
2:F:116:THR:HG22	2:F:158:ASN:HA	1.93	0.50
1:A:190:TRP:CH2	2:C:9:HIS:HA	2.46	0.50
1:A:450:ILE:HG22	2:D:171:VAL:HG13	1.91	0.50
4:O:168:VAL:HG11	4:Q:190:SER:OG	2.11	0.50
4:Q:209:GLU:HB3	4:Q:226:GLU:HG2	1.94	0.50
3:H:520:THR:CA	3:L:311:THR:HA	2.42	0.49
1:A:468:TYR:O	2:G:2:ALA:HB3	2.12	0.49
1:A:240:ILE:HG21	3:N:33:GLN:HB3	1.94	0.49
3:L:291:ASP:OD1	3:L:337:SER:HA	2.12	0.49
3:L:560:ARG:HH21	3:L:560:ARG:HA	1.77	0.49
2:E:101:VAL:HB	2:E:171:VAL:CG2	2.42	0.49
3:H:497:GLY:CA	3:L:344:SER:OG	2.61	0.49
1:A:236:ASN:HA	3:J:31:LEU:O	2.13	0.49
4:P:233:GLU:HG2	4:P:240:ILE:HD12	1.94	0.48
3:J:318:LYS:HE3	3:J:320:TYR:CD2	2.47	0.48
1:A:306:GLU:CD	1:A:432:LYS:HZ3	2.22	0.48
1:A:461:LEU:O	2:F:163:THR:HA	2.13	0.48
2:G:129:LYS:HE3	2:G:142:VAL:O	2.13	0.48
3:L:872:GLU:OE2	3:L:875:LYS:HE2	2.13	0.48
1:A:245:VAL:CG1	3:N:28:ASP:HA	2.43	0.48
1:A:460:TYR:OH	2:F:161:GLU:O	2.29	0.48
3:J:19:ASP:HB2	3:N:144:LYS:HE3	1.94	0.48
1:A:320:ASN:C	1:A:321:ASN:HD22	2.21	0.48
2:E:156:PHE:CD1	2:F:158:ASN:CG	2.92	0.48
1:A:196:LYS:CG	2:C:172:GLU:HG3	2.42	0.47
1:A:197:ILE:CG2	2:C:150:PHE:CE1	2.97	0.47
2:B:172:GLU:C	2:B:173:VAL:HG22	2.40	0.47
3:I:943:PHE:CD2	3:L:339:GLN:HG3	2.49	0.47
3:K:998:TRP:CD1	3:K:999:GLU:H	2.32	0.47
1:A:127:LYS:HB3	3:K:131:PRO:HB2	1.97	0.47
4:P:225:LYS:HG2	4:P:228:GLU:HB2	1.96	0.47
1:A:153:TYR:CE2	2:B:155:GLN:HB2	2.50	0.46
2:G:116:THR:HG22	2:G:158:ASN:HA	1.98	0.46
3:I:1105:ASN:HB2	3:L:291:ASP:HB2	1.97	0.46
2:E:91:GLU:H	2:E:91:GLU:CD	2.24	0.46
3:H:520:THR:HA	3:L:311:THR:CA	2.42	0.46
1:A:296:TYR:C	1:A:298:SER:H	2.24	0.46
3:N:309:THR:HG23	3:N:320:TYR:CD1	2.51	0.46
3:H:885:ASN:HD21	3:H:887:ASP:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:HA	3:N:29:ARG:C	2.42	0.45
3:J:318:LYS:HE3	3:J:320:TYR:CE2	2.51	0.45
1:A:204:ASP:CG	2:D:168:ARG:HH11	2.23	0.45
2:C:61:VAL:HG12	2:C:103:LEU:HA	1.98	0.45
3:J:995:GLN:C	3:J:997:LYS:H	2.24	0.45
4:P:213:ILE:HD13	4:P:215:LYS:HE3	1.97	0.45
1:A:127:LYS:HB3	3:K:131:PRO:CG	2.47	0.45
1:A:127:LYS:CB	3:K:131:PRO:HB2	2.47	0.45
1:A:443:TYR:CE1	2:C:161:GLU:HB2	2.51	0.45
2:E:101:VAL:HB	2:E:171:VAL:HG22	1.99	0.45
2:G:91:GLU:N	2:G:91:GLU:CD	2.75	0.45
1:A:153:TYR:CZ	1:A:181:THR:HB	2.52	0.45
1:A:190:TRP:CH2	2:C:12:LEU:HB2	2.52	0.45
2:E:129:LYS:HE3	2:E:142:VAL:O	2.17	0.44
3:H:996:LEU:H	3:H:996:LEU:CD1	2.30	0.44
3:L:291:ASP:CG	3:L:337:SER:HA	2.43	0.44
2:C:56:LYS:HZ2	2:C:111:GLU:CD	2.26	0.44
3:H:520:THR:HG22	3:L:310:GLU:O	2.18	0.44
2:G:14:LYS:HE2	2:G:90:PRO:O	2.18	0.44
4:P:123:ASN:HA	4:P:126:ILE:HG22	2.00	0.44
4:O:144:ILE:HG22	4:Q:144:ILE:HD12	2.00	0.44
1:A:465:ARG:HA	2:E:162:GLN:O	2.16	0.44
1:A:469:VAL:HG22	2:G:2:ALA:C	2.43	0.44
3:L:186:TYR:CE1	3:L:223:LYS:HE2	2.53	0.44
2:C:104:GLU:CD	2:C:168:ARG:HE	2.26	0.44
1:A:196:LYS:CG	2:C:172:GLU:CG	2.95	0.43
1:A:206:PHE:CE1	2:D:80:TYR:HB2	2.53	0.43
1:A:245:VAL:CG2	3:N:28:ASP:HA	2.47	0.43
3:K:560:ARG:HE	3:K:560:ARG:HA	1.81	0.43
1:A:281:SER:N	3:J:130:VAL:CG1	2.81	0.43
2:C:157:GLN:CD	2:D:158:ASN:H	2.26	0.43
3:H:996:LEU:H	3:H:996:LEU:HD12	1.82	0.43
4:Q:209:GLU:H	4:Q:226:GLU:CD	2.26	0.43
4:P:198:LEU:HD22	4:Q:202:THR:HB	2.00	0.43
1:A:192:ASP:H	2:B:173:VAL:HG23	1.82	0.43
4:P:381:LYS:HZ2	4:P:411:ASP:CG	2.25	0.43
1:A:193:GLY:HA3	2:B:9:HIS:ND1	2.33	0.43
1:A:209:TYR:CE1	1:A:446:GLY:HA2	2.54	0.43
1:A:280:ALA:HB1	3:J:130:VAL:CB	2.46	0.43
3:H:318:LYS:HE3	3:H:320:TYR:CZ	2.54	0.43
1:A:452:PRO:CG	2:D:173:VAL:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:497:GLY:HA2	3:L:344:SER:OG	2.17	0.43
1:A:233:PHE:CE2	3:N:31:LEU:HB3	2.53	0.43
1:A:176:TYR:OH	1:A:181:THR:HG21	2.19	0.42
3:N:981:LYS:HZ3	3:N:981:LYS:N	2.17	0.42
1:A:469:VAL:CG2	2:G:2:ALA:CB	2.85	0.42
2:F:14:LYS:HE2	2:F:93:ALA:HB3	2.01	0.42
3:J:92:ASN:HD22	3:J:94:ASP:HB2	1.85	0.42
1:A:192:ASP:N	2:B:173:VAL:CB	2.83	0.42
2:B:129:LYS:HE3	2:B:143:GLU:HA	2.02	0.42
3:K:60:LYS:HE3	3:K:60:LYS:H	1.85	0.42
1:A:206:PHE:CB	2:D:80:TYR:CD1	3.03	0.42
1:A:469:VAL:CG1	2:G:3:ILE:CA	2.92	0.42
3:H:497:GLY:C	3:L:344:SER:OG	2.62	0.42
3:J:60:LYS:HE2	3:J:173:GLU:OE1	2.20	0.42
1:A:196:LYS:N	2:C:172:GLU:HB3	2.35	0.41
1:A:265:TYR:CE2	1:A:285:ARG:HB3	2.55	0.41
3:I:869:MET:HE1	3:I:877:TYR:CE1	2.55	0.41
1:A:232:ILE:O	1:A:234:LYS:HE2	2.19	0.41
1:A:453:TYR:HE2	2:D:9:HIS:CE1	2.38	0.41
2:G:129:LYS:HE3	2:G:142:VAL:C	2.45	0.41
3:J:504:ARG:HD3	3:L:483:TYR:CD1	2.55	0.41
1:A:465:ARG:NH2	2:F:155:GLN:O	2.51	0.41
3:H:497:GLY:HA2	3:L:344:SER:CB	2.50	0.41
4:P:190:SER:HB3	4:Q:186:PHE:CD1	2.54	0.41
2:E:156:PHE:CD1	2:E:156:PHE:N	2.89	0.41
2:F:11:GLU:OE2	2:F:94:LYS:HE3	2.19	0.41
3:N:48:LYS:HE2	3:N:52:ASP:OD2	2.20	0.41
4:O:240:ILE:HG12	4:Q:235:TYR:CD1	2.56	0.41
1:A:192:ASP:H	2:B:173:VAL:HG21	1.82	0.41
2:B:172:GLU:HB2	2:B:173:VAL:HG22	2.03	0.41
1:A:457:ILE:HD13	2:E:150:PHE:CD1	2.55	0.41
3:N:996:LEU:H	3:N:996:LEU:CD1	2.34	0.41
1:A:196:LYS:C	2:C:172:GLU:CB	2.94	0.41
1:A:450:ILE:HG21	2:D:171:VAL:HG22	2.02	0.41
2:C:157:GLN:HE21	2:C:157:GLN:HB3	1.75	0.41
2:G:125:ASP:O	2:G:146:GLY:HA3	2.21	0.41
3:L:311:THR:HG23	3:L:317:THR:OG1	2.21	0.41
3:I:369:THR:HG21	3:I:376:LYS:HE3	2.02	0.40
3:L:999:GLU:H	3:L:999:GLU:CD	2.29	0.40
1:A:196:LYS:O	1:A:197:ILE:HG23	2.21	0.40
3:I:999:GLU:H	3:I:999:GLU:CD	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:402:VAL:HG13	4:P:424:ARG:HD2	2.01	0.40
1:A:137:MET:HE1	3:H:134:PHE:O	2.22	0.40
1:A:190:TRP:CH2	2:C:12:LEU:HD13	2.57	0.40
4:Q:214:LYS:HE2	4:Q:218:GLY:O	2.22	0.40
2:C:152:ASP:CG	2:C:154:LYS:HZ3	2.29	0.40
3:H:996:LEU:HD12	3:H:996:LEU:N	2.36	0.40
1:A:130:LEU:HB2	3:H:29:ARG:O	2.21	0.40
3:I:56:LYS:HE3	3:I:175:ASP:HB2	2.04	0.40
4:P:342:LEU:HB3	4:P:358:LEU:HD22	2.02	0.40
4:Q:130:TYR:HE1	4:Q:144:ILE:HD11	1.87	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	358/1019 (35%)	318 (89%)	37 (10%)	3 (1%)	16	52
2	B	168/173 (97%)	156 (93%)	9 (5%)	3 (2%)	6	35
2	C	170/173 (98%)	160 (94%)	10 (6%)	0	100	100
2	D	168/173 (97%)	156 (93%)	9 (5%)	3 (2%)	6	35
2	E	170/173 (98%)	152 (89%)	11 (6%)	7 (4%)	2	20
2	F	170/173 (98%)	152 (89%)	13 (8%)	5 (3%)	3	26
2	G	170/173 (98%)	157 (92%)	9 (5%)	4 (2%)	4	30
3	H	900/1152 (78%)	846 (94%)	52 (6%)	2 (0%)	43	76
3	I	900/1152 (78%)	857 (95%)	42 (5%)	1 (0%)	48	81
3	J	900/1152 (78%)	842 (94%)	52 (6%)	6 (1%)	18	55
3	K	900/1152 (78%)	852 (95%)	48 (5%)	0	100	100
3	L	900/1152 (78%)	843 (94%)	48 (5%)	9 (1%)	12	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	900/1152 (78%)	833 (93%)	59 (7%)	8 (1%)	14	49
4	O	456/458 (100%)	431 (94%)	25 (6%)	0	100	100
4	P	456/458 (100%)	431 (94%)	23 (5%)	2 (0%)	30	65
4	Q	456/458 (100%)	428 (94%)	28 (6%)	0	100	100
All	All	8142/10343 (79%)	7614 (94%)	475 (6%)	53 (1%)	20	55

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	70	PRO
2	E	93	ALA
2	F	93	ALA
2	G	93	ALA
2	G	111	GLU
4	P	227	PHE
1	A	190	TRP
2	B	161	GLU
2	D	29	LYS
2	G	73	ASP
3	J	996	LEU
3	L	311	THR
3	L	913	LEU
3	N	313	PRO
3	N	360	GLU
2	B	76	ASN
2	E	92	ASN
2	E	98	ALA
2	F	92	ASN
3	I	996	LEU
3	L	869	MET
3	L	996	LEU
3	L	1116	VAL
3	N	461	PHE
3	N	519	ILE
1	A	297	THR
1	A	313	SER
2	D	159	ARG
2	E	73	ASP
2	E	111	GLU
2	E	156	PHE
2	F	70	PRO

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Mol	Chain	Res	Type
3	J	1010	LEU
2	D	69	SER
2	F	69	SER
2	F	73	ASP
2	G	143	GLU
3	H	1003	ASN
3	J	340	GLY
3	L	28	ASP
3	L	340	GLY
3	N	93	ASP
3	N	833	GLN
3	N	1040	THR
4	P	432	SER
2	E	70	PRO
3	J	1043	LEU
3	L	337	SER
3	N	493	GLY
3	H	340	GLY
3	J	557	ILE
3	J	337	SER
3	L	583	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	332/928 (36%)	320 (96%)	12 (4%)	31	53
2	B	151/153 (99%)	144 (95%)	7 (5%)	24	47
2	C	152/153 (99%)	142 (93%)	10 (7%)	15	39
2	D	151/153 (99%)	149 (99%)	2 (1%)	61	72
2	E	152/153 (99%)	141 (93%)	11 (7%)	13	37
2	F	152/153 (99%)	137 (90%)	15 (10%)	7	26
2	G	152/153 (99%)	142 (93%)	10 (7%)	15	39
3	H	800/1010 (79%)	786 (98%)	14 (2%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	800/1010 (79%)	791 (99%)	9 (1%)	65	74
3	J	800/1010 (79%)	781 (98%)	19 (2%)	43	63
3	K	800/1010 (79%)	790 (99%)	10 (1%)	61	72
3	L	800/1010 (79%)	781 (98%)	19 (2%)	43	63
3	N	800/1010 (79%)	785 (98%)	15 (2%)	50	67
4	O	405/405 (100%)	400 (99%)	5 (1%)	63	73
4	P	405/405 (100%)	396 (98%)	9 (2%)	45	64
4	Q	405/405 (100%)	395 (98%)	10 (2%)	42	62
All	All	7257/9121 (80%)	7080 (98%)	177 (2%)	43	63

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	TYR
1	A	189	LYS
1	A	190	TRP
1	A	191	LEU
1	A	212	THR
1	A	236	ASN
1	A	277	GLN
1	A	292	ASP
1	A	306	GLU
1	A	320	ASN
1	A	367	GLU
1	A	470	GLU
2	B	9	HIS
2	B	70	PRO
2	B	150	PHE
2	B	151	PHE
2	B	157	GLN
2	B	159	ARG
2	B	166	LYS
2	C	9	HIS
2	C	41	GLN
2	C	71	GLU
2	C	75	LYS
2	C	78	ILE
2	C	80	TYR
2	C	91	GLU

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Mol	Chain	Res	Type
2	C	101	VAL
2	C	157	GLN
2	C	172	GLU
2	D	75	LYS
2	D	91	GLU
2	E	11	GLU
2	E	51	GLU
2	E	88	VAL
2	E	91	GLU
2	E	101	VAL
2	E	111	GLU
2	E	125	ASP
2	E	126	LEU
2	E	136	ASN
2	E	143	GLU
2	E	156	PHE
2	F	3	ILE
2	F	38	ASN
2	F	51	GLU
2	F	68	LYS
2	F	88	VAL
2	F	101	VAL
2	F	108	VAL
2	F	111	GLU
2	F	125	ASP
2	F	127	VAL
2	F	136	ASN
2	F	142	VAL
2	F	143	GLU
2	F	154	LYS
2	F	162	GLN
2	G	38	ASN
2	G	51	GLU
2	G	68	LYS
2	G	88	VAL
2	G	91	GLU
2	G	101	VAL
2	G	111	GLU
2	G	125	ASP
2	G	127	VAL
2	G	157	GLN
3	H	97	LYS

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Mol	Chain	Res	Type
3	H	103	LYS
3	H	144	LYS
3	H	198	GLU
3	H	257	ASN
3	H	342	GLU
3	H	358	ARG
3	H	366	GLU
3	H	465	ARG
3	H	560	ARG
3	H	942	LYS
3	H	945	GLU
3	H	1014	ARG
3	H	1075	LYS
3	I	33	GLN
3	I	269	GLU
3	I	291	ASP
3	I	342	GLU
3	I	358	ARG
3	I	833	GLN
3	I	981	LYS
3	I	1045	GLU
3	I	1134	GLU
3	J	19	ASP
3	J	97	LYS
3	J	144	LYS
3	J	269	GLU
3	J	283	ARG
3	J	822	ASN
3	J	861	THR
3	J	869	MET
3	J	884	GLU
3	J	892	VAL
3	J	981	LYS
3	J	987	MET
3	J	995	GLN
3	J	997	LYS
3	J	1045	GLU
3	J	1078	LYS
3	J	1087	ASP
3	J	1092	LYS
3	J	1143	ARG
3	K	33	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	K	97	LYS
3	K	170	THR
3	K	269	GLU
3	K	560	ARG
3	K	945	GLU
3	K	981	LYS
3	K	1007	LEU
3	K	1078	LYS
3	K	1133	THR
3	L	33	GLN
3	L	185	THR
3	L	257	ASN
3	L	283	ARG
3	L	339	GLN
3	L	342	GLU
3	L	515	ASP
3	L	520	THR
3	L	541	GLU
3	L	584	ASN
3	L	822	ASN
3	L	833	GLN
3	L	942	LYS
3	L	1045	GLU
3	L	1075	LYS
3	L	1078	LYS
3	L	1086	ASP
3	L	1087	ASP
3	L	1134	GLU
3	N	4	ASN
3	N	32	GLN
3	N	33	GLN
3	N	97	LYS
3	N	144	LYS
3	N	170	THR
3	N	283	ARG
3	N	294	ASP
3	N	322	GLN
3	N	526	ILE
3	N	942	LYS
3	N	981	LYS
3	N	1075	LYS
3	N	1078	LYS

*Continued on next page...*

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Mol	Chain	Res	Type
3	N	1133	THR
4	O	10	GLU
4	O	70	ARG
4	O	192	ASP
4	O	209	GLU
4	O	320	ASN
4	P	26	GLU
4	P	32	ARG
4	P	40	ASP
4	P	70	ARG
4	P	83	ARG
4	P	192	ASP
4	P	225	LYS
4	P	231	ASP
4	P	414	ASP
4	Q	26	GLU
4	Q	40	ASP
4	Q	70	ARG
4	Q	83	ARG
4	Q	95	GLU
4	Q	192	ASP
4	Q	224	LYS
4	Q	226	GLU
4	Q	227	PHE
4	Q	356	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	129	HIS
1	A	268	ASN
1	A	303	ASN
1	A	321	ASN
2	B	76	ASN
2	B	92	ASN
2	B	162	GLN
2	C	50	GLN
2	C	158	ASN
2	D	157	GLN
2	E	153	ASN
2	F	7	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
2	F	38	ASN
2	F	45	ASN
2	F	158	ASN
2	G	45	ASN
2	G	153	ASN
2	G	157	GLN
3	H	49	ASN
3	H	92	ASN
3	H	248	ASN
3	H	258	ASN
3	H	441	ASN
3	H	443	GLN
3	H	576	GLN
3	H	590	ASN
3	H	799	GLN
3	H	885	ASN
3	H	910	ASN
3	H	1126	GLN
3	I	92	ASN
3	I	254	ASN
3	I	258	ASN
3	I	393	GLN
3	I	799	GLN
3	I	833	GLN
3	J	92	ASN
3	J	126	GLN
3	J	386	ASN
3	J	441	ASN
3	J	556	HIS
3	J	590	ASN
3	J	822	ASN
3	J	914	GLN
3	K	248	ASN
3	K	258	ASN
3	K	264	ASN
3	K	276	GLN
3	K	293	GLN
3	K	332	GLN
3	K	393	GLN
3	K	576	GLN
3	K	837	ASN
3	K	910	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	K	1003	ASN
3	K	1105	ASN
3	L	195	ASN
3	L	257	ASN
3	L	289	GLN
3	L	339	GLN
3	L	441	ASN
3	L	799	GLN
3	L	833	GLN
3	L	944	ASN
3	L	995	GLN
3	N	195	ASN
3	N	276	GLN
3	N	356	ASN
3	N	443	GLN
3	N	499	ASN
3	N	576	GLN
3	N	590	ASN
3	N	1003	ASN
3	N	1105	ASN
4	O	20	GLN
4	O	281	GLN
4	P	23	ASN
4	Q	20	GLN
4	Q	102	HIS

### 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.

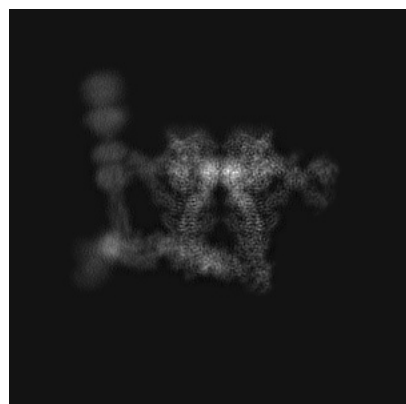
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55968. These allow visual inspection of the internal detail of the map and identification of artifacts.

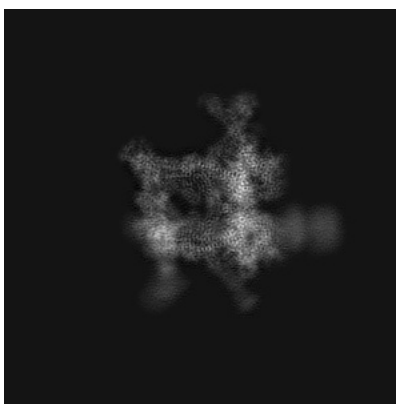
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

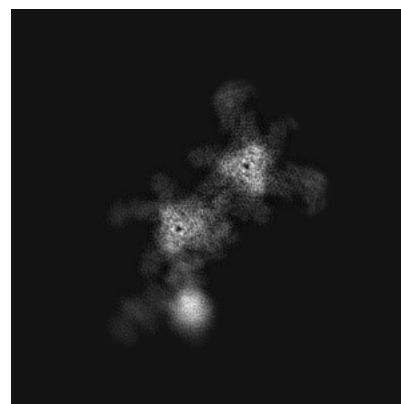
#### 6.1.1 Primary map



X

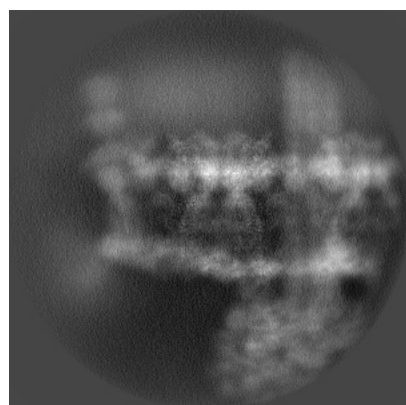


Y

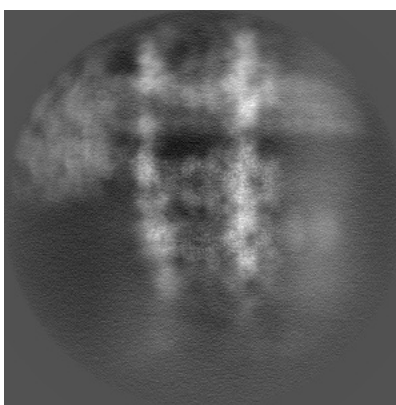


Z

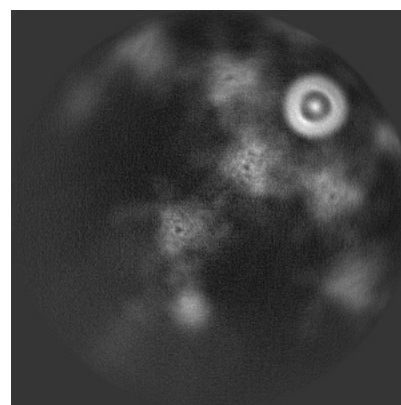
#### 6.1.2 Raw map



X



Y

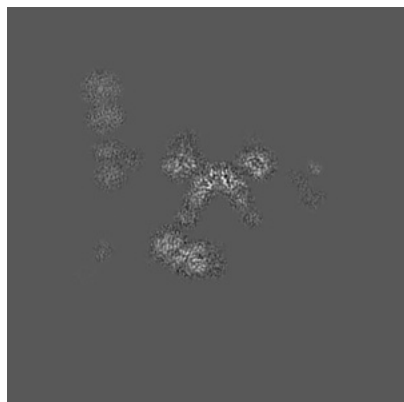


Z

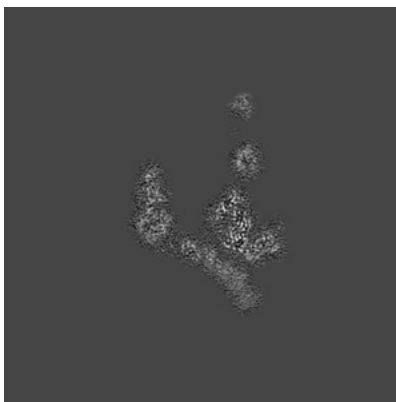
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

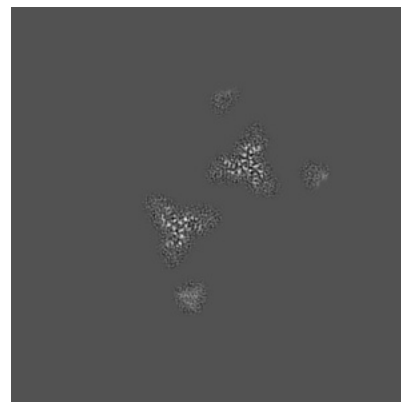
### 6.2.1 Primary map



X Index: 240

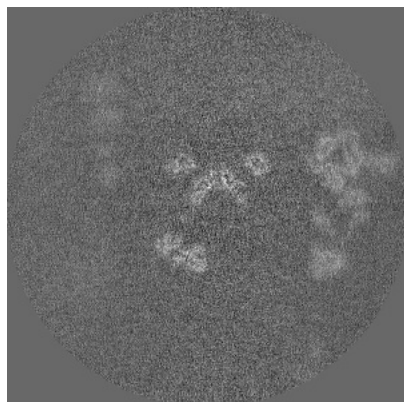


Y Index: 240

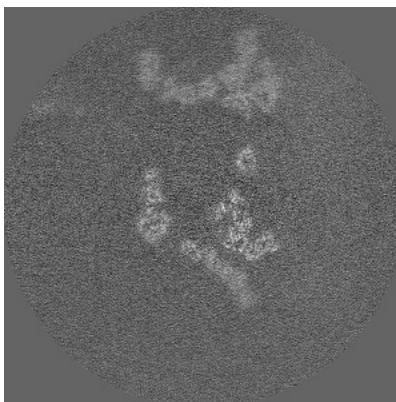


Z Index: 240

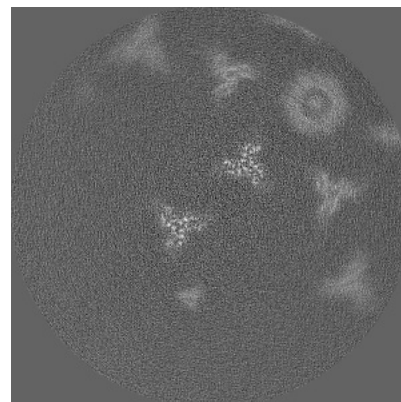
### 6.2.2 Raw map



X Index: 240



Y Index: 240

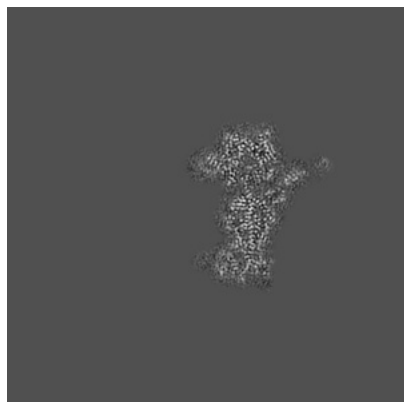


Z Index: 240

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

## 6.3 Largest variance slices [i](#)

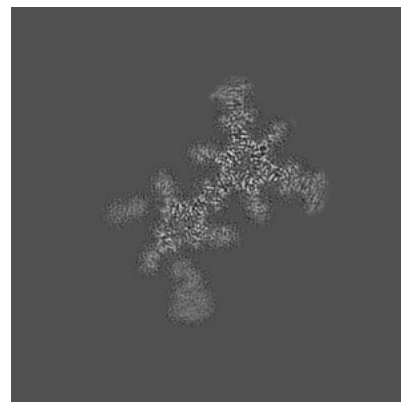
### 6.3.1 Primary map



X Index: 290

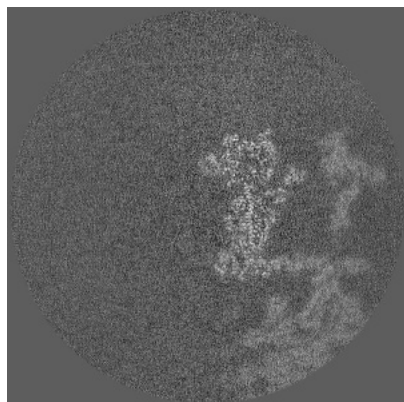


Y Index: 297

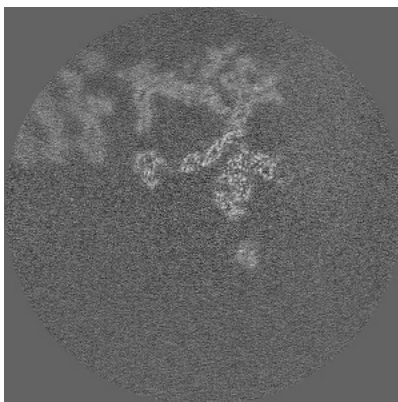


Z Index: 283

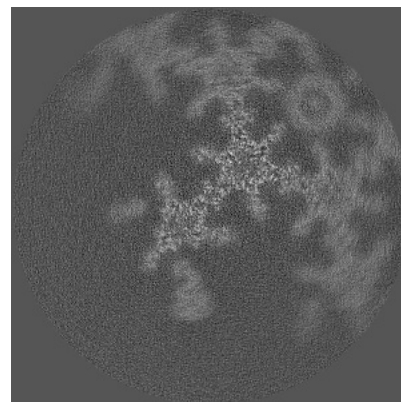
### 6.3.2 Raw map



X Index: 289



Y Index: 269

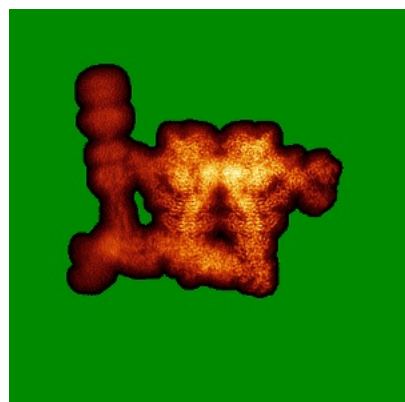


Z Index: 283

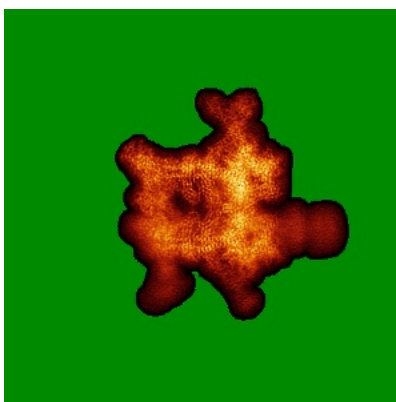
The images above show the largest variance slices of the map in three orthogonal directions.

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

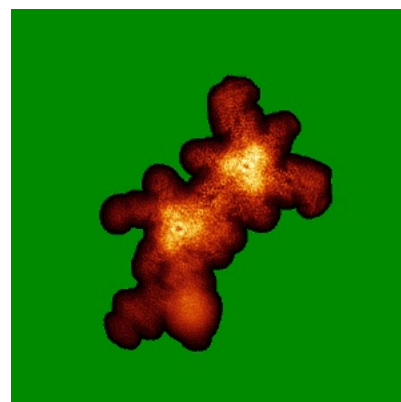
### 6.4.1 Primary map



X

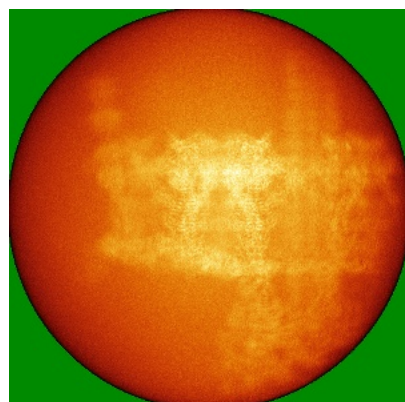


Y

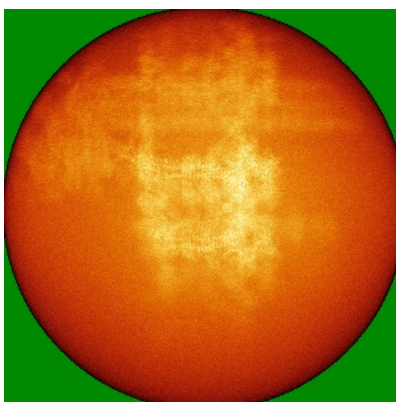


Z

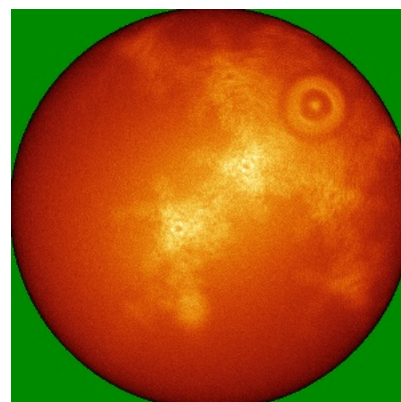
### 6.4.2 Raw map



X



Y

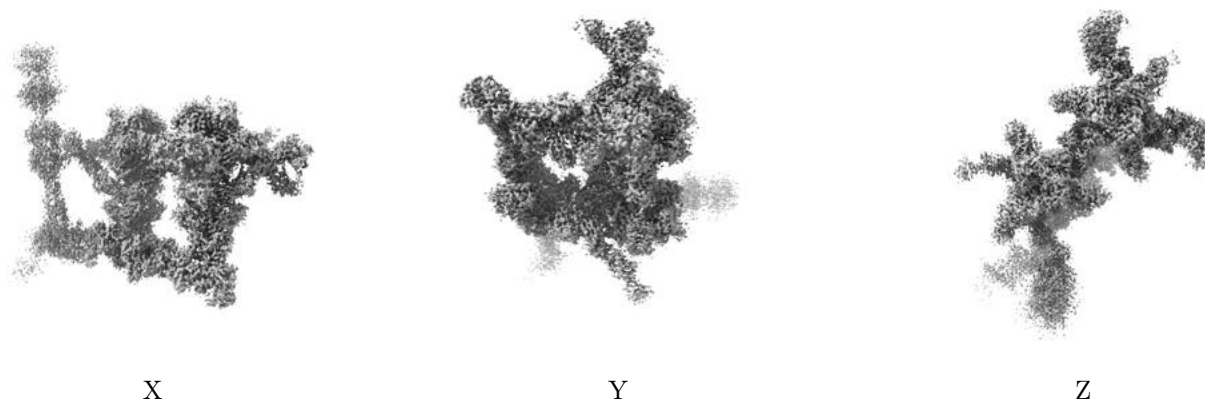


Z

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.

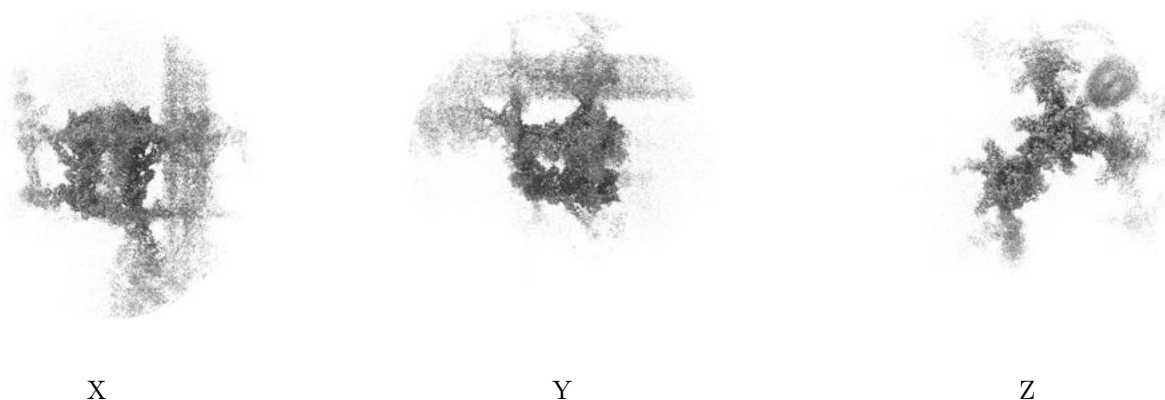
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.



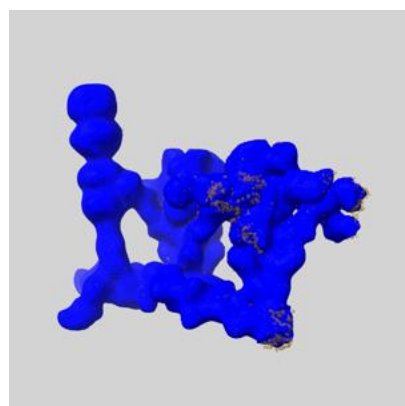
## 6.6 Mask visualisation [i](#)

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

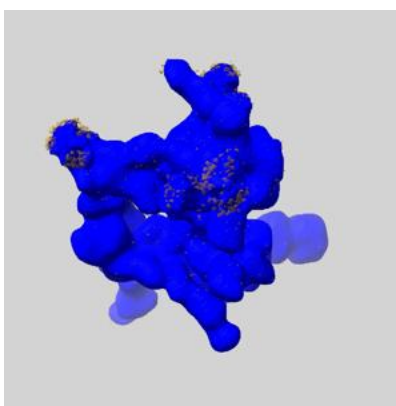
A mask typically either:

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

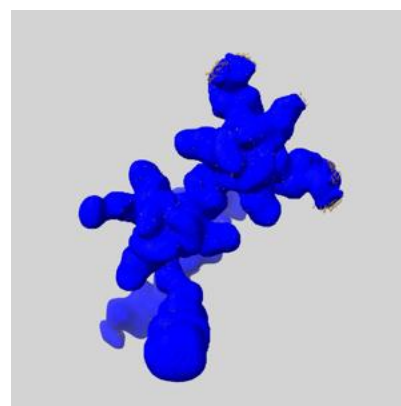
### 6.6.1 emd\_55968\_msk\_1.map [i](#)



X



Y

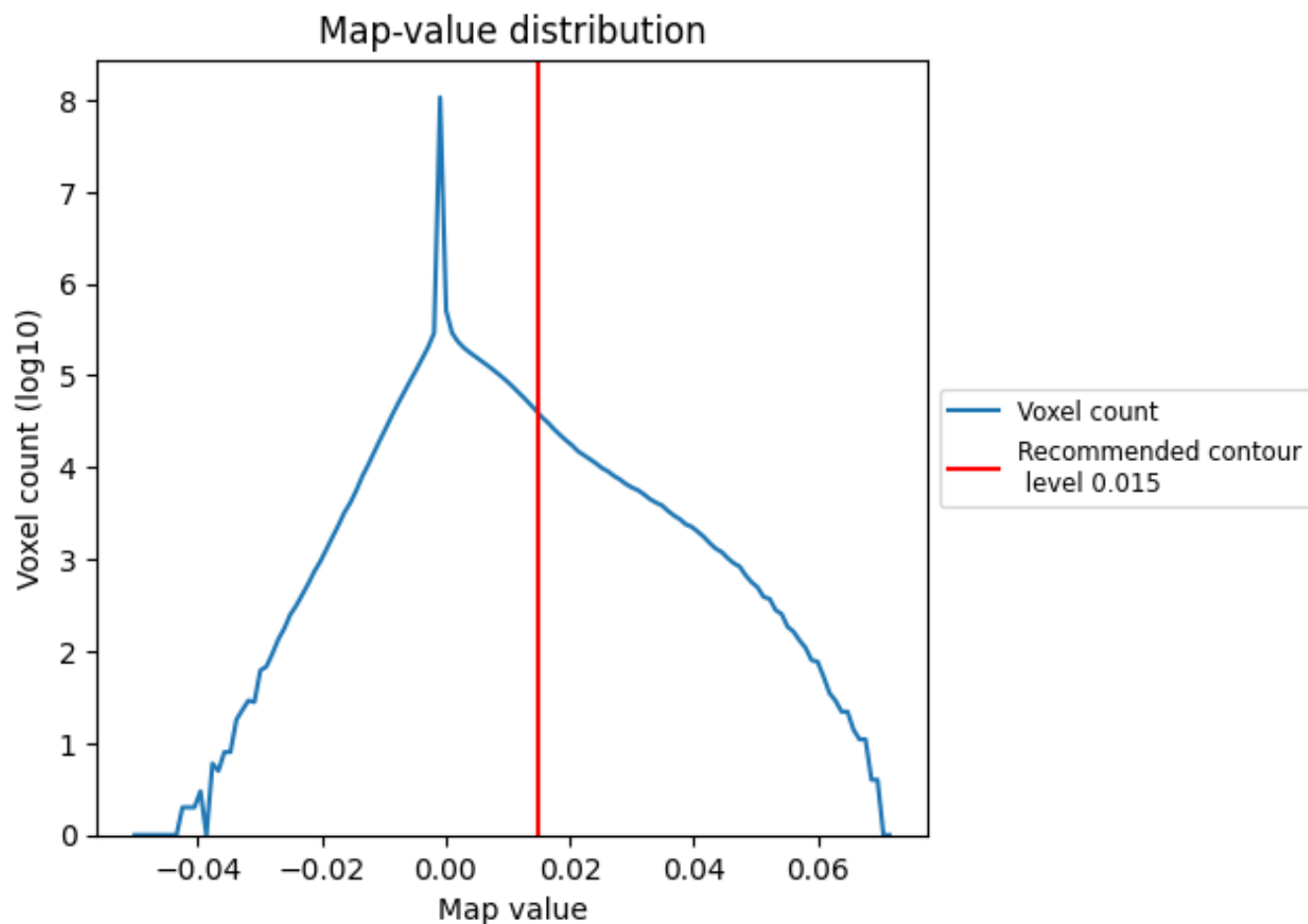


Z

## 7 Map analysis [i](#)

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

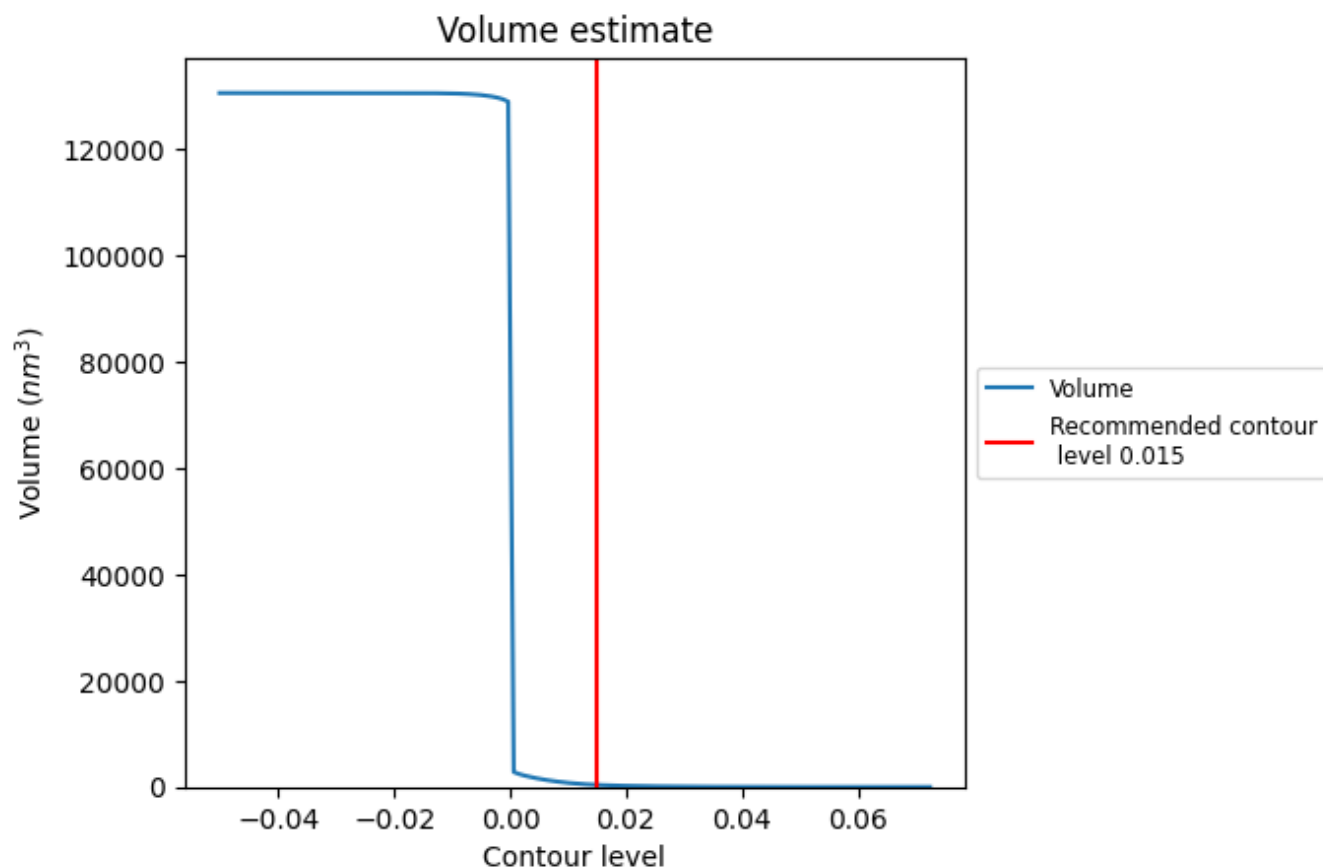
### 7.1 Map-value distribution [i](#)



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.



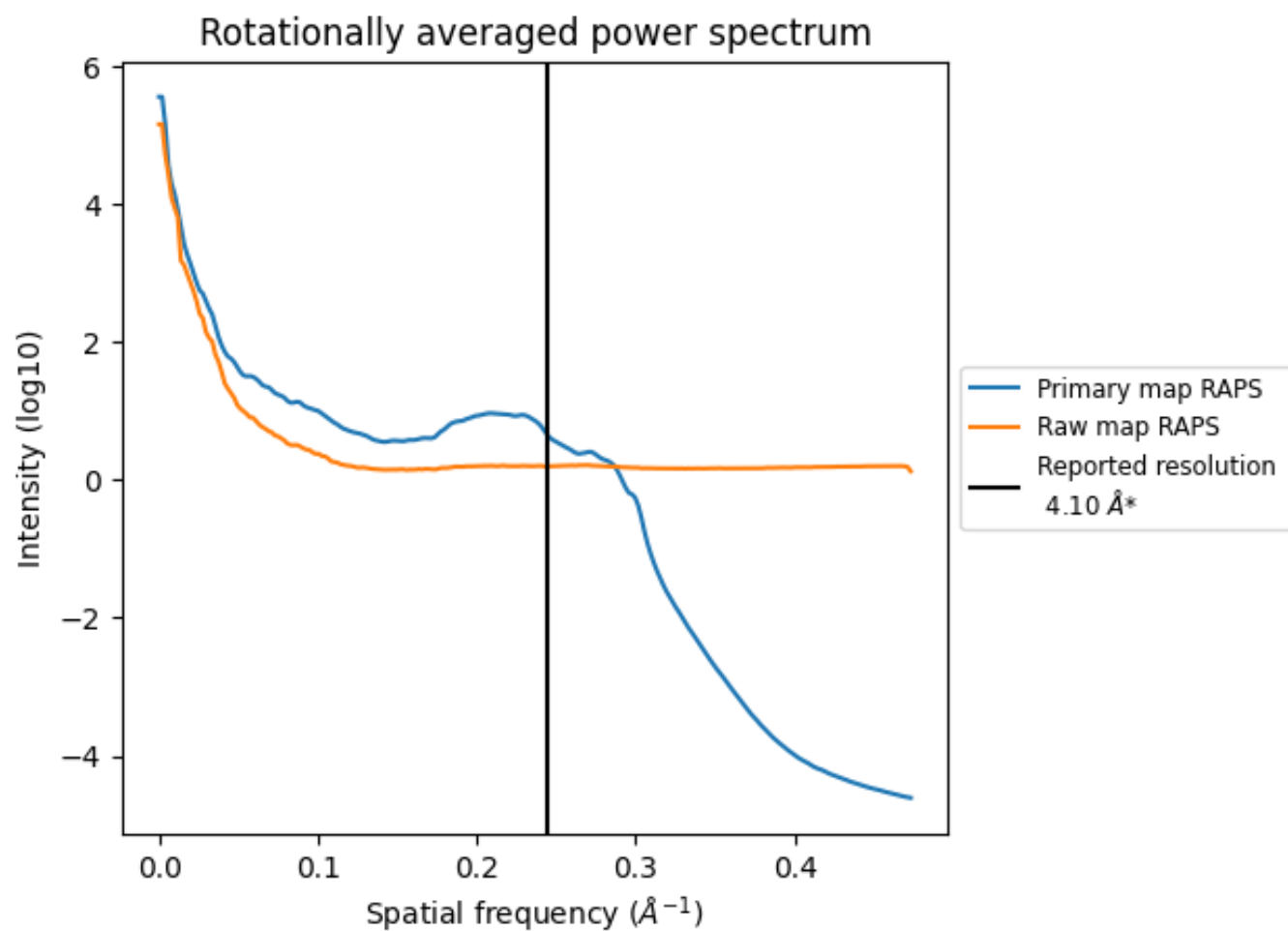
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm<sup>3</sup>; this corresponds to an approximate mass of 347 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

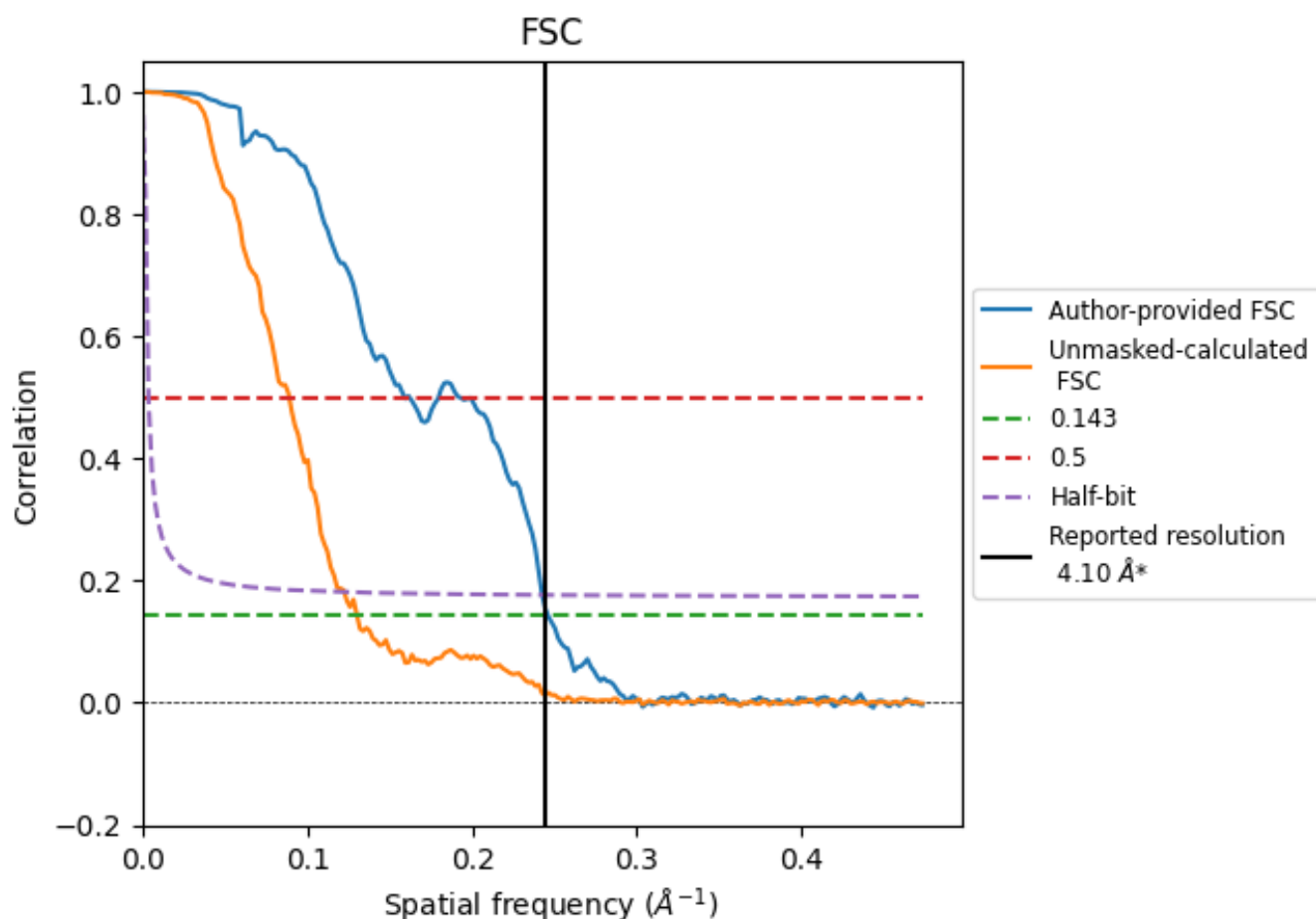


\*Reported resolution corresponds to spatial frequency of 0.244  $\text{\AA}^{-1}$

## 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  $0.244 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

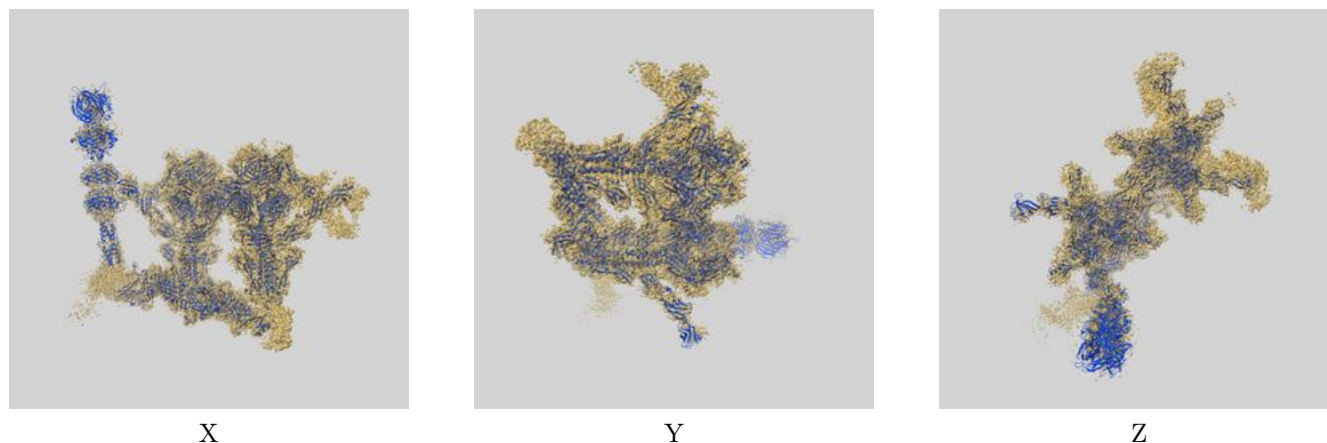
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.07	6.28	4.12
Unmasked-calculated*	7.67	11.22	8.16

\*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 7.67 differs from the reported value 4.1 by more than 10 %

## 9 Map-model fit [i](#)

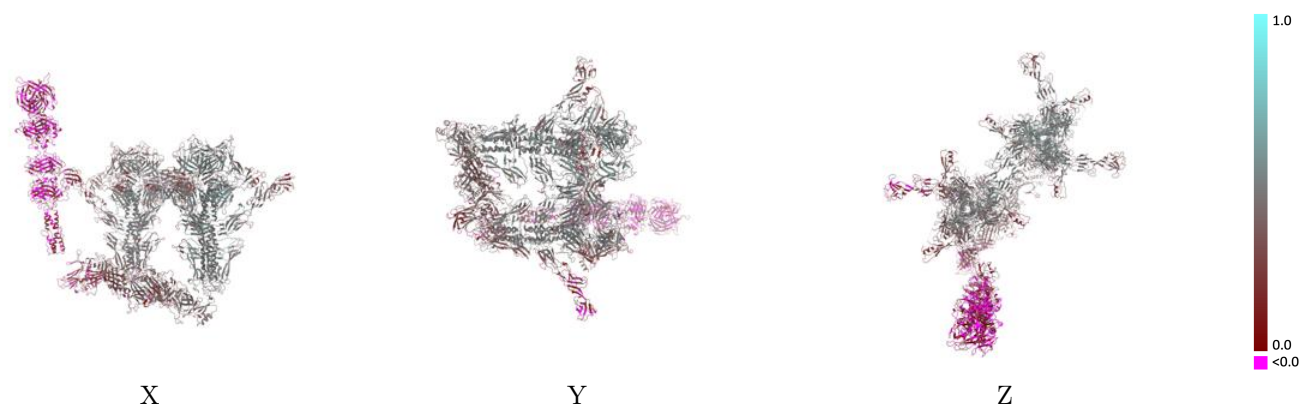
This section contains information regarding the fit between EMDB map EMD-55968 and PDB model 9TIS. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



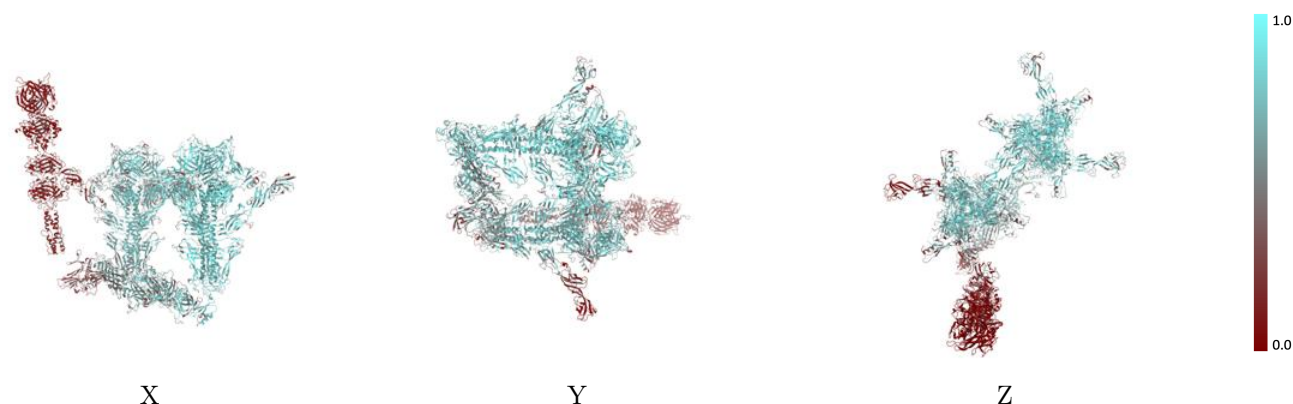
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



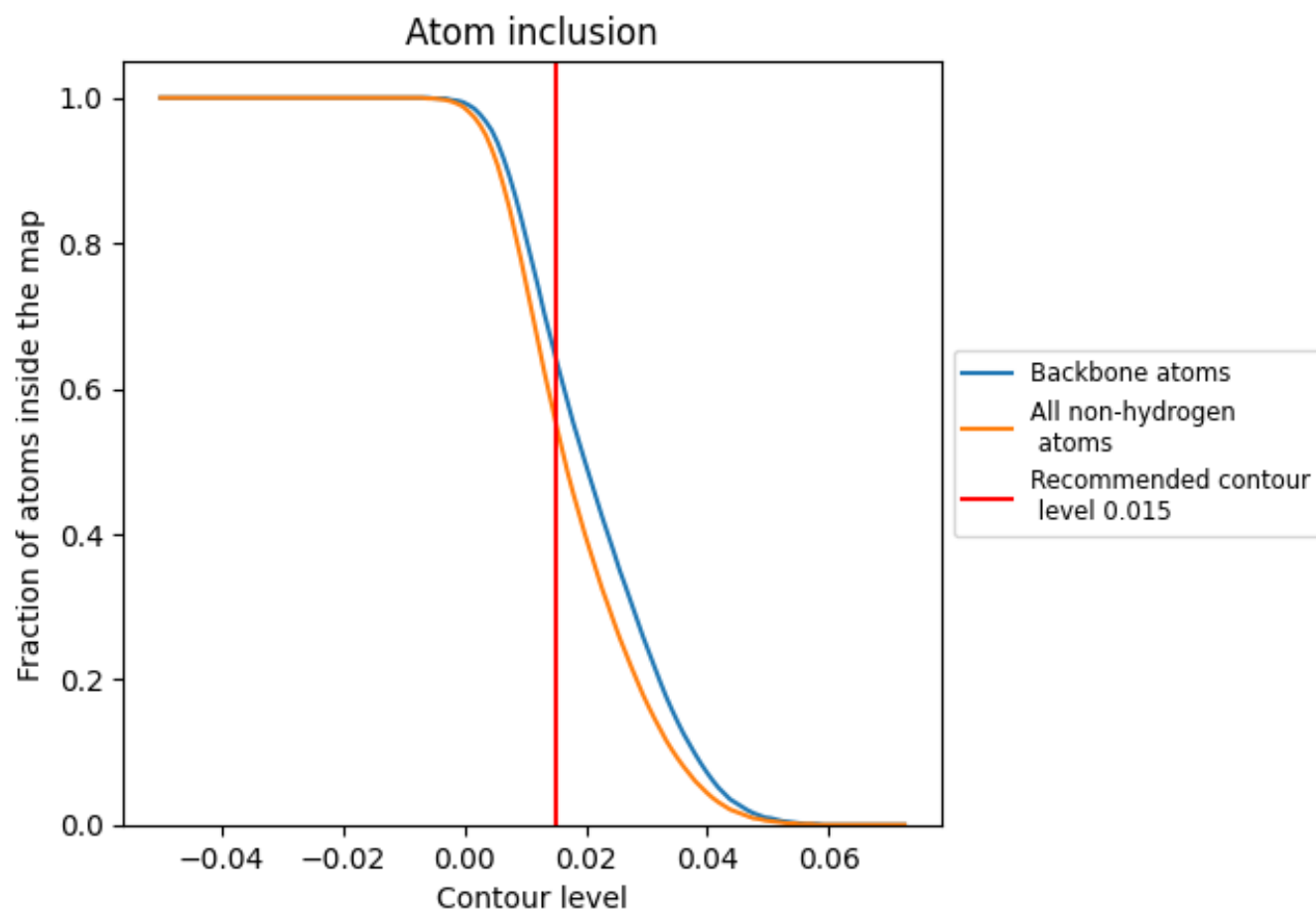
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 55% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.3370
A	 0.5790	 0.3360
B	 0.6210	 0.3800
C	 0.6030	 0.3490
D	 0.6150	 0.3630
E	 0.4950	 0.2940
F	 0.4060	 0.2440
G	 0.2260	 0.1460
H	 0.7280	 0.4460
I	 0.7290	 0.4480
J	 0.5780	 0.3540
K	 0.7530	 0.4710
L	 0.6940	 0.4150
N	 0.6040	 0.3770
O	 0.0820	 0.0430
P	 0.0680	 0.0380
Q	 0.0760	 0.0390

