



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 10:02 PM UTC

PDB ID : 9M8O / pdb_00009m8o
EMDB ID : EMD-63716
Title : Cryo-EM structure of bacteriophage NF5 baseplate
Authors : Peng, Y.N.; Liu, H.R.
Deposited on : 2025-03-12
Resolution : 3.44 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

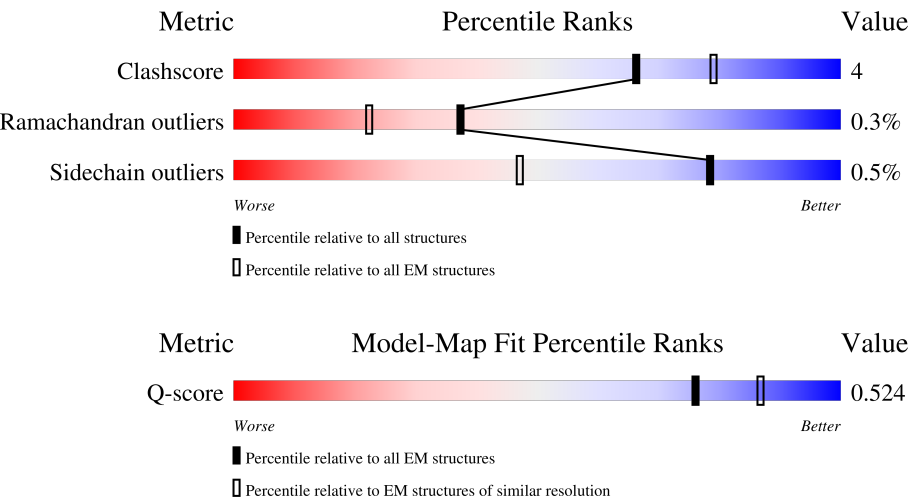
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.44 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.



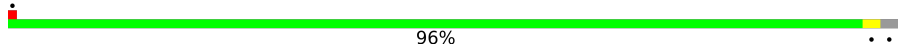
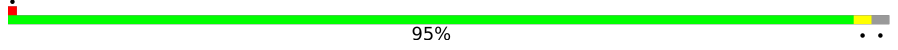
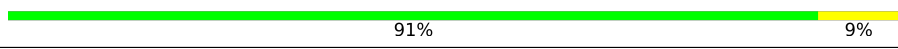
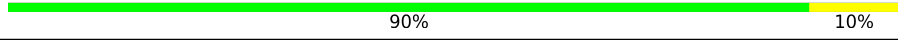
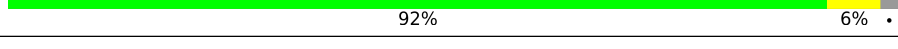
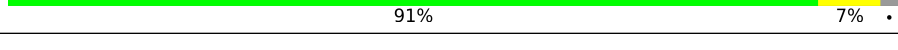
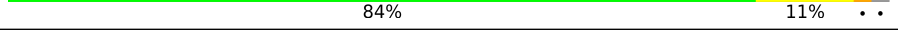
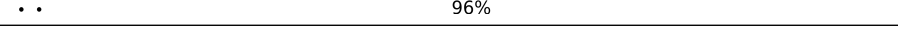
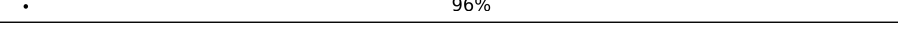
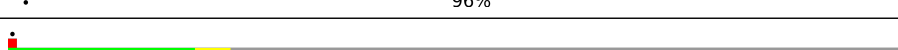
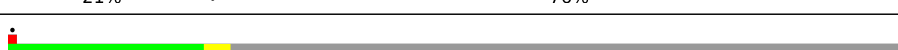
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13877 (2.94 - 3.94)

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

Mol	Chain	Length	Quality of chain
1	A	169	92%6%.
1	B	169	95%..
1	C	169	92%6%.
1	D	169	92%5%.

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Mol	Chain	Length	Quality of chain
1	E	169	
1	F	169	
2	G	255	
2	H	255	
2	I	255	
2	J	255	
2	K	255	
2	L	255	
3	M	674	
3	N	674	
3	O	674	
4	P	639	
4	Q	639	
4	R	639	
4	S	639	
4	T	639	
4	U	639	
4	V	639	
4	W	639	
4	X	639	
4	Y	639	
4	Z	639	
4	a	639	
4	b	639	
4	c	639	

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Mol	Chain	Length	Quality of chain
4	d	639	13%84%
4	e	639	21%76%
4	f	639	22%75%
4	g	639	12%84%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 40205 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 Gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	166	Total	C	N	O	S	0	0
			1297	817	206	272	2		
1	B	166	Total	C	N	O	S	0	0
			1297	817	206	272	2		
1	C	165	Total	C	N	O	S	0	0
			1285	808	205	270	2		
1	D	164	Total	C	N	O	S	0	0
			1281	807	204	268	2		
1	E	166	Total	C	N	O	S	0	0
			1297	817	206	272	2		
1	F	165	Total	C	N	O	S	0	0
			1292	814	205	271	2		

- Molecule 2 is a protein called Gp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	255	Total	C	N	O	S	0	0
			2023	1289	327	397	10		
2	H	255	Total	C	N	O	S	0	0
			2023	1289	327	397	10		
2	I	254	Total	C	N	O	S	0	0
			2015	1284	326	396	9		
2	J	250	Total	C	N	O	S	0	0
			1986	1266	322	389	9		
2	K	250	Total	C	N	O	S	0	0
			1986	1266	322	389	9		
2	L	250	Total	C	N	O	S	0	0
			1986	1266	322	389	9		

- Molecule 3 is a protein called Gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	27	Total	C	N	O	S	0	0
			220	139	35	45	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	27	Total	C	N	O	S	0	0
			220	139	35	45	1		
3	O	26	Total	C	N	O	S	0	0
			209	130	34	44	1		

- Molecule 4 is a protein called Gp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	Q	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	R	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	S	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	T	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	U	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	V	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	W	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	X	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	Y	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	Z	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	a	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	b	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	c	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		
4	d	100	Total	C	N	O	S	0	0
			793	505	133	154	1		
4	e	156	Total	C	N	O	S	0	0
			1246	791	209	243	3		
4	f	158	Total	C	N	O	S	0	0
			1259	800	211	245	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	100	Total	C	N	O	S	0	0
			793	505	133	154	1		

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: Gp11



- Molecule 1: Gp11



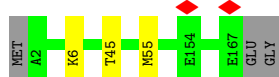
- Molecule 1: Gp11



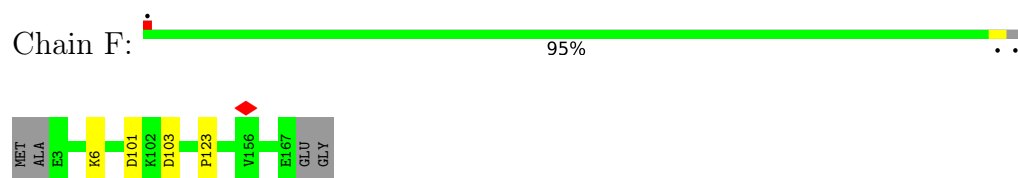
- Molecule 1: Gp11



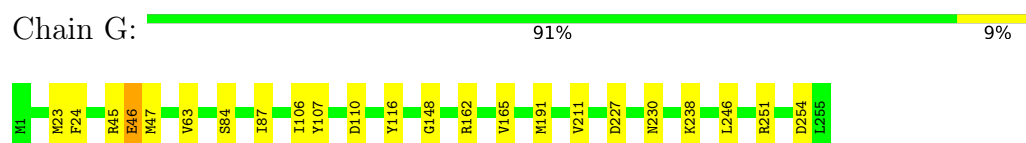
- Molecule 1: Gp11



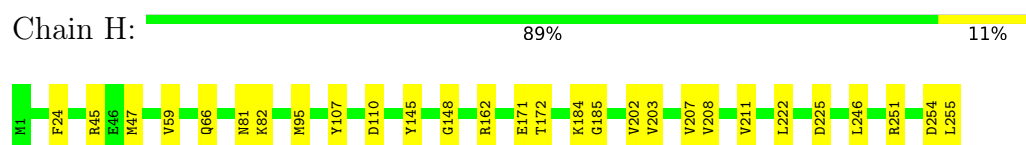
● Molecule 1: Gp11



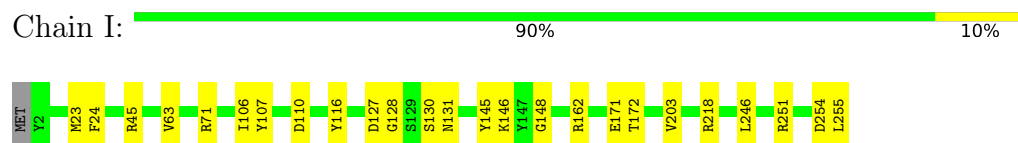
● Molecule 2: Gp15



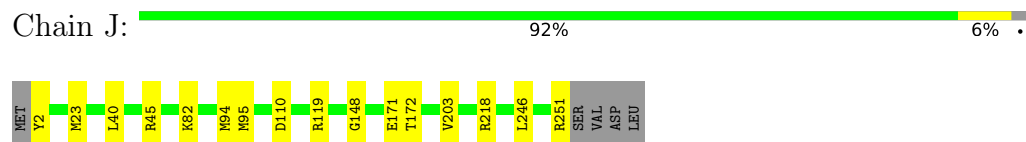
● Molecule 2: Gp15



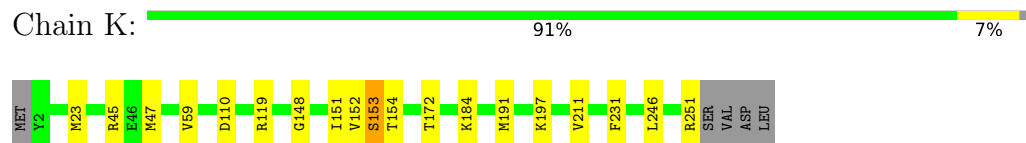
● Molecule 2: Gp15



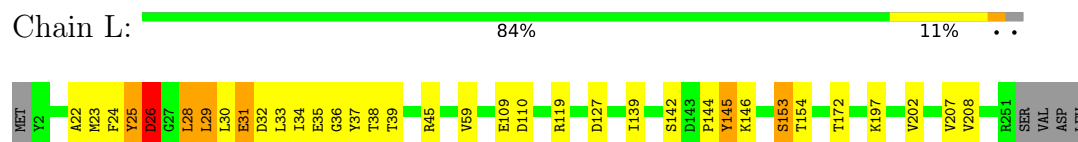
● Molecule 2: Gp15



● Molecule 2: Gp15



● Molecule 2: Gp15



Chain M: 96%

Chain N: 96%

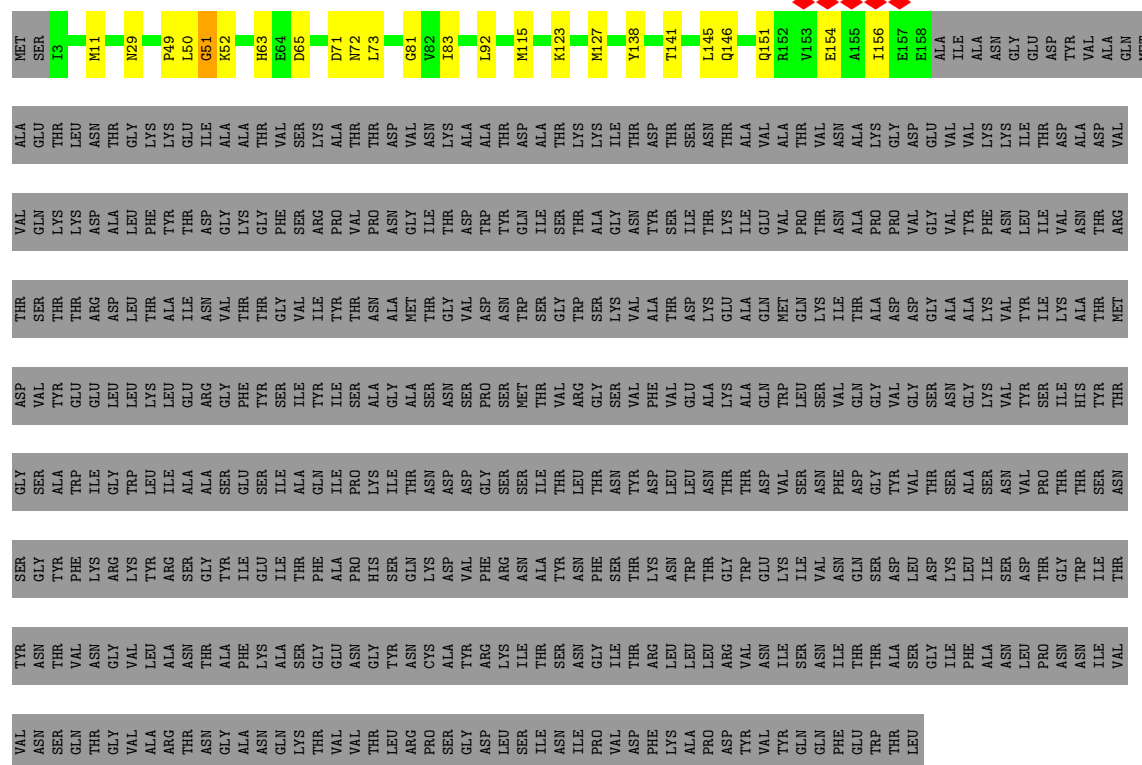


- Molecule 3: Gp14

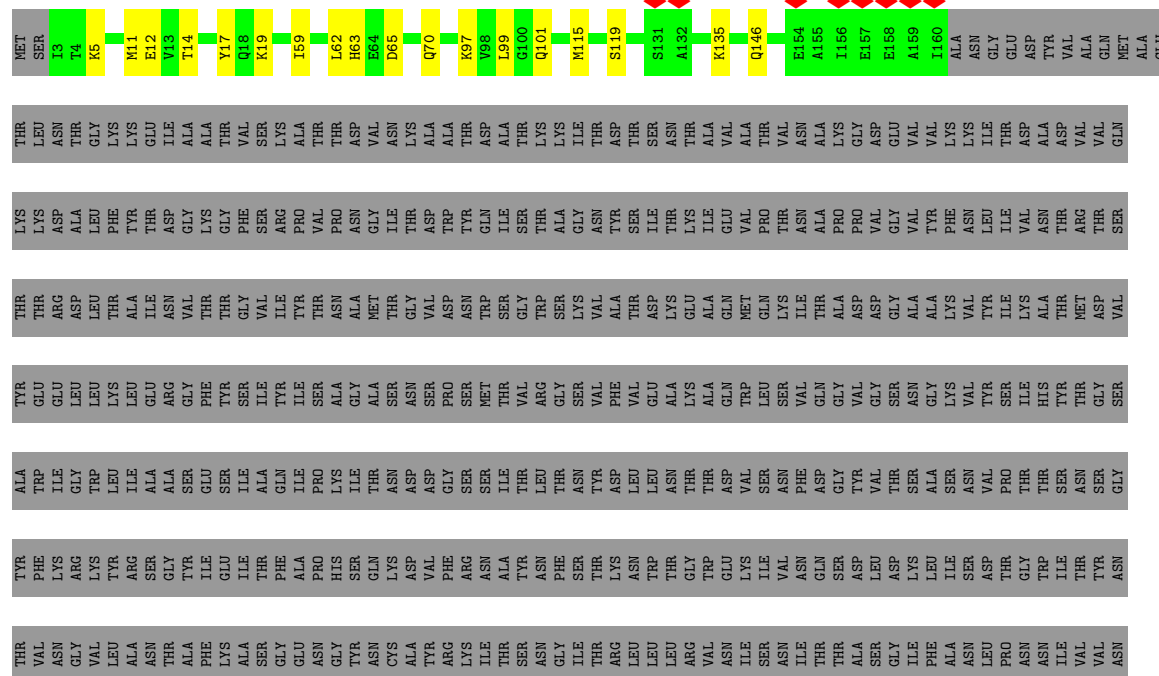
Chain 0: 96%

[illegible]

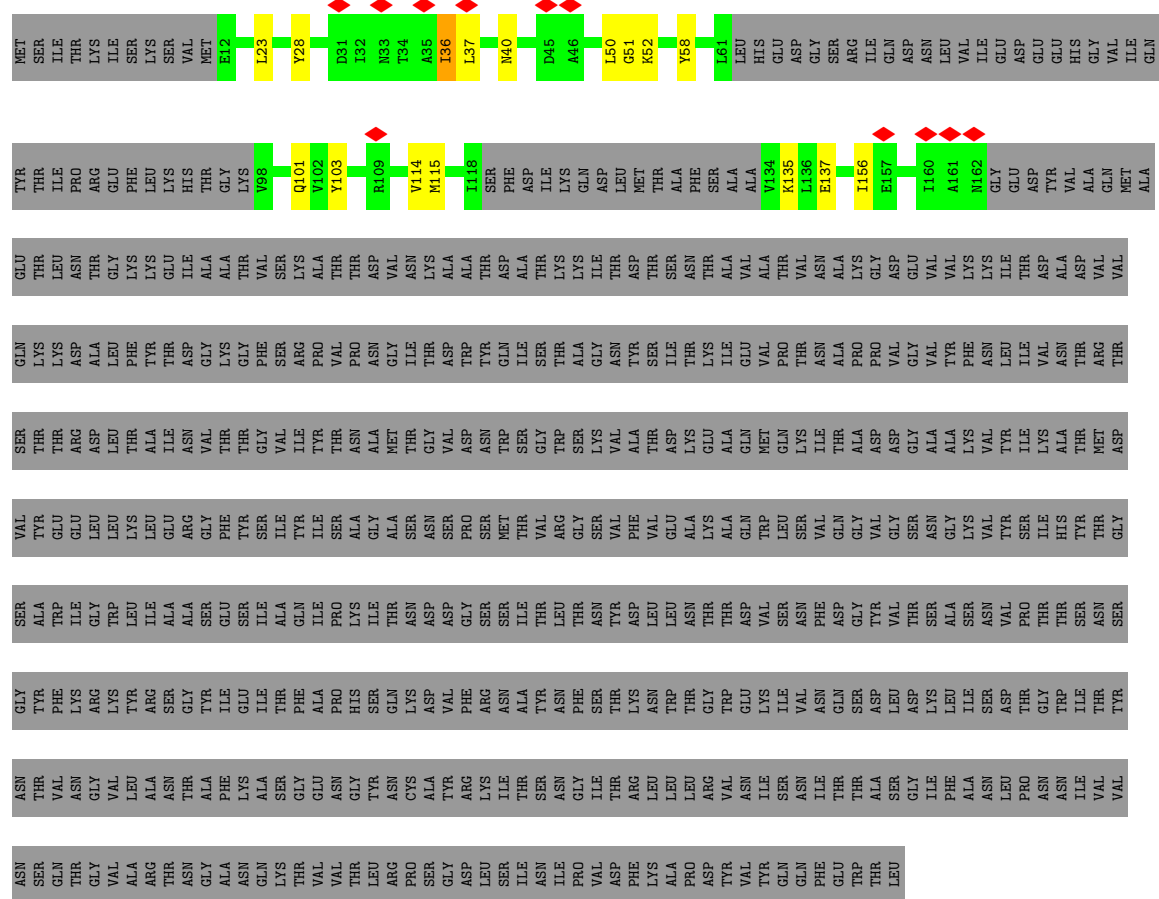
- Molecule 4: Gp18



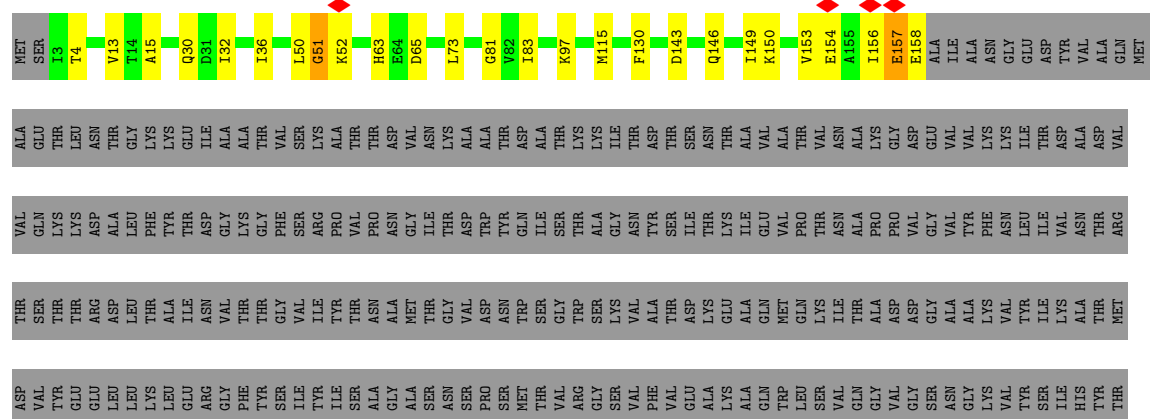
Chain Q:



Chain R: 13% 84%



Chain S: 20% . 76%



[illegible]

- Molecule 4: Gp18

[illegible]

- Molecule 4: Gp18



VAL	ILE	GLN	TYR	THR	ILE	PRO	ARG	GLU	PHE	LEU	LVS	HIS	THR	GLY	LVS	V98	Y103	I104	R109	D110	M115	R116	K117	I118	SER	PHE	ASP	ILE	LVS	GLN	ASP	LEU	MET	THR	ALA	ALA	ALA	V134	K135	L136	T141	F142	D143	K150	Q151	R152	V153	I156	E157	E158
MET	SER	ILE	THR	LVS	ILE	SER	LVS	SER	VAL	MET	E12	K19	D22	V25	Y28	D31	I32	N33	T34	N40	V41	T42	R43	L50	G51	K52	S53	N54	Y58	L61	LEU	HIS	GLU	ASP	GLY	SER	ARG	ILE	GLN	ASP	ASN	LEU	VAL	ILE	GLU	ASP	GLU	GLU	HIS	





Chain d: 13% 84%



SER	GLN	THR	GLY	VAL	ALA	ARG	THR	ASN	GLY	ALA	ASN	GLN	LYS	THR	VAL	VAL	THR	LEU	ARG	PRO	SER	SER	GLY	ASP	LEU	SER	ASN	ILE	PRO	VAL	ASP	PHE	LYS	ALA	PRO	ASP	TYR	VAL	TYR	GLN	GLN	PHE	GLU	TRP	THR	LEU
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- Molecule 4: Gp18

[illegible]

MET	ALA	GLU	THR	LEU	ASN	THR	GLY	LYS	GLU	ILE	ALA	ALA	THR	VAL	SER	LYS	ALA	THR	THR	ASP	VAL	ASN	LYS	ALA	ALA	THR	THR	ASP	ALA	ALA	LYS	THR	THR	SER	ASN	THR	THR	ALA	VAL	VAL	ALA	ALA	GLY	ASP	GLU	VAL	VAL	LYS	LYS	ILE	THR	THR	ASP	ALA	STR
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VAL	VAL	GLN	LYS	LYS	ASP	ALA	LEU	PHE	THR	THR	ASP	GLY	GLY	PHE	SER	ARG	PRO	PRO	PRO	ASN	ILE	GLY	THR	ASP	TRP	GLN	ILE	SER	THR	ALA	GLY	ASN	TYR	SER	ILE	THR	THR	LYS	ILE	GLU	VAL	PRO	THR	ASN	ALA	PRO	PRO	VAL	GLY	VAL	TYR	PHE	ASN	LEU	ILE	ILE	VAL	ASN	THR
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ARG	THR	SER	THR	THR	THR	ARG	ASP	LEU	THR	ALA	ASN	VAL	THR	THR	GLY	VAL	ILE	TYR	THR	ASN	ALA	ALA	MET	THR	GLY	VAL	ASP	ASN	TRP	SER	GLY	TRP	LYS	VAL	ALA	THR	ASP	LYS	GLU	ALA	GLN	MET	GLN	LYS	ILE	THR	ALA	ASP	GLY	ALA	LYS	VAL	TYR	ILE	LYS	ALA	THR
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NET	ASP	VAL	TYR	GLU	LEU	LYS	LEU	GLU	ARG	GLY	PHE	TYR	SER	SER	ILE	TYR	SER	SER	ALA	ALA	ALA	SER	ASN	PRO	SER	SER	MET	THR	THR	VAL	ARG	GLY	SER	SER	VAL	PHE	VAL	VAL	GLU	ALA	LYS	GLN	ALA	GLN	TRP	LEU	SER	VAL	VAL	GLY	SER	ASN	GLY	LYS	VAL	TYR	SER	ILE	THR	ASP	NET
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[illegible]

ASN SER GLY TYR PHE PHE LYS ARG LYS TYR ARG ARG SER SER GLY TYR ILE GLU ILE THR PHE ALA PRO HIS SER GLN LYS ASP VAL PHE PHE SER SER THR THR LYS ASN ASN TRP THR GLY GLU LYS ILE VAL ASN ASN GLN SER ASP ASP LYS LYS LEU LEU ILE SER ASP THR GLY TRP ILE

THR	TYR	ASN	THR	VAL	ASN	GLY	VAL	LEU	ALA	ASN	THR	ALA	PHE	LYS	ALA	SER	GLY	GLU	ASN	GLY	TYR	ASN	CYS	ALA	TYR	ARG	ARG	LEU	LEU	LEU	ARG	VAL	ASN	ASN	ILE	SER	THR	THR	ALA	SER	GLY	ILE	PHE	ALA	ASN	PRO	LEU	ASN	THR	ILE
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VAL	VAL	ASN	SER	GLN	THR	GLY	VAL	ALA	ARG	THR	ASN	GLY	ALA	ASN	GLN	LYS	THR	VAL	VAL	THR	THR	LEU	ARG	PRO	SER	SER	GLY	ASP	LEU	SER	ILE	ILE	ILE	PRO	PRO	VAL	ASP	PHE	LYS	ALA	PRO	ASP	TYR	VAL	TYR	GLN	GLN	PHE	GLU	TRP	THR	LEU
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- Molecule 4: Gp18



MET	LEU	LEU	THR	THR	LYS	LYS	LYS	VAL	MET	E12	V25	Y28	D31	N40	R43	A46	L50	G51	K52	S53	N54	L61	LEU	HIS	GLU	ASP	GLY	GLY	ARG	ARG	ILE	GLN	ASP	ASN	LEU	VAL	VAL	ILE	GLU	GLY	GLY	GLY	GLY	GLY	THR	THR	PRO
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GLU
 PHE
 LEU
 LYS
 HIS
 THR
 GLY
 LYS
 V98
 I104
 R109
 R116
 K117
 I118
 SER
 PHE
 ASP
 ILE
 LYS
 GLN
 ASP
 LEU
 MET
 THR
 ALA
 PHE
 SER
 ALA
 ALA
 V134
 K135
 L136
 I137
 T141
 F142
 D143
 K150
 V153
 E154
 E157
 E158
 A159
 I160
 A161
 N162
 GLY
 GLU
 ASP
 TYR
 VAL
 ALA
 GLN
 MET

[illegible]

VAL	GLN	LYS	LYS	ASP	ASP	ALA	LEU	PHE	TYR	THR	THR	ASP	GLY	LYS	GLY	PHE	SER	ARG	PRO	VAL	VAL	PRO	ASN	GLY	ILE	THR	ASP	TRP	TYR	GLN	ILE	SER	THR	GLY	ALA	ASN	TYR	LYS	ILE	GLU	VAL	PRO	THR	ASN	ALA	ALA	PRO	PRO	VAL	GLY	VAL	THR	PHE	ASN	LEU	ILE	ASN	VAL	THR	ARG
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[illegible]

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.561	Depositor
Minimum map value	-0.797	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.26	Depositor
Map size ($\text{\AA}$)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	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	0.30	2/1318 (0.2%)	0.36	2/1780 (0.1%)
1	B	0.13	0/1318	0.28	0/1780
1	C	0.13	0/1304	0.27	0/1759
1	D	0.44	4/1302 (0.3%)	0.47	3/1758 (0.2%)
1	E	0.13	0/1318	0.27	0/1780
1	F	0.30	2/1313 (0.2%)	0.29	0/1773
2	G	0.13	0/2059	0.33	2/2779 (0.1%)
2	H	0.12	0/2059	0.26	0/2779
2	I	0.12	0/2051	0.25	0/2769
2	J	0.12	0/2022	0.27	0/2729
2	K	0.30	2/2022 (0.1%)	0.35	2/2729 (0.1%)
2	L	0.99	24/2022 (1.2%)	0.76	9/2729 (0.3%)
3	M	0.14	0/223	0.32	0/296
3	N	0.10	0/223	0.22	0/296
3	O	0.12	0/211	0.21	0/280
4	P	0.41	0/1263	0.53	0/1706
4	Q	0.24	0/1276	0.32	0/1724
4	R	0.34	0/800	0.59	0/1081
4	S	0.49	1/1263 (0.1%)	0.59	2/1706 (0.1%)
4	T	0.14	0/1276	0.31	0/1724
4	U	0.37	0/800	0.50	1/1081 (0.1%)
4	V	0.29	0/1263	0.50	1/1706 (0.1%)
4	W	0.13	0/1276	0.29	0/1724
4	X	0.27	0/800	0.57	0/1081
4	Y	0.34	1/1263 (0.1%)	0.58	4/1706 (0.2%)
4	Z	0.14	0/1276	0.31	0/1724
4	a	0.33	0/800	0.53	0/1081
4	b	0.29	0/1263	0.53	1/1706 (0.1%)
4	c	0.13	0/1276	0.29	0/1724
4	d	0.29	0/800	0.55	0/1081
4	e	0.34	2/1263 (0.2%)	0.62	4/1706 (0.2%)
4	f	0.14	0/1276	0.30	0/1724
4	g	0.30	0/800	0.47	0/1081
All	All	0.33	38/40799 (0.1%)	0.43	31/55082 (0.1%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	26	ASP	CA-C	-10.25	1.43	1.53
2	L	144	PRO	CA-CB	-7.48	1.44	1.53
2	L	24	PHE	C-O	-7.33	1.15	1.24
2	L	142	SER	CA-C	-7.06	1.43	1.52
2	L	39	THR	C-O	-7.00	1.15	1.23
2	L	154	THR	CA-C	-6.97	1.46	1.53
2	L	37	TYR	CA-C	-6.92	1.44	1.52
1	D	89	GLU	C-O	-6.77	1.15	1.24
1	D	111	TYR	C-O	-6.58	1.16	1.24
2	L	39	THR	CA-C	-6.55	1.44	1.52
2	L	25	TYR	CA-C	-6.53	1.45	1.52
2	L	34	ILE	C-O	-6.52	1.17	1.24
1	D	111	TYR	CA-CB	-6.46	1.43	1.53
2	K	153	SER	CA-C	-6.45	1.44	1.52
2	L	153	SER	CA-C	-6.40	1.44	1.52
2	L	37	TYR	C-O	-6.29	1.16	1.23
2	L	35	GLU	C-O	-6.24	1.16	1.24
2	K	154	THR	CA-C	-6.11	1.46	1.53
2	L	38	THR	C-O	-6.08	1.17	1.23
1	F	6	LYS	CA-C	-6.06	1.45	1.52
1	D	111	TYR	CA-C	-5.94	1.45	1.52
4	Y	156	ILE	CA-C	-5.78	1.45	1.52
2	L	29	LEU	C-O	-5.75	1.17	1.24
2	L	142	SER	C-O	-5.69	1.16	1.24
4	S	154	GLU	CA-C	5.64	1.60	1.52
2	L	25	TYR	C-O	-5.62	1.17	1.24
2	L	23	MET	C-O	-5.49	1.16	1.23
1	A	3	GLU	CA-C	-5.43	1.45	1.52
2	L	146	LYS	CA-CB	-5.39	1.45	1.53
2	L	38	THR	CA-CB	-5.27	1.44	1.53
1	A	3	GLU	N-CA	-5.24	1.39	1.46
1	F	6	LYS	C-O	-5.18	1.17	1.23
2	L	146	LYS	C-O	-5.13	1.18	1.24
4	e	154	GLU	CA-C	5.10	1.59	1.52
2	L	30	LEU	C-O	-5.08	1.17	1.24
2	L	145	TYR	CA-C	-5.04	1.46	1.52
4	e	154	GLU	N-CA	5.02	1.52	1.46
2	L	26	ASP	CA-CB	-5.01	1.43	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	154	GLU	N-CA-C	10.68	122.92	111.28
2	L	35	GLU	N-CA-C	9.94	122.12	111.28
4	e	153	VAL	CA-C-N	8.35	131.47	120.28
4	e	153	VAL	C-N-CA	8.35	131.47	120.28
4	Y	154	GLU	N-CA-C	7.72	120.44	111.02
2	L	32	ASP	N-CA-C	7.59	119.64	111.36
2	L	36	GLY	N-CA-C	7.50	122.37	112.77
4	Y	156	ILE	CB-CA-C	-7.07	102.46	112.22
4	V	154	GLU	N-CA-C	6.91	119.66	111.71
2	L	33	LEU	N-CA-C	6.90	118.80	111.28
2	L	154	THR	CB-CA-C	-6.90	101.86	112.07
4	b	154	GLU	N-CA-C	6.82	119.55	111.71
2	L	154	THR	N-CA-C	6.33	118.63	109.71
2	L	139	ILE	O-C-N	-5.98	117.04	123.14
4	S	157	GLU	N-CA-C	-5.97	104.77	111.28
4	Y	151	GLN	O-C-N	-5.94	115.27	122.22
2	G	46	GLU	CA-C-N	5.93	132.86	121.54
2	G	46	GLU	C-N-CA	5.93	132.86	121.54
2	L	26	ASP	N-CA-C	-5.54	99.90	108.31
4	Y	156	ILE	N-CA-C	-5.40	105.26	110.72
1	A	2	ALA	CA-C-N	-5.36	114.06	122.73
1	A	2	ALA	C-N-CA	-5.36	114.06	122.73
1	D	89	GLU	CA-C-O	-5.34	115.05	120.71
4	U	136	LEU	N-CA-C	5.32	117.68	110.35
1	D	89	GLU	CA-C-N	5.30	130.31	122.94
1	D	89	GLU	C-N-CA	5.30	130.31	122.94
2	K	154	THR	N-CA-C	5.22	117.22	110.65
2	L	144	PRO	CA-C-O	-5.17	114.29	122.82
4	S	154	GLU	N-CA-C	5.16	116.90	111.28
2	K	151	ILE	O-C-N	-5.07	117.73	123.20
4	e	153	VAL	N-CA-C	5.04	119.82	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1297	0	1249	8	0
1	B	1297	0	1249	3	0
1	C	1285	0	1239	6	0
1	D	1281	0	1234	6	0
1	E	1297	0	1249	3	0
1	F	1292	0	1244	3	0
2	G	2023	0	2032	15	0
2	H	2023	0	2032	18	0
2	I	2015	0	2020	15	0
2	J	1986	0	1991	13	0
2	K	1986	0	1991	10	0
2	L	1986	0	1991	11	0
3	M	220	0	201	5	0
3	N	220	0	201	1	0
3	O	209	0	192	1	0
4	P	1246	0	1261	14	0
4	Q	1259	0	1277	12	0
4	R	793	0	808	10	0
4	S	1246	0	1261	18	0
4	T	1259	0	1277	11	0
4	U	793	0	808	18	0
4	V	1246	0	1261	18	0
4	W	1259	0	1277	8	0
4	X	793	0	808	10	0
4	Y	1246	0	1261	19	0
4	Z	1259	0	1277	9	0
4	a	793	0	808	15	0
4	b	1246	0	1261	25	0
4	c	1259	0	1277	13	0
4	d	793	0	808	13	0
4	e	1246	0	1261	14	0
4	f	1259	0	1277	11	0
4	g	793	0	808	12	0
All	All	40205	0	40191	317	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 4.

All (317) 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)
4:V:154:GLU:HA	4:V:157:GLU:HB2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:154:GLU:HA	4:b:157:GLU:HB2	1.56	0.86
4:S:149:ILE:HD11	4:T:153:VAL:HG11	1.62	0.80
4:b:127:MET:HE1	4:c:70:GLN:HG3	1.64	0.79
4:P:127:MET:HE1	4:Q:70:GLN:HG3	1.72	0.72
4:V:127:MET:HE1	4:W:70:GLN:HG3	1.75	0.67
4:Y:21:SER:HB2	4:Y:116:ARG:HH12	1.60	0.66
2:H:184:LYS:HG2	2:H:185:GLY:H	1.59	0.66
4:U:150:LYS:HA	4:U:153:VAL:HG12	1.79	0.65
2:G:46:GLU:O	2:G:47:MET:HG2	1.97	0.64
3:M:660:ILE:HG22	3:M:664:MET:HE2	1.79	0.64
2:H:45:ARG:NH2	2:H:110:ASP:OD2	2.30	0.64
2:I:45:ARG:NH2	2:I:110:ASP:OD2	2.31	0.64
4:d:22:ASP:OD1	4:d:43:ARG:NH1	2.32	0.63
4:b:71:ASP:OD2	4:b:72:ASN:N	2.31	0.62
4:Z:97:LYS:NZ	4:Z:121:ASP:OD1	2.31	0.61
4:g:25:VAL:HG21	4:g:104:ILE:HD13	1.82	0.61
4:Y:29:ASN:ND2	4:Y:92:LEU:O	2.34	0.60
2:K:191:MET:HE1	2:K:211:VAL:HG11	1.83	0.60
2:L:45:ARG:NH2	2:L:110:ASP:OD2	2.35	0.60
4:e:101:GLN:NE2	4:e:115:MET:O	2.32	0.60
2:K:197:LYS:HE3	2:K:197:LYS:HA	1.83	0.60
4:e:50:LEU:HD23	4:e:81:GLY:HA2	1.84	0.60
4:Y:50:LEU:HD23	4:Y:81:GLY:HA2	1.83	0.59
4:S:146:GLN:HG3	4:U:156:ILE:HD11	1.85	0.59
4:R:101:GLN:HG2	4:R:115:MET:HE3	1.84	0.59
4:S:157:GLU:O	4:S:158:GLU:C	2.46	0.59
4:P:145:LEU:HD22	4:Q:146:GLN:HG3	1.85	0.58
4:b:32:ILE:HG23	4:b:89:ARG:HD3	1.86	0.58
2:I:145:TYR:HE1	2:I:255:LEU:HD12	1.69	0.57
4:e:12:GLU:HG2	4:e:14:THR:HG23	1.85	0.57
4:a:28:TYR:HB2	4:a:40:ASN:HB2	1.86	0.57
4:d:28:TYR:HB2	4:d:40:ASN:HB2	1.87	0.57
2:G:148:GLY:O	2:G:251:ARG:NH1	2.36	0.56
2:I:24:PHE:HB2	2:I:107:TYR:HB2	1.87	0.56
4:a:114:VAL:HG12	4:a:136:LEU:HD22	1.88	0.56
4:Q:11:MET:HB3	4:Q:115:MET:HE3	1.86	0.56
4:V:71:ASP:OD1	4:V:72:ASN:N	2.38	0.56
4:g:109:ARG:CZ	4:g:109:ARG:HA	2.36	0.56
4:g:50:LEU:HB3	4:g:54:ASN:OD1	2.07	0.55
2:H:211:VAL:HG21	2:H:222:LEU:HD11	1.89	0.55
4:Y:146:GLN:HG3	4:a:156:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:156:ILE:HG12	4:Z:157:GLU:OE2	2.07	0.55
4:d:58:TYR:HB3	4:d:103:TYR:HB2	1.88	0.55
2:H:148:GLY:O	2:H:251:ARG:NH1	2.37	0.54
4:Y:157:GLU:O	4:Y:158:GLU:C	2.50	0.54
4:b:146:GLN:HG3	4:d:156:ILE:HD11	1.89	0.54
4:W:62:LEU:HD23	4:W:99:LEU:HD12	1.88	0.54
4:S:4:THR:HG21	4:S:36:ILE:HD12	1.89	0.54
4:e:4:THR:HG21	4:e:36:ILE:HD12	1.89	0.54
4:X:36:ILE:HG22	4:X:37:LEU:H	1.73	0.53
2:H:66:GLN:OE1	2:J:119:ARG:NH1	2.34	0.53
4:c:11:MET:HB3	4:c:115:MET:HE2	1.89	0.53
4:g:50:LEU:O	4:g:52:LYS:N	2.42	0.53
1:B:89:GLU:OE2	1:B:111:TYR:OH	2.27	0.53
4:U:109:ARG:HA	4:U:109:ARG:CZ	2.39	0.53
4:V:123:LYS:HE2	4:W:17:TYR:HE1	1.73	0.53
4:U:25:VAL:O	4:U:116:ARG:NE	2.42	0.53
4:U:43:ARG:NH2	4:U:110:ASP:OD2	2.42	0.52
4:a:34:THR:HG22	4:a:35:ALA:H	1.75	0.52
1:A:55:MET:HE3	1:D:115:TYR:HB2	1.91	0.52
2:H:24:PHE:HB2	2:H:107:TYR:HB2	1.91	0.52
4:U:50:LEU:O	4:U:52:LYS:N	2.41	0.52
4:S:150:LYS:O	4:S:153:VAL:HG12	2.09	0.52
4:Y:153:VAL:O	4:Y:156:ILE:HG13	2.10	0.52
2:J:45:ARG:NH2	2:J:110:ASP:OD2	2.43	0.52
2:J:148:GLY:O	2:J:251:ARG:NH1	2.41	0.52
4:f:12:GLU:HG2	4:f:14:THR:HG23	1.91	0.52
4:X:58:TYR:HB3	4:X:103:TYR:HB2	1.92	0.52
4:a:25:VAL:HG21	4:a:104:ILE:HD13	1.91	0.52
4:a:50:LEU:O	4:a:52:LYS:N	2.41	0.52
1:D:28:MET:HG3	1:D:29:ALA:N	2.24	0.51
4:U:25:VAL:HG22	4:U:41:VAL:HG12	1.92	0.51
2:I:63:VAL:HG11	2:L:119:ARG:NH2	2.25	0.51
4:R:50:LEU:O	4:R:52:LYS:N	2.43	0.51
2:G:45:ARG:NH2	2:G:110:ASP:OD2	2.43	0.51
2:I:172:THR:HG22	2:I:246:LEU:HD23	1.93	0.51
4:P:29:ASN:ND2	4:P:92:LEU:O	2.43	0.51
4:P:71:ASP:OD1	4:P:72:ASN:N	2.39	0.51
4:R:36:ILE:HG22	4:R:37:LEU:H	1.75	0.51
4:Y:4:THR:HG21	4:Y:36:ILE:HD12	1.93	0.51
4:b:152:ARG:O	4:b:153:VAL:C	2.50	0.51
4:P:146:GLN:HG3	4:R:156:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:50:LEU:HD23	4:S:81:GLY:HA2	1.92	0.51
4:V:146:GLN:HG3	4:X:156:ILE:HD11	1.92	0.51
4:b:123:LYS:HE3	4:c:17:TYR:CE1	2.46	0.51
4:Q:63:HIS:ND1	4:Q:65:ASP:OD1	2.43	0.51
4:e:145:LEU:HD22	4:f:146:GLN:HG3	1.92	0.51
2:K:59:VAL:O	2:K:59:VAL:HG12	2.10	0.50
4:T:97:LYS:NZ	4:T:121:ASP:OD1	2.35	0.50
4:R:23:LEU:HB3	4:R:114:VAL:HG21	1.93	0.50
4:Y:130:PHE:HE1	4:Z:68:ARG:HD2	1.76	0.50
4:d:36:ILE:O	4:d:37:LEU:HG	2.11	0.50
4:X:28:TYR:HB2	4:X:40:ASN:HB2	1.93	0.50
4:Y:130:PHE:CE1	4:Z:68:ARG:HD2	2.46	0.50
4:c:62:LEU:HD23	4:c:99:LEU:HD12	1.94	0.50
4:a:60:VAL:HB	4:a:101:GLN:HB2	1.94	0.50
2:G:84:SER:O	2:G:87:ILE:HG22	2.11	0.50
2:I:71:ARG:HH22	2:I:146:LYS:HE2	1.76	0.50
4:U:31:ASP:OD2	4:U:34:THR:OG1	2.23	0.50
4:Q:12:GLU:HG2	4:Q:14:THR:HG23	1.94	0.50
4:d:36:ILE:HG22	4:d:37:LEU:H	1.77	0.50
4:T:61:LEU:HD12	4:T:69:ILE:HD11	1.94	0.49
4:U:25:VAL:HG21	4:U:104:ILE:HD13	1.93	0.49
4:c:63:HIS:ND1	4:c:65:ASP:OD1	2.45	0.49
4:b:89:ARG:NH2	4:d:141:THR:HG21	2.26	0.49
1:F:101:ASP:OD1	1:F:101:ASP:N	2.45	0.49
2:L:28:LEU:HD22	2:L:28:LEU:H	1.78	0.49
4:b:49:PRO:HB2	4:b:52:LYS:HE3	1.95	0.49
4:c:5:LYS:HB3	4:e:15:ALA:HB2	1.94	0.49
2:I:71:ARG:HH12	2:I:146:LYS:HE3	1.78	0.49
4:e:130:PHE:HE1	4:f:68:ARG:HD2	1.77	0.49
4:X:36:ILE:O	4:X:37:LEU:HG	2.13	0.48
2:G:46:GLU:O	2:G:46:GLU:HG2	2.13	0.48
2:H:145:TYR:HE1	2:H:255:LEU:HD12	1.77	0.48
4:Q:5:LYS:HB3	4:S:15:ALA:HB2	1.95	0.48
2:L:22:ALA:HB3	2:L:109:GLU:HG3	1.95	0.48
4:S:130:PHE:HE1	4:T:68:ARG:HD2	1.76	0.48
4:P:73:LEU:HD13	4:P:83:ILE:HG21	1.95	0.48
4:g:117:LYS:NZ	4:g:137:GLU:OE1	2.38	0.48
4:d:23:LEU:HB3	4:d:114:VAL:HG21	1.95	0.48
4:g:150:LYS:HA	4:g:153:VAL:HG22	1.95	0.48
4:U:28:TYR:HB2	4:U:40:ASN:HB2	1.93	0.48
4:Y:153:VAL:O	4:Y:157:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:123:LYS:HE2	4:Q:17:TYR:HE1	1.78	0.48
4:b:73:LEU:HD13	4:b:83:ILE:HG21	1.95	0.48
1:F:103:ASP:OD1	1:F:103:ASP:N	2.44	0.47
2:G:63:VAL:HG11	2:K:119:ARG:NH2	2.29	0.47
2:G:238:LYS:HB3	2:G:238:LYS:HE3	1.70	0.47
4:a:109:ARG:HA	4:a:109:ARG:CZ	2.44	0.47
2:J:94:MET:HE3	2:J:95:MET:HE3	1.96	0.47
4:Q:97:LYS:NZ	4:Q:119:SER:OG	2.42	0.47
4:X:23:LEU:HB3	4:X:114:VAL:HG21	1.96	0.47
4:d:50:LEU:O	4:d:52:LYS:N	2.47	0.47
4:V:58:TYR:HB2	4:V:103:TYR:HB2	1.96	0.47
4:P:50:LEU:HD23	4:P:81:GLY:HA2	1.97	0.47
1:D:118:SER:HB3	1:D:134:GLU:HB2	1.95	0.47
4:R:28:TYR:HB2	4:R:40:ASN:HB2	1.96	0.47
4:S:143:ASP:OD2	4:U:58:TYR:OH	2.27	0.47
4:T:71:ASP:OD2	4:T:85:TYR:OH	2.31	0.47
4:V:49:PRO:HB2	4:V:52:LYS:HE3	1.97	0.47
4:W:63:HIS:ND1	4:W:65:ASP:OD1	2.48	0.47
4:b:156:ILE:HA	4:b:156:ILE:HD12	1.70	0.47
4:e:63:HIS:ND1	4:e:65:ASP:OD1	2.47	0.47
4:g:141:THR:HG22	4:g:143:ASP:H	1.80	0.47
2:G:23:MET:HE2	2:G:23:MET:HB3	1.83	0.47
2:H:172:THR:OG1	2:H:202:VAL:O	2.32	0.47
4:R:36:ILE:O	4:R:37:LEU:HG	2.15	0.47
4:R:135:LYS:HD2	4:R:135:LYS:HA	1.74	0.47
4:V:154:GLU:CA	4:V:157:GLU:HB2	2.33	0.47
4:g:28:TYR:HB2	4:g:40:ASN:HB2	1.96	0.47
2:L:207:VAL:HG13	2:L:208:VAL:HG13	1.97	0.46
4:T:62:LEU:HD13	4:T:68:ARG:NH1	2.31	0.46
4:b:145:LEU:HD22	4:c:146:GLN:HG3	1.97	0.46
2:G:165:VAL:HG21	2:G:251:ARG:O	2.16	0.46
1:A:113:GLN:HB2	2:J:2:TYR:CE1	2.51	0.46
4:c:69:ILE:HD11	4:c:136:LEU:HD23	1.97	0.46
1:C:55:MET:HA	1:C:55:MET:HE2	1.97	0.46
2:H:225:ASP:OD1	2:H:225:ASP:N	2.49	0.46
4:a:25:VAL:O	4:a:116:ARG:NE	2.49	0.46
1:B:118:SER:HB3	1:B:134:GLU:HB2	1.98	0.46
4:V:63:HIS:ND1	4:V:65:ASP:OD1	2.49	0.46
4:e:149:ILE:HG13	4:g:160:ILE:HD11	1.98	0.46
2:G:162:ARG:HD2	2:G:254:ASP:OD1	2.16	0.46
4:S:149:ILE:HD12	4:S:149:ILE:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:103:TYR:CE1	4:U:115:MET:HE3	2.50	0.46
4:Q:62:LEU:HD23	4:Q:99:LEU:HD12	1.98	0.45
4:e:73:LEU:HD13	4:e:83:ILE:HG21	1.98	0.45
2:I:106:ILE:HB	2:I:116:TYR:HB2	1.99	0.45
2:H:171:GLU:HG2	2:H:203:VAL:HG22	1.98	0.45
2:I:127:ASP:OD1	2:I:128:GLY:N	2.49	0.45
4:a:141:THR:HG22	4:a:143:ASP:H	1.82	0.45
4:S:130:PHE:CE1	4:T:68:ARG:HD2	2.51	0.45
4:Y:63:HIS:ND1	4:Y:65:ASP:OD1	2.49	0.45
4:b:129:ALA:HB3	4:c:68:ARG:HH12	1.81	0.45
1:C:118:SER:HB3	1:C:134:GLU:HB2	1.99	0.45
3:M:664:MET:CE	3:O:664:MET:HE1	2.46	0.45
4:f:11:MET:HB3	4:f:115:MET:HE3	1.98	0.45
1:E:6:LYS:HA	1:E:6:LYS:HD3	1.71	0.45
2:I:218:ARG:HD3	2:I:218:ARG:HA	1.79	0.45
4:U:19:LYS:HB3	4:U:19:LYS:HE3	1.81	0.45
4:X:50:LEU:O	4:X:52:LYS:N	2.50	0.45
4:S:50:LEU:HB3	4:S:51:GLY:H	1.66	0.45
4:V:73:LEU:HD13	4:V:83:ILE:HG21	1.97	0.45
4:e:50:LEU:O	4:e:52:LYS:N	2.50	0.45
4:f:73:LEU:HD13	4:f:83:ILE:HG21	1.99	0.45
2:L:172:THR:OG1	2:L:202:VAL:O	2.28	0.45
4:T:73:LEU:HD13	4:T:83:ILE:HG21	1.99	0.45
4:W:12:GLU:HG2	4:W:14:THR:HG23	1.99	0.45
4:b:89:ARG:HH22	4:d:141:THR:HG21	1.81	0.45
4:c:135:LYS:HE2	4:c:135:LYS:HB3	1.78	0.45
2:J:218:ARG:HD3	2:J:218:ARG:HA	1.73	0.45
2:G:24:PHE:HB2	2:G:107:TYR:HB2	1.99	0.44
4:P:49:PRO:HB2	4:P:52:LYS:HE3	1.98	0.44
4:V:145:LEU:HD22	4:W:146:GLN:HG3	1.98	0.44
1:D:28:MET:HG3	1:D:29:ALA:H	1.83	0.44
2:K:148:GLY:O	2:K:251:ARG:NH1	2.43	0.44
2:H:207:VAL:HG23	2:H:208:VAL:HG23	2.00	0.44
4:S:63:HIS:ND1	4:S:65:ASP:OD1	2.50	0.44
4:R:58:TYR:HB3	4:R:103:TYR:HB2	2.00	0.44
4:a:152:ARG:O	4:a:156:ILE:HG12	2.17	0.44
2:L:25:TYR:O	2:L:26:ASP:C	2.58	0.44
2:L:197:LYS:HE3	2:L:197:LYS:HA	2.00	0.44
4:Q:19:LYS:HE3	4:Q:19:LYS:HB3	1.78	0.44
4:b:152:ARG:C	4:b:154:GLU:N	2.75	0.44
4:f:62:LEU:HD13	4:f:68:ARG:NH1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:13:VAL:HG22	4:S:115:MET:SD	2.57	0.44
4:T:97:LYS:HB2	4:T:97:LYS:HE2	1.73	0.44
4:b:149:ILE:HD12	4:c:153:VAL:HG21	1.99	0.44
4:b:50:LEU:CD2	4:b:81:GLY:HA2	2.47	0.44
2:H:95:MET:HG2	2:K:47:MET:HG2	2.00	0.44
4:P:50:LEU:CD2	4:P:81:GLY:HA2	2.47	0.44
4:R:115:MET:HB3	4:R:137:GLU:HB2	2.00	0.44
4:g:154:GLU:HA	4:g:157:GLU:HG3	2.00	0.44
2:H:172:THR:HG22	2:H:246:LEU:HD23	1.99	0.43
4:Q:135:LYS:HE2	4:Q:135:LYS:HB3	1.72	0.43
4:Y:152:ARG:HH11	4:Z:157:GLU:HG3	1.83	0.43
4:S:50:LEU:O	4:S:52:LYS:N	2.51	0.43
4:d:43:ARG:HG2	4:d:44:ASN:OD1	2.18	0.43
4:T:152:ARG:HB3	4:T:152:ARG:NH1	2.33	0.43
4:U:116:ARG:CZ	4:U:136:LEU:HD11	2.48	0.43
2:L:59:VAL:HG12	2:L:59:VAL:O	2.18	0.43
4:P:138:TYR:HA	4:P:141:THR:HG22	2.01	0.43
4:Y:50:LEU:O	4:Y:52:LYS:N	2.51	0.43
2:H:59:VAL:HG12	2:H:59:VAL:O	2.18	0.43
4:V:50:LEU:CD2	4:V:81:GLY:HA2	2.49	0.43
4:Y:89:ARG:NH2	4:a:141:THR:HG21	2.33	0.43
4:Z:73:LEU:HD13	4:Z:83:ILE:HG21	1.99	0.43
1:A:40:ARG:HH21	1:A:58:ILE:HD11	1.84	0.43
2:H:47:MET:SD	2:J:95:MET:HE3	2.59	0.43
2:J:172:THR:HG22	2:J:246:LEU:HD23	1.99	0.43
2:L:31:GLU:H	2:L:31:GLU:HG2	1.38	0.43
4:Y:50:LEU:HB3	4:Y:51:GLY:H	1.69	0.43
4:b:123:LYS:HE3	4:c:17:TYR:HE1	1.83	0.43
4:Y:73:LEU:HD13	4:Y:83:ILE:HG21	1.99	0.43
4:Y:143:ASP:OD2	4:a:58:TYR:OH	2.33	0.43
4:b:138:TYR:HA	4:b:141:THR:HG22	2.00	0.43
4:W:69:ILE:HD11	4:W:136:LEU:HD23	2.01	0.43
4:Z:16:ASP:OD2	4:Z:16:ASP:N	2.52	0.43
4:b:50:LEU:HD23	4:b:81:GLY:HA2	2.01	0.43
4:f:4:THR:HG21	4:f:36:ILE:HD12	2.00	0.43
2:G:227:ASP:HB3	2:G:230:ASN:HB2	2.01	0.43
2:L:127:ASP:OD1	2:L:127:ASP:N	2.43	0.42
4:U:152:ARG:O	4:U:156:ILE:HG12	2.19	0.42
4:a:150:LYS:HA	4:a:153:VAL:HG22	2.00	0.42
4:g:25:VAL:O	4:g:116:ARG:NE	2.48	0.42
2:I:162:ARG:HD2	2:I:254:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:63:HIS:ND1	4:P:65:ASP:OD1	2.52	0.42
4:b:63:HIS:CE1	4:b:94:HIS:HB3	2.54	0.42
4:V:156:ILE:HA	4:V:156:ILE:HD12	1.72	0.42
4:U:40:ASN:OD1	4:U:41:VAL:N	2.52	0.42
4:e:152:ARG:O	4:e:153:VAL:C	2.62	0.42
1:A:115:TYR:HB2	1:E:55:MET:HE3	2.00	0.42
2:H:162:ARG:HD2	2:H:254:ASP:OD1	2.20	0.42
2:K:45:ARG:NH2	2:K:110:ASP:OD2	2.51	0.42
4:T:152:ARG:HB3	4:T:152:ARG:HH11	1.84	0.42
4:V:77:ASP:OD2	4:V:80:HIS:ND1	2.42	0.42
4:e:123:LYS:HE3	4:f:17:TYR:CZ	2.55	0.42
2:I:171:GLU:HG2	2:I:203:VAL:HG22	2.02	0.42
2:J:82:LYS:HE3	2:J:82:LYS:HB3	1.88	0.42
2:K:184:LYS:HD3	2:K:231:PHE:CZ	2.55	0.42
4:Z:99:LEU:HD23	4:Z:119:SER:HB3	2.01	0.42
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.93	0.42
4:U:141:THR:HG22	4:U:143:ASP:H	1.84	0.42
4:V:138:TYR:HA	4:V:141:THR:HG22	2.01	0.42
4:X:135:LYS:HD2	4:X:135:LYS:HA	1.72	0.42
4:b:129:ALA:HB3	4:c:68:ARG:NH1	2.35	0.42
4:Z:62:LEU:HD13	4:Z:68:ARG:NE	2.35	0.41
2:G:106:ILE:HB	2:G:116:TYR:HB2	2.03	0.41
4:d:24:ASN:OD1	4:d:25:VAL:N	2.53	0.41
4:d:135:LYS:HD2	4:d:135:LYS:HA	1.87	0.41
4:f:99:LEU:HD23	4:f:119:SER:HB3	2.01	0.41
2:I:148:GLY:O	2:I:251:ARG:NH1	2.52	0.41
1:A:34:HIS:O	1:D:123:PRO:HD2	2.20	0.41
1:C:5:LYS:NZ	1:C:94:ASP:OD2	2.44	0.41
4:S:73:LEU:HD13	4:S:83:ILE:HG21	2.02	0.41
2:I:23:MET:HE2	2:I:23:MET:HB3	1.94	0.41
1:C:12:LEU:HD21	1:C:62:PHE:HZ	1.85	0.41
1:C:13:LEU:HB2	1:C:91:TRP:HB2	2.02	0.41
4:S:97:LYS:HB2	4:S:97:LYS:HE2	1.79	0.41
4:V:50:LEU:HD23	4:V:81:GLY:HA2	2.02	0.41
1:A:113:GLN:HB2	2:J:2:TYR:CZ	2.55	0.41
4:Q:59:ILE:HG13	4:Q:101:GLN:O	2.21	0.41
4:Y:149:ILE:HG21	4:a:156:ILE:HD12	2.03	0.41
4:b:13:VAL:HG22	4:b:115:MET:SD	2.61	0.41
4:e:50:LEU:HB3	4:e:51:GLY:H	1.69	0.41
4:f:29:ASN:HB2	4:f:125:ASP:OD1	2.21	0.41
1:B:26:TRP:HZ3	1:B:28:MET:SD	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:110:ASP:OD1	2:H:110:ASP:N	2.54	0.41
2:K:172:THR:HG22	2:K:246:LEU:HD23	2.03	0.41
4:V:152:ARG:O	4:V:153:VAL:C	2.62	0.41
4:g:43:ARG:O	4:g:46:ALA:N	2.47	0.41
1:C:34:HIS:O	1:F:123:PRO:HD2	2.20	0.41
3:M:654:LYS:O	3:M:658:GLU:HG2	2.21	0.41
3:M:669:GLN:OE1	3:M:669:GLN:HA	2.21	0.41
4:U:50:LEU:HB3	4:U:54:ASN:OD1	2.21	0.41
4:V:29:ASN:ND2	4:V:92:LEU:O	2.53	0.41
4:b:154:GLU:CA	4:b:157:GLU:HB2	2.38	0.41
4:f:61:LEU:HD12	4:f:69:ILE:HD11	2.01	0.41
1:A:53:GLN:HE21	1:D:136:ALA:HB1	1.86	0.41
2:G:246:LEU:HD23	2:G:246:LEU:H	1.86	0.41
2:I:130:SER:OG	2:I:131:ASN:N	2.54	0.41
3:M:667:ASP:O	3:M:670:ILE:HG22	2.21	0.41
4:P:50:LEU:HB3	4:P:51:GLY:H	1.62	0.41
4:W:19:LYS:HE3	4:W:19:LYS:HB3	1.78	0.41
4:X:32:ILE:O	4:X:33:ASN:OD1	2.39	0.41
2:H:81:ASN:OD1	2:H:82:LYS:N	2.52	0.40
2:J:171:GLU:HG2	2:J:203:VAL:HG22	2.03	0.40
2:K:23:MET:HE2	2:K:23:MET:HB3	1.89	0.40
4:P:11:MET:HB3	4:P:115:MET:HE2	2.04	0.40
4:X:40:ASN:OD1	4:X:41:VAL:N	2.55	0.40
1:E:45:THR:HG21	2:J:40:LEU:HD13	2.04	0.40
2:G:191:MET:HE1	2:G:211:VAL:HG11	2.03	0.40
2:J:23:MET:HE2	2:J:23:MET:HB3	1.85	0.40
3:N:666:GLY:O	3:N:670:ILE:HG12	2.20	0.40
4:b:4:THR:HG21	4:b:36:ILE:HD12	2.03	0.40
4:S:30:GLN:O	4:S:32:ILE:HD12	2.22	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	
1	A	164/169 (97%)	156 (95%)	8 (5%)	0	100	100
1	B	164/169 (97%)	156 (95%)	8 (5%)	0	100	100
1	C	161/169 (95%)	156 (97%)	5 (3%)	0	100	100
1	D	162/169 (96%)	156 (96%)	6 (4%)	0	100	100
1	E	164/169 (97%)	159 (97%)	5 (3%)	0	100	100
1	F	163/169 (96%)	159 (98%)	4 (2%)	0	100	100
2	G	253/255 (99%)	247 (98%)	6 (2%)	0	100	100
2	H	253/255 (99%)	247 (98%)	6 (2%)	0	100	100
2	I	252/255 (99%)	247 (98%)	5 (2%)	0	100	100
2	J	248/255 (97%)	240 (97%)	8 (3%)	0	100	100
2	K	248/255 (97%)	240 (97%)	8 (3%)	0	100	100
2	L	248/255 (97%)	242 (98%)	6 (2%)	0	100	100
3	M	25/674 (4%)	25 (100%)	0	0	100	100
3	N	25/674 (4%)	24 (96%)	1 (4%)	0	100	100
3	O	24/674 (4%)	24 (100%)	0	0	100	100
4	P	154/639 (24%)	150 (97%)	3 (2%)	1 (1%)	21	52
4	Q	156/639 (24%)	155 (99%)	1 (1%)	0	100	100
4	R	94/639 (15%)	86 (92%)	6 (6%)	2 (2%)	5	28
4	S	154/639 (24%)	151 (98%)	2 (1%)	1 (1%)	21	52
4	T	156/639 (24%)	155 (99%)	1 (1%)	0	100	100
4	U	94/639 (15%)	90 (96%)	3 (3%)	1 (1%)	11	40
4	V	154/639 (24%)	151 (98%)	2 (1%)	1 (1%)	21	52
4	W	156/639 (24%)	155 (99%)	1 (1%)	0	100	100
4	X	94/639 (15%)	88 (94%)	4 (4%)	2 (2%)	5	28
4	Y	154/639 (24%)	152 (99%)	1 (1%)	1 (1%)	21	52
4	Z	156/639 (24%)	152 (97%)	4 (3%)	0	100	100
4	a	94/639 (15%)	88 (94%)	5 (5%)	1 (1%)	11	40
4	b	154/639 (24%)	151 (98%)	2 (1%)	1 (1%)	21	52
4	c	156/639 (24%)	155 (99%)	1 (1%)	0	100	100
4	d	94/639 (15%)	87 (93%)	5 (5%)	2 (2%)	5	28
4	e	154/639 (24%)	150 (97%)	3 (2%)	1 (1%)	21	52
4	f	156/639 (24%)	154 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	g	94/639 (15%)	91 (97%)	2 (2%)	1 (1%)	11	40
All	All	4978/16068 (31%)	4839 (97%)	124 (2%)	15 (0%)	37	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	R	36	ILE
4	R	51	GLY
4	X	36	ILE
4	X	51	GLY
4	d	36	ILE
4	d	51	GLY
4	P	51	GLY
4	S	51	GLY
4	U	51	GLY
4	V	51	GLY
4	Y	51	GLY
4	a	51	GLY
4	b	51	GLY
4	e	51	GLY
4	g	51	GLY

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	138/140 (99%)	138 (100%)	0	100	100
1	B	138/140 (99%)	138 (100%)	0	100	100
1	C	137/140 (98%)	137 (100%)	0	100	100
1	D	136/140 (97%)	136 (100%)	0	100	100
1	E	138/140 (99%)	138 (100%)	0	100	100
1	F	138/140 (99%)	138 (100%)	0	100	100
2	G	233/233 (100%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	233/233 (100%)	233 (100%)	0	100	100
2	I	232/233 (100%)	232 (100%)	0	100	100
2	J	228/233 (98%)	228 (100%)	0	100	100
2	K	228/233 (98%)	226 (99%)	2 (1%)	70	76
2	L	228/233 (98%)	222 (97%)	6 (3%)	40	63
3	M	23/523 (4%)	23 (100%)	0	100	100
3	N	23/523 (4%)	23 (100%)	0	100	100
3	O	22/523 (4%)	22 (100%)	0	100	100
4	P	139/543 (26%)	136 (98%)	3 (2%)	45	65
4	Q	140/543 (26%)	140 (100%)	0	100	100
4	R	87/543 (16%)	87 (100%)	0	100	100
4	S	139/543 (26%)	138 (99%)	1 (1%)	76	78
4	T	140/543 (26%)	140 (100%)	0	100	100
4	U	87/543 (16%)	85 (98%)	2 (2%)	44	64
4	V	139/543 (26%)	138 (99%)	1 (1%)	76	78
4	W	140/543 (26%)	140 (100%)	0	100	100
4	X	87/543 (16%)	87 (100%)	0	100	100
4	Y	139/543 (26%)	137 (99%)	2 (1%)	59	71
4	Z	140/543 (26%)	140 (100%)	0	100	100
4	a	87/543 (16%)	86 (99%)	1 (1%)	65	74
4	b	139/543 (26%)	137 (99%)	2 (1%)	59	71
4	c	140/543 (26%)	140 (100%)	0	100	100
4	d	87/543 (16%)	86 (99%)	1 (1%)	65	74
4	e	139/543 (26%)	137 (99%)	2 (1%)	59	71
4	f	140/543 (26%)	140 (100%)	0	100	100
4	g	87/543 (16%)	86 (99%)	1 (1%)	65	74
All	All	4471/13581 (33%)	4447 (100%)	24 (0%)	78	81

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	152	VAL
2	K	153	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	26	ASP
2	L	28	LEU
2	L	29	LEU
2	L	31	GLU
2	L	145	TYR
2	L	153	SER
4	P	151	GLN
4	P	154	GLU
4	P	156	ILE
4	S	156	ILE
4	U	134	VAL
4	U	136	LEU
4	V	156	ILE
4	Y	156	ILE
4	Y	158	GLU
4	a	34	THR
4	b	152	ARG
4	b	156	ILE
4	d	134	VAL
4	e	153	VAL
4	e	156	ILE
4	g	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	152	GLN
1	B	138	ASN
1	C	138	ASN
1	C	152	GLN
1	F	138	ASN
4	P	29	ASN
4	P	38	GLN
4	P	70	GLN
4	P	151	GLN
4	R	24	ASN
4	R	54	ASN
4	S	38	GLN
4	S	151	GLN
4	T	38	GLN
4	Y	29	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Y	30	GLN
4	Z	29	ASN
4	b	38	GLN
4	e	84	GLN
4	e	94	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.

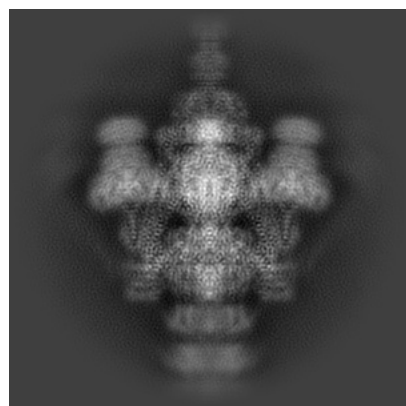
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63716. These allow visual inspection of the internal detail of the map and identification of artifacts.

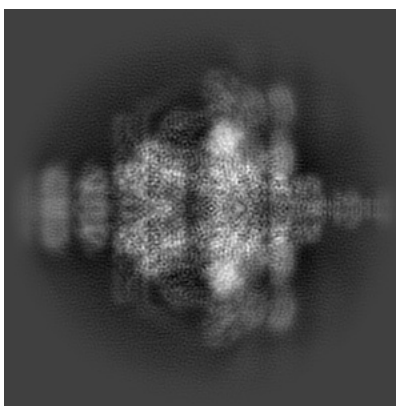
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

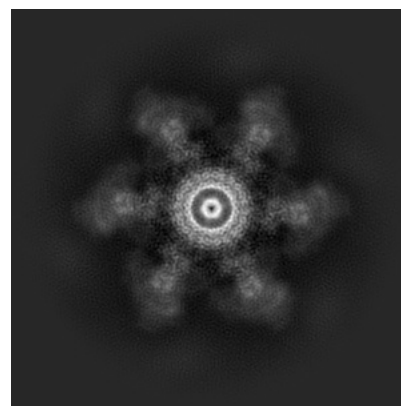
6.1.1 Primary map



X

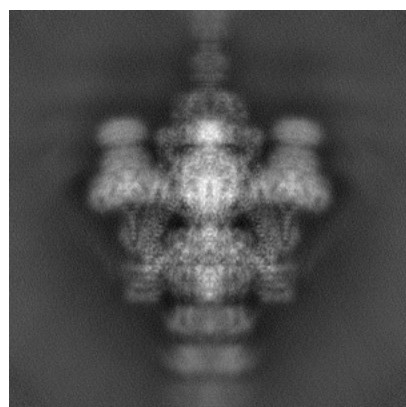


Y

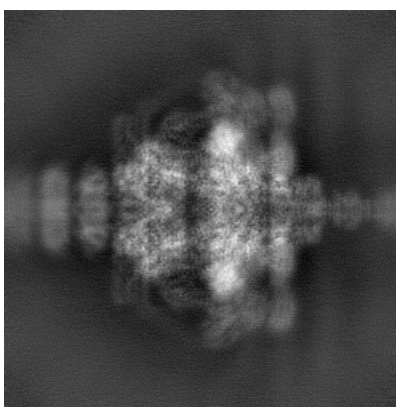


Z

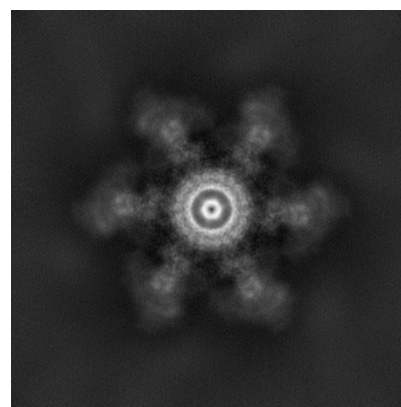
6.1.2 Raw map



X



Y

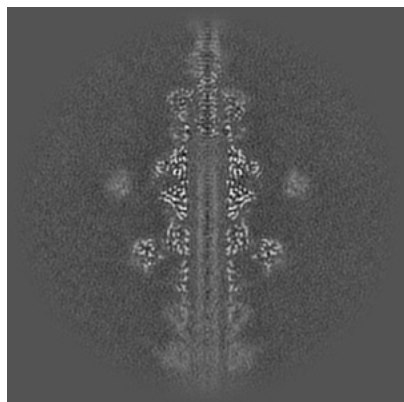


Z

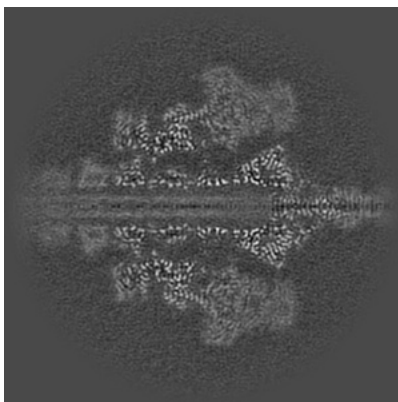
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

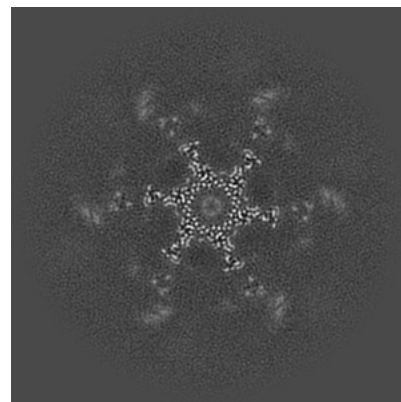
6.2.1 Primary map



X Index: 180

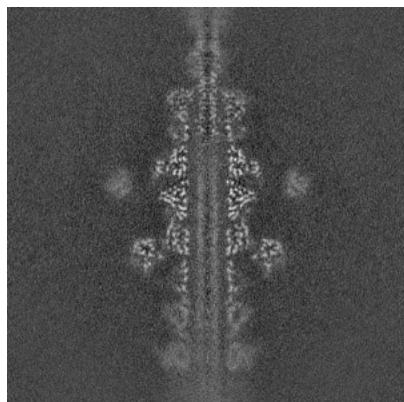


Y Index: 180

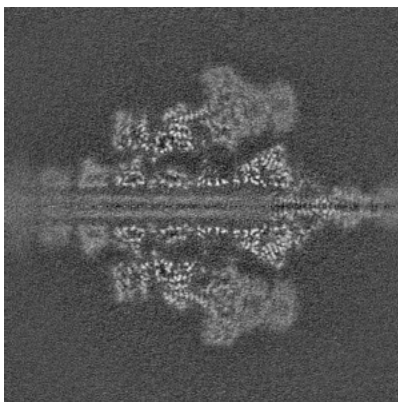


Z Index: 180

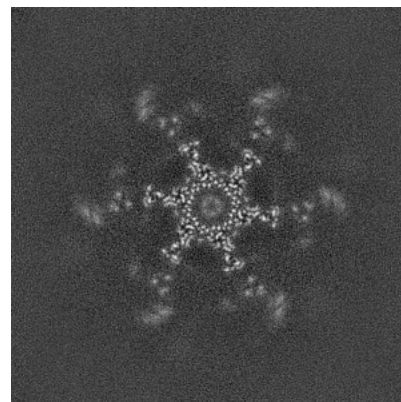
6.2.2 Raw map



X Index: 180



Y Index: 180

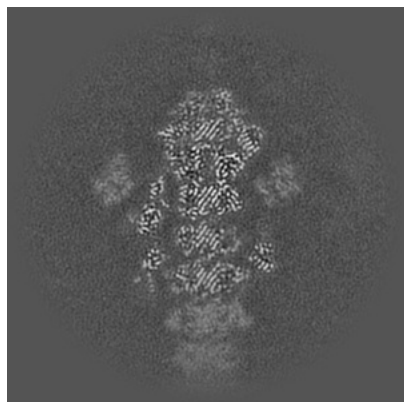


Z Index: 180

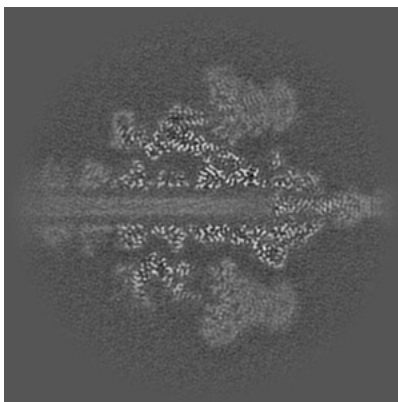
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

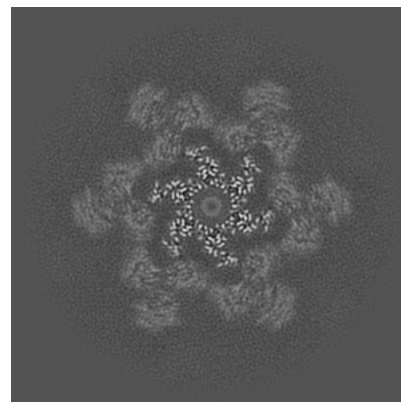
6.3.1 Primary map



X Index: 199

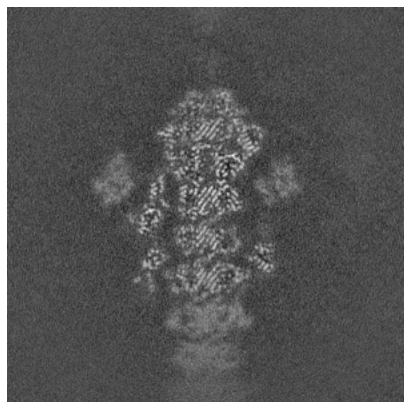


Y Index: 175

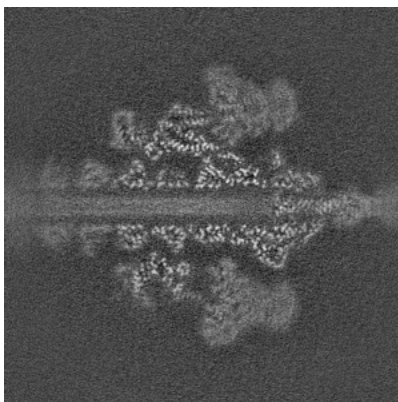


Z Index: 192

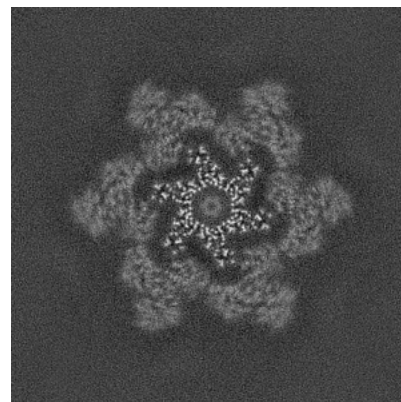
6.3.2 Raw map



X Index: 199



Y Index: 175

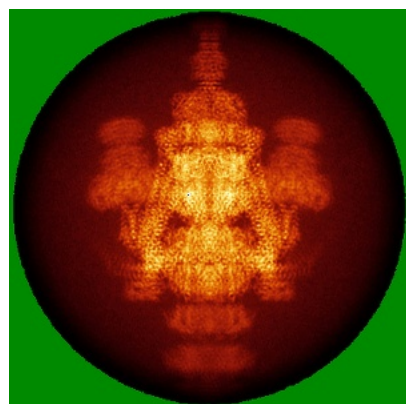


Z Index: 194

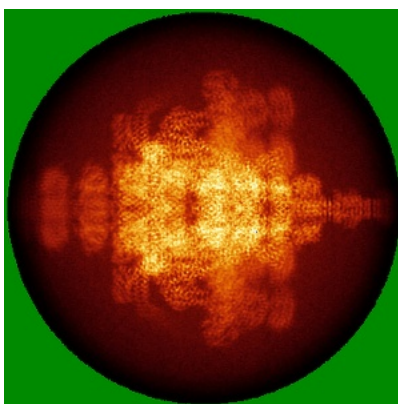
The images above show the largest variance slices of the map in three orthogonal directions.

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

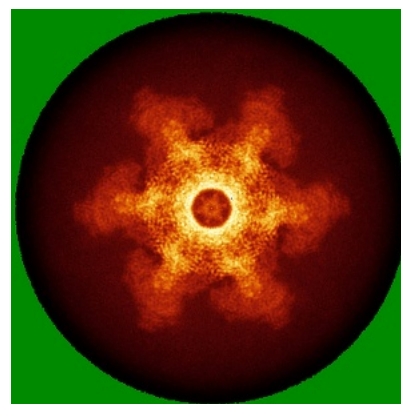
6.4.1 Primary map



X

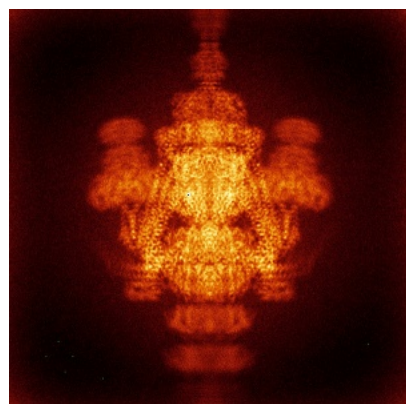


Y

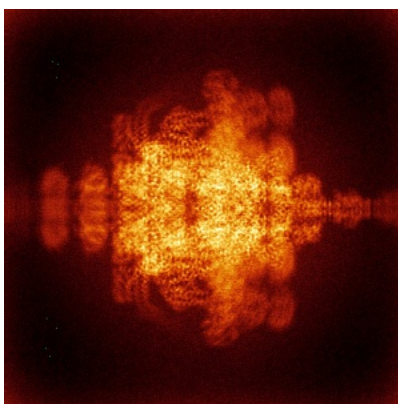


Z

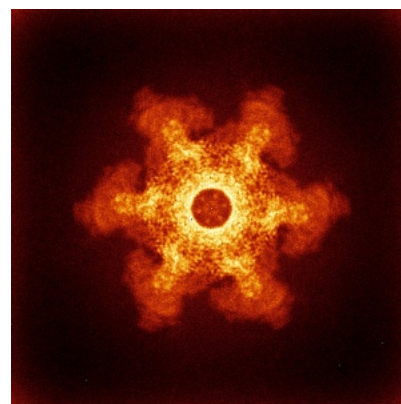
6.4.2 Raw map



X



Y

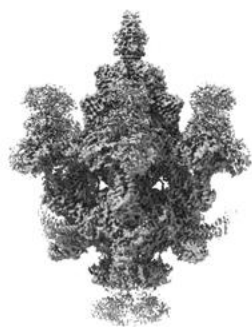


Z

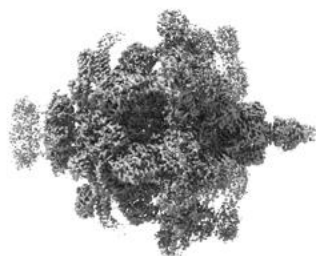
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

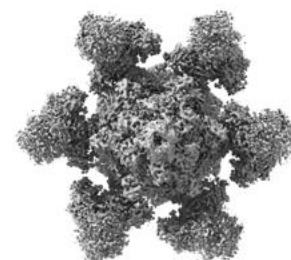
6.5.1 Primary map



X



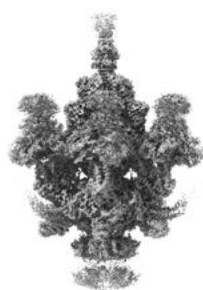
Y



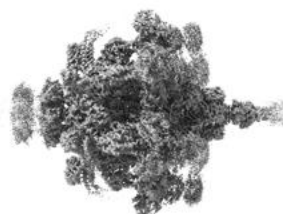
Z

The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

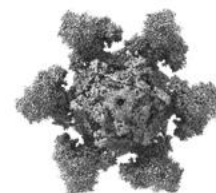
6.5.2 Raw map



X



Y



Z

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.

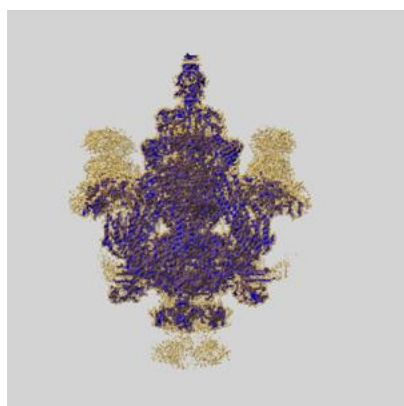
6.6 Mask visualisation [i](#)

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

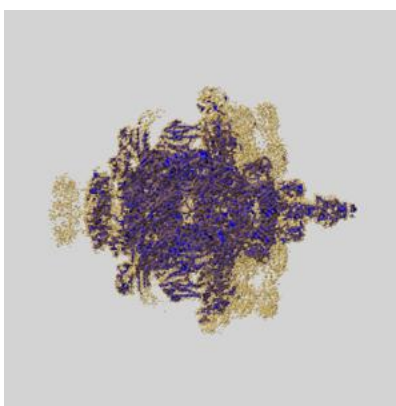
A mask typically either:

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

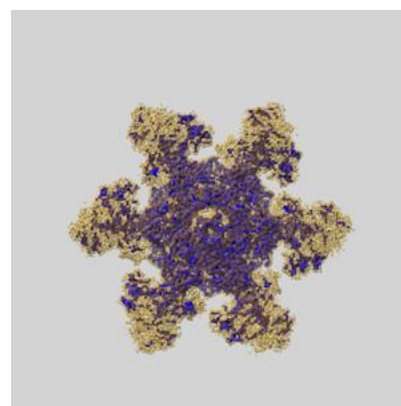
6.6.1 emd_63716_msk_1.map [i](#)



X



Y

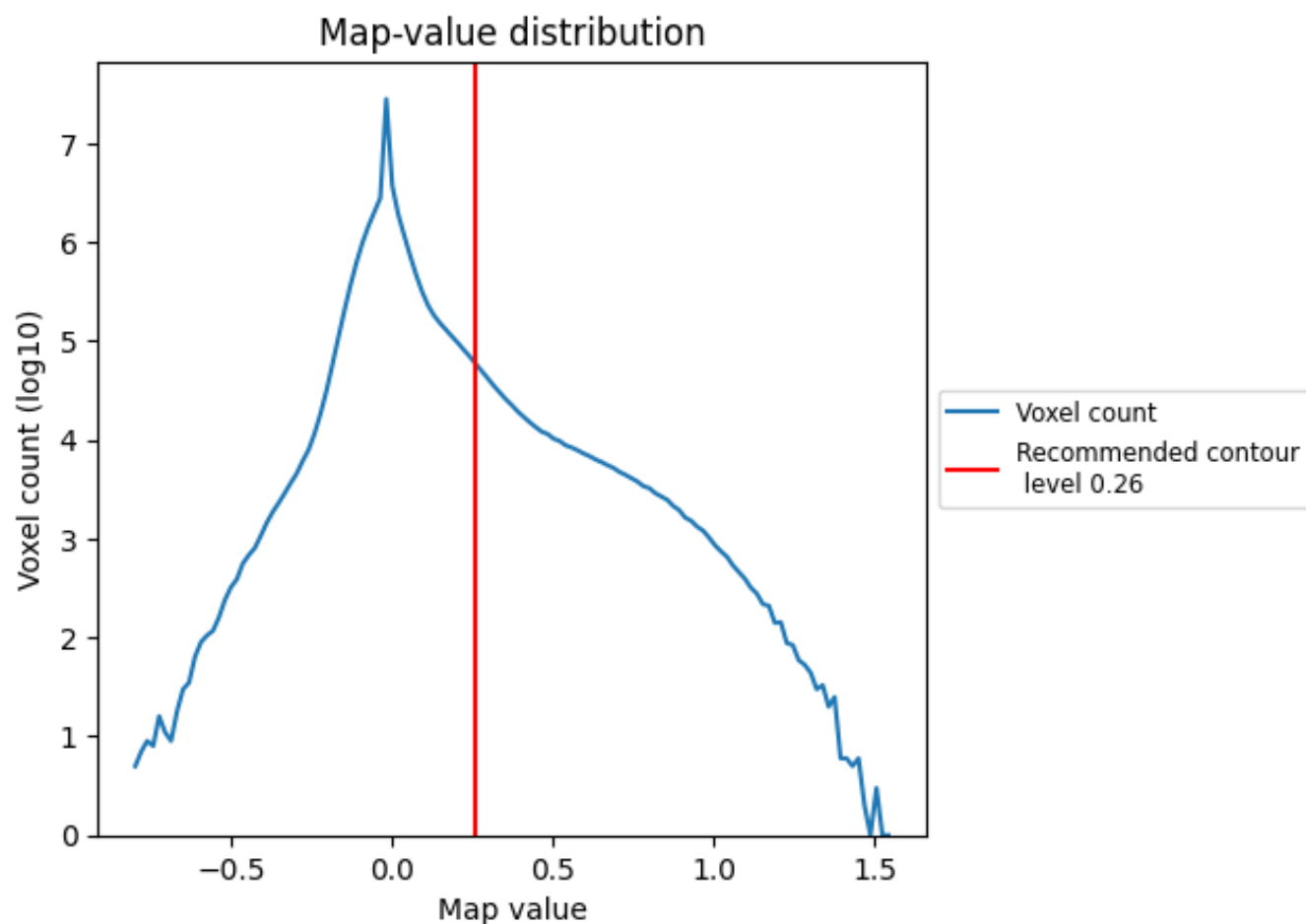


Z

7 Map analysis [i](#)

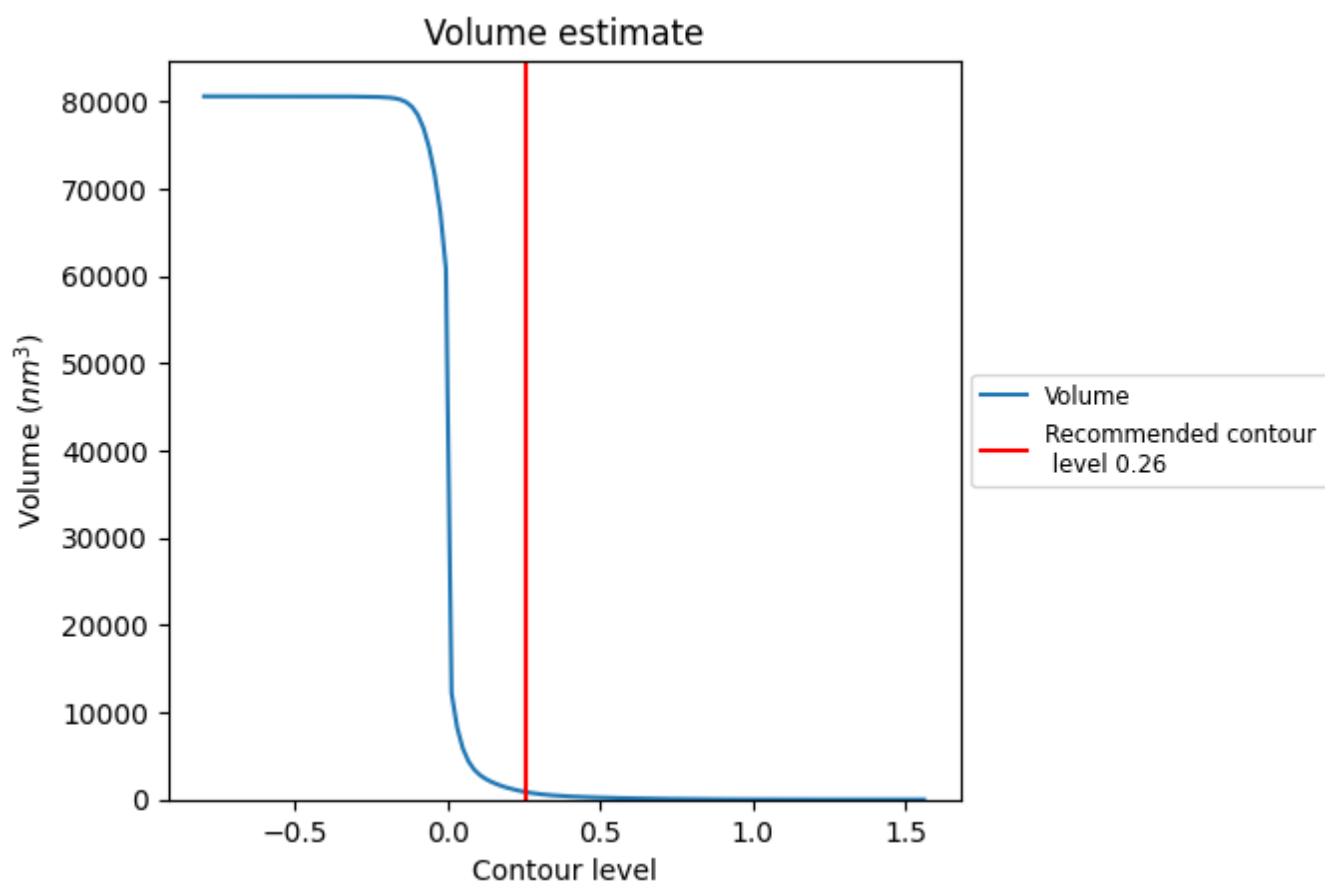
This section contains the results of statistical analysis of the map.

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.

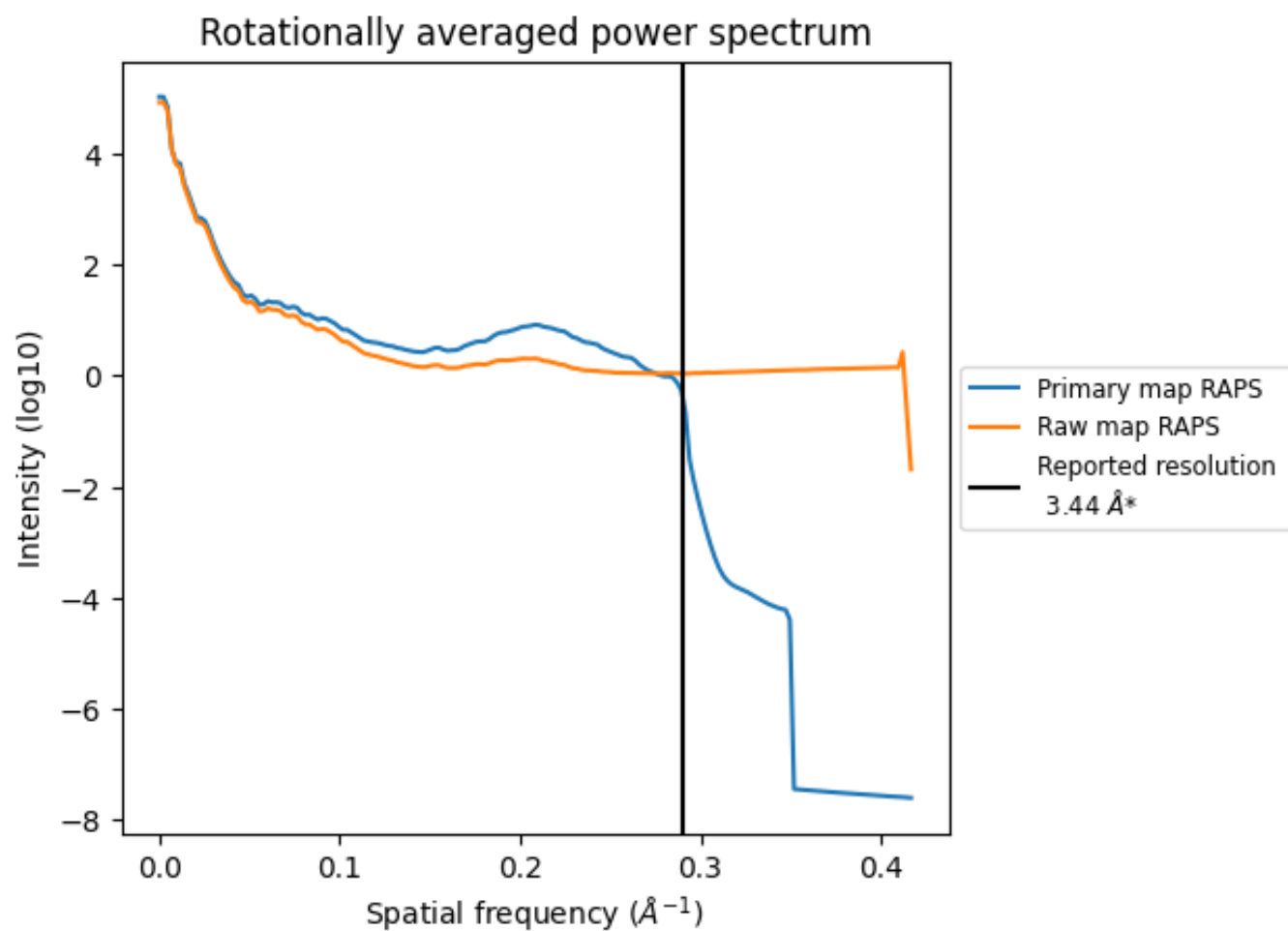
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 844 nm³; this corresponds to an approximate mass of 763 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 ⓘ

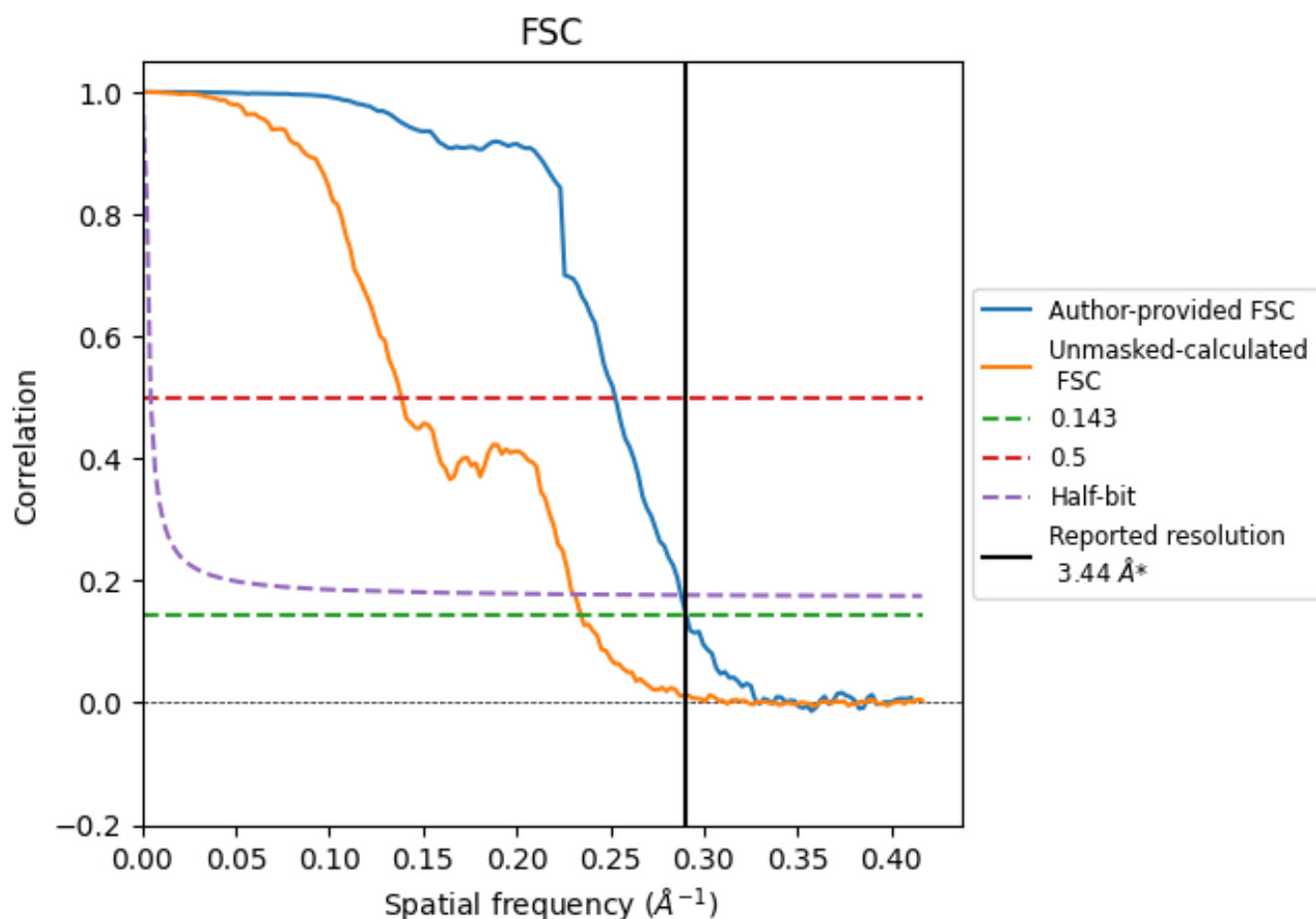


*Reported resolution corresponds to spatial frequency of $0.291 \text{ \AA}^{-1}$

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 0.291 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

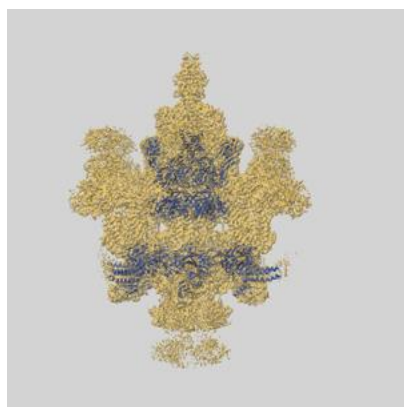
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	3.96	3.47
Unmasked-calculated*	4.26	7.23	4.33

*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 4.26 differs from the reported value 3.44 by more than 10 %

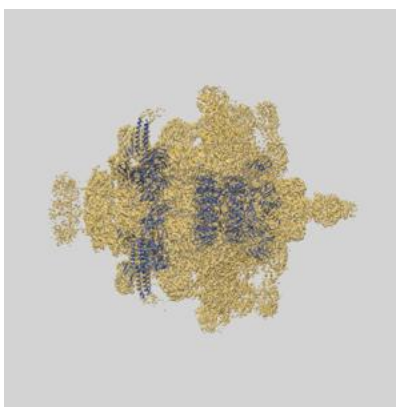
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63716 and PDB model 9M8O. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

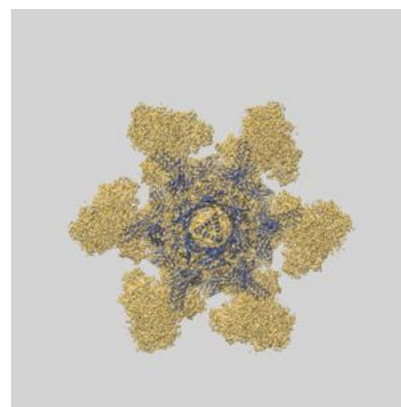
9.1 Map-model overlay [i](#)



X



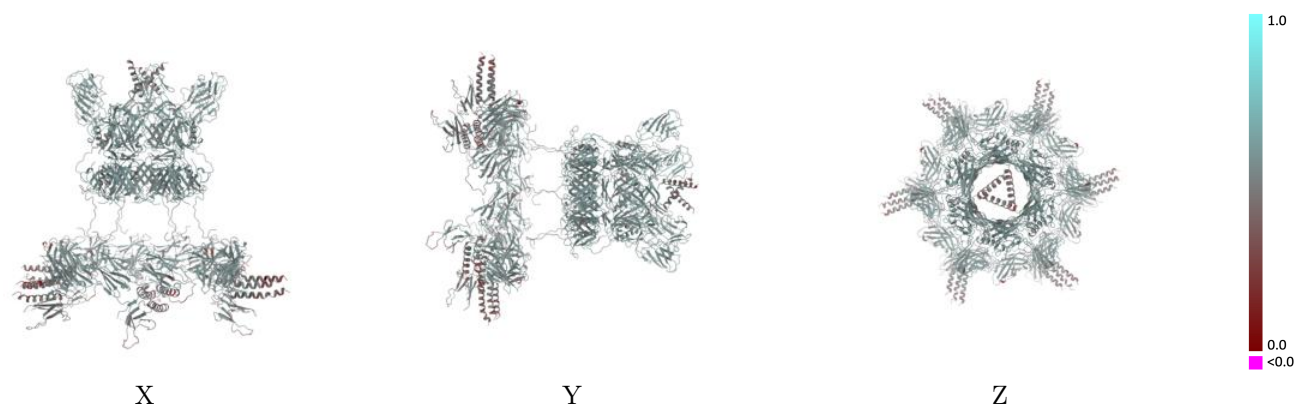
Y



Z

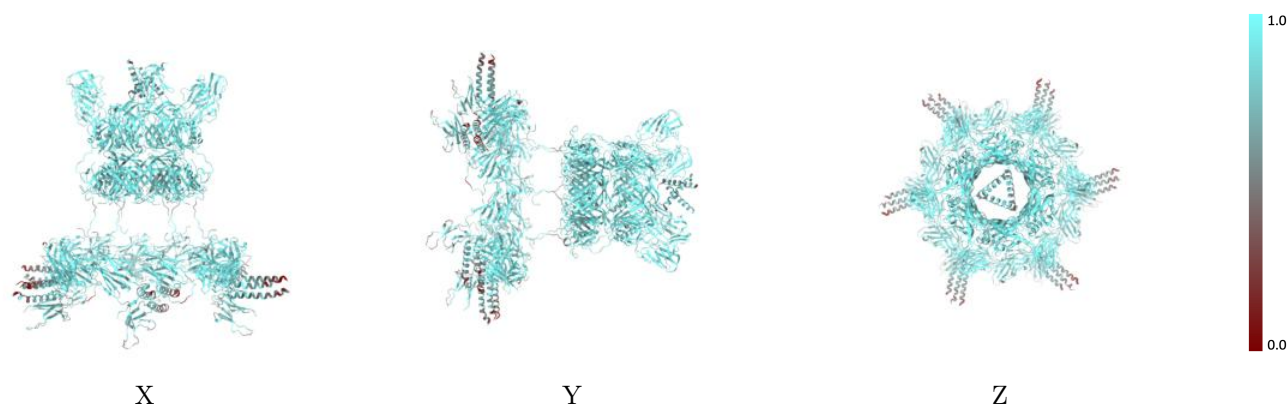
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



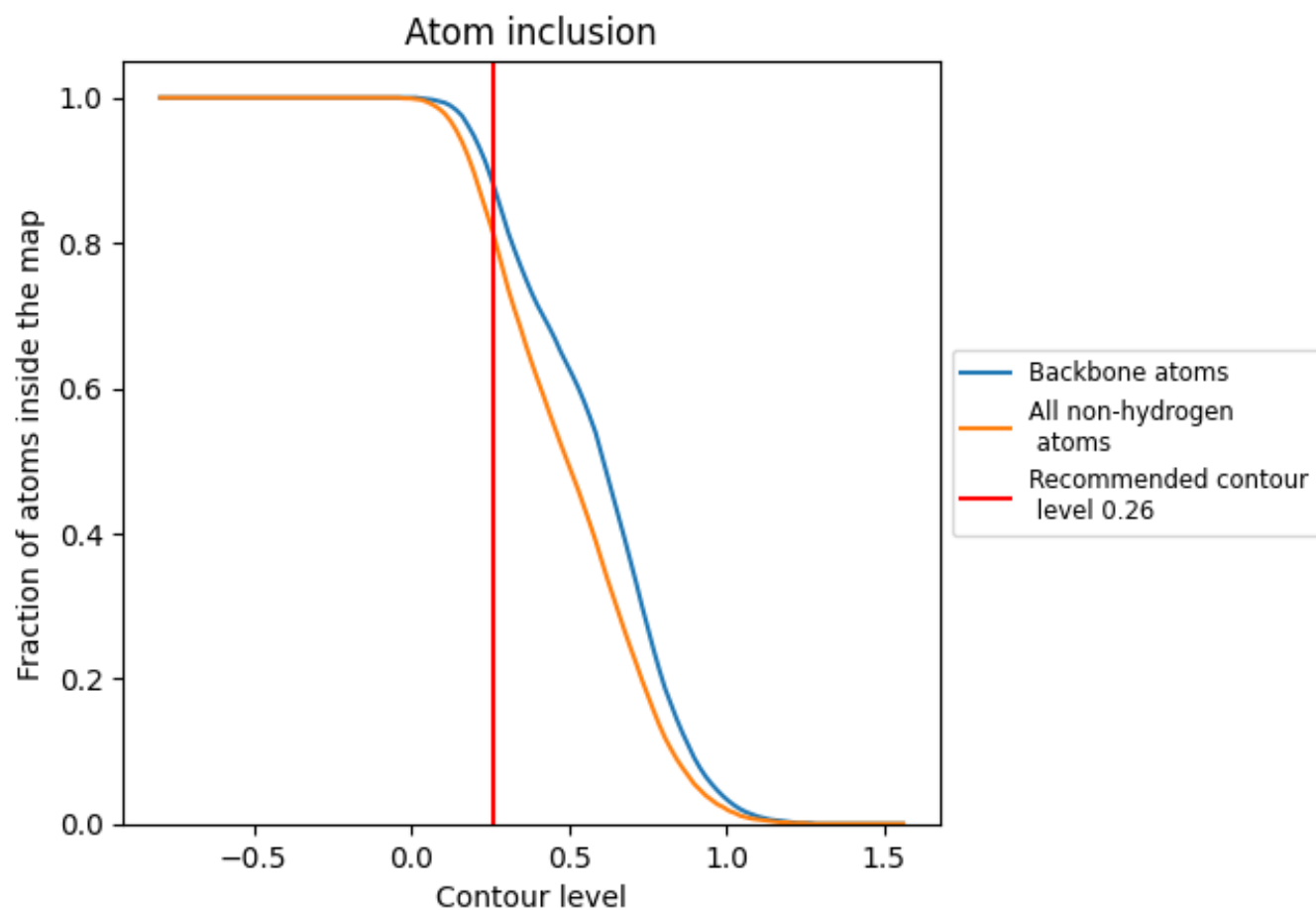
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.26).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.5240
A	 0.8260	 0.5430
B	 0.8290	 0.5380
C	 0.8330	 0.5460
D	 0.8270	 0.5460
E	 0.8290	 0.5460
F	 0.8340	 0.5390
G	 0.8730	 0.5460
H	 0.8740	 0.5470
I	 0.8750	 0.5460
J	 0.8720	 0.5450
K	 0.8740	 0.5470
L	 0.8740	 0.5500
M	 0.6710	 0.4630
N	 0.6710	 0.4600
O	 0.6590	 0.4350
P	 0.8070	 0.5180
Q	 0.8020	 0.5220
R	 0.6810	 0.4710
S	 0.7990	 0.5080
T	 0.7880	 0.5140
U	 0.6890	 0.4730
V	 0.8140	 0.5180
W	 0.7980	 0.5220
X	 0.6890	 0.4680
Y	 0.8120	 0.5090
Z	 0.7860	 0.5120
a	 0.6920	 0.4680
b	 0.8090	 0.5140
c	 0.8010	 0.5230
d	 0.6920	 0.4680
e	 0.8040	 0.5070
f	 0.7790	 0.5090
g	 0.7000	 0.4770

