



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:32 AM UTC

PDB ID : 7QOH / pdb_00007qoh
EMDB ID : EMD-14090
Title : Unique vertex of the phicrAss001 virion with C5 symmetry imposed
Authors : Bayfield, O.W.; Shkoporov, A.N.; Yutin, N.; Khokhlova, E.V.; Smith, J.L.R.;
Hawkins, D.E.D.P.; Koonin, E.V.; Hill, C.; Antson, A.A.
Deposited on : 2021-12-24
Resolution : 3.32 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

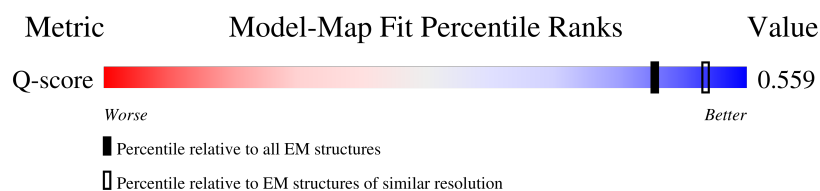
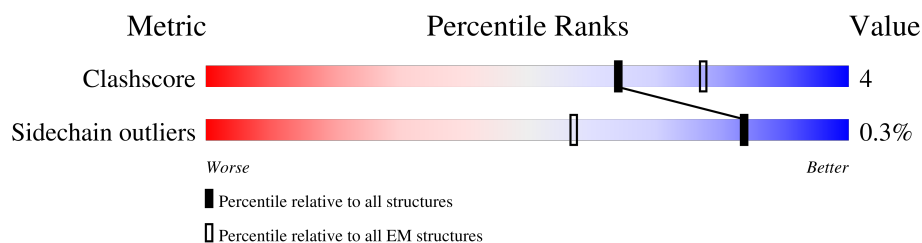
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14518 (2.82 - 3.82)

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	504	19% 84% 12% .
1	B	504	13% 85% 15%
1	C	504	12% 86% 14%
1	D	504	13% 77% 13% 10%
1	E	504	15% 90% 9%

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Mol	Chain	Length	Quality of chain
1	F	504	
2	a	333	
2	b	333	
2	d	333	
2	e	333	
2	f	333	
3	g	104	
3	h	104	
4	i	97	
4	j	97	
4	k	97	
5	l	806	
5	m	806	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37079 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 Major capsid protein gp32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	484	Total	C	N	O	S	0	0
			3861	2451	668	723	19		
1	B	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	C	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	D	456	Total	C	N	O	S	0	0
			3649	2329	631	671	18		
1	E	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	F	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		

- Molecule 2 is a protein called Auxiliary capsid protein gp36.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	b	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	d	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	e	267	Total	C	N	O	S	0	0
			2077	1335	332	401	9		
2	f	185	Total	C	N	O	S	0	0
			1434	919	226	283	6		

- Molecule 3 is a protein called Portal vertex capsid protein gp57.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	g	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	h	73	Total	C	N	O	S	0	0
			563	359	91	105	8		

- Molecule 4 is a protein called Head fiber trimer protein gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	i	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	j	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	k	38	Total	C	N	O	S	0	0
			310	201	51	56	2		

- Molecule 5 is a protein called Portal protein gp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	l	16	Total	C	N	O	S	0	0
			126	75	22	28	1		
5	m	17	Total	C	N	O	S	0	0
			140	85	24	30	1		

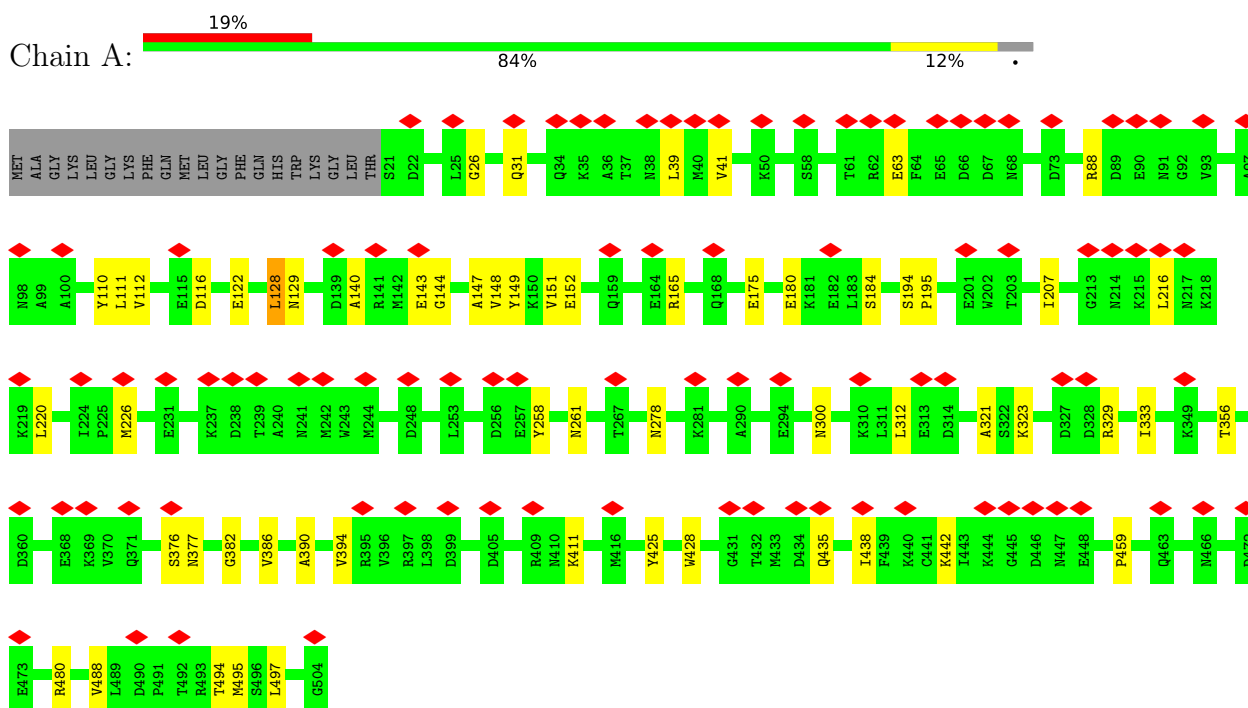
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	

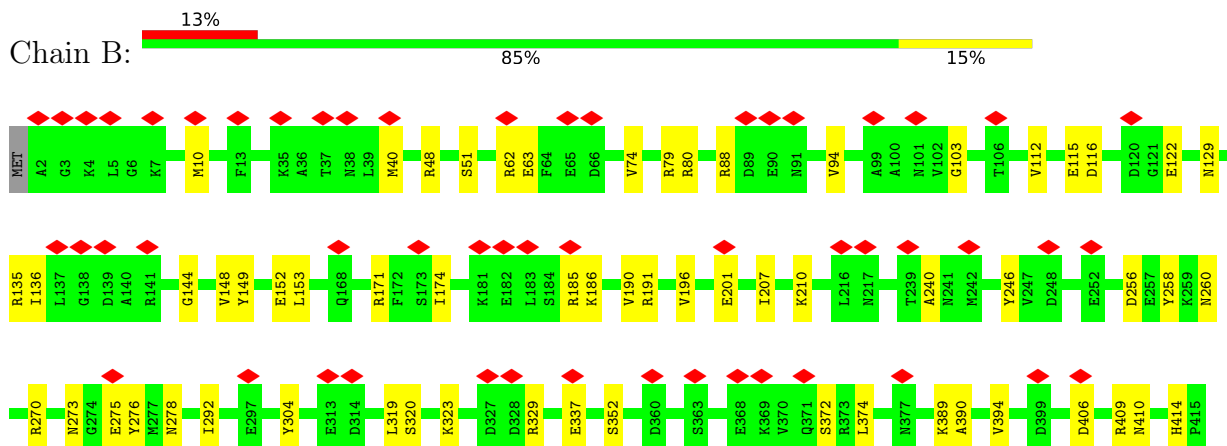
3 Residue-property plots

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

• Molecule 1: Major capsid protein gp32

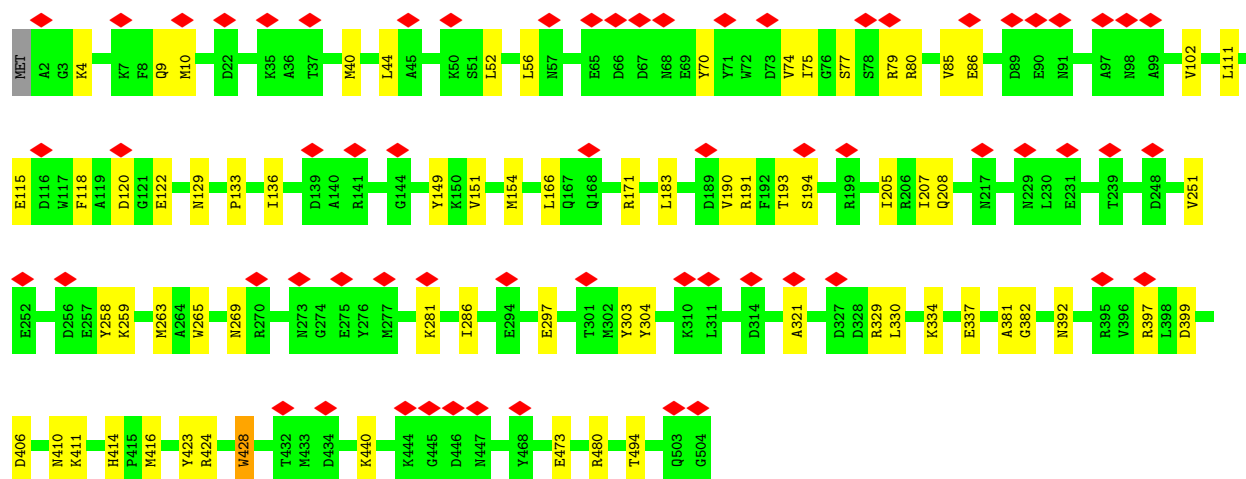
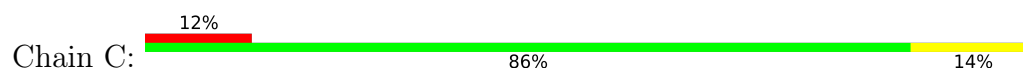


• Molecule 1: Major capsid protein gp32

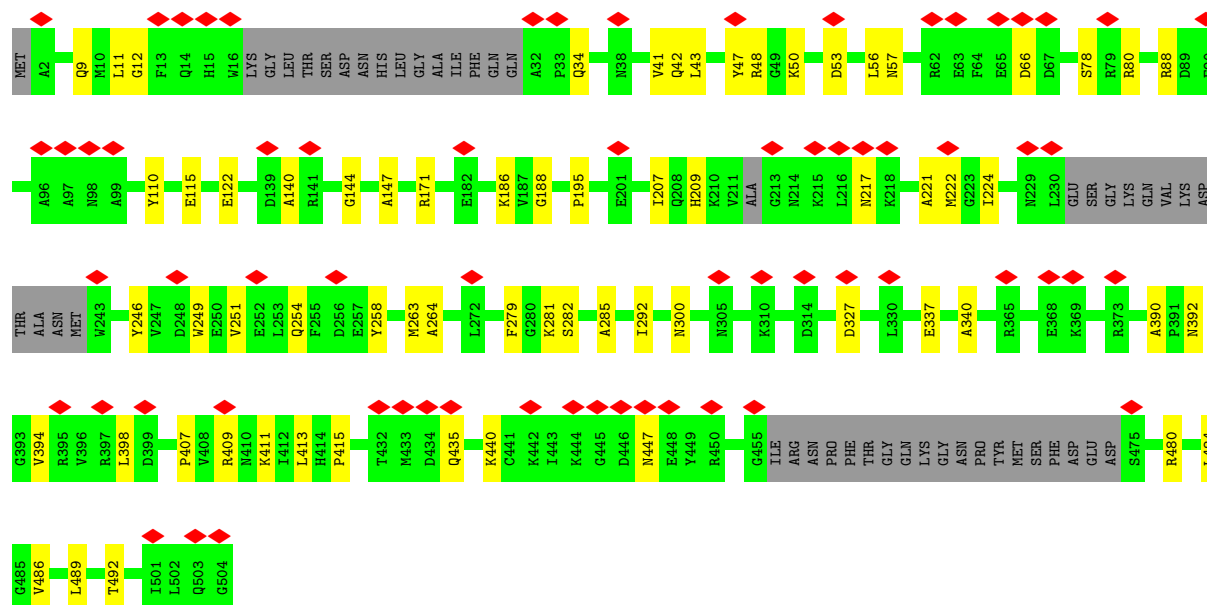
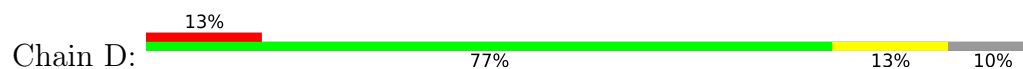




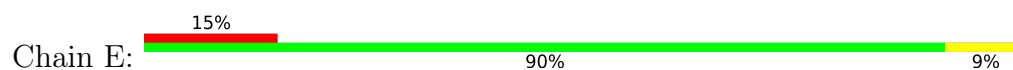
• Molecule 1: Major capsid protein gp32

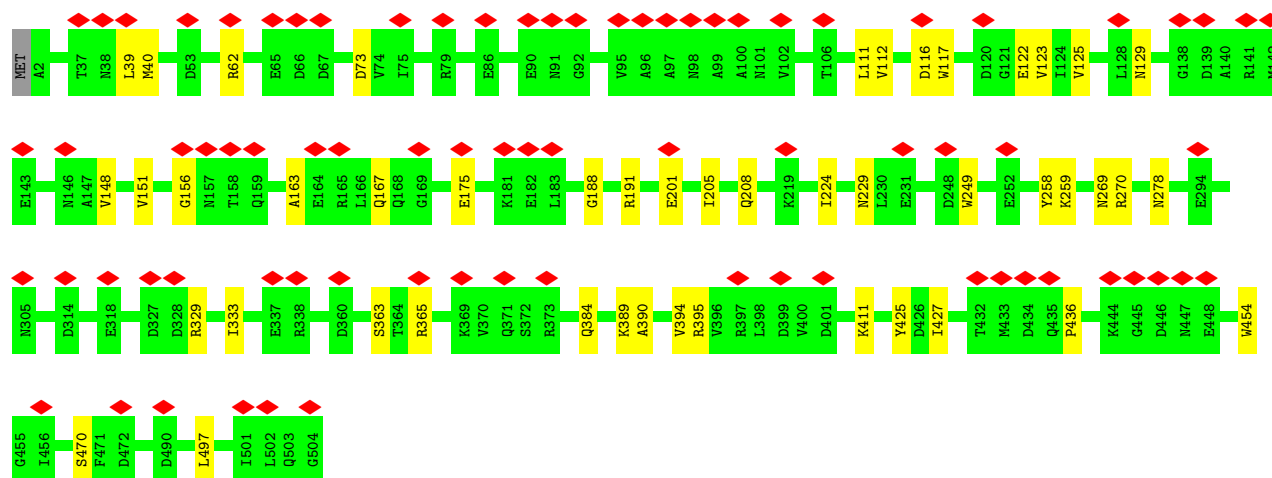


• Molecule 1: Major capsid protein gp32

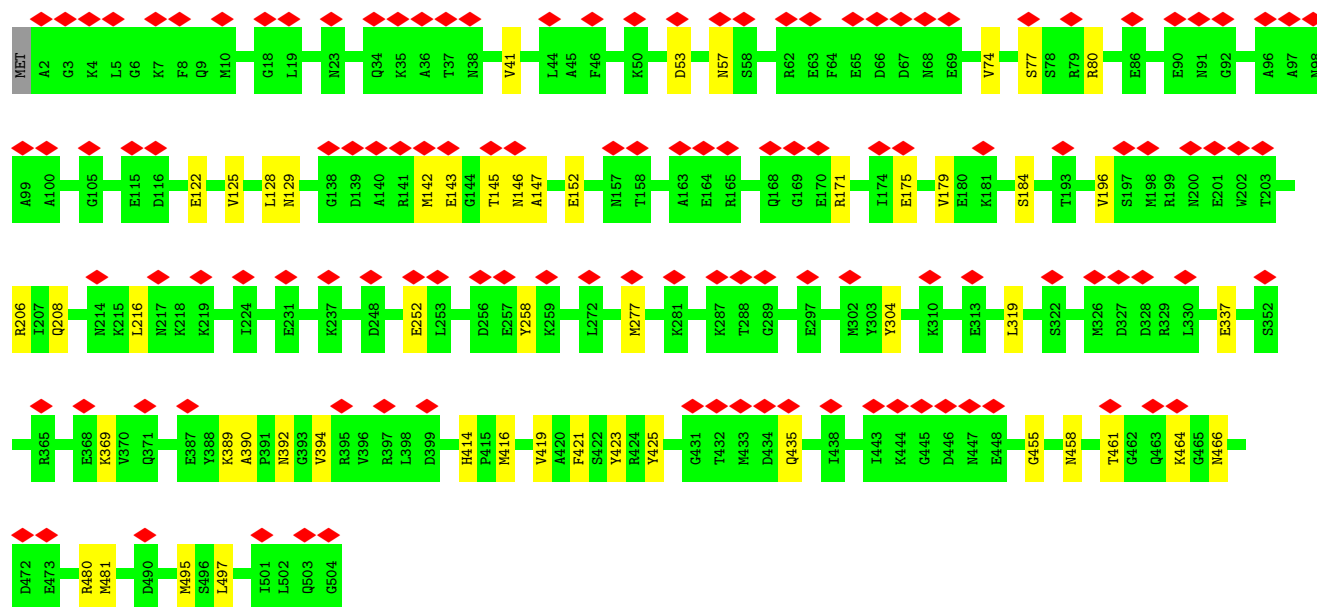
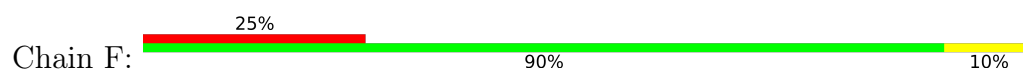


• Molecule 1: Major capsid protein gp32

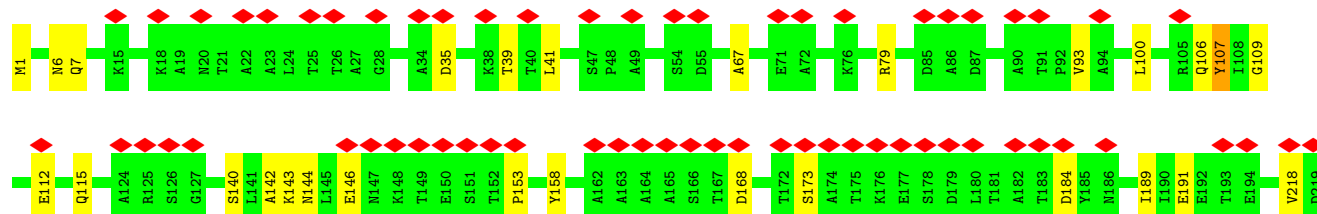
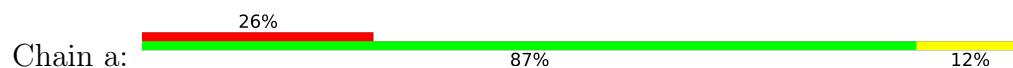


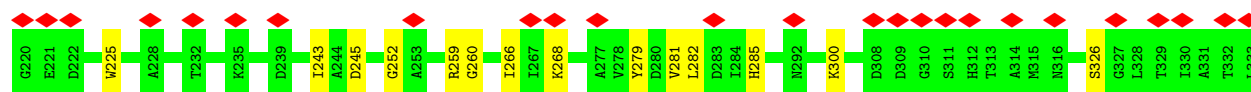


- Molecule 1: Major capsid protein gp32

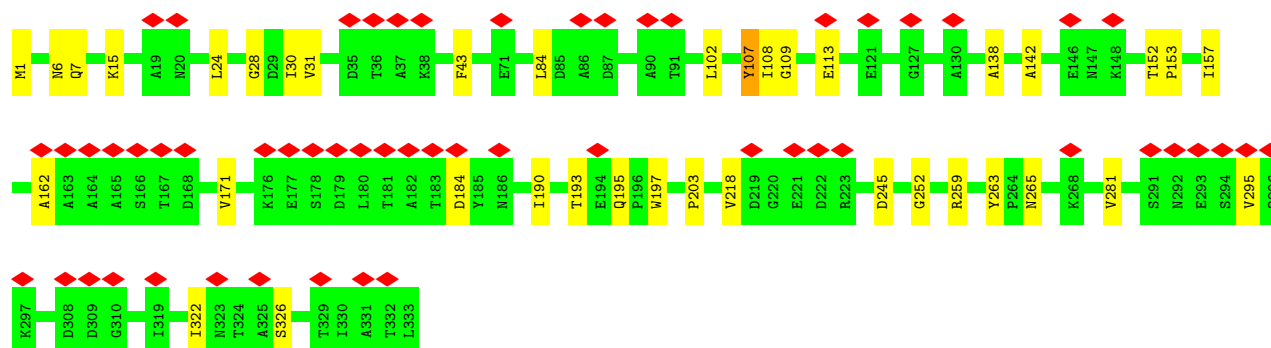
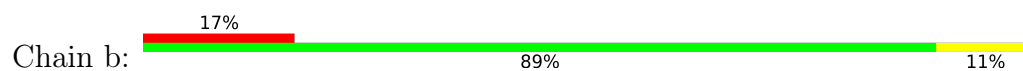


- Molecule 2: Auxiliary capsid protein gp36

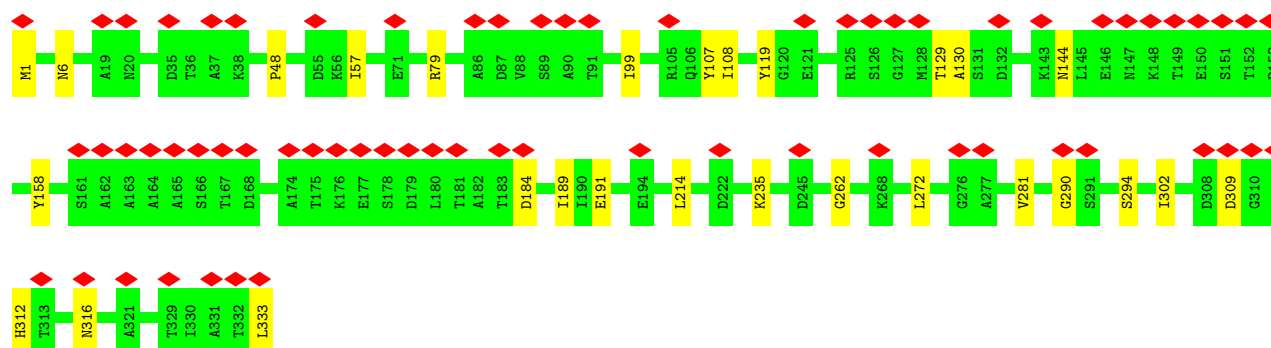
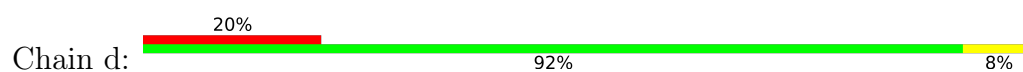




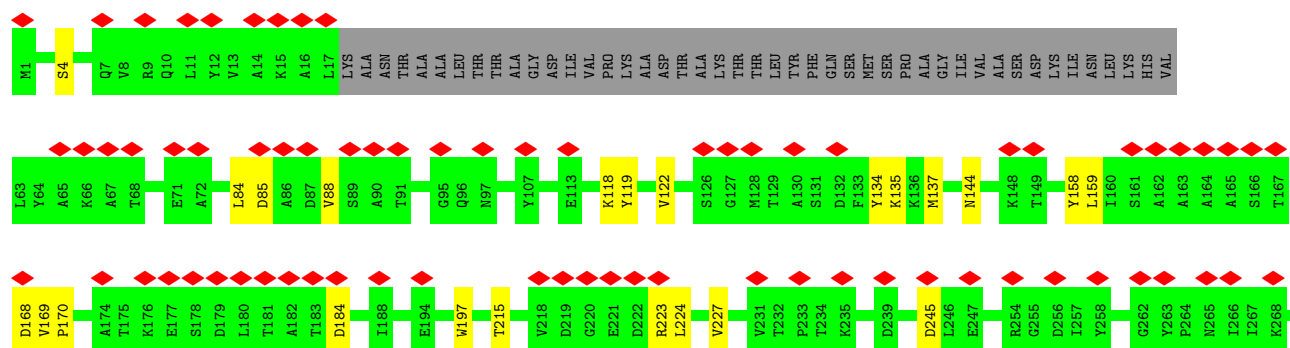
• Molecule 2: Auxiliary capsid protein gp36



• Molecule 2: Auxiliary capsid protein gp36



• Molecule 2: Auxiliary capsid protein gp36



ASN	LEU	ALA	THR	GLY	ALA	GLU	LEU	THR	THR	VAL	VAL	THR	THR	LYS	VAL	ASN	ALA	ILE	LEU	SER	ALA	LYS	VAL	ALA	ASP	ILE	MET	VAL	GLU	ALA	ASN
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• Molecule 4: Head fiber trimer protein gp21



M1	K2	T3	L4	H5	T6	L7	K8	I9	S10	P11	M12	A13	P14	D15	I16	M17	I21	Y22	K23	G24	T25	M26	N30	N31	G32	E33	W34	E35	T36	I37	G38	GLY	GLU	SER	LEU	PRO	TYR	VAL	LEU	PRO	ALA	THR	THR	SER	THR	ILE	GLY	VAL	LYS	LYS	THR	ASN	VAL	GLY
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ASN	LEU	ALA	THR	GLY	ALA	GLU	LEU	THR	THR	VAL	VAL	THR	THR	LYS	VAL	ASN	ALA	ILE	LEU	SER	ALA	LYS	VAL	ALA	ASP	ILE	MET	VAL	GLU	ASP	ALA	ASN
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• Molecule 4: Head fiber trimer protein gp21



M1	K2	T3	L4	H5	T6	L7	S10	P11	M12	A13	P14	D15	I16	M17	Y22	K23	G24	T25	M26	N31	G32	E33	W34	T36	I37	G38	GLU	GLU	SER	GLY	PRO	TYR	VAL	LEU	PRO	ALA	THR	THR	SER	THR	ILE	GLY	VAL	LYS	LYS	THR	ASN	VAL	GLY	LEU	ALA
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THR	GLY	ALA	GLU	LEU	THR	VAL	THR	LYS	VAL	ASN	ALA	VAL	LYS	THR	LYS	THR	GLN	TRP	ASP	ILE	MET	VAL	ASP	ALA	ASN
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• Molecule 5: Portal protein gp20



MET	ALA	ASP	PHE	LEU	LEU	ASN	PHE	PRO	ARG	GLN	LEU	PRO	PHE	SER	LYS	LYS	THR	THR	GLN	TRP	ASP	ILE	MET	LEU	ALA	ASN	GLN	LYS	THR	PHE	ASP	GLY	TYR	SER	LEU	VAL	GLN	LYS	VAL	ARG	LYS	VAL	ILE	THR	ASN	TYR	ASP	LEU	ALA	ASN	GLY	ARG	LEU	HIS	ASP	MET
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SER	ASP	LEU	GLY	LEU	VAL	ASN	LEU	ASN	PRO	GLY	ILE	LYS	ALA	ALA	TYR	ILE	PRO	ASP	ARG	ILE	ASN	TRP	LEU	ASN	LYS	LYS	ASN	VAL	ASN	VAL	ARG	LEU	GLY	GLU	SER	LEU	GLN	LYS	VAL	ARG	LYS	VAL	PHE	ASP	VAL	THR	ASN	PRO	ASN	ALA	ALA	ILE	ASN	GLY	GLU	ILE	HIS	ASP
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ASN	LYS	LYS	ASN	GLY	LEU	GLN	ARG	GLY	THR	ILE	MET	GLY	THR	THR	ASP	GLY	GLU	ASP	GLY	TYR	ASN	PRO	GLY	LYS	LEU	ASN	VAL	ASN	TYR	THR	THR	THR	GLY	TRP	ASN	GLY	VAL	ARG	VAL	ASN	GLY	LEU	THR	ASN	PRO	ASN	GLY	GLU	ILE	LYS	THR	ASN	GLY	ASP	ILE
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PRO	LEU	ILE	PHE	ASN	ASN	GLY	PHE	ASP	MET	ALA	ASP	MET	THR	CYS	GLY	GLY	THR	GLY	VAL	GLY	GLY	GLY	VAL	GLY	ILE	GLY	VAL	ASN	VAL	ASN	VAL	ASP	PRO	GLY	GLY	GLY	VAL	ASN	GLY	VAL	ARG	VAL	THR	ASN	PRO	ASN	GLY	GLU	ILE	LYS	THR	ASN	GLY	ASP	ILE
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TRP	SER	PRO	GLY	ARG	VAL	ILE	ASP	THR	TYR	ASP	VAL	LEU	VAL	ASP	PRO	LYS	ILE	LYS	TYR	THR	GLY	GLN	GLY	ALA	VAL	VAL	ASP	GLN	GLY	ASP	ASN	ASN	ILE	ASP	ASP	GLY	ARG	TYR	GLY	VAL	VAL	ASN	PRO	ASP	VAL	H298	Q289	H290	H291	I292	G293	D294	E295	I296	R299	D300	G301
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T302	Y303	PHE	ASP	PRO	ALA	ASN	LEU	THR	GLY	GLY	ILE	ALA	ASN	THR	ASN	SER	LEU	LEU	PRO	TYR	ASP	GLY	ALA	GLY	LEU	VAL	VAL	VAL	GLY	ARG	LEU	TYR	TRP	ILE	ILE	ILE	LYS	VAL	VAL	LYS	VAL	SER	TYR	ASN	PRO	GLY	THR	GLY	GLY	GLY	GLY	GLY	TRP	ASN	PHE	TYR	PRO	GLY
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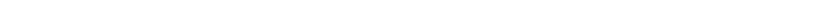
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LEU	ASN	ASP	SER	ARG	PRO	PHE	SER	VAL	GLY	GLY	GLY	THR	LYS	PRO	TYR	ASN	SER	LEU	TYR	ASP	TYR	ASP	GLY	ALA	GLY	ALA	LYS	ILE	PHE	VAL	ASN	GLY	THR	ARG	ILE	GLY	ASN	GLY	VAL	ASN	GLY	VAL	ASN	PRO	PRO	GLY	GLY	LEU	LEU	PHE	ASP	ILE	LYS	GLY	GLY	GLY	TRP	ASP	ALA
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VAL	ASN	HIS	ILE	ALA	VAL	ILE	ASP	SER	PHE	GLY	GLY	THR	ILE	GLY	GLY	SER	THR	GLY	LYS	TRP	ALA	ILE	GLY	GLY	GLY	LYS	GLY	ILE	ALA	GLY	VAL	ASN	GLY	THR	ARG	ILE	GLY	ASN	GLY	VAL	ASN	GLY	VAL	ASN	PRO	PRO	GLY	GLY	LEU	LEU	PHE	ILE	LYS	LYS	MET	GLY	TRP	MET	ALA	ASP	VAL	VAL	ALA
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[illegible]

- Molecule 5: Portal protein gp20

Chain m:  98%

[illegible]

ALA
GLU
THR
ASP
ALA
SER
ILE
LYS
ARG
GLN
ALA
LEU
ARG
LYS
LYS
SER
SER
THR
THR
ASN
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	122709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.944	Depositor
Minimum map value	-0.669	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	398.71204, 398.71204, 398.71204	wwPDB
Map dimensions	286, 286, 286	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.394098, 1.394098, 1.394098	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/3950	0.46	0/5346
1	B	0.24	0/4106	0.45	0/5553
1	C	0.26	0/4106	0.47	0/5553
1	D	0.25	0/3732	0.46	0/5044
1	E	0.23	0/4106	0.45	0/5553
1	F	0.23	0/4106	0.46	0/5553
2	a	0.22	0/2591	0.51	2/3533 (0.1%)
2	b	0.25	0/2591	0.52	2/3533 (0.1%)
2	d	0.23	0/2591	0.47	0/3533
2	e	0.21	0/2119	0.48	0/2887
2	f	0.18	0/1465	0.45	0/2001
3	g	0.27	0/629	0.46	0/852
3	h	0.27	0/572	0.53	0/773
4	i	0.18	0/318	0.40	0/430
4	j	0.18	0/318	0.45	0/430
4	k	0.21	0/318	0.54	0/430
5	l	0.28	0/126	0.76	0/169
5	m	0.23	0/141	0.49	0/189
All	All	0.24	0/37885	0.47	4/51362 (0.0%)

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	1
1	F	0	1
2	a	0	1
2	b	0	2
2	d	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	h	0	1
4	k	0	1
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	6	ASN	CA-C-N	5.33	131.72	121.54
2	a	6	ASN	C-N-CA	5.33	131.72	121.54
2	b	6	ASN	CA-C-N	5.05	131.19	121.54
2	b	6	ASN	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	LEU	Peptide
1	F	128	LEU	Peptide
2	a	107	TYR	Peptide
2	b	107	TYR	Peptide
2	b	263	TYR	Peptide
2	d	107	TYR	Peptide
2	d	262	GLY	Peptide
2	d	6	ASN	Peptide
3	h	85	VAL	Peptide
4	k	22	TYR	Peptide

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	3861	0	3765	41	0
1	B	4012	0	3921	54	0
1	C	4012	0	3921	53	0
1	D	3649	0	3574	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4012	0	3920	36	0
1	F	4012	0	3921	33	0
2	a	2542	0	2558	25	0
2	b	2542	0	2558	24	0
2	d	2542	0	2558	15	0
2	e	2077	0	2075	17	0
2	f	1434	0	1419	9	0
3	g	619	0	619	8	0
3	h	563	0	570	7	0
4	i	310	0	313	4	0
4	j	310	0	313	5	0
4	k	310	0	313	4	0
5	l	126	0	115	0	0
5	m	140	0	122	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	37079	0	36555	302	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 (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:198:VAL:H	2:f:202:MET:HB2	1.55	0.71
1:A:39:LEU:HA	1:F:435:GLN:HE22	1.58	0.67
1:C:191:ARG:H	1:D:254:GLN:HE22	1.43	0.64
2:f:88:VAL:HG22	2:f:223:ARG:HE	1.63	0.63
2:b:138:ALA:HB1	2:b:171:VAL:HG11	1.80	0.63
1:C:10:MET:SD	1:C:10:MET:N	2.73	0.62
1:C:194:SER:HB3	1:D:222:MET:HG2	1.82	0.62
1:E:390:ALA:HB3	1:E:394:VAL:HB	1.81	0.61
1:B:374:LEU:HD12	1:F:392:ASN:HD22	1.65	0.61
2:e:278:VAL:HG23	2:e:308:ASP:HB3	1.82	0.61
1:A:63:GLU:HG2	1:A:442:LYS:HB2	1.82	0.60
2:b:15:LYS:HD3	2:b:28:GLY:HA3	1.84	0.60
1:C:133:PRO:HB2	1:C:154:MET:HB3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:425:TYR:HB2	1:F:497:LEU:HB2	1.83	0.60
1:A:175:GLU:OE2	1:B:409:ARG:NH1	2.35	0.59
1:C:414:HIS:HD2	1:C:416:MET:H	1.49	0.59
1:B:129:ASN:OD1	1:C:411:LYS:NZ	2.36	0.59
1:B:435:GLN:NE2	1:C:40:MET:O	2.36	0.59
1:B:80:ARG:NH2	1:B:115:GLU:OE2	2.36	0.59
1:F:216:LEU:HD21	1:F:464:LYS:HG2	1.84	0.58
1:C:190:VAL:HG21	1:D:251:VAL:HG12	1.84	0.58
1:D:9:GLN:NE2	3:g:89:ASN:O	2.37	0.58
1:D:246:TYR:HD2	1:D:249:TRP:HB2	1.68	0.57
1:B:435:GLN:HE22	1:C:40:MET:H	1.50	0.57
1:C:321:ALA:O	1:C:329:ARG:NH2	2.37	0.57
1:C:80:ARG:NH2	1:C:115:GLU:OE1	2.38	0.57
1:A:300:ASN:HB3	1:A:495:MET:HG3	1.87	0.57
2:a:146:GLU:HG3	2:a:153:PRO:HG3	1.86	0.57
1:A:329:ARG:NH2	1:B:337:GLU:OE2	2.38	0.56
1:A:88:ARG:HB2	1:A:110:TYR:HB2	1.88	0.56
2:e:119:TYR:O	2:e:144:ASN:ND2	2.39	0.56
1:C:129:ASN:ND2	1:D:409:ARG:O	2.39	0.56
1:F:179:VAL:HG22	1:F:184:SER:HB2	1.88	0.56
1:D:53:ASP:OD1	1:D:57:ASN:ND2	2.38	0.56
1:B:79:ARG:NH1	2:b:113:GLU:OE2	2.39	0.55
2:d:119:TYR:O	2:d:144:ASN:ND2	2.39	0.55
1:E:156:GLY:HA2	1:F:277:MET:HE1	1.88	0.55
2:a:158:TYR:HB3	2:a:168:ASP:HB2	1.88	0.55
1:F:458:ASN:ND2	1:F:461:THR:OG1	2.39	0.55
1:D:11:LEU:HD13	1:D:224:ILE:HD13	1.89	0.55
2:e:281:VAL:HG22	2:e:305:VAL:HG12	1.88	0.55
1:D:56:LEU:HD12	1:D:440:LYS:HD3	1.86	0.55
2:a:158:TYR:HB2	2:a:189:ILE:HB	1.89	0.55
1:C:473:GLU:OE2	2:b:7:GLN:NE2	2.39	0.55
1:F:53:ASP:O	1:F:57:ASN:ND2	2.39	0.55
2:b:152:THR:OG1	2:b:195:GLN:OE1	2.25	0.55
3:g:51:LYS:NZ	3:h:84:ILE:O	2.38	0.55
1:B:171:ARG:HB2	1:C:411:LYS:HD3	1.89	0.55
3:g:36:MET:HB2	3:g:48:ALA:HB3	1.89	0.55
1:C:70:TYR:HB3	1:D:34:GLN:HG3	1.90	0.54
1:F:206:ARG:HG3	1:F:481:MET:HB3	1.88	0.54
1:A:261:ASN:HD22	1:F:175:GLU:HA	1.72	0.54
2:a:140:SER:O	2:a:144:ASN:ND2	2.40	0.54
1:B:390:ALA:HB3	1:B:394:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:ARG:NH2	1:F:337:GLU:OE2	2.38	0.54
1:E:229:ASN:O	1:E:249:TRP:NE1	2.37	0.54
2:b:1:MET:HB3	2:b:203:PRO:HB3	1.89	0.54
1:C:428:TRP:HA	1:C:494:THR:HG23	1.89	0.54
2:a:1:MET:HG2	2:a:245:ASP:HB3	1.88	0.54
1:B:273:ASN:ND2	1:B:275:GLU:OE2	2.41	0.53
2:e:88:VAL:HG22	2:e:223:ARG:HE	1.72	0.53
3:g:79:ARG:NH2	3:g:95:GLN:OE1	2.41	0.53
1:A:377:ASN:OD1	1:E:389:LYS:NZ	2.41	0.53
1:D:489:LEU:HD11	1:E:39:LEU:HD22	1.90	0.53
1:A:41:VAL:HB	1:F:74:VAL:HG22	1.90	0.53
1:D:435:GLN:NE2	1:E:40:MET:O	2.40	0.53
1:F:80:ARG:HD2	2:f:110:LEU:HD12	1.90	0.53
1:C:207:ILE:HG22	1:C:480:ARG:HB2	1.89	0.53
1:B:406:ASP:O	1:B:410:ASN:ND2	2.42	0.53
1:A:144:GLY:HA2	2:a:281:VAL:HG11	1.90	0.52
1:A:140:ALA:HB1	1:A:147:ALA:HB1	1.91	0.52
1:B:320:SER:HB2	1:B:329:ARG:HG2	1.90	0.52
1:E:205:ILE:HD11	1:E:259:LYS:HG3	1.91	0.52
1:F:419:VAL:HG12	1:F:421:PHE:H	1.74	0.52
1:A:333:ILE:HD12	1:A:425:TYR:HD2	1.75	0.52
4:i:3:THR:HG22	4:j:8:LYS:HG2	1.91	0.52
1:B:389:LYS:HB2	1:C:382:GLY:HA3	1.92	0.52
1:A:323:LYS:NZ	2:a:115:GLN:O	2.43	0.52
1:D:88:ARG:HB2	1:D:110:TYR:HB2	1.91	0.52
1:B:207:ILE:HG22	1:B:480:ARG:HB2	1.92	0.51
1:A:207:ILE:HG22	1:A:480:ARG:HB2	1.91	0.51
1:C:10:MET:HG2	2:b:265:ASN:HA	1.92	0.51
1:C:406:ASP:O	1:C:410:ASN:ND2	2.43	0.51
1:D:43:LEU:O	1:D:48:ARG:NH2	2.43	0.51
1:D:300:ASN:ND2	1:D:492:THR:O	2.43	0.51
1:B:186:LYS:HD2	1:C:208:GLN:HG3	1.93	0.51
1:E:116:ASP:HB3	2:e:4:SER:HB3	1.92	0.51
1:A:425:TYR:HB2	1:A:497:LEU:HB3	1.93	0.51
1:D:263:MET:HG3	1:D:484:LEU:HD13	1.93	0.51
2:b:107:TYR:O	2:b:109:GLY:N	2.44	0.51
1:B:438:ILE:HG23	1:B:488:VAL:HG22	1.93	0.51
1:C:171:ARG:HB2	1:D:411:LYS:HD2	1.92	0.51
2:a:35:ASP:OD2	2:a:39:THR:OG1	2.29	0.51
3:h:79:ARG:NH2	3:h:92:MET:O	2.42	0.51
4:i:20:TRP:HB3	4:i:27:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:GLU:OE1	1:E:270:ARG:NH1	2.44	0.50
2:b:142:ALA:HB2	2:b:157:ILE:HD11	1.94	0.50
3:g:41:THR:HA	4:i:12:ASN:HD21	1.76	0.50
1:C:330:LEU:HD11	1:C:397:ARG:HD3	1.93	0.50
2:d:57:ILE:HD11	2:d:302:ILE:HD12	1.94	0.50
1:A:390:ALA:HB3	1:A:394:VAL:HB	1.94	0.49
1:A:122:GLU:OE2	1:B:258:TYR:OH	2.30	0.49
1:B:122:GLU:OE2	1:C:258:TYR:OH	2.30	0.49
1:D:340:ALA:HA	1:D:398:LEU:HD21	1.94	0.49
2:b:162:ALA:HB3	2:b:184:ASP:HB2	1.95	0.49
1:A:428:TRP:HA	1:A:494:THR:HG23	1.93	0.49
1:E:122:GLU:OE2	1:F:258:TYR:OH	2.26	0.49
1:A:435:GLN:NE2	1:B:40:MET:O	2.46	0.49
1:E:425:TYR:HB2	1:E:497:LEU:HB2	1.94	0.49
3:h:52:ALA:HB1	3:h:57:GLN:HB3	1.94	0.49
1:F:304:TYR:OH	1:F:423:TYR:O	2.28	0.49
1:A:411:LYS:HG2	1:F:171:ARG:HB2	1.94	0.49
1:B:135:ARG:NH2	1:B:152:GLU:OE1	2.45	0.49
1:D:209:HIS:CE1	1:D:217:ASN:HD22	2.31	0.49
1:A:312:LEU:HD13	1:A:497:LEU:HD22	1.96	0.48
1:D:47:TYR:HB2	1:D:407:PRO:HG2	1.95	0.48
1:F:390:ALA:HB3	1:F:394:VAL:HB	1.95	0.48
1:D:207:ILE:HG22	1:D:480:ARG:HB2	1.94	0.48
1:E:112:VAL:HG22	1:E:148:VAL:HG22	1.96	0.48
1:B:10:MET:HE1	2:a:268:LYS:HB3	1.94	0.48
1:D:392:ASN:H	1:E:384:GLN:HE22	1.61	0.48
1:F:319:LEU:HD13	1:F:495:MET:HE2	1.95	0.48
2:f:94:ALA:HB3	4:j:32:GLY:HA3	1.95	0.48
1:C:118:PHE:HA	1:C:191:ARG:HH21	1.77	0.48
3:g:37:GLU:OE2	3:g:95:GLN:NE2	2.46	0.48
3:h:59:GLU:HG2	3:h:77:VAL:HG21	1.96	0.48
1:C:85:VAL:HG12	1:C:86:GLU:HG2	1.96	0.48
1:E:73:ASP:OD1	1:E:73:ASP:N	2.45	0.48
1:B:292:ILE:HG13	1:B:486:VAL:HG11	1.95	0.48
1:D:186:LYS:HB2	1:E:208:GLN:HG2	1.96	0.48
2:f:100:LEU:HD21	2:f:211:PRO:HB3	1.94	0.48
1:D:78:SER:OG	1:E:229:ASN:ND2	2.47	0.48
4:j:26:MET:HG2	4:j:37:ILE:HD12	1.96	0.48
2:b:218:VAL:O	4:k:31:ASN:ND2	2.47	0.48
1:F:77:SER:OG	2:f:114:ASP:OD2	2.29	0.47
2:b:184:ASP:OD1	2:b:184:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG13	1:A:148:VAL:HG12	1.96	0.47
1:A:128:LEU:HD12	1:A:165:ARG:HD2	1.96	0.47
1:C:297:GLU:OE2	1:C:424:ARG:NH2	2.46	0.47
3:h:36:MET:HE1	3:h:62:LEU:HB2	1.97	0.47
4:j:30:ASN:HB3	4:j:35:GLU:HG3	1.96	0.47
1:E:454:TRP:O	1:E:470:SER:OG	2.33	0.47
1:D:144:GLY:HA2	2:d:281:VAL:HG11	1.96	0.47
1:D:327:ASP:OD1	1:D:327:ASP:N	2.44	0.47
1:B:499:PRO:HD2	1:B:502:LEU:HD12	1.97	0.47
2:a:260:GLY:HA2	2:a:266:ILE:HG21	1.95	0.47
1:A:321:ALA:O	1:B:48:ARG:NH2	2.41	0.47
1:C:111:LEU:HD12	1:C:151:VAL:HG21	1.97	0.47
2:a:106:GLN:NE2	2:a:112:GLU:OE2	2.45	0.47
1:B:201:GLU:OE1	1:B:276:TYR:OH	2.32	0.46
2:a:184:ASP:OD1	2:a:184:ASP:N	2.46	0.46
1:A:129:ASN:ND2	1:B:409:ARG:O	2.47	0.46
1:A:152:GLU:OE2	1:B:278:ASN:ND2	2.44	0.46
2:d:309:ASP:OD1	2:d:309:ASP:N	2.47	0.46
1:F:414:HIS:HD2	1:F:416:MET:H	1.64	0.46
1:D:489:LEU:HD21	1:E:39:LEU:HD13	1.97	0.46
2:a:41:LEU:HD13	2:a:326:SER:HB2	1.97	0.46
2:d:158:TYR:OH	2:d:235:LYS:NZ	2.49	0.46
2:e:184:ASP:N	2:e:184:ASP:OD1	2.49	0.46
1:D:390:ALA:HB3	1:D:394:VAL:HB	1.97	0.46
1:B:185:ARG:HB2	1:C:281:LYS:HE3	1.97	0.46
1:B:455:GLY:O	1:B:466:ASN:ND2	2.37	0.46
1:E:117:TRP:CE2	1:E:191:ARG:HD3	2.51	0.46
2:a:79:ARG:HG2	2:a:191:GLU:HG3	1.96	0.46
1:A:220:LEU:HD13	1:A:226:MET:HE3	1.98	0.46
1:B:74:VAL:HB	1:B:196:VAL:HG23	1.97	0.46
1:D:292:ILE:HG12	1:D:486:VAL:HG11	1.98	0.46
2:d:312:HIS:O	2:d:316:ASN:ND2	2.49	0.46
2:a:243:ILE:HG13	2:a:279:TYR:HB2	1.96	0.45
1:C:74:VAL:HG12	1:D:41:VAL:HB	1.98	0.45
1:D:409:ARG:O	1:D:411:LYS:NZ	2.42	0.45
2:d:290:GLY:HA3	2:d:294:SER:HB2	1.97	0.45
1:B:103:GLY:HA3	1:B:153:LEU:HD12	1.98	0.45
1:E:188:GLY:O	1:F:208:GLN:NE2	2.39	0.45
2:d:108:ILE:H	2:d:108:ILE:HG13	1.49	0.45
1:C:122:GLU:OE2	1:D:258:TYR:OH	2.34	0.45
1:C:183:LEU:O	1:D:282:SER:OG	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASP:OD1	1:B:149:TYR:OH	2.33	0.45
1:C:77:SER:HA	5:m:282:GLU:HG3	1.99	0.45
1:E:62:ARG:HH21	1:E:436:PRO:HD2	1.81	0.45
1:B:304:TYR:OH	1:B:423:TYR:O	2.32	0.45
2:e:197:TRP:NE1	2:e:245:ASP:OD2	2.41	0.45
1:C:269:ASN:ND2	1:C:286:ILE:O	2.44	0.45
1:D:171:ARG:HB2	1:E:411:LYS:HG2	1.98	0.45
1:F:142:MET:HA	1:F:147:ALA:HA	1.99	0.45
2:a:93:VAL:HG21	2:a:218:VAL:HG22	1.99	0.45
1:A:26:GLY:HA2	1:A:31:GLN:HB2	1.98	0.45
1:C:4:LYS:HG2	1:C:9:GLN:HB3	1.99	0.45
1:C:102:VAL:HG21	1:C:166:LEU:HD12	1.98	0.45
1:C:205:ILE:HD11	1:C:259:LYS:HG3	1.98	0.45
1:F:145:THR:HG22	2:f:73:LEU:HD22	1.98	0.45
1:A:88:ARG:NH2	1:A:143:GLU:OE1	2.48	0.45
1:C:56:LEU:HD13	1:C:263:MET:HE2	1.98	0.45
1:D:66:ASP:N	1:D:66:ASP:OD1	2.50	0.45
1:B:323:LYS:HB3	1:C:44:LEU:HG	1.99	0.44
1:A:111:LEU:HD12	1:A:151:VAL:HG21	1.99	0.44
1:D:56:LEU:HD21	1:D:264:ALA:HB2	1.99	0.44
4:k:26:MET:HB3	4:k:37:ILE:HG12	1.98	0.44
1:B:190:VAL:HG21	1:C:251:VAL:HG22	1.99	0.44
1:F:143:GLU:N	1:F:146:ASN:O	2.42	0.44
2:e:122:VAL:HG12	2:e:137:MET:HE3	1.99	0.44
1:D:447:ASN:OD1	1:D:447:ASN:N	2.42	0.44
1:E:125:VAL:HB	1:E:129:ASN:HA	1.98	0.44
4:i:9:ILE:HD11	4:k:4:LEU:HD11	2.00	0.44
2:b:162:ALA:N	2:b:184:ASP:O	2.50	0.44
2:e:85:ASP:OD1	2:e:85:ASP:N	2.51	0.44
3:g:31:MET:HE2	3:g:31:MET:HB3	1.86	0.44
2:f:79:ARG:NH1	2:f:234:THR:OG1	2.49	0.44
2:a:252:GLY:HA3	2:a:259:ARG:HH21	1.83	0.44
2:b:157:ILE:HG22	2:b:190:ILE:HG23	2.00	0.44
1:A:278:ASN:ND2	1:F:152:GLU:OE2	2.43	0.44
1:D:122:GLU:OE2	1:E:258:TYR:OH	2.36	0.43
1:D:413:LEU:H	3:h:69:ASN:HB3	1.81	0.43
2:e:84:LEU:H	2:e:134:TYR:HH	1.64	0.43
1:B:174:ILE:HD13	1:B:191:ARG:HH22	1.84	0.43
1:F:252:GLU:HA	1:F:480:ARG:HH12	1.83	0.43
1:F:277:MET:HE3	1:F:277:MET:HB2	1.88	0.43
2:e:286:TYR:HE1	2:e:302:ILE:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:HG3	1:B:94:VAL:HA	2.00	0.43
1:C:52:LEU:HD11	1:C:265:TRP:HE1	1.83	0.43
1:E:123:VAL:HG23	1:E:175:GLU:HB2	2.00	0.43
1:F:455:GLY:O	1:F:466:ASN:ND2	2.43	0.43
2:d:99:ILE:HB	2:d:214:LEU:HD12	2.00	0.43
1:D:188:GLY:O	1:E:208:GLN:NE2	2.50	0.43
1:A:376:SER:H	1:E:395:ARG:HH22	1.66	0.43
2:b:197:TRP:NE1	2:b:245:ASP:OD2	2.47	0.43
1:B:210:LYS:NZ	2:a:7:GLN:OE1	2.39	0.43
1:C:263:MET:HE3	1:C:440:LYS:HG2	1.99	0.43
1:C:75:ILE:HD11	1:C:193:THR:HG23	2.00	0.43
1:D:12:GLY:HA2	1:D:221:ALA:HA	1.99	0.43
2:e:85:ASP:HB3	2:e:227:VAL:HG23	2.01	0.43
1:E:363:SER:O	1:F:369:LYS:NZ	2.42	0.43
2:b:252:GLY:HA3	2:b:259:ARG:HH21	1.83	0.43
2:e:158:TYR:HB3	2:e:168:ASP:HB2	2.00	0.43
1:B:48:ARG:O	1:B:51:SER:OG	2.32	0.42
1:D:195:PRO:HD2	1:E:224:ILE:HD12	2.00	0.42
2:a:100:LEU:HB2	2:a:225:TRP:HZ2	1.84	0.42
2:a:107:TYR:O	2:a:109:GLY:N	2.52	0.42
1:C:10:MET:HE3	2:b:265:ASN:HB3	2.00	0.42
1:A:438:ILE:HG23	1:A:488:VAL:HG22	2.00	0.42
1:C:79:ARG:NH1	1:D:50:LYS:O	2.43	0.42
1:C:392:ASN:ND2	1:D:337:GLU:HG2	2.34	0.42
1:B:270:ARG:NH2	1:B:276:TYR:OH	2.52	0.42
1:E:163:ALA:O	1:E:167:GLN:NE2	2.51	0.42
1:E:333:ILE:HG12	1:E:427:ILE:HG12	2.01	0.42
1:A:216:LEU:HD13	1:A:459:PRO:HA	2.01	0.42
1:B:414:HIS:HD2	1:B:416:MET:HB2	1.84	0.42
2:a:79:ARG:NH1	2:a:191:GLU:OE1	2.52	0.42
2:b:24:LEU:HD21	2:b:31:VAL:HG23	2.02	0.42
1:A:180:GLU:O	1:A:184:SER:OG	2.37	0.42
4:j:37:ILE:HD13	4:k:26:MET:HB2	2.01	0.42
1:B:112:VAL:HG13	1:B:148:VAL:HG22	2.02	0.42
2:a:143:LYS:HA	2:a:143:LYS:HD3	1.90	0.42
2:d:129:THR:OG1	2:d:130:ALA:N	2.53	0.42
2:e:118:LYS:HD2	2:e:118:LYS:HA	1.87	0.42
1:A:356:THR:HG23	1:B:352:SER:HA	2.02	0.42
2:d:48:PRO:HG3	2:d:272:LEU:HD21	2.02	0.42
1:C:304:TYR:OH	1:C:423:TYR:O	2.37	0.41
1:A:116:ASP:OD1	1:A:149:TYR:OH	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:NH1	1:B:63:GLU:O	2.54	0.41
1:B:389:LYS:N	1:C:381:ALA:O	2.50	0.41
1:D:415:PRO:HA	3:h:67:ILE:HG22	2.02	0.41
2:d:184:ASP:OD1	2:d:184:ASP:N	2.52	0.41
1:B:319:LEU:HD22	1:B:495:MET:HE2	2.03	0.41
1:D:392:ASN:H	1:E:384:GLN:NE2	2.19	0.41
1:A:194:SER:HA	1:A:195:PRO:HD3	1.93	0.41
2:e:169:VAL:HA	2:e:170:PRO:HD3	1.92	0.41
1:E:365:ARG:HA	1:E:365:ARG:HD3	1.90	0.41
2:e:215:THR:HG22	2:e:224:LEU:HD12	2.01	0.41
1:D:80:ARG:NH2	1:D:115:GLU:OE1	2.38	0.41
2:b:108:ILE:H	2:b:108:ILE:HG12	1.66	0.41
2:f:237:VAL:HA	2:f:238:PRO:HD3	1.90	0.41
1:C:334:LYS:NZ	1:C:399:ASP:OD2	2.46	0.41
1:D:42:GLN:NE2	5:m:281:ASP:OD1	2.53	0.41
1:D:140:ALA:HB1	1:D:147:ALA:HB1	2.01	0.41
2:a:67:ALA:HB2	2:a:282:LEU:HD13	2.02	0.41
2:a:142:ALA:O	2:a:173:SER:OG	2.36	0.41
2:d:79:ARG:HG2	2:d:191:GLU:HG3	2.02	0.41
2:b:30:ILE:HD11	2:b:43:PHE:HB3	2.02	0.41
1:B:144:GLY:HA2	2:b:281:VAL:HG11	2.03	0.41
1:C:303:TYR:HB2	3:g:80:ILE:HB	2.02	0.41
1:F:125:VAL:HB	1:F:129:ASN:HA	2.03	0.41
2:e:135:LYS:HA	2:e:159:LEU:HD11	2.02	0.41
1:A:382:GLY:HA3	1:F:389:LYS:HB2	2.02	0.41
1:B:136:ILE:HG23	1:B:149:TYR:HB3	2.03	0.41
1:B:240:ALA:O	1:B:246:TYR:OH	2.35	0.41
1:B:256:ASP:O	1:B:260:ASN:ND2	2.53	0.41
1:C:136:ILE:HG23	1:C:149:TYR:HB3	2.02	0.41
2:d:1:MET:HE2	2:d:1:MET:HB3	1.95	0.41
2:d:79:ARG:HH21	2:d:189:ILE:HD13	1.86	0.41
1:B:471:PHE:HD1	1:B:473:GLU:H	1.67	0.40
1:C:120:ASP:OD2	1:D:281:LYS:NZ	2.41	0.40
2:b:322:ILE:O	2:b:326:SER:OG	2.33	0.40
1:B:329:ARG:NH2	1:C:337:GLU:OE2	2.54	0.40
1:D:279:PHE:HA	1:D:285:ALA:HA	2.03	0.40
1:A:258:TYR:OH	1:F:122:GLU:OE2	2.39	0.40
1:A:386:VAL:HG21	1:B:372:SER:HB2	2.04	0.40
2:a:285:HIS:ND1	2:a:300:LYS:O	2.54	0.40
2:b:102:LEU:HD21	2:b:190:ILE:HG21	2.01	0.40
1:E:269:ASN:HD22	1:E:278:ASN:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:153:PRO:HB2	2:b:193:THR:HG21	2.04	0.40
1:E:111:LEU:HD12	1:E:151:VAL:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	B	4/427 (1%)	4 (100%)	0	100	100
1	C	207/427 (48%)	206 (100%)	1 (0%)	81	82
1	D	387/427 (91%)	387 (100%)	0	100	100
1	E	426/427 (100%)	426 (100%)	0	100	100
1	F	426/427 (100%)	424 (100%)	2 (0%)	81	82
2	a	275/275 (100%)	275 (100%)	0	100	100
2	b	275/275 (100%)	273 (99%)	2 (1%)	76	79
2	d	275/275 (100%)	274 (100%)	1 (0%)	84	83
2	e	225/275 (82%)	225 (100%)	0	100	100
2	f	157/275 (57%)	155 (99%)	2 (1%)	61	73
3	g	68/86 (79%)	67 (98%)	1 (2%)	57	71
3	h	62/86 (72%)	61 (98%)	1 (2%)	55	71
4	i	34/78 (44%)	34 (100%)	0	100	100
4	j	34/78 (44%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	k	34/78 (44%)	34 (100%)	0	100	100
5	l	14/714 (2%)	14 (100%)	0	100	100
5	m	15/714 (2%)	15 (100%)	0	100	100
All	All	2918/5344 (55%)	2908 (100%)	10 (0%)	84	85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	428	TRP
1	F	41	VAL
1	F	196	VAL
2	b	84	LEU
2	b	295	VAL
2	d	333	LEU
2	f	218	VAL
2	f	237	VAL
3	g	23	VAL
3	h	67	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	295	GLN
1	C	362	ASN
1	C	414	HIS
1	C	435	GLN
1	D	15	HIS
1	D	42	GLN
1	D	159	GLN
1	D	167	GLN
1	D	217	ASN
1	D	254	GLN
1	E	9	GLN
1	E	14	GLN
1	E	34	GLN
1	E	127	ASN
1	E	129	ASN
1	E	157	ASN
1	E	214	ASN
1	E	229	ASN

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Mol	Chain	Res	Type
1	E	245	HIS
1	E	284	ASN
1	E	377	ASN
1	E	384	GLN
1	E	410	ASN
1	E	435	GLN
1	F	57	ASN
1	F	159	GLN
1	F	229	ASN
1	F	278	ASN
1	F	284	ASN
1	F	362	ASN
1	F	377	ASN
1	F	392	ASN
1	F	414	HIS
1	F	435	GLN
1	F	458	ASN
1	F	479	HIS
2	a	97	ASN
2	a	115	GLN
2	a	241	HIS
2	b	61	HIS
2	b	75	HIS
2	b	106	GLN
2	b	265	ASN
2	d	20	ASN
2	d	156	ASN
2	e	97	ASN
2	e	212	GLN
3	g	32	GLN
3	g	65	ASN
3	g	82	GLN
3	h	82	GLN
4	i	12	ASN
4	i	17	ASN
4	k	31	ASN

5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

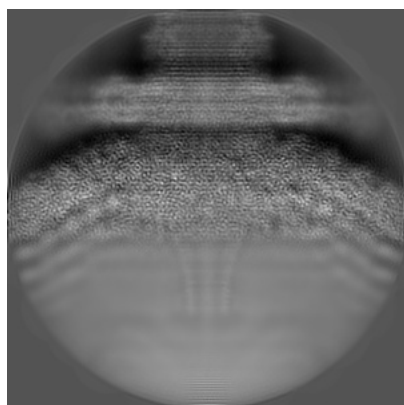
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14090. These allow visual inspection of the internal detail of the map and identification of artifacts.

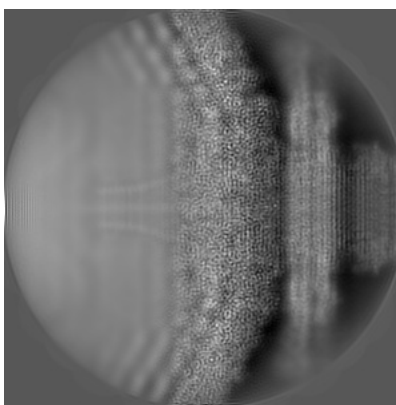
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

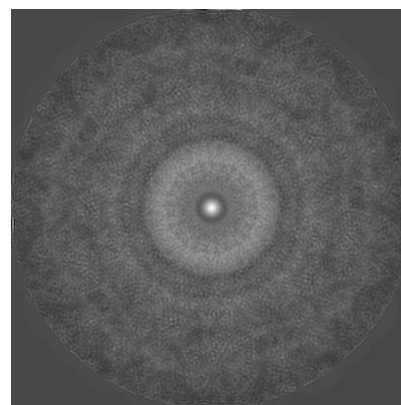
6.1.1 Primary map



X



Y

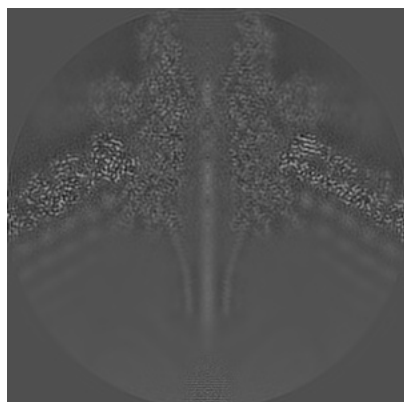


Z

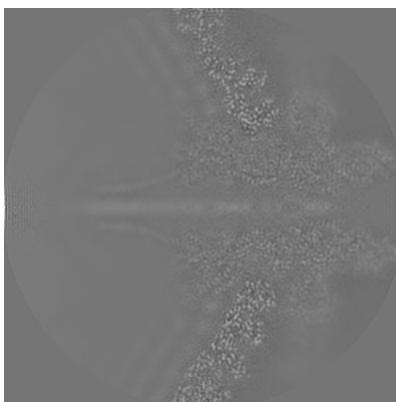
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

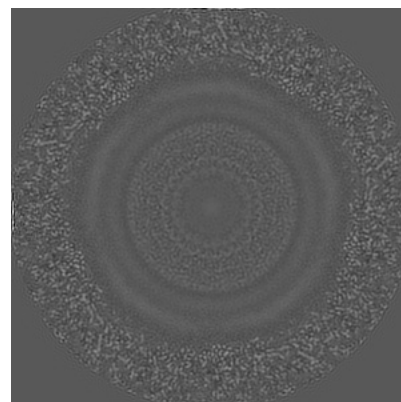
6.2.1 Primary map



X Index: 143



Y Index: 143

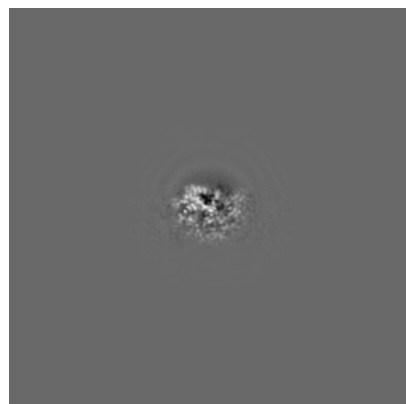


Z Index: 143

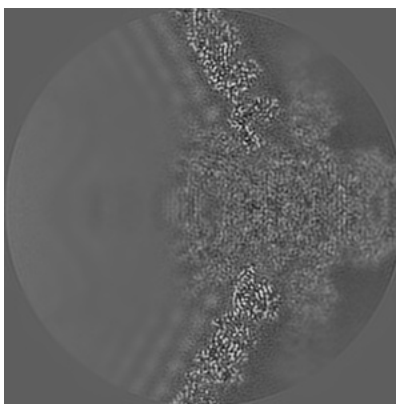
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

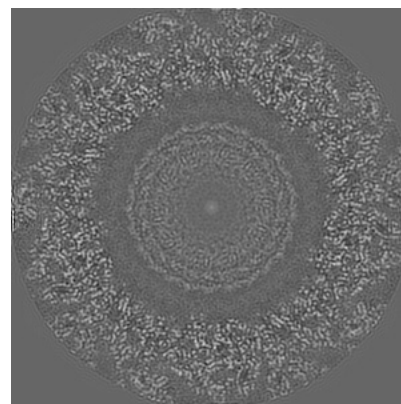
6.3.1 Primary map



X Index: 1



Y Index: 120

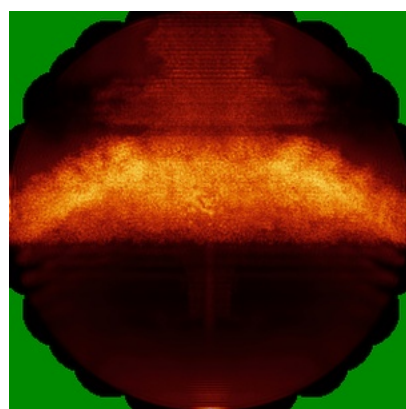


Z Index: 154

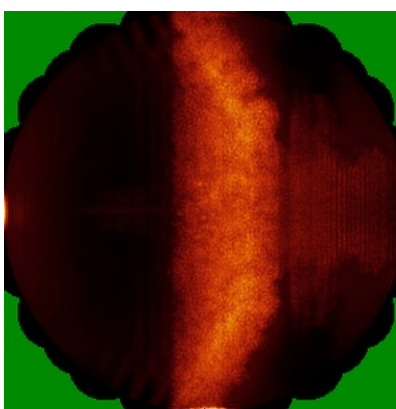
The images above show the largest variance slices of the map in three orthogonal directions.

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

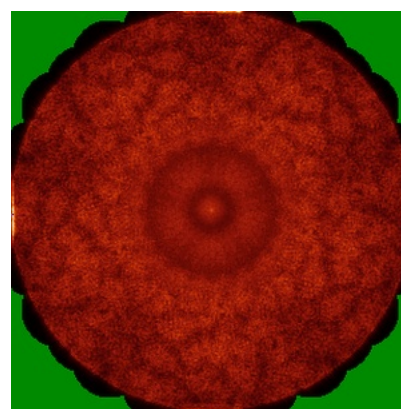
6.4.1 Primary map



X



Y

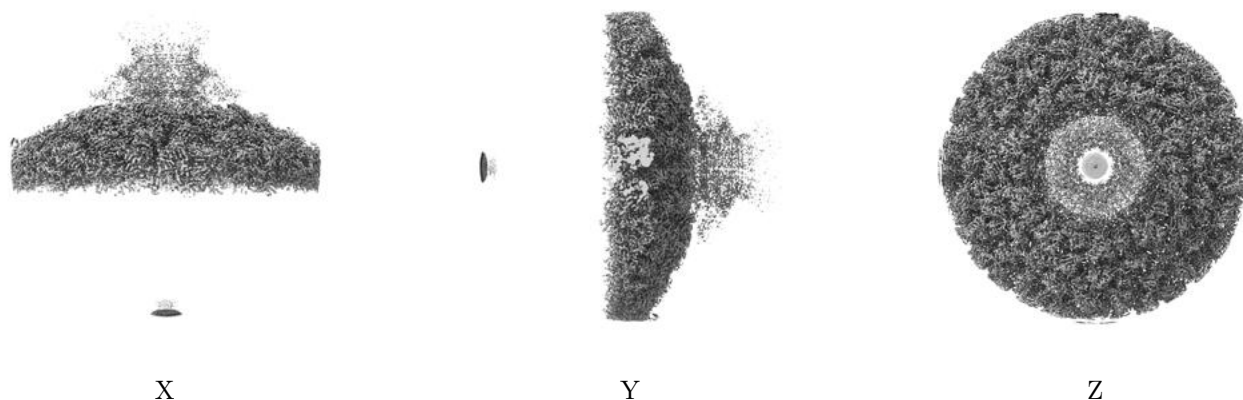


Z

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

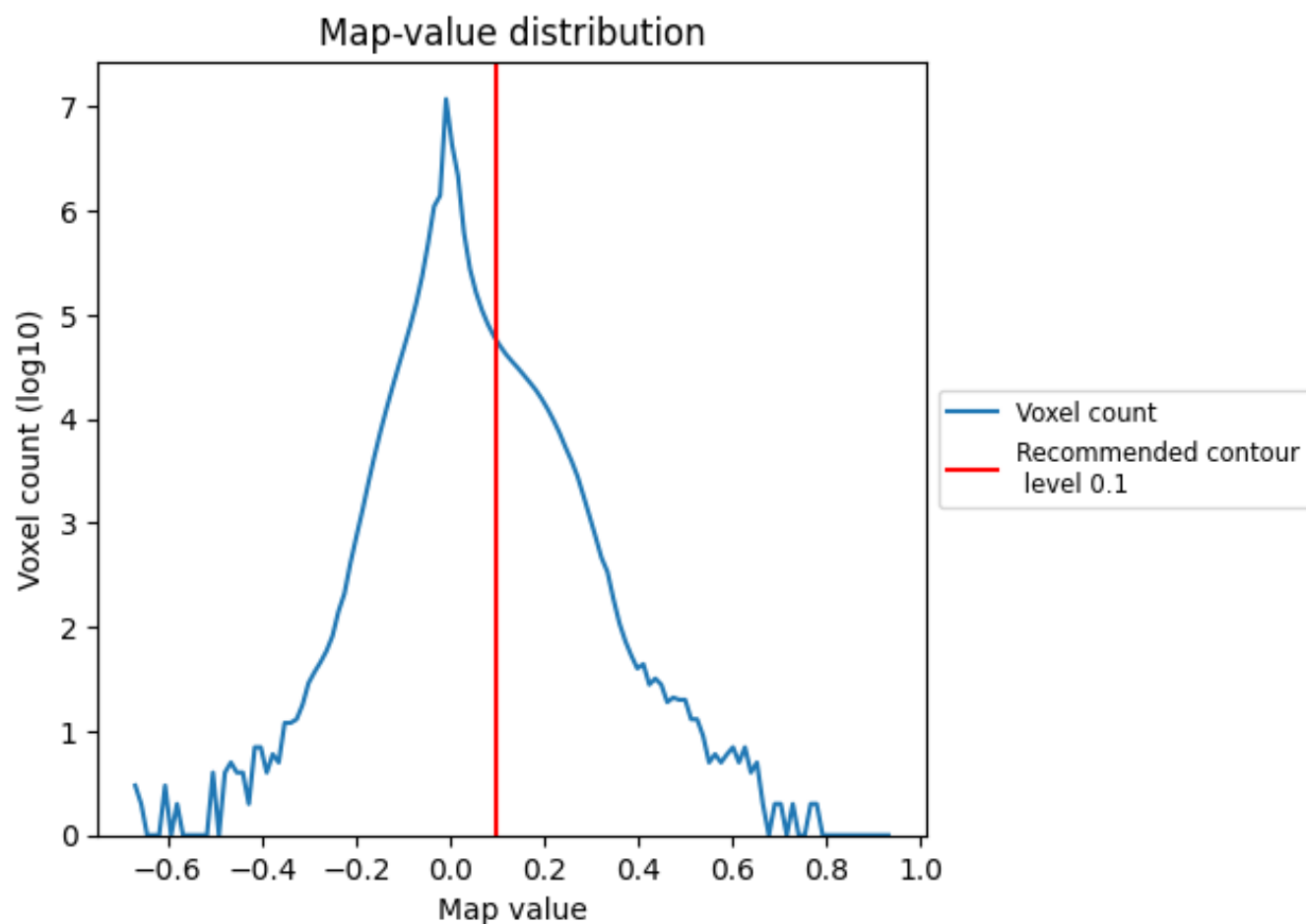
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

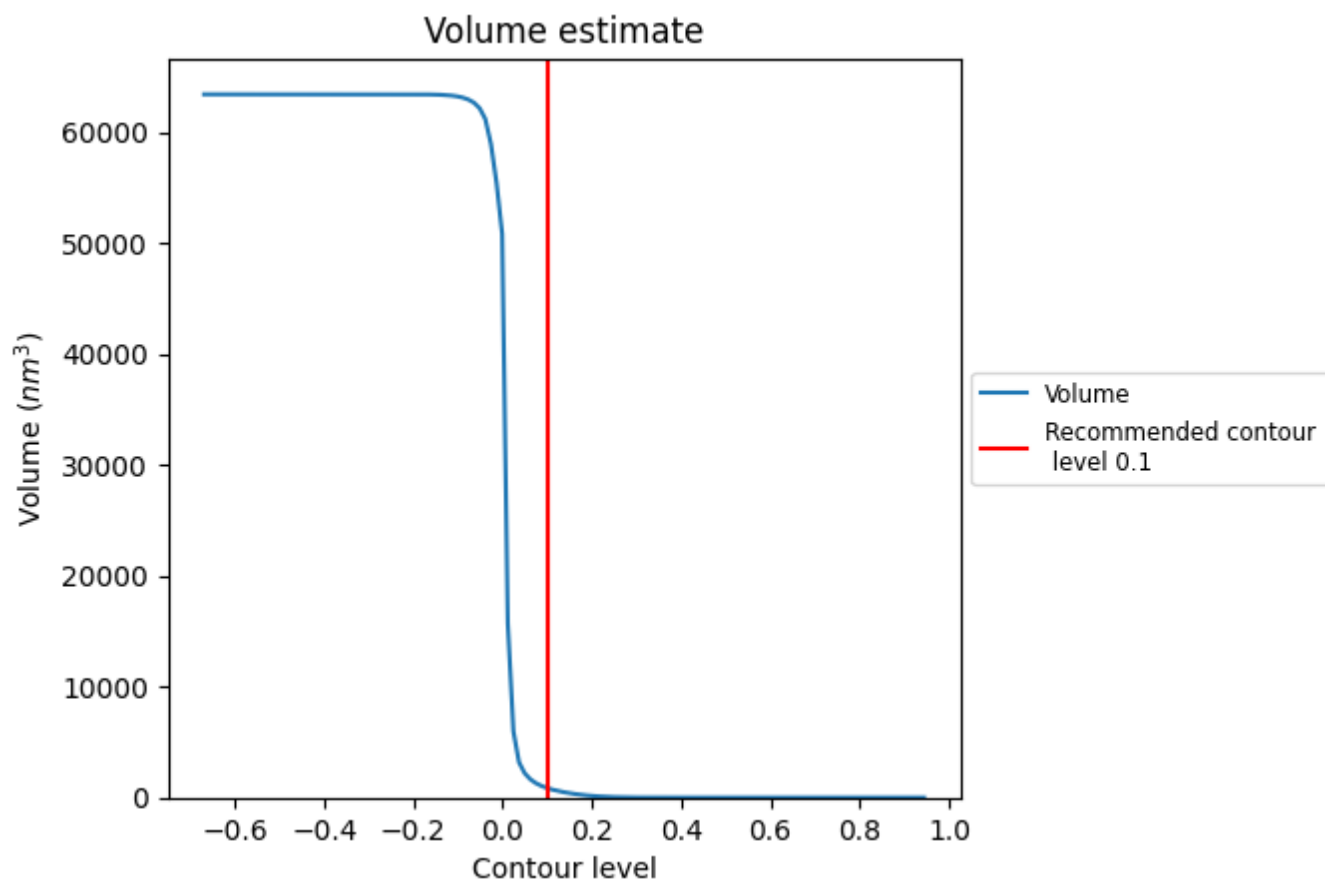
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

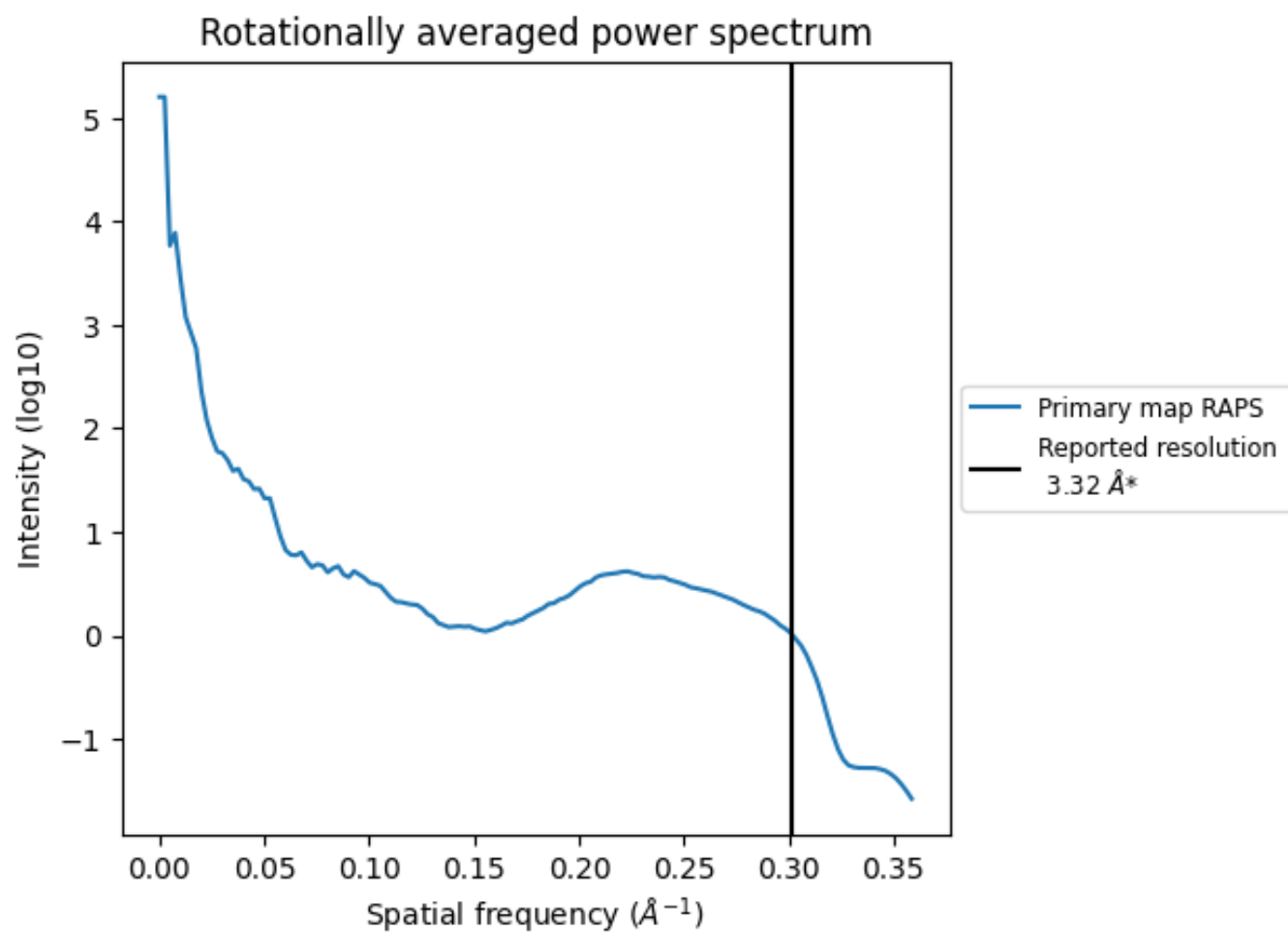
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 857 nm³; this corresponds to an approximate mass of 774 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 ⓘ

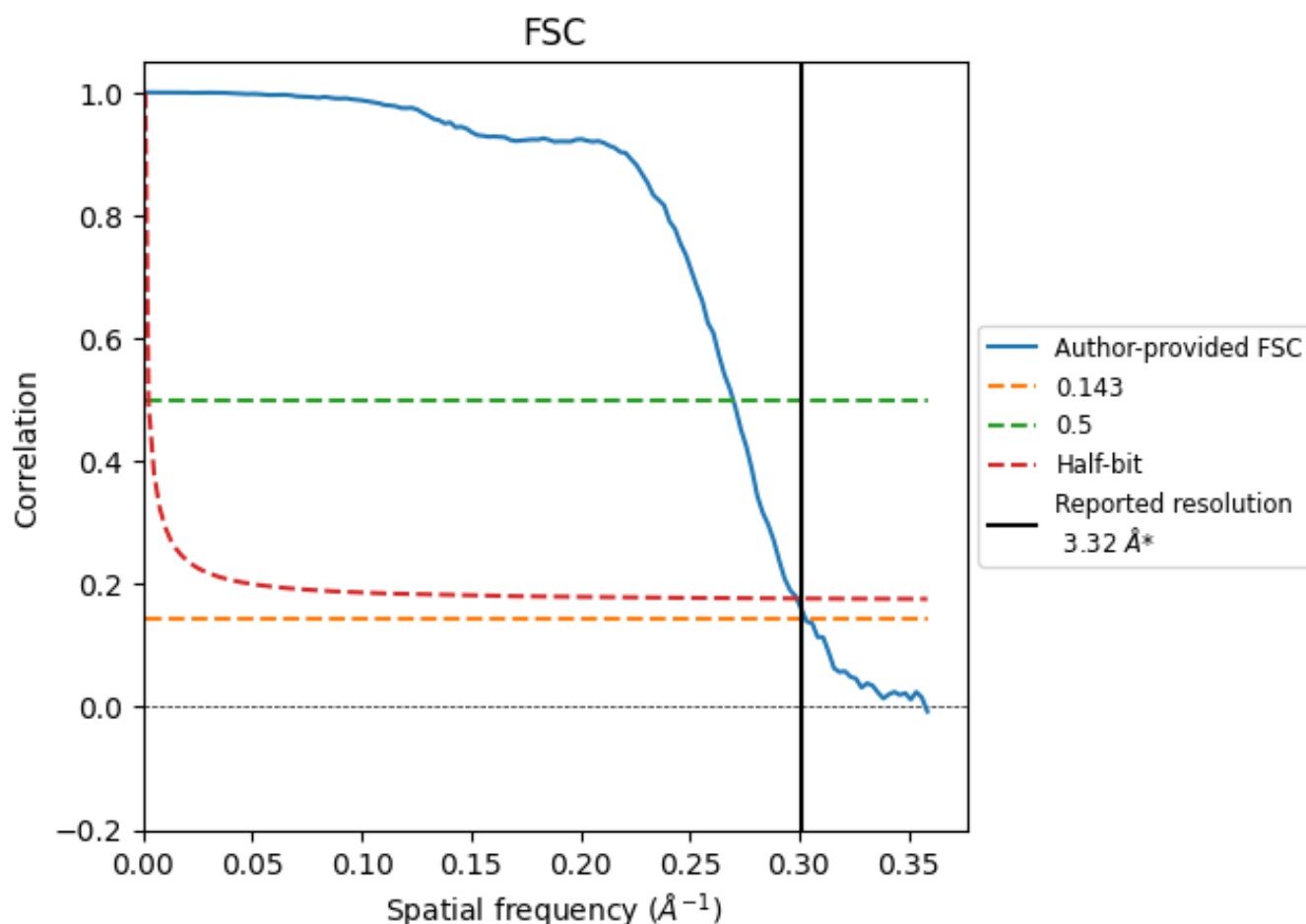


*Reported resolution corresponds to spatial frequency of 0.301 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.301 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	3.30	3.71	3.35
Unmasked-calculated*	-	-	-

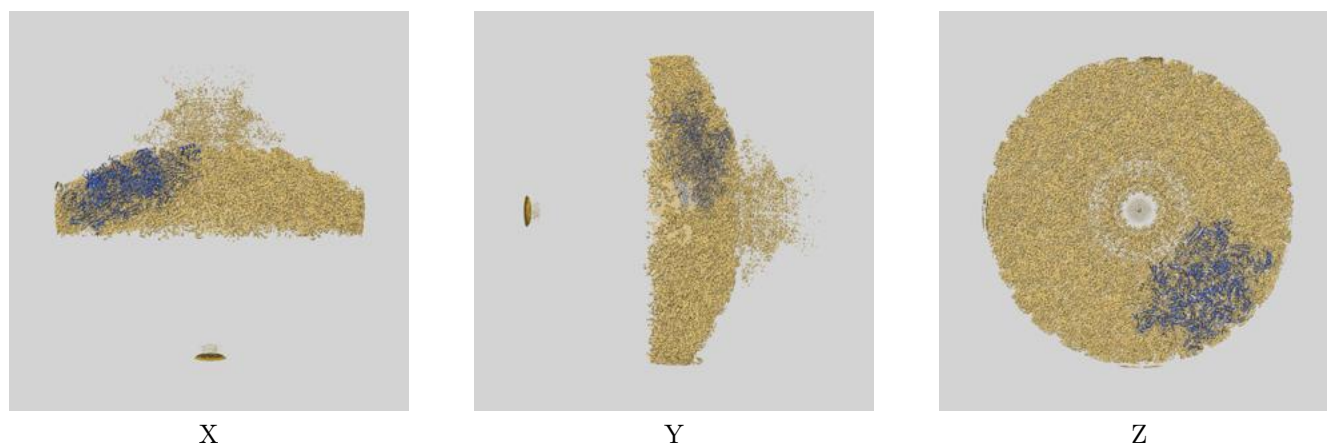
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

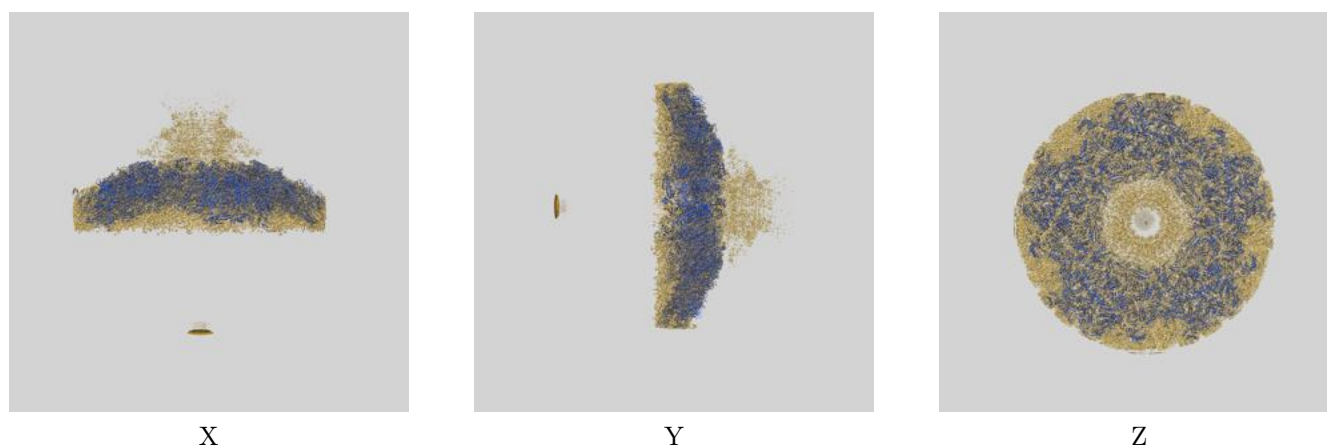
This section contains information regarding the fit between EMDB map EMD-14090 and PDB model 7QOH. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

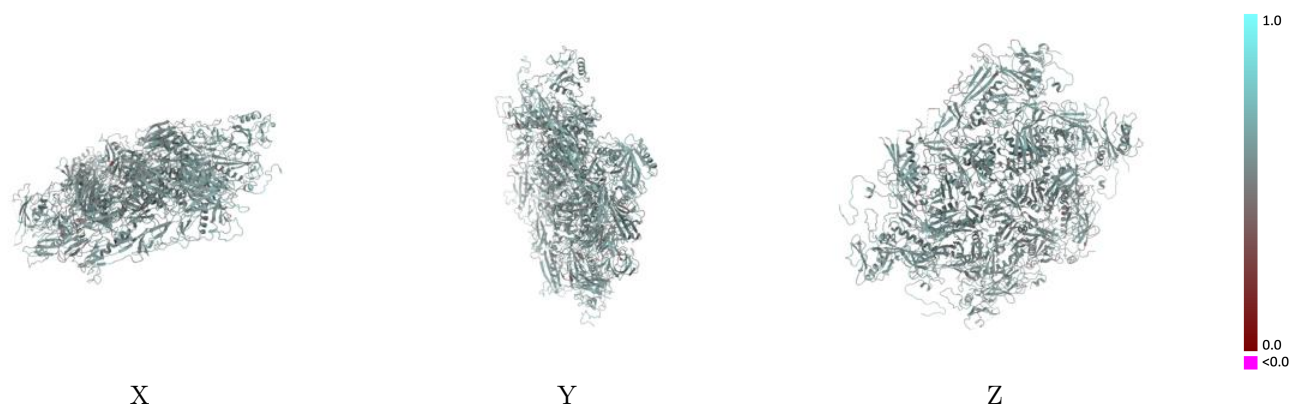


9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

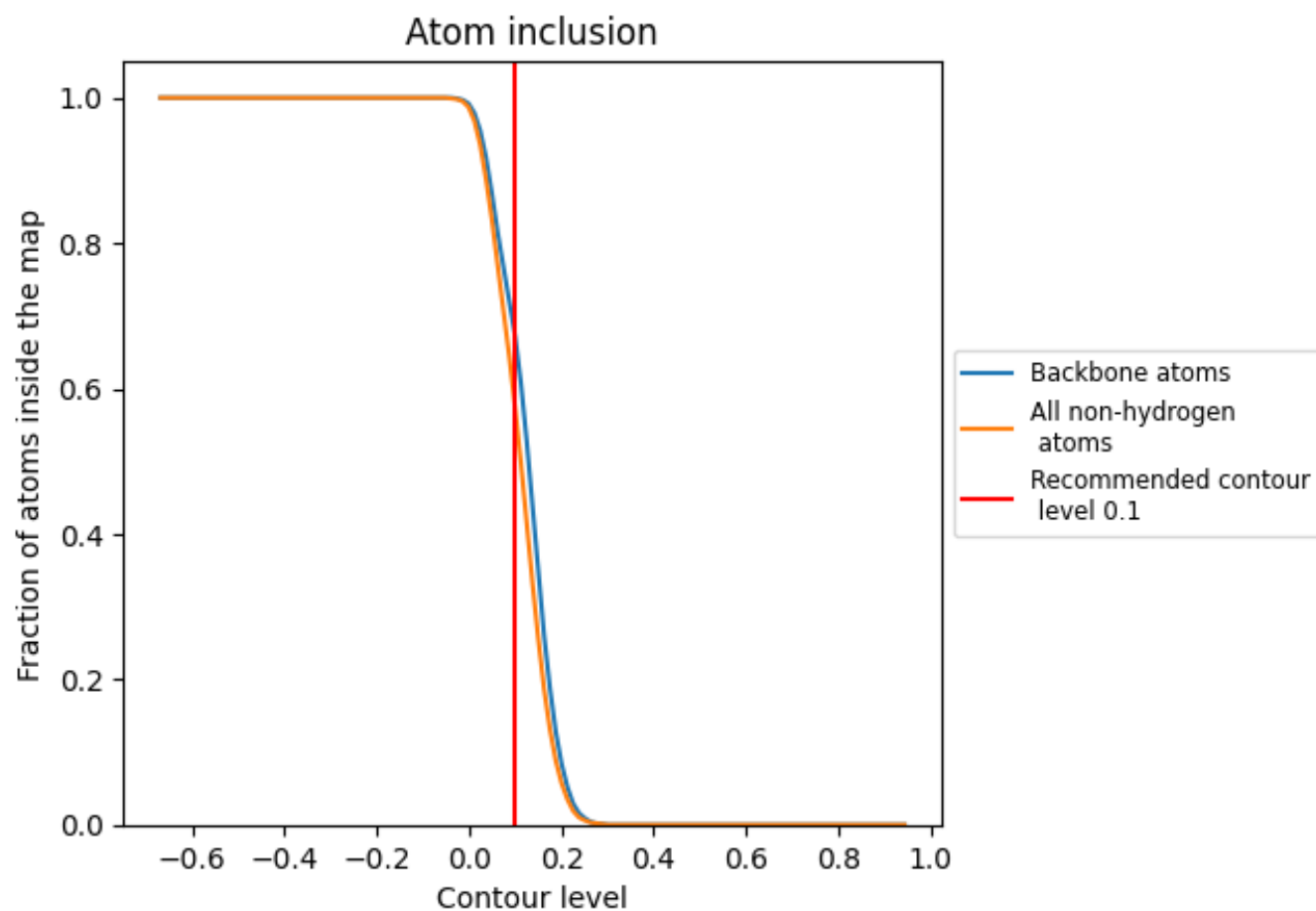


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5730	 0.5590
A	 0.5730	 0.5610
B	 0.6250	 0.5710
C	 0.6320	 0.5670
D	 0.6090	 0.5610
E	 0.6070	 0.5710
F	 0.5420	 0.5550
a	 0.5350	 0.5480
b	 0.6010	 0.5600
d	 0.5930	 0.5550
e	 0.5120	 0.5530
f	 0.3970	 0.5290
g	 0.6140	 0.5600
h	 0.5640	 0.5420
i	 0.3820	 0.5510
j	 0.3160	 0.5410
k	 0.3850	 0.5410
l	 0.2600	 0.4610
m	 0.4670	 0.5400

