



Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 06:07 AM JST

PDB ID : 8YS4 / pdb_00008ys4
EMDB ID : EMD-38377
Title : Overall structure of Eastern Equine Encephalitis virus VLP in complex with the receptor VLDLR LA3-5
Authors : Cao, D.; Ma, B.; Cao, Z.; Xu, X.; Zhang, X.; Xiang, Y.
Deposited on : 2024-03-22
Resolution : 4.80 Å(reported)

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

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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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

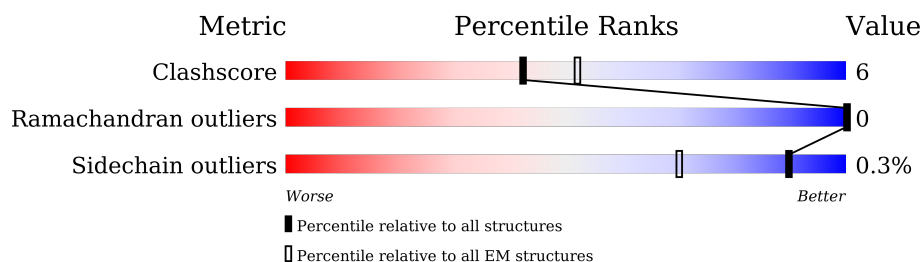
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	441	 85% 15%
1	D	441	 90% 10%
1	G	441	 89% 11%
1	J	441	 88% 11%
2	B	420	 6% 85% 15%
2	E	420	 6% 87% 13%
2	H	420	 5% 79% 20%
2	K	420	 5% 86% 13%

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Mol	Chain	Length	Quality of chain
3	C	261	
3	F	261	
3	I	261	
3	L	261	
4	M	41	
4	N	41	
4	O	41	
4	P	41	
5	Q	41	
5	R	41	
5	S	41	
5	T	41	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33820 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 Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		
1	D	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		
1	G	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		
1	J	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	SER	THR	conflict	UNP Q4QXJ7
A	237	VAL	ALA	conflict	UNP Q4QXJ7
A	246	LYS	ARG	conflict	UNP Q4QXJ7
A	311	PHE	SER	conflict	UNP Q4QXJ7
A	411	ILE	LEU	conflict	UNP Q4QXJ7
D	82	SER	THR	conflict	UNP Q4QXJ7
D	237	VAL	ALA	conflict	UNP Q4QXJ7
D	246	LYS	ARG	conflict	UNP Q4QXJ7
D	311	PHE	SER	conflict	UNP Q4QXJ7
D	411	ILE	LEU	conflict	UNP Q4QXJ7
G	82	SER	THR	conflict	UNP Q4QXJ7
G	237	VAL	ALA	conflict	UNP Q4QXJ7
G	246	LYS	ARG	conflict	UNP Q4QXJ7
G	311	PHE	SER	conflict	UNP Q4QXJ7
G	411	ILE	LEU	conflict	UNP Q4QXJ7
J	82	SER	THR	conflict	UNP Q4QXJ7
J	237	VAL	ALA	conflict	UNP Q4QXJ7
J	246	LYS	ARG	conflict	UNP Q4QXJ7
J	311	PHE	SER	conflict	UNP Q4QXJ7
J	411	ILE	LEU	conflict	UNP Q4QXJ7

- Molecule 2 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	420	Total	C	N	O	S	0	0
			3300	2088	599	589	24		
2	E	420	Total	C	N	O	S	0	0
			3300	2088	599	589	24		
2	H	420	Total	C	N	O	S	0	0
			3300	2088	599	589	24		
2	K	420	Total	C	N	O	S	0	0
			3300	2088	599	589	24		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	LYS	GLU	conflict	UNP Q4QXJ7
E	206	LYS	GLU	conflict	UNP Q4QXJ7
H	206	LYS	GLU	conflict	UNP Q4QXJ7
K	206	LYS	GLU	conflict	UNP Q4QXJ7

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	151	Total	C	N	O	S	0	0
			1165	734	207	220	4		
3	F	151	Total	C	N	O	S	0	0
			1165	734	207	220	4		
3	I	151	Total	C	N	O	S	0	0
			1165	734	207	220	4		
3	L	151	Total	C	N	O	S	0	0
			1165	734	207	220	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	50	SER	ASN	conflict	UNP Q4QXJ7
C	67	ASN	LYS	engineered mutation	UNP Q4QXJ7
F	50	SER	ASN	conflict	UNP Q4QXJ7
F	67	ASN	LYS	engineered mutation	UNP Q4QXJ7
I	50	SER	ASN	conflict	UNP Q4QXJ7
I	67	ASN	LYS	engineered mutation	UNP Q4QXJ7
L	50	SER	ASN	conflict	UNP Q4QXJ7
L	67	ASN	LYS	engineered mutation	UNP Q4QXJ7

- Molecule 4 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	41	Total	C	N	O	S	0	0
			303	176	50	71	6		
4	N	41	Total	C	N	O	S	0	0
			303	176	50	71	6		
4	O	41	Total	C	N	O	S	0	0
			303	176	50	71	6		
4	P	41	Total	C	N	O	S	0	0
			303	176	50	71	6		

- Molecule 5 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	41	Total	C	N	O	S	0	0
			310	176	59	69	6		
5	R	41	Total	C	N	O	S	0	0
			310	176	59	69	6		
5	S	41	Total	C	N	O	S	0	0
			310	176	59	69	6		
5	T	41	Total	C	N	O	S	0	0
			310	176	59	69	6		

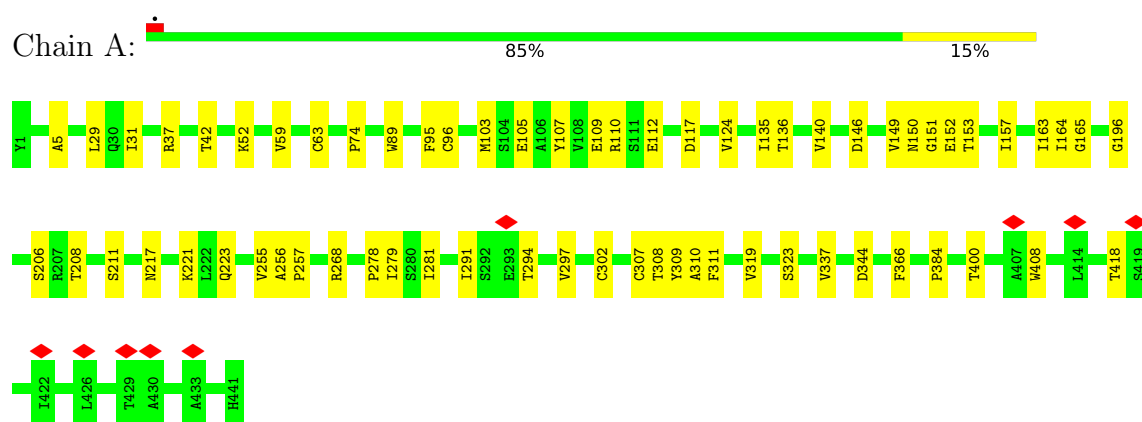
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	M	1	Total	Ca	0
			1	1	
6	N	1	Total	Ca	0
			1	1	
6	O	1	Total	Ca	0
			1	1	
6	P	1	Total	Ca	0
			1	1	
6	Q	1	Total	Ca	0
			1	1	
6	R	1	Total	Ca	0
			1	1	
6	S	1	Total	Ca	0
			1	1	
6	T	1	Total	Ca	0
			1	1	

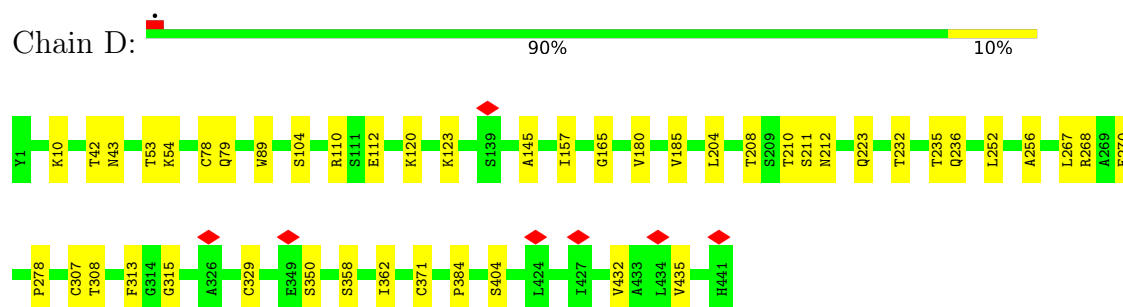
3 Residue-property plots [i](#)

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.

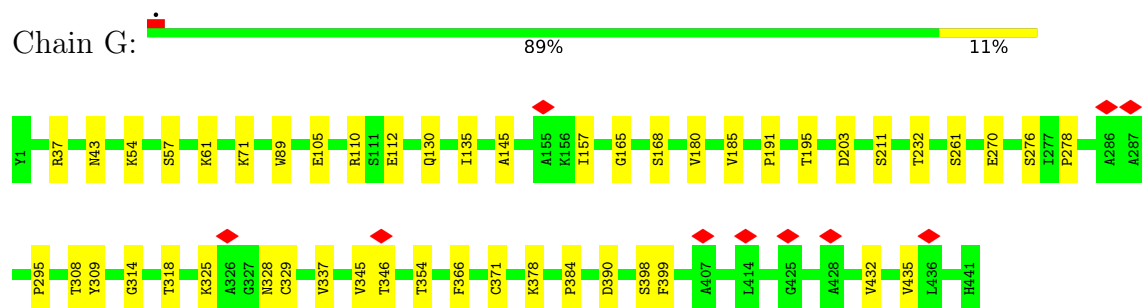
- Molecule 1: Spike glycoprotein E1




- Molecule 1: Spike glycoprotein E1

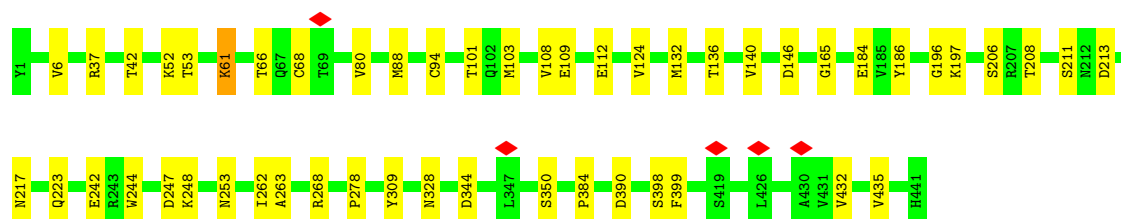


- Molecule 1: Spike glycoprotein E1




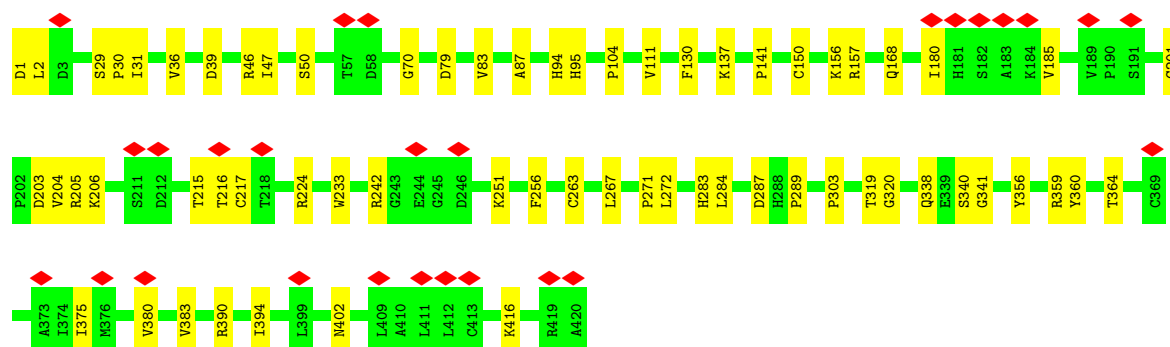
- Molecule 1: Spike glycoprotein E1

Chain J:  88% 11%




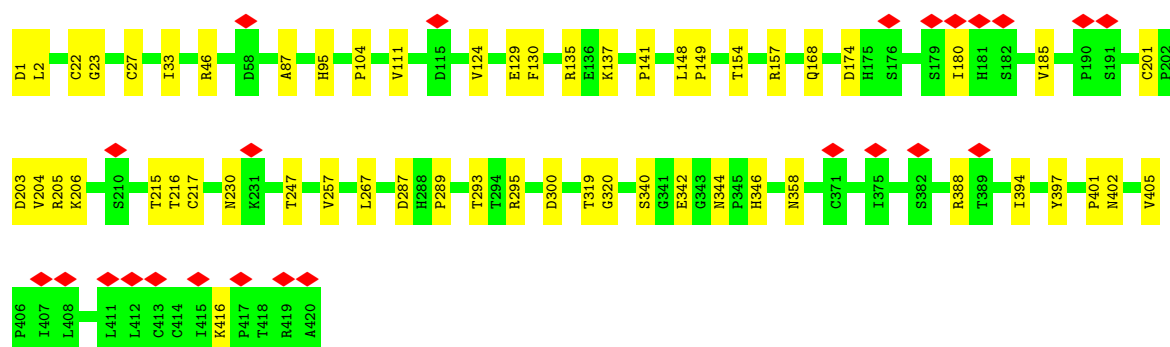
• Molecule 2: Spike glycoprotein E2

Chain B:  6% 85% 15%




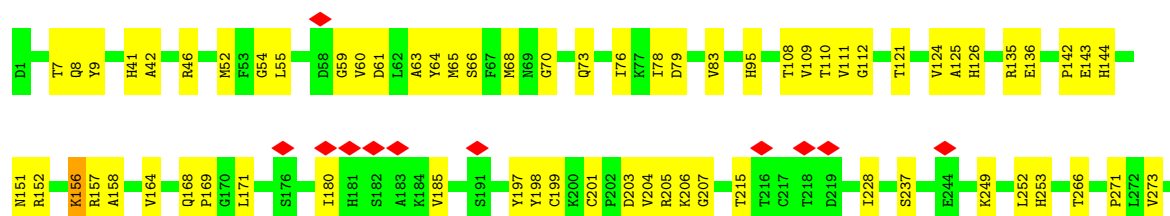
• Molecule 2: Spike glycoprotein E2

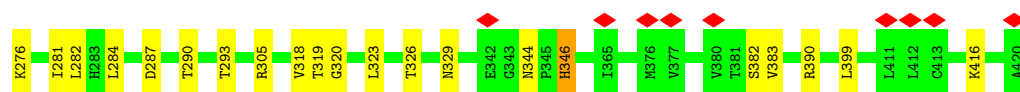
Chain E:  6% 87% 13%



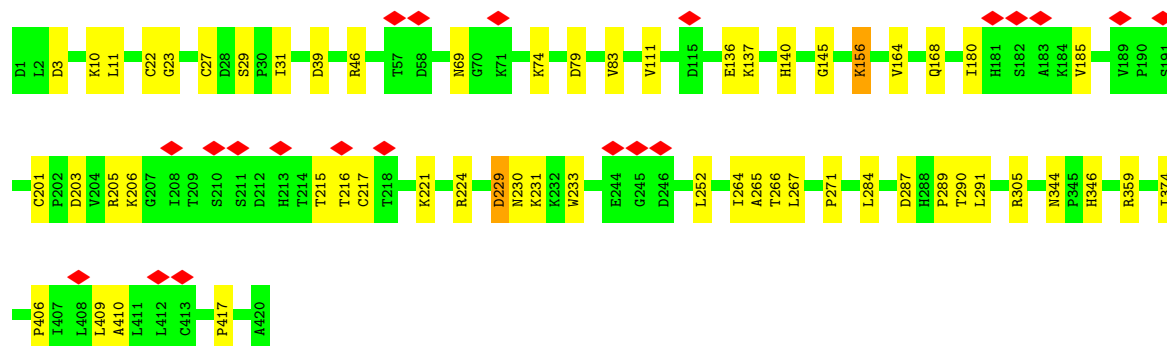
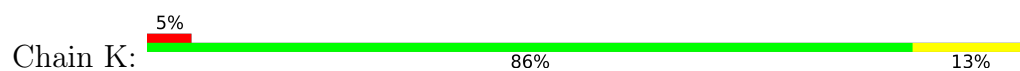
• Molecule 2: Spike glycoprotein E2

Chain H:  5% 79% 20%

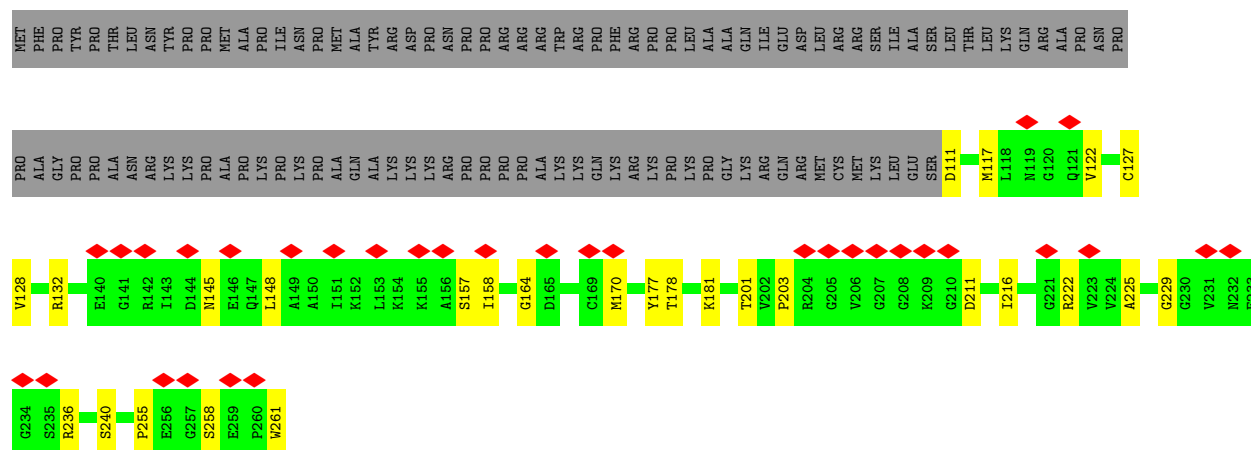




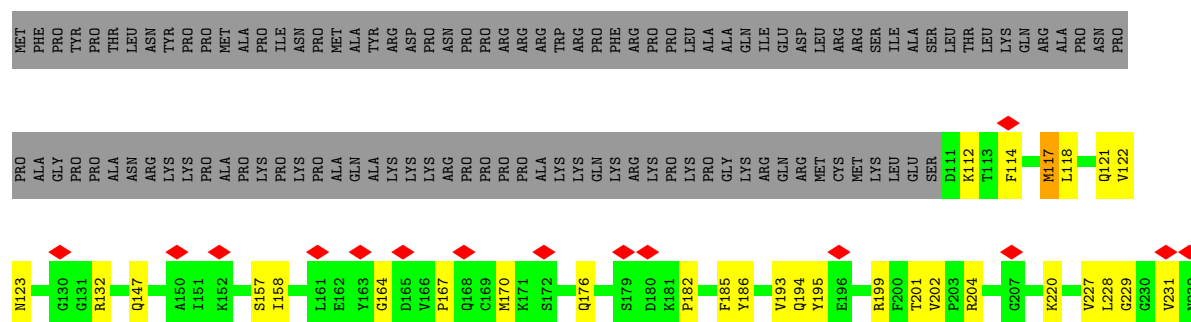
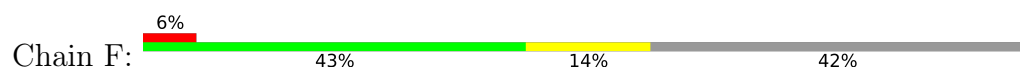
• Molecule 2: Spike glycoprotein E2

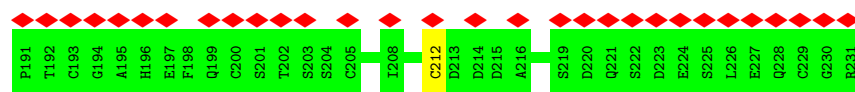


• Molecule 3: Capsid protein

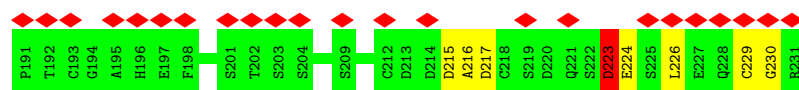
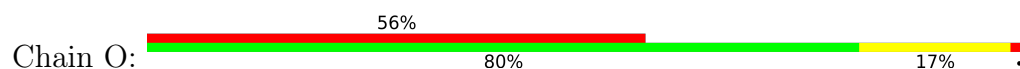


• Molecule 3: Capsid protein

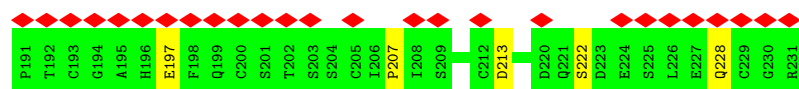
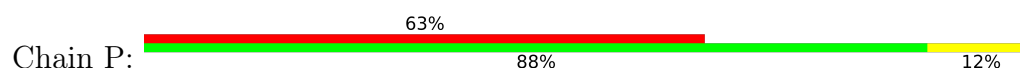




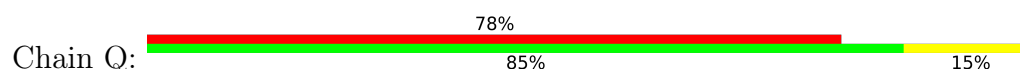
- Molecule 4: Very low-density lipoprotein receptor



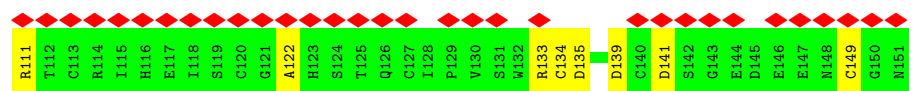
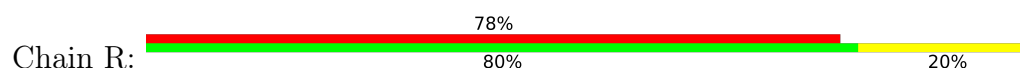
- Molecule 4: Very low-density lipoprotein receptor



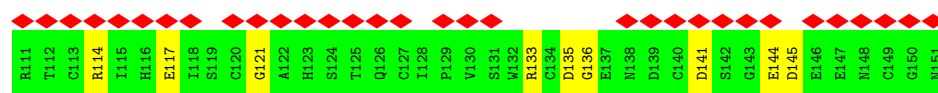
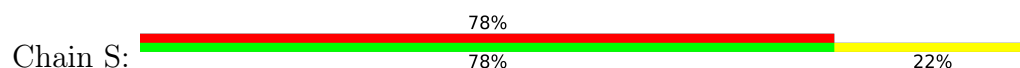
- Molecule 5: Very low-density lipoprotein receptor



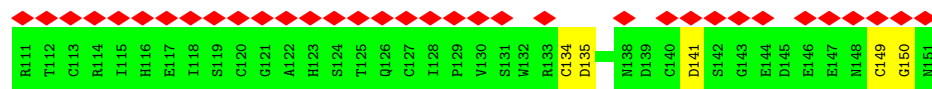
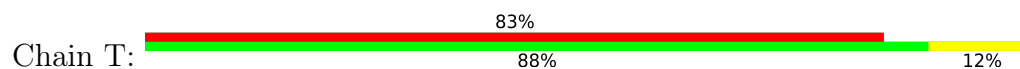
- Molecule 5: Very low-density lipoprotein receptor



- Molecule 5: Very low-density lipoprotein receptor



- Molecule 5: Very low-density lipoprotein receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	776.72003, 776.72003, 776.72003	wwPDB
Map dimensions	584, 584, 584	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.21	0/3469	0.49	2/4734 (0.0%)
1	D	0.21	0/3469	0.45	0/4734
1	G	0.20	0/3469	0.45	0/4734
1	J	0.23	0/3469	0.52	1/4734 (0.0%)
2	B	0.22	0/3395	0.47	0/4630
2	E	0.21	0/3395	0.44	0/4630
2	H	0.22	0/3395	0.55	3/4630 (0.1%)
2	K	0.21	0/3395	0.45	2/4630 (0.0%)
3	C	0.18	0/1192	0.48	0/1615
3	F	0.15	0/1192	0.42	0/1615
3	I	0.18	0/1192	0.47	2/1615 (0.1%)
3	L	0.19	0/1192	0.53	0/1615
4	M	0.17	0/308	0.46	0/417
4	N	0.16	0/308	0.43	0/417
4	O	0.25	0/308	0.61	1/417 (0.2%)
4	P	0.22	0/308	0.53	0/417
5	Q	0.17	0/314	0.44	0/423
5	R	0.19	0/314	0.55	0/423
5	S	0.17	0/314	0.45	0/423
5	T	0.17	0/314	0.48	0/423
All	All	0.21	0/34712	0.48	11/47276 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	61	LYS	N-CA-C	-9.25	92.38	108.20
1	A	153	THR	N-CA-C	7.41	118.98	109.72
2	H	156	LYS	N-CA-C	7.20	121.41	109.46
1	A	152	GLU	N-CA-C	7.03	118.94	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	229	ASP	O-C-N	-6.00	115.91	123.05
2	K	156	LYS	N-CA-C	5.88	118.53	109.07
2	H	64	TYR	N-CA-C	5.87	118.77	110.50
4	O	223	ASP	N-CA-C	5.82	117.63	111.28
3	I	114	PHE	CA-C-N	5.41	125.88	120.52
3	I	114	PHE	C-N-CA	5.41	125.88	120.52
2	H	59	GLY	N-CA-C	5.02	119.00	112.68

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	3375	0	3281	43	0
1	D	3375	0	3281	30	0
1	G	3375	0	3281	40	0
1	J	3375	0	3281	35	0
2	B	3300	0	3268	51	0
2	E	3300	0	3268	42	0
2	H	3300	0	3268	68	0
2	K	3300	0	3268	38	0
3	C	1165	0	1146	19	0
3	F	1165	0	1146	24	0
3	I	1165	0	1146	15	0
3	L	1165	0	1146	16	0
4	M	303	0	250	4	0
4	N	303	0	250	1	0
4	O	303	0	250	11	0
4	P	303	0	250	3	0
5	Q	310	0	258	6	0
5	R	310	0	260	15	0
5	S	310	0	258	13	0
5	T	310	0	258	4	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	1	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
All	All	33820	0	32814	431	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 6.

All (431) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:HB2	2:B:224:ARG:HG3	1.46	0.97
1:J:66:THR:HG22	1:J:101:THR:HG21	1.49	0.95
2:H:156:LYS:HE3	4:O:217:ASP:OD2	1.65	0.95
2:E:1:ASP:OD2	2:E:2:LEU:N	2.01	0.93
1:A:31:ILE:HG23	1:A:135:ILE:CD1	2.02	0.90
1:J:184:GLU:OE1	1:J:184:GLU:N	2.08	0.87
2:H:199:CYS:HB2	2:H:205:ARG:HB3	1.59	0.85
1:A:31:ILE:HG23	1:A:135:ILE:HD11	1.58	0.85
1:G:61:LYS:CE	5:S:136:GLY:O	2.26	0.84
1:G:308:THR:HG22	1:G:314:GLY:O	1.78	0.84
2:H:142:PRO:HG3	2:H:266:THR:HG22	1.59	0.83
2:K:156:LYS:NZ	4:P:213:ASP:OD2	2.11	0.82
2:B:1:ASP:OD2	2:B:2:LEU:N	2.13	0.81
2:H:206:LYS:NZ	5:S:135:ASP:OD2	2.12	0.81
3:C:255:PRO:HG2	3:C:258:SER:HB3	1.62	0.81
5:R:133:ARG:O	5:R:134:CYS:SG	2.39	0.79
1:G:61:LYS:HZ3	5:S:136:GLY:HA3	1.50	0.77
1:G:61:LYS:NZ	5:S:136:GLY:HA3	2.00	0.76
2:H:197:TYR:CZ	2:H:207:GLY:HA3	2.20	0.75
1:J:66:THR:HG22	1:J:101:THR:CG2	2.16	0.75
2:H:273:VAL:HG22	2:H:282:LEU:HD23	1.68	0.75
2:E:203:ASP:OD2	5:Q:126:GLN:NE2	2.19	0.74
2:B:203:ASP:OD1	2:B:204:VAL:N	2.21	0.74
2:H:54:GLY:C	2:H:55:LEU:HD12	2.13	0.72
2:E:203:ASP:OD1	2:E:204:VAL:N	2.21	0.72
2:H:203:ASP:OD1	2:H:204:VAL:N	2.24	0.71
2:B:156:LYS:HE2	4:M:217:ASP:OD2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:197:TYR:CE2	2:H:207:GLY:HA3	2.27	0.69
1:G:61:LYS:HE3	5:S:136:GLY:O	1.93	0.69
1:G:308:THR:CG2	1:G:314:GLY:HA3	2.22	0.69
5:R:134:CYS:CB	5:R:149:CYS:SG	2.81	0.68
2:H:197:TYR:CE2	2:H:207:GLY:CA	2.78	0.67
1:G:37:ARG:HH21	1:G:130:GLN:HE21	1.42	0.67
2:H:108:THR:HG22	2:H:125:ALA:HA	1.77	0.65
1:A:59:VAL:HG22	1:A:103:MET:HB2	1.78	0.65
4:O:226:LEU:H	4:O:226:LEU:HD23	1.61	0.65
1:G:308:THR:HG22	1:G:314:GLY:HA3	1.78	0.64
2:K:206:LYS:NZ	5:T:135:ASP:OD2	2.28	0.64
4:O:226:LEU:HD23	4:O:226:LEU:N	2.12	0.64
2:H:197:TYR:CZ	2:H:207:GLY:CA	2.81	0.64
2:E:206:LYS:NZ	5:Q:135:ASP:OD2	2.27	0.64
2:H:108:THR:HB	2:H:124:VAL:O	1.98	0.63
2:H:390:ARG:HH22	2:H:416:LYS:HE2	1.64	0.63
4:O:223:ASP:OD1	4:O:223:ASP:N	2.32	0.62
2:E:1:ASP:CG	2:E:2:LEU:H	2.02	0.62
2:H:52:MET:HE3	2:H:55:LEU:HD22	1.81	0.62
1:J:244:TRP:HA	1:J:247:ASP:OD2	1.99	0.62
2:H:54:GLY:O	2:H:55:LEU:HD12	2.00	0.61
2:H:273:VAL:HG22	2:H:282:LEU:CD2	2.30	0.61
2:E:267:LEU:HD23	1:J:223:GLN:HE22	1.65	0.61
2:H:108:THR:HG21	2:K:140:HIS:CG	2.35	0.60
2:H:198:TYR:CD2	2:H:206:LYS:HB3	2.37	0.60
2:H:60:VAL:HG12	2:H:60:VAL:O	2.01	0.60
1:J:68:CYS:HB3	1:J:103:MET:HE1	1.83	0.60
2:E:401:PRO:HD2	3:F:176:GLN:HE22	1.67	0.60
2:H:54:GLY:HA2	2:H:61:ASP:O	2.02	0.59
3:L:151:ILE:HG23	3:L:165:ASP:HB2	1.83	0.59
4:O:226:LEU:H	4:O:226:LEU:CD2	2.15	0.59
2:H:65:MET:HE2	2:H:78:ILE:HG12	1.84	0.59
1:J:112:GLU:OE2	2:K:46:ARG:NH2	2.36	0.59
2:H:197:TYR:CE2	2:H:207:GLY:N	2.71	0.59
1:A:149:VAL:O	1:A:149:VAL:HG12	2.01	0.59
1:G:295:PRO:HB3	1:G:325:LYS:HG3	1.84	0.58
1:G:309:TYR:HB3	1:G:384:PRO:HD3	1.85	0.58
2:K:83:VAL:HG22	2:K:111:VAL:HG12	1.85	0.58
2:H:136:GLU:HG2	2:H:290:THR:HG23	1.85	0.58
2:H:79:ASP:OD1	2:H:79:ASP:N	2.37	0.58
2:K:406:PRO:HG2	2:K:409:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:THR:HA	2:H:126:HIS:H	1.68	0.58
3:I:182:PRO:O	3:I:186:TYR:OH	2.21	0.58
5:R:134:CYS:HB3	5:R:149:CYS:CB	2.33	0.58
5:T:149:CYS:SG	5:T:150:GLY:N	2.78	0.57
1:D:180:VAL:HG22	1:D:185:VAL:HG12	1.86	0.57
2:K:229:ASP:OD2	2:K:231:LYS:HG2	2.05	0.57
1:D:362:ILE:HG21	1:D:404:SER:HA	1.86	0.57
1:G:89:TRP:CZ3	2:H:70:GLY:HA2	2.40	0.57
3:L:157:SER:OG	3:L:158:ILE:N	2.37	0.57
2:B:206:LYS:HZ1	5:R:139:ASP:CG	2.12	0.56
3:I:137:LEU:H	3:I:160:ASP:HB3	1.70	0.56
2:K:22:CYS:SG	2:K:23:GLY:N	2.79	0.56
1:D:268:ARG:NH1	1:D:270:GLU:OE2	2.38	0.56
3:F:231:VAL:HG22	3:F:261:TRP:HB2	1.87	0.56
4:O:226:LEU:O	4:O:230:GLY:HA2	2.06	0.56
1:A:221:LYS:NZ	1:A:223:GLN:OE1	2.38	0.56
1:G:112:GLU:OE2	2:H:46:ARG:NH2	2.35	0.56
3:C:255:PRO:HG2	3:C:258:SER:CB	2.35	0.56
3:I:157:SER:OG	3:I:158:ILE:N	2.38	0.56
1:A:89:TRP:CZ3	2:B:70:GLY:HA2	2.40	0.56
1:D:307:CYS:SG	1:D:308:THR:N	2.78	0.56
1:G:165:GLY:HA3	1:G:278:PRO:HG2	1.86	0.56
2:H:205:ARG:O	2:H:205:ARG:HG3	2.05	0.56
2:K:287:ASP:OD1	2:K:287:ASP:N	2.37	0.56
4:M:213:ASP:OD1	4:M:213:ASP:N	2.39	0.56
1:J:196:GLY:O	1:J:217:ASN:ND2	2.38	0.55
5:R:134:CYS:HB3	5:R:149:CYS:SG	2.47	0.55
1:A:95:PHE:HB2	2:B:224:ARG:CG	2.29	0.55
2:B:79:ASP:OD1	2:B:79:ASP:N	2.37	0.55
1:J:398:SER:OG	1:J:399:PHE:N	2.38	0.55
1:J:309:TYR:HB3	1:J:384:PRO:HD3	1.88	0.55
3:L:168:GLN:HA	3:L:171:LYS:HG3	1.89	0.55
1:A:149:VAL:HG22	1:A:164:ILE:HG21	1.89	0.54
2:B:205:ARG:NH2	2:B:217:CYS:SG	2.80	0.54
2:K:205:ARG:NH2	2:K:217:CYS:SG	2.80	0.54
5:Q:141:ASP:N	5:Q:141:ASP:OD1	2.41	0.54
1:A:112:GLU:OE2	2:B:46:ARG:NH2	2.40	0.54
5:R:134:CYS:HB3	5:R:149:CYS:HB3	1.89	0.54
3:C:132:ARG:HA	3:C:164:GLY:HA3	1.90	0.54
3:F:157:SER:OG	3:F:158:ILE:N	2.41	0.54
2:E:205:ARG:NH2	2:E:217:CYS:SG	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:344:ASN:ND2	2:K:346:HIS:O	2.41	0.53
3:F:185:PHE:HA	3:F:194:GLN:HG3	1.90	0.53
1:G:308:THR:HG22	1:G:314:GLY:C	2.32	0.53
2:H:197:TYR:CZ	2:H:207:GLY:C	2.86	0.53
2:B:29:SER:OG	2:B:31:ILE:O	2.26	0.53
1:D:53:THR:HG21	1:D:236:GLN:HE22	1.74	0.53
2:E:135:ARG:NH2	2:E:293:THR:OG1	2.41	0.53
2:H:344:ASN:ND2	2:H:346:HIS:O	2.42	0.53
2:K:168:GLN:NE2	2:K:230:ASN:OD1	2.41	0.53
1:A:308:THR:HG23	1:A:310:ALA:H	1.73	0.53
2:E:22:CYS:SG	2:E:27:CYS:N	2.67	0.52
1:J:42:THR:HG22	1:J:124:VAL:HG12	1.91	0.52
2:B:94:HIS:O	2:B:157:ARG:NH1	2.43	0.52
2:E:33:ILE:HG21	2:E:124:VAL:HG11	1.90	0.52
2:E:22:CYS:SG	2:E:23:GLY:N	2.82	0.52
3:L:235:SER:OG	3:L:236:ARG:NH1	2.41	0.52
5:T:141:ASP:OD1	5:T:141:ASP:N	2.40	0.52
2:H:287:ASP:OD1	2:H:287:ASP:N	2.38	0.52
1:A:337:VAL:HB	1:A:366:PHE:HB3	1.92	0.52
2:H:52:MET:HB2	2:H:66:SER:HB2	1.92	0.52
1:J:186:TYR:OH	1:J:248:LYS:HD2	2.10	0.52
2:B:390:ARG:HH12	2:B:416:LYS:HB2	1.75	0.52
2:H:158:ALA:O	2:H:253:HIS:ND1	2.41	0.52
1:A:105:GLU:OE2	2:B:242:ARG:NH2	2.43	0.52
2:B:137:LYS:HB2	2:B:289:PRO:HG2	1.91	0.51
2:K:410:ALA:HB1	2:K:417:PRO:HA	1.91	0.51
1:A:52:LYS:NZ	1:A:109:GLU:OE2	2.41	0.51
2:H:136:GLU:OE1	2:H:266:THR:OG1	2.25	0.51
3:L:195:TYR:HE1	3:L:197:ASN:HB2	1.75	0.51
5:R:141:ASP:OD1	5:R:141:ASP:N	2.40	0.51
3:C:145:ASN:HB3	3:C:148:LEU:HB2	1.93	0.51
3:F:132:ARG:HA	3:F:164:GLY:HA3	1.93	0.51
5:S:141:ASP:N	5:S:141:ASP:OD1	2.43	0.51
3:F:199:ARG:HH11	3:F:241:VAL:HG21	1.75	0.51
1:G:329:CYS:SG	1:G:371:CYS:N	2.84	0.51
5:R:111:ARG:NH1	5:R:122:ALA:O	2.44	0.51
1:D:384:PRO:HD2	2:E:340:SER:HA	1.92	0.50
2:E:87:ALA:HB3	2:E:104:PRO:HG3	1.92	0.50
1:G:135:ILE:HG13	1:G:157:ILE:HG21	1.93	0.50
2:H:276:LYS:HD3	2:H:281:ILE:HD11	1.93	0.50
3:C:157:SER:OG	3:C:158:ILE:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:HG23	1:D:252:LEU:HB3	1.92	0.50
1:D:223:GLN:NE2	1:D:235:THR:OG1	2.45	0.50
1:G:61:LYS:HE2	5:S:136:GLY:O	2.09	0.50
2:H:112:GLY:HA3	2:H:121:THR:HG22	1.92	0.50
2:B:319:THR:OG1	2:B:320:GLY:N	2.45	0.50
2:E:344:ASN:ND2	2:E:346:HIS:O	2.45	0.50
1:G:191:PRO:O	1:G:195:THR:OG1	2.30	0.50
2:H:197:TYR:OH	2:H:207:GLY:HA3	2.11	0.50
3:C:127:CYS:SG	3:C:128:VAL:N	2.84	0.50
2:E:1:ASP:HA	4:N:212:CYS:O	2.12	0.50
3:F:123:ASN:N	3:F:123:ASN:OD1	2.45	0.50
2:H:63:ALA:O	2:H:78:ILE:HG13	2.12	0.50
3:L:233:GLU:HB2	3:L:237:THR:HA	1.93	0.50
2:H:135:ARG:NH2	2:H:326:THR:OG1	2.45	0.50
1:G:308:THR:HG22	1:G:314:GLY:CA	2.40	0.49
3:I:132:ARG:HA	3:I:164:GLY:HA3	1.93	0.49
4:P:222:SER:O	4:P:228:GLN:NE2	2.45	0.49
3:C:201:THR:O	3:C:236:ARG:NH2	2.45	0.49
1:J:253:ASN:HB3	1:J:262:ILE:HB	1.93	0.49
3:C:240:SER:HB3	3:C:255:PRO:HD2	1.93	0.49
2:K:203:ASP:OD1	2:K:203:ASP:N	2.44	0.49
2:B:206:LYS:NZ	5:R:135:ASP:OD2	2.40	0.49
2:H:7:THR:OG1	2:H:8:GLN:OE1	2.31	0.49
2:E:168:GLN:HB3	2:E:247:THR:HG22	1.95	0.49
2:K:136:GLU:HG2	2:K:290:THR:HG23	1.95	0.49
3:F:158:ILE:HB	3:F:252:LYS:HD2	1.94	0.49
1:D:211:SER:OG	1:D:212:ASN:N	2.44	0.49
1:A:146:ASP:OD2	1:A:146:ASP:N	2.40	0.49
2:B:87:ALA:HB3	2:B:104:PRO:HG3	1.94	0.49
3:I:118:LEU:O	3:I:121:GLN:NE2	2.46	0.49
1:A:165:GLY:HA3	1:A:278:PRO:HG2	1.94	0.49
2:B:206:LYS:NZ	5:R:139:ASP:CG	2.71	0.49
2:K:221:LYS:O	2:K:221:LYS:HG2	2.13	0.49
1:D:208:THR:HG22	1:D:210:THR:H	1.78	0.49
3:F:147:GLN:HG3	3:L:120:GLY:HA3	1.95	0.49
1:A:309:TYR:HB2	1:A:384:PRO:HD3	1.94	0.48
3:C:117:MET:HE1	3:C:122:VAL:HG22	1.95	0.48
3:C:177:TYR:HD1	3:C:222:ARG:HD3	1.78	0.48
3:L:145:ASN:HB3	3:L:148:LEU:HB2	1.95	0.48
3:F:186:TYR:HB2	3:F:193:VAL:HG23	1.95	0.48
1:A:135:ILE:HG13	1:A:157:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:PRO:HB3	2:B:284:LEU:HD23	1.95	0.48
1:J:165:GLY:HA3	1:J:278:PRO:HG2	1.95	0.48
2:E:1:ASP:CG	2:E:2:LEU:N	2.62	0.48
3:F:118:LEU:O	3:F:121:GLN:NE2	2.46	0.48
3:L:199:ARG:HB2	3:L:239:LEU:HB2	1.95	0.48
1:D:112:GLU:OE1	2:E:46:ARG:NH2	2.39	0.48
2:H:266:THR:O	2:H:329:ASN:ND2	2.46	0.48
1:A:302:CYS:HB2	1:A:319:VAL:HG22	1.96	0.48
3:C:111:ASP:N	3:C:111:ASP:OD1	2.45	0.48
3:F:195:TYR:O	3:F:199:ARG:NH2	2.40	0.48
3:F:228:LEU:HD11	3:F:242:VAL:HG13	1.95	0.48
1:J:432:VAL:HA	1:J:435:VAL:HG22	1.96	0.48
1:J:94:CYS:C	2:K:224:ARG:HE	2.22	0.47
2:E:319:THR:OG1	2:E:320:GLY:N	2.46	0.47
1:A:42:THR:HG22	1:A:124:VAL:HG12	1.95	0.47
2:H:319:THR:OG1	2:H:320:GLY:N	2.47	0.47
1:A:110:ARG:NH2	1:A:211:SER:O	2.44	0.47
1:A:29:LEU:HD11	1:A:281:ILE:HD13	1.96	0.47
3:F:202:VAL:O	3:F:237:THR:OG1	2.33	0.47
1:G:203:ASP:OD1	1:G:203:ASP:N	2.47	0.47
1:G:318:THR:HG22	1:G:354:THR:HG22	1.96	0.47
2:H:55:LEU:O	2:H:66:SER:OG	2.29	0.47
2:K:22:CYS:SG	2:K:27:CYS:N	2.80	0.47
3:L:202:VAL:HG23	3:L:237:THR:HG23	1.96	0.47
4:O:215:ASP:O	4:O:224:GLU:OE1	2.33	0.47
2:B:340:SER:OG	2:B:341:GLY:N	2.47	0.47
2:E:394:ILE:HG23	2:E:416:LYS:HD3	1.97	0.47
2:E:402:ASN:OD1	2:E:402:ASN:N	2.48	0.47
3:F:182:PRO:O	3:F:186:TYR:OH	2.26	0.47
2:H:83:VAL:HG22	2:H:111:VAL:HG12	1.97	0.47
1:A:311:PHE:H	2:B:338:GLN:HE21	1.62	0.47
3:I:154:LYS:HB2	3:I:163:TYR:HB2	1.96	0.47
1:J:211:SER:OG	1:J:213:ASP:OD1	2.32	0.47
2:K:271:PRO:HB3	2:K:284:LEU:HD23	1.96	0.47
2:B:168:GLN:HA	2:B:233:TRP:HD1	1.80	0.47
2:E:203:ASP:CG	2:E:204:VAL:H	2.20	0.47
3:I:123:ASN:ND2	3:I:140:GLU:OE1	2.48	0.47
2:B:206:LYS:NZ	5:R:139:ASP:OD1	2.48	0.46
3:F:229:GLY:HA2	3:F:261:TRP:H	1.80	0.46
1:G:110:ARG:NH2	1:G:211:SER:O	2.48	0.46
3:C:170:MET:HE2	3:C:170:MET:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:227:VAL:HA	3:F:241:VAL:HG12	1.97	0.46
3:I:245:ASN:HB3	3:I:249:VAL:HG23	1.97	0.46
2:E:397:TYR:HE1	2:E:405:VAL:HA	1.79	0.46
2:H:399:LEU:HB3	3:I:250:THR:HG21	1.98	0.46
5:Q:118:ILE:HG12	5:Q:130:VAL:HG12	1.96	0.46
2:B:30:PRO:O	2:B:50:SER:OG	2.32	0.46
1:D:165:GLY:HA3	1:D:278:PRO:HG2	1.96	0.46
2:E:33:ILE:HD11	2:E:111:VAL:HG22	1.96	0.46
2:H:151:ASN:OD1	2:H:151:ASN:N	2.48	0.46
3:I:243:THR:OG1	3:I:244:TRP:N	2.48	0.46
2:K:39:ASP:OD1	2:K:39:ASP:N	2.49	0.46
1:A:307:CYS:SG	1:A:308:THR:N	2.88	0.46
1:A:344:ASP:OD2	1:A:344:ASP:N	2.49	0.46
2:H:293:THR:HG22	2:H:305:ARG:HB2	1.97	0.46
3:C:203:PRO:HA	3:C:236:ARG:HH12	1.80	0.46
1:G:61:LYS:NZ	5:S:136:GLY:CA	2.77	0.46
1:A:135:ILE:HG13	1:A:157:ILE:CD1	2.45	0.46
2:B:46:ARG:HD3	2:B:256:PHE:HB2	1.97	0.46
1:A:255:VAL:HG13	2:B:303:PRO:HG3	1.98	0.46
2:B:402:ASN:OD1	2:B:402:ASN:N	2.47	0.46
1:G:168:SER:HB3	1:G:276:SER:H	1.81	0.46
1:G:180:VAL:HG22	1:G:185:VAL:HG12	1.98	0.46
1:J:80:VAL:HG13	1:J:101:THR:HG23	1.98	0.46
4:O:226:LEU:N	4:O:226:LEU:CD2	2.76	0.46
2:E:168:GLN:NE2	2:E:230:ASN:OD1	2.49	0.45
3:F:201:THR:O	3:F:201:THR:OG1	2.30	0.45
3:L:128:VAL:O	3:L:174:THR:OG1	2.32	0.45
1:A:196:GLY:O	1:A:217:ASN:ND2	2.40	0.45
2:E:300:ASP:OD2	2:E:300:ASP:N	2.49	0.45
1:J:263:ALA:HB1	1:J:268:ARG:HH21	1.81	0.45
4:O:224:GLU:HA	4:O:229:CYS:SG	2.56	0.45
5:S:121:GLY:N	5:S:144:GLU:OE2	2.47	0.45
2:B:95:HIS:HD2	2:B:157:ARG:HE	1.65	0.45
3:F:112:LYS:HZ1	3:F:114:PHE:HB2	1.80	0.45
1:J:53:THR:HG22	1:J:108:VAL:HG22	1.98	0.45
1:G:57:SER:OG	2:H:237:SER:O	2.33	0.45
1:G:398:SER:OG	1:G:399:PHE:N	2.50	0.45
5:S:114:ARG:HB3	5:S:117:GLU:HG3	1.98	0.45
2:K:11:LEU:HD23	2:K:233:TRP:HZ3	1.82	0.45
5:R:135:ASP:OD1	5:R:135:ASP:N	2.40	0.45
1:A:151:GLY:O	1:A:163:ILE:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:THR:O	1:G:232:THR:OG1	2.33	0.45
3:L:179:SER:OG	3:L:245:ASN:O	2.35	0.45
4:M:229:CYS:HB3	4:M:231:ARG:HG2	1.99	0.45
5:R:134:CYS:CB	5:R:149:CYS:HG	2.29	0.45
1:D:313:PHE:HA	1:D:358:SER:HB2	1.98	0.45
2:E:185:VAL:HG23	2:E:215:THR:HB	1.99	0.45
2:H:382:SER:OG	2:H:383:VAL:N	2.48	0.45
1:J:6:VAL:HA	1:J:278:PRO:HA	1.99	0.45
2:B:150:CYS:HB3	2:B:263:CYS:HB2	1.80	0.45
2:E:287:ASP:OD1	2:E:287:ASP:N	2.49	0.45
2:H:42:ALA:HB3	2:H:152:ARG:HH12	1.82	0.45
2:H:143:GLU:HG3	2:H:144:HIS:N	2.32	0.45
2:K:29:SER:OG	2:K:31:ILE:O	2.35	0.45
2:K:185:VAL:HG23	2:K:215:THR:HB	1.99	0.45
5:S:133:ARG:NH2	5:S:145:ASP:OD1	2.49	0.45
1:G:61:LYS:HZ3	5:S:136:GLY:CA	2.26	0.44
2:H:9:TYR:HD1	2:H:52:MET:HE1	1.82	0.44
2:B:36:VAL:HG22	2:B:47:ILE:HG23	1.99	0.44
2:B:203:ASP:CG	2:B:204:VAL:H	2.20	0.44
1:D:78:CYS:SG	1:D:79:GLN:N	2.89	0.44
1:D:145:ALA:HB3	1:D:157:ILE:HG12	1.99	0.44
2:H:168:GLN:HG2	2:H:169:PRO:HD2	1.99	0.44
1:A:136:THR:OG1	1:A:140:VAL:O	2.36	0.44
3:F:117:MET:HE1	3:F:122:VAL:HG22	1.99	0.44
1:J:390:ASP:OD1	1:J:390:ASP:N	2.49	0.44
3:L:194:GLN:H	3:L:200:PHE:HB2	1.82	0.44
4:M:211:VAL:HA	4:M:223:ASP:HB2	1.99	0.44
2:H:76:ILE:HD13	2:H:76:ILE:HA	1.89	0.44
1:J:328:ASN:ND2	1:J:344:ASP:OD1	2.47	0.44
1:A:117:ASP:OD2	1:A:117:ASP:N	2.49	0.44
2:E:154:THR:OG1	2:E:257:VAL:O	2.35	0.44
2:E:203:ASP:CG	2:E:204:VAL:N	2.75	0.44
2:H:171:LEU:HD22	2:H:228:ILE:HG12	2.00	0.44
2:H:185:VAL:HG23	2:H:215:THR:HB	1.99	0.44
2:B:185:VAL:HG23	2:B:215:THR:HB	1.99	0.44
2:B:203:ASP:CG	2:B:204:VAL:N	2.75	0.44
2:B:39:ASP:OD2	2:B:39:ASP:N	2.51	0.44
1:J:88:MET:HE3	1:J:88:MET:HB3	1.92	0.44
3:C:216:ILE:HD12	3:C:225:ALA:HB3	1.99	0.44
2:E:95:HIS:HD1	2:E:157:ARG:HE	1.65	0.44
2:E:388:ARG:HE	2:E:388:ARG:HB3	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:309:TYR:OH	2:K:359:ARG:NH1	2.47	0.44
1:G:54:LYS:HB2	1:G:54:LYS:HE2	1.70	0.43
3:L:127:CYS:SG	3:L:128:VAL:N	2.91	0.43
1:A:400:THR:O	1:A:400:THR:OG1	2.33	0.43
1:D:110:ARG:HG3	1:D:204:LEU:HD21	1.99	0.43
3:I:168:GLN:NE2	3:I:169:CYS:SG	2.90	0.43
1:J:52:LYS:NZ	1:J:109:GLU:OE2	2.51	0.43
1:A:150:ASN:OD1	1:A:150:ASN:N	2.50	0.43
2:H:271:PRO:HB3	2:H:284:LEU:HD23	2.00	0.43
1:G:337:VAL:HB	1:G:366:PHE:HB3	2.01	0.43
2:E:204:VAL:HG21	5:Q:139:ASP:OD1	2.18	0.43
3:F:220:LYS:HD2	3:F:220:LYS:HA	1.85	0.43
2:H:249:LYS:HB3	2:H:249:LYS:HE3	1.76	0.43
2:K:79:ASP:OD2	2:K:79:ASP:N	2.49	0.43
2:K:267:LEU:HD12	2:K:267:LEU:HA	1.89	0.43
2:K:374:ILE:HD13	2:K:374:ILE:HA	1.93	0.43
1:D:54:LYS:HB2	1:D:54:LYS:HE2	1.72	0.43
2:E:130:PHE:HZ	2:E:141:PRO:HD3	1.84	0.43
1:J:132:MET:HA	1:J:146:ASP:HA	2.00	0.43
1:J:217:ASN:OD1	1:J:217:ASN:N	2.52	0.43
3:L:201:THR:O	3:L:201:THR:OG1	2.36	0.43
1:D:123:LYS:HB3	1:D:123:LYS:HE3	1.87	0.43
1:G:261:SER:O	1:G:270:GLU:N	2.52	0.43
2:K:164:VAL:O	2:K:252:LEU:N	2.51	0.43
2:K:180:ILE:HA	2:K:185:VAL:HA	2.01	0.43
5:S:135:ASP:OD1	5:S:135:ASP:N	2.43	0.43
1:G:378:LYS:HE3	1:G:378:LYS:HB2	1.82	0.43
2:B:206:LYS:CE	5:R:139:ASP:OD1	2.67	0.43
3:F:167:PRO:HG2	3:F:170:MET:HE1	2.00	0.43
1:A:291:ILE:O	1:A:294:THR:OG1	2.36	0.42
3:C:229:GLY:HA2	3:C:261:TRP:HB3	2.01	0.42
2:K:145:GLY:N	2:K:264:ILE:CG2	2.82	0.42
5:T:134:CYS:HB3	5:T:149:CYS:HB2	1.67	0.42
1:A:297:VAL:HG12	1:A:323:SER:HB2	2.00	0.42
1:J:197:LYS:HA	1:J:197:LYS:HD3	1.88	0.42
1:A:309:TYR:HE1	2:B:359:ARG:HH22	1.65	0.42
2:B:272:LEU:HB2	2:B:283:HIS:HB2	2.01	0.42
3:C:181:LYS:H	3:C:181:LYS:HG3	1.68	0.42
1:G:71:LYS:NZ	1:G:105:GLU:OE2	2.51	0.42
2:H:109:VAL:CG1	2:H:110:THR:N	2.82	0.42
2:B:402:ASN:HD22	3:C:178:THR:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:TRP:CH2	2:E:174:ASP:OD2	2.72	0.42
4:P:197:GLU:HA	4:P:207:PRO:HA	2.01	0.42
2:B:287:ASP:OD1	2:B:287:ASP:N	2.41	0.42
3:F:240:SER:HB2	3:F:254:THR:HG22	2.01	0.42
2:H:68:MET:HB3	2:H:73:GLN:HA	2.01	0.42
2:K:3:ASP:OD2	2:K:10:LYS:NZ	2.44	0.42
1:A:37:ARG:HD2	1:A:268:ARG:HD2	2.01	0.42
1:D:256:ALA:O	2:E:295:ARG:NH1	2.50	0.42
2:H:108:THR:HG21	2:K:140:HIS:ND1	2.35	0.42
1:D:120:LYS:HE2	1:D:120:LYS:HB2	1.89	0.42
1:D:432:VAL:HA	1:D:435:VAL:HG12	2.01	0.42
2:H:180:ILE:HA	2:H:185:VAL:HA	2.01	0.42
2:H:318:VAL:HG22	2:H:323:LEU:HD22	2.02	0.42
2:K:145:GLY:HA3	2:K:265:ALA:O	2.20	0.42
1:D:350:SER:O	1:D:350:SER:OG	2.35	0.42
1:G:43:ASN:OD1	1:G:43:ASN:N	2.53	0.42
1:J:37:ARG:HD2	1:J:268:ARG:HD2	2.02	0.42
3:L:230:GLY:O	3:L:237:THR:OG1	2.38	0.42
1:A:63:CYS:HB3	1:A:96:CYS:HB2	1.75	0.41
2:B:130:PHE:HZ	2:B:141:PRO:HD3	1.84	0.41
3:I:132:ARG:HG2	3:I:161:LEU:HD11	2.02	0.41
2:K:69:ASN:HD21	2:K:74:LYS:HD2	1.85	0.41
1:J:146:ASP:OD2	1:J:146:ASP:N	2.53	0.41
2:E:342:GLU:HB3	2:E:358:ASN:HD22	1.85	0.41
1:G:328:ASN:HD21	1:G:346:THR:HA	1.84	0.41
2:K:136:GLU:OE2	2:K:266:THR:OG1	2.31	0.41
5:R:133:ARG:C	5:R:134:CYS:SG	3.03	0.41
2:B:267:LEU:HD12	2:B:267:LEU:HA	1.92	0.41
2:E:205:ARG:NH2	2:E:216:THR:OG1	2.54	0.41
1:A:5:ALA:HB3	1:A:279:ILE:HD11	2.02	0.41
2:B:180:ILE:HA	2:B:185:VAL:HA	2.01	0.41
3:C:211:ASP:OD2	3:C:211:ASP:N	2.52	0.41
1:D:42:THR:HG21	1:D:267:LEU:HD23	2.03	0.41
1:G:135:ILE:HG13	1:G:157:ILE:CG2	2.50	0.41
3:I:242:VAL:HA	3:I:252:LYS:HA	2.03	0.41
3:F:204:ARG:NH2	3:F:235:SER:O	2.46	0.41
1:G:328:ASN:ND2	1:G:345:VAL:O	2.54	0.41
2:K:137:LYS:HB2	2:K:289:PRO:HG2	2.02	0.41
5:Q:135:ASP:OD1	5:Q:135:ASP:N	2.40	0.41
1:A:256:ALA:HA	1:A:257:PRO:HD3	1.94	0.41
3:C:201:THR:HB	3:C:236:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:137:LYS:HB2	2:E:289:PRO:HG2	2.02	0.41
2:B:380:VAL:HA	2:B:383:VAL:HG22	2.02	0.41
1:D:43:ASN:OD1	1:D:43:ASN:N	2.53	0.41
1:D:307:CYS:HA	1:D:315:GLY:HA2	2.02	0.41
2:E:180:ILE:HA	2:E:185:VAL:HA	2.01	0.41
1:A:206:SER:OG	1:A:208:THR:O	2.39	0.41
2:B:251:LYS:HB3	2:B:251:LYS:HE2	1.85	0.41
2:B:360:TYR:HB2	2:B:364:THR:HG23	2.03	0.41
2:B:394:ILE:HD12	2:B:416:LYS:HD2	2.03	0.41
2:H:95:HIS:HB2	2:H:157:ARG:HE	1.86	0.41
2:H:164:VAL:O	2:H:252:LEU:N	2.53	0.41
3:I:181:LYS:HE3	3:I:181:LYS:HB3	1.85	0.41
1:J:61:LYS:HD2	1:J:66:THR:HB	2.03	0.41
1:A:418:THR:HG21	2:B:375:ILE:HG12	2.02	0.41
2:B:356:TYR:HB3	2:B:364:THR:HG21	2.03	0.41
1:J:350:SER:O	1:J:350:SER:OG	2.37	0.41
1:D:10:LYS:HD3	1:D:10:LYS:HA	1.94	0.40
2:H:203:ASP:CG	2:H:204:VAL:N	2.79	0.40
4:O:226:LEU:O	4:O:230:GLY:CA	2.69	0.40
2:B:83:VAL:HG22	2:B:111:VAL:HG12	2.03	0.40
1:D:104:SER:O	1:D:104:SER:OG	2.38	0.40
2:E:148:LEU:HD23	2:E:149:PRO:HD2	2.02	0.40
1:G:145:ALA:HB3	1:G:157:ILE:HD12	2.02	0.40
1:G:432:VAL:HA	1:G:435:VAL:HG12	2.01	0.40
1:J:206:SER:OG	1:J:208:THR:O	2.39	0.40
1:A:74:PRO:HD2	1:A:107:TYR:HE1	1.86	0.40
1:D:329:CYS:SG	1:D:371:CYS:N	2.94	0.40
3:I:168:GLN:HA	3:I:171:LYS:HD2	2.02	0.40
2:K:205:ARG:NH2	2:K:216:THR:OG1	2.55	0.40
2:B:205:ARG:NH2	2:B:216:THR:OG1	2.55	0.40
2:H:109:VAL:HG12	2:H:110:THR:N	2.37	0.40
1:D:104:SER:HB2	1:D:232:THR:HG23	2.03	0.40
1:J:136:THR:OG1	1:J:140:VAL:O	2.39	0.40
2:K:291:LEU:HD11	2:K:305:ARG:HG3	2.03	0.40
4:O:216:ALA:HA	4:O:224:GLU:OE2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/441 (100%)	412 (94%)	27 (6%)	0	100	100
1	D	439/441 (100%)	413 (94%)	26 (6%)	0	100	100
1	G	439/441 (100%)	414 (94%)	25 (6%)	0	100	100
1	J	439/441 (100%)	416 (95%)	23 (5%)	0	100	100
2	B	418/420 (100%)	377 (90%)	41 (10%)	0	100	100
2	E	418/420 (100%)	388 (93%)	30 (7%)	0	100	100
2	H	418/420 (100%)	378 (90%)	40 (10%)	0	100	100
2	K	418/420 (100%)	383 (92%)	35 (8%)	0	100	100
3	C	149/261 (57%)	130 (87%)	19 (13%)	0	100	100
3	F	149/261 (57%)	127 (85%)	22 (15%)	0	100	100
3	I	149/261 (57%)	132 (89%)	17 (11%)	0	100	100
3	L	149/261 (57%)	131 (88%)	18 (12%)	0	100	100
4	M	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
4	N	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
4	O	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
4	P	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
5	Q	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
5	R	39/41 (95%)	32 (82%)	7 (18%)	0	100	100
5	S	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
5	T	39/41 (95%)	39 (100%)	0	0	100	100
All	All	4336/4816 (90%)	3993 (92%)	343 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/371 (100%)	370 (100%)	1 (0%)	91	92
1	D	371/371 (100%)	371 (100%)	0	100	100
1	G	371/371 (100%)	370 (100%)	1 (0%)	91	92
1	J	371/371 (100%)	370 (100%)	1 (0%)	91	92
2	B	367/367 (100%)	366 (100%)	1 (0%)	91	92
2	E	367/367 (100%)	365 (100%)	2 (0%)	86	90
2	H	367/367 (100%)	364 (99%)	3 (1%)	79	85
2	K	367/367 (100%)	366 (100%)	1 (0%)	91	92
3	C	125/221 (57%)	125 (100%)	0	100	100
3	F	125/221 (57%)	124 (99%)	1 (1%)	79	85
3	I	125/221 (57%)	125 (100%)	0	100	100
3	L	125/221 (57%)	125 (100%)	0	100	100
4	M	37/37 (100%)	37 (100%)	0	100	100
4	N	37/37 (100%)	37 (100%)	0	100	100
4	O	37/37 (100%)	36 (97%)	1 (3%)	40	59
4	P	37/37 (100%)	37 (100%)	0	100	100
5	Q	36/36 (100%)	36 (100%)	0	100	100
5	R	36/36 (100%)	36 (100%)	0	100	100
5	S	36/36 (100%)	36 (100%)	0	100	100
5	T	36/36 (100%)	36 (100%)	0	100	100
All	All	3744/4128 (91%)	3732 (100%)	12 (0%)	90	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	TRP
2	B	201	CYS
2	E	129	GLU

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Mol	Chain	Res	Type
2	E	201	CYS
3	F	117	MET
1	G	390	ASP
2	H	41	HIS
2	H	201	CYS
2	H	346	HIS
1	J	242	GLU
2	K	201	CYS
4	O	223	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	125	HIS
1	A	361	ASN
1	A	387	HIS
2	B	8	GLN
2	B	21	ASN
2	B	80	ASN
2	B	82	HIS
2	B	168	GLN
2	B	175	HIS
2	B	315	ASN
2	B	338	GLN
2	B	350	HIS
3	C	168	GLN
1	D	3	HIS
1	D	100	ASN
1	D	223	GLN
1	D	253	ASN
1	D	271	ASN
1	D	369	GLN
2	E	80	ASN
2	E	94	HIS
2	E	144	HIS
2	E	162	HIS
2	E	168	GLN
2	E	175	HIS
2	E	253	HIS
2	E	275	HIS
2	E	288	HIS

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Mol	Chain	Res	Type
2	E	306	GLN
2	E	338	GLN
2	E	346	HIS
2	E	358	ASN
3	F	119	ASN
3	F	176	GLN
3	F	189	HIS
3	F	190	HIS
3	F	232	ASN
1	G	100	ASN
1	G	130	GLN
1	G	217	ASN
1	G	328	ASN
1	G	332	HIS
2	H	5	HIS
2	H	21	ASN
2	H	80	ASN
2	H	114	HIS
2	H	160	GLN
2	H	175	HIS
2	H	306	GLN
2	H	315	ASN
2	H	404	GLN
3	I	119	ASN
3	I	121	GLN
3	I	168	GLN
3	I	187	ASN
1	J	3	HIS
1	J	35	ASN
1	J	73	HIS
1	J	223	GLN
1	J	356	HIS
1	J	439	HIS
2	K	24	HIS
2	K	120	HIS
2	K	175	HIS
2	K	346	HIS
3	L	119	ASN
3	L	121	GLN
3	L	246	GLN
5	R	151	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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.

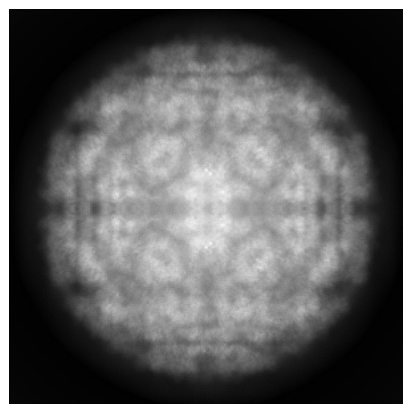
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38377. These allow visual inspection of the internal detail of the map and identification of artifacts.

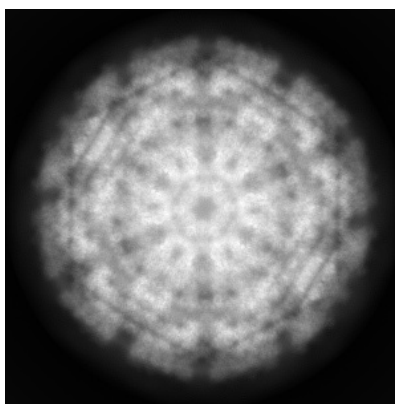
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

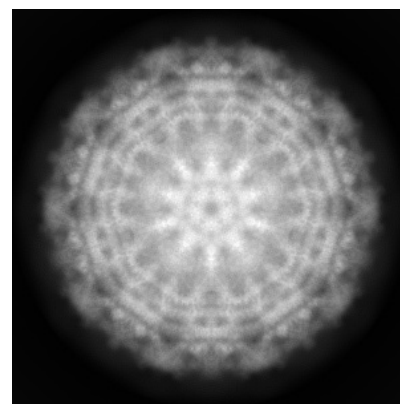
6.1.1 Primary map



X

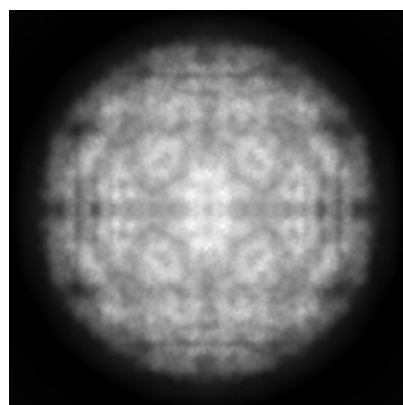


Y

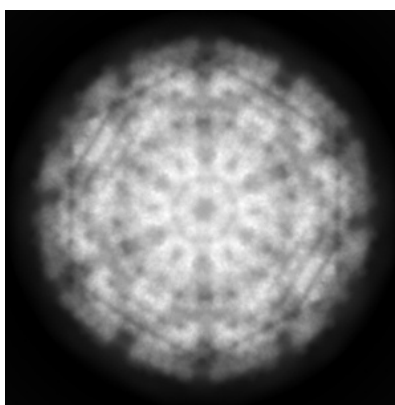


Z

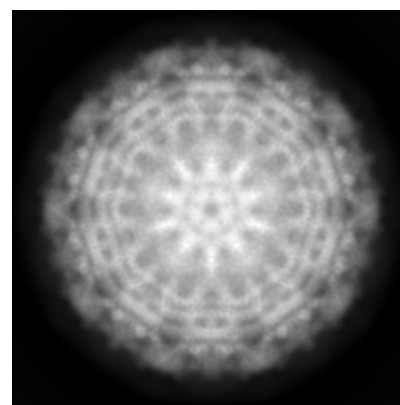
6.1.2 Raw map



X



Y

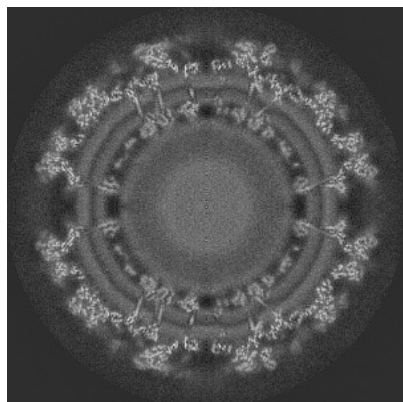


Z

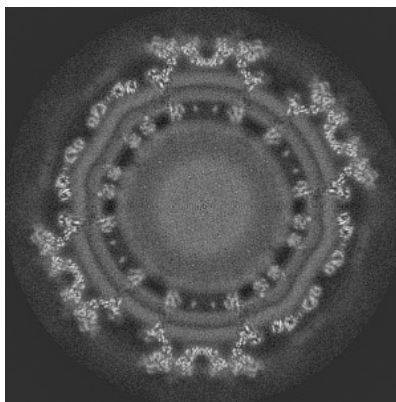
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

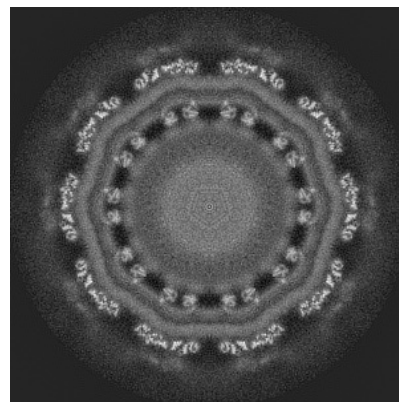
6.2.1 Primary map



X Index: 292

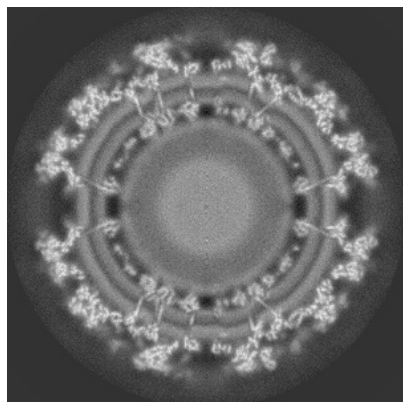


Y Index: 292

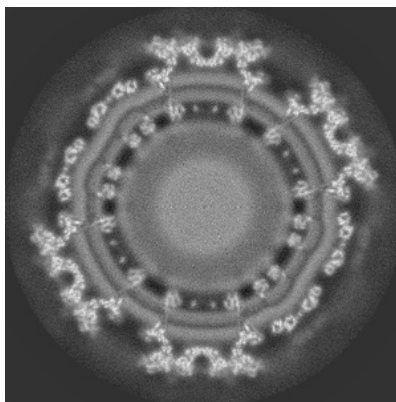


Z Index: 292

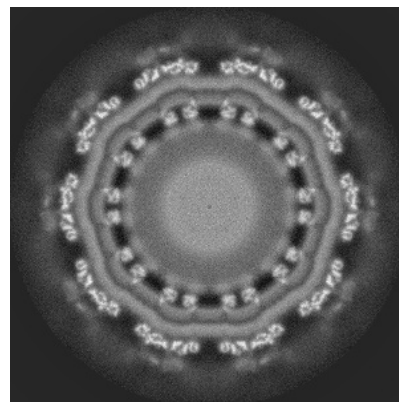
6.2.2 Raw map



X Index: 292



Y Index: 292

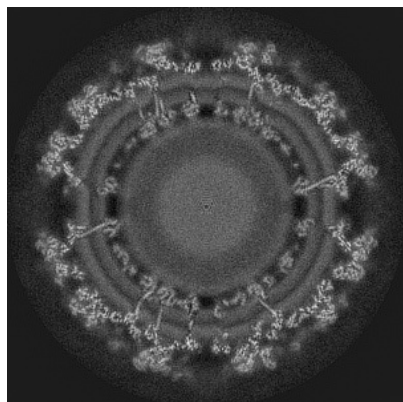


Z Index: 292

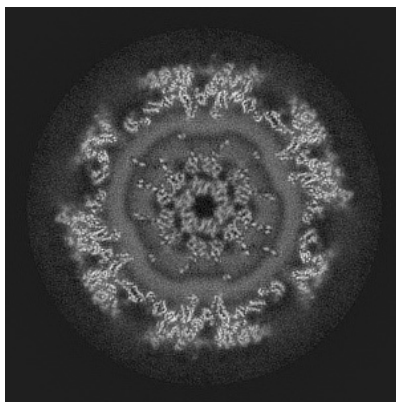
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

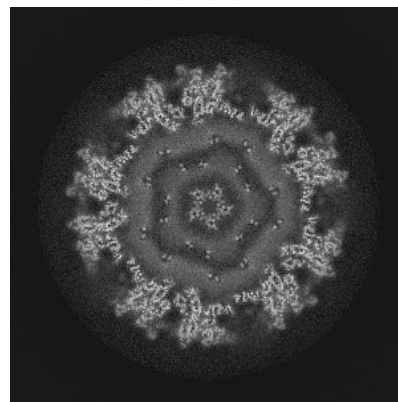
6.3.1 Primary map



X Index: 290

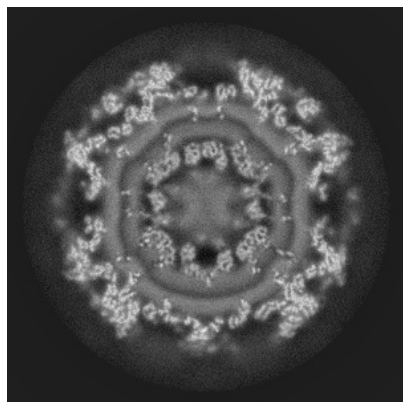


Y Index: 427

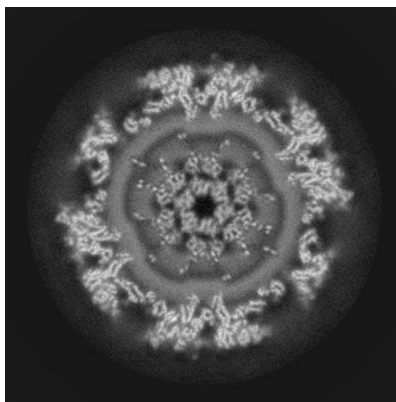


Z Index: 442

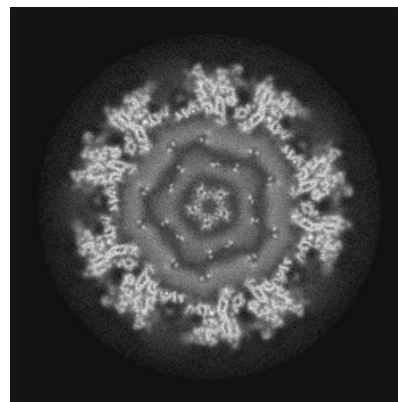
6.3.2 Raw map



X Index: 175



Y Index: 427

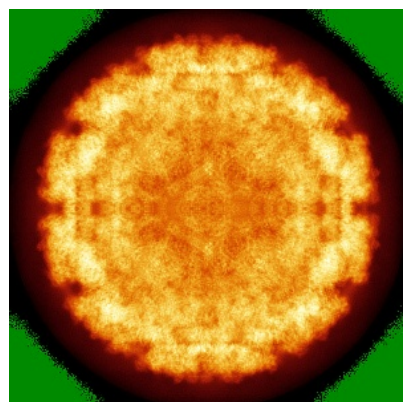


Z Index: 142

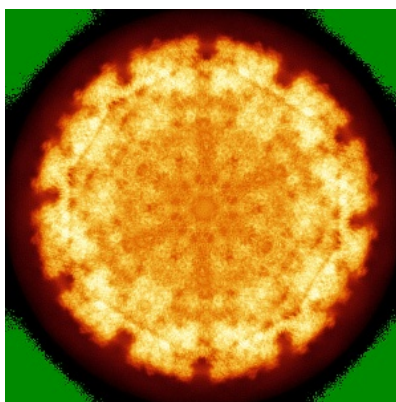
The images above show the largest variance slices of the map in three orthogonal directions.

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

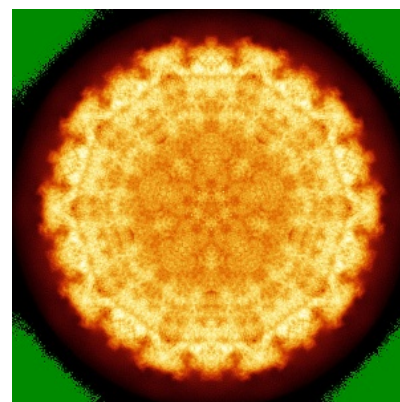
6.4.1 Primary map



X

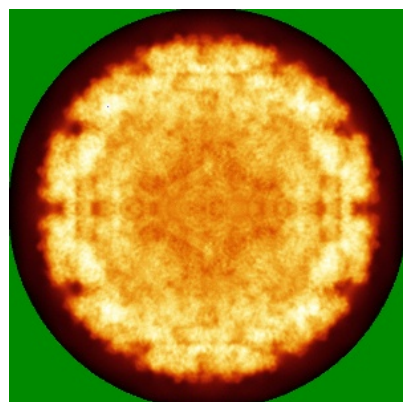


Y

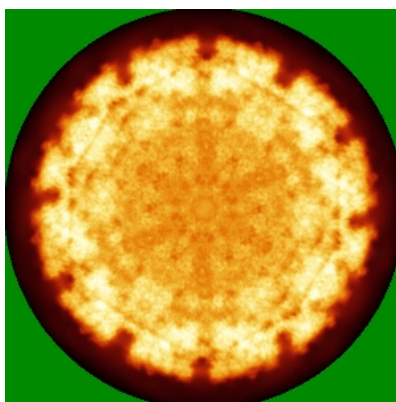


Z

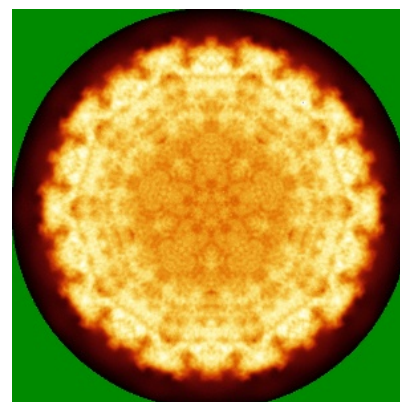
6.4.2 Raw map



X



Y

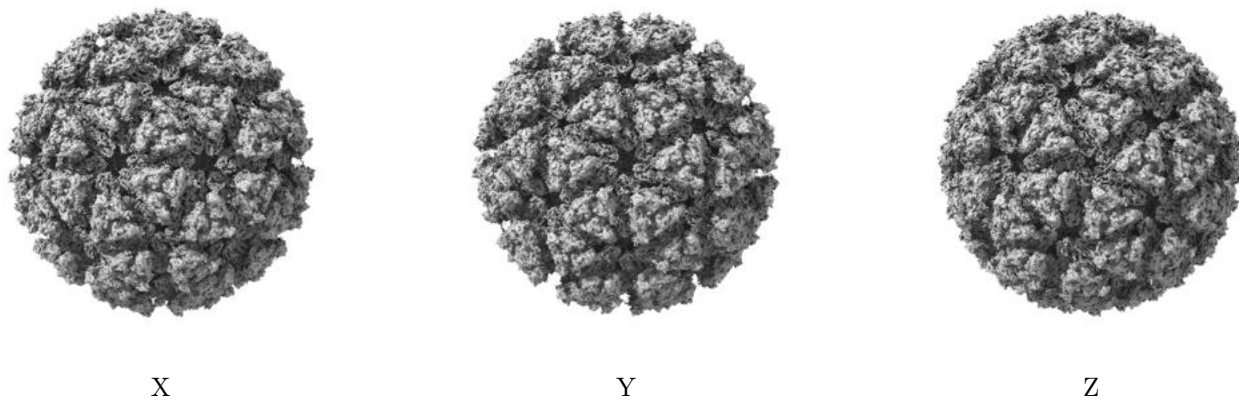


Z

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

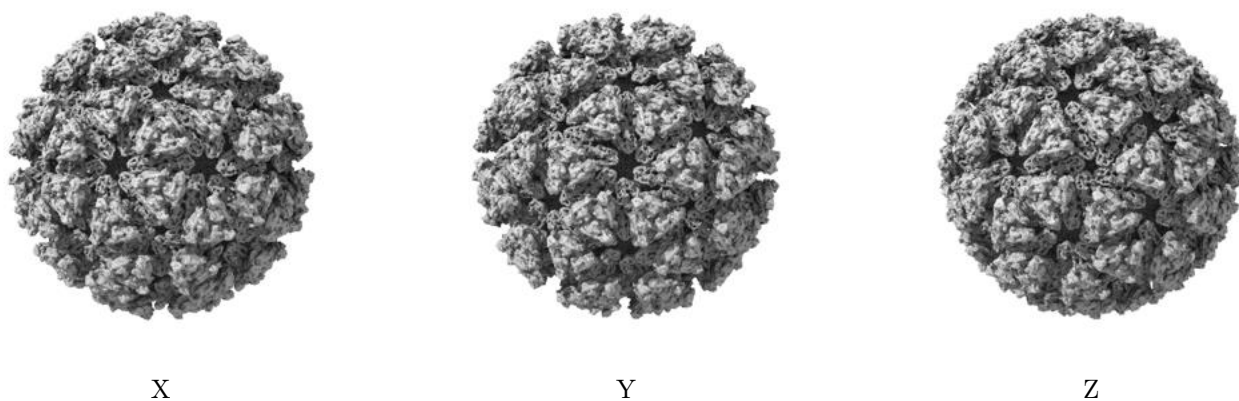
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

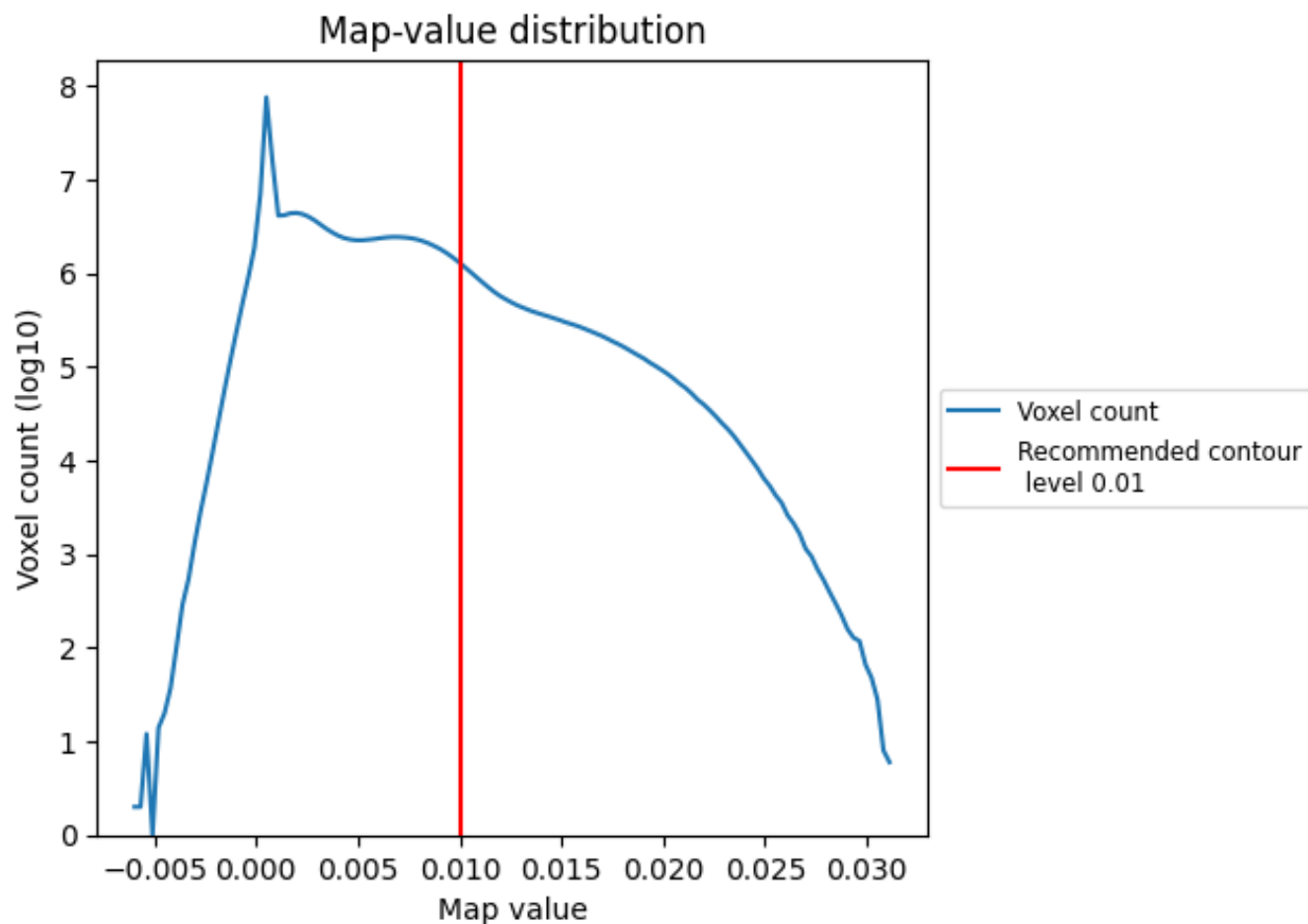
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

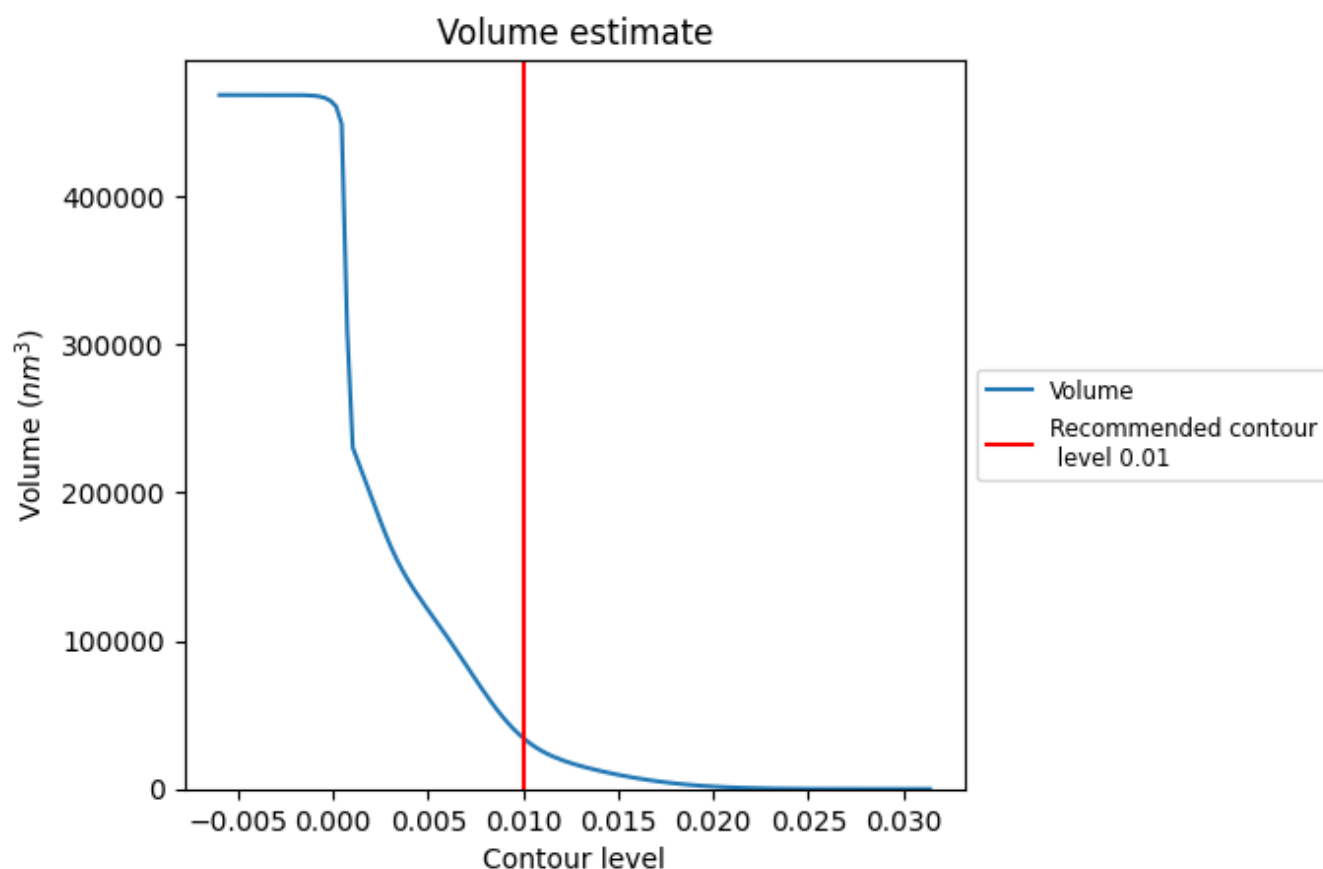
This section contains the results of statistical analysis of the map.

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.

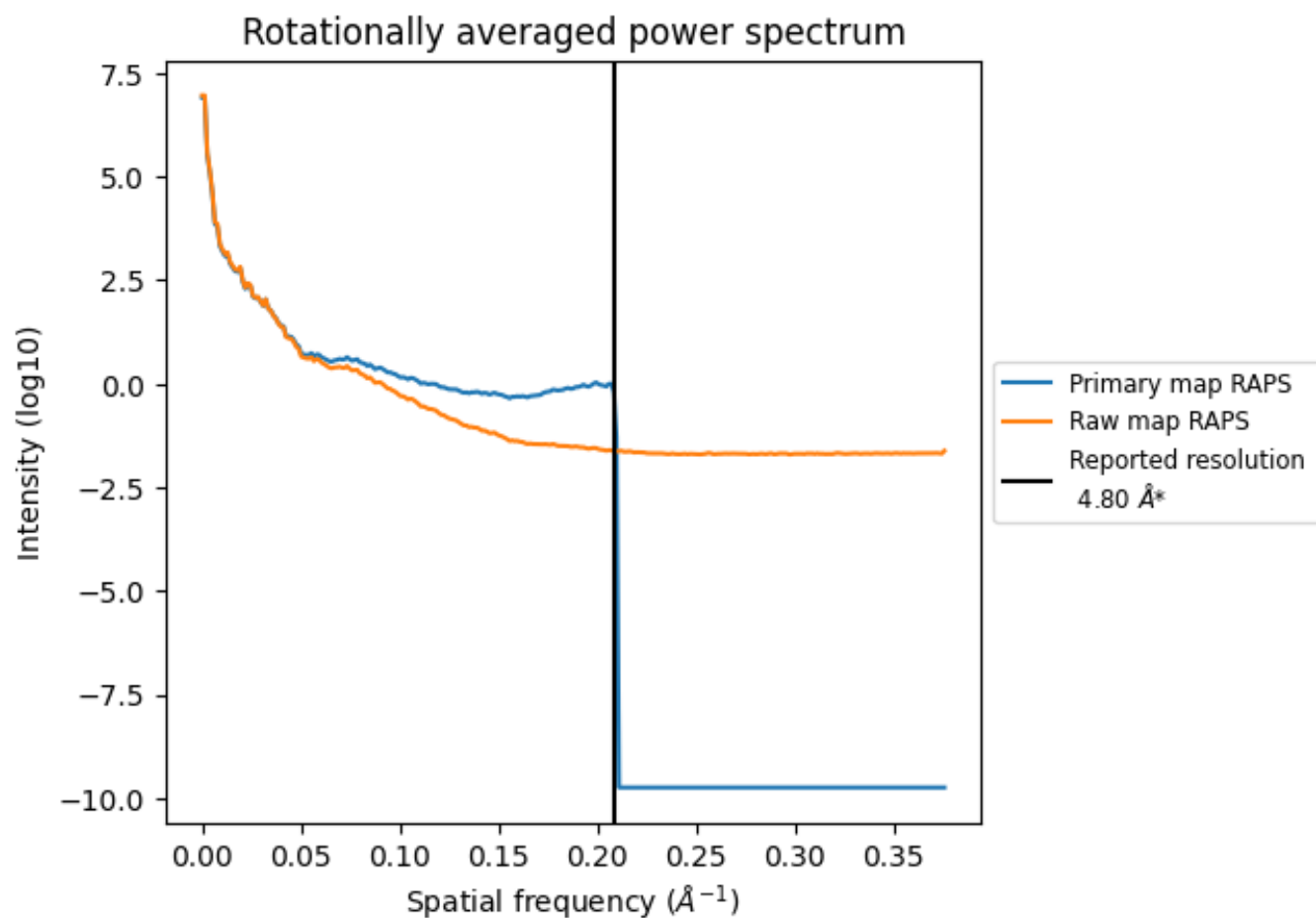
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34542 nm³; this corresponds to an approximate mass of 31203 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 ⓘ

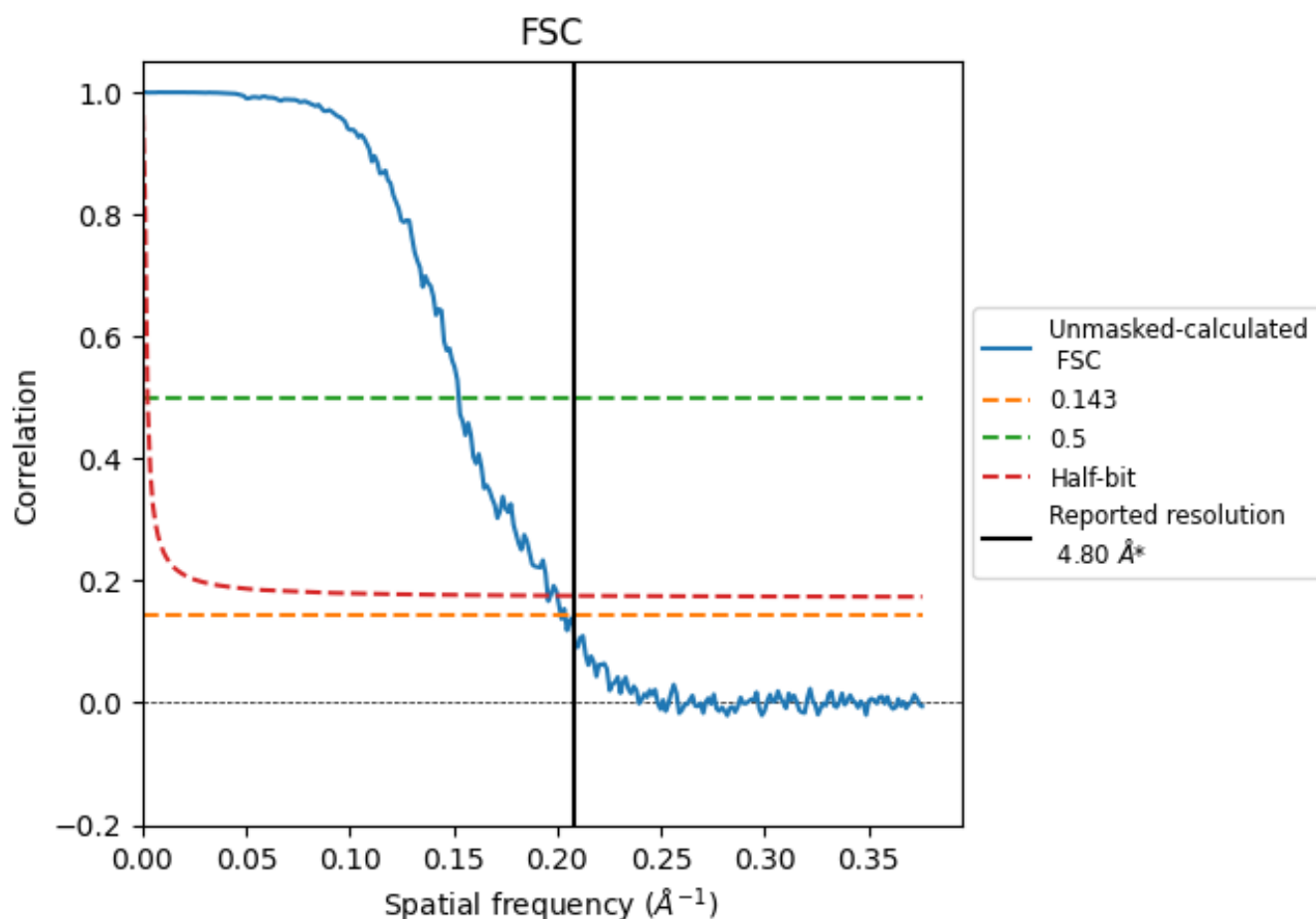


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.96	6.55	5.12

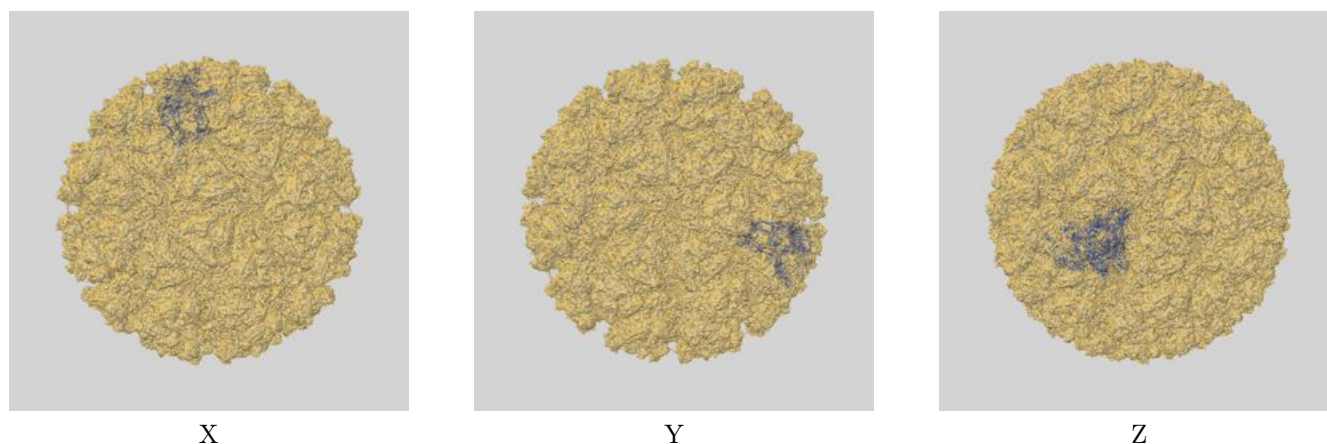
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

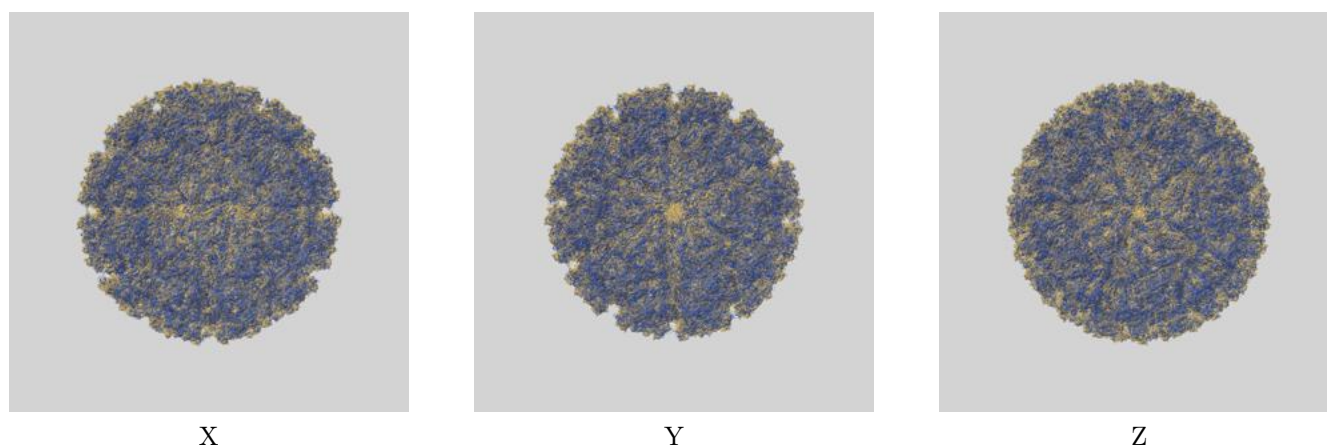
This section contains information regarding the fit between EMDB map EMD-38377 and PDB model 8YS4. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

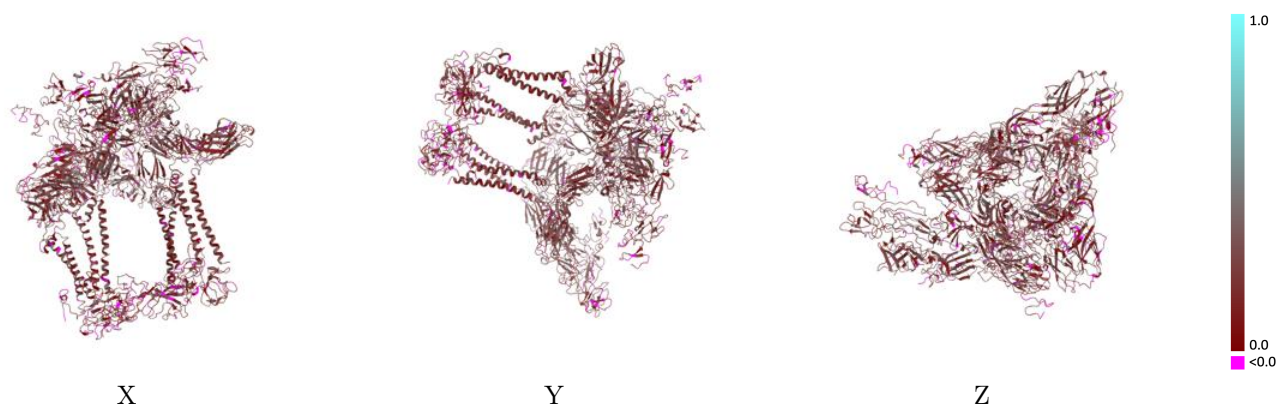


9.1.2 Map-model assembly overlay [i](#)



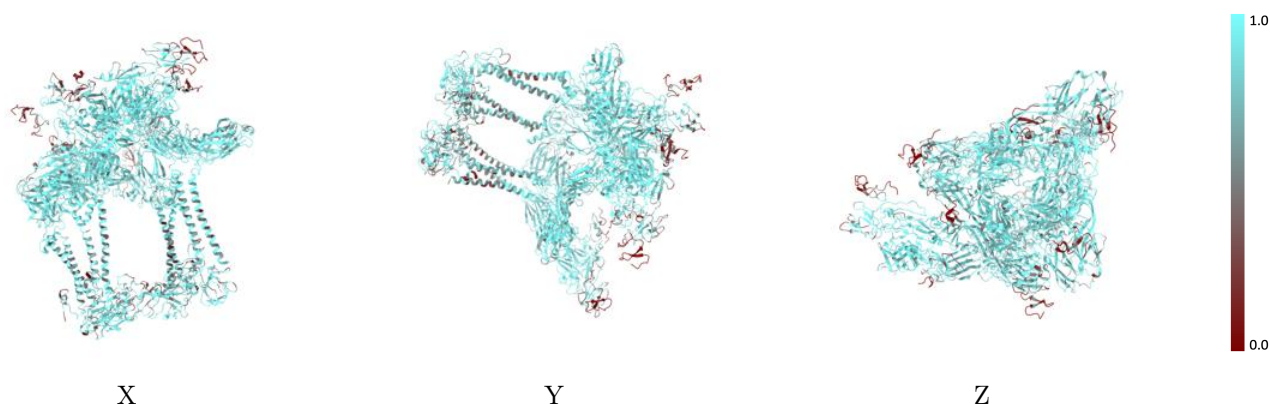
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



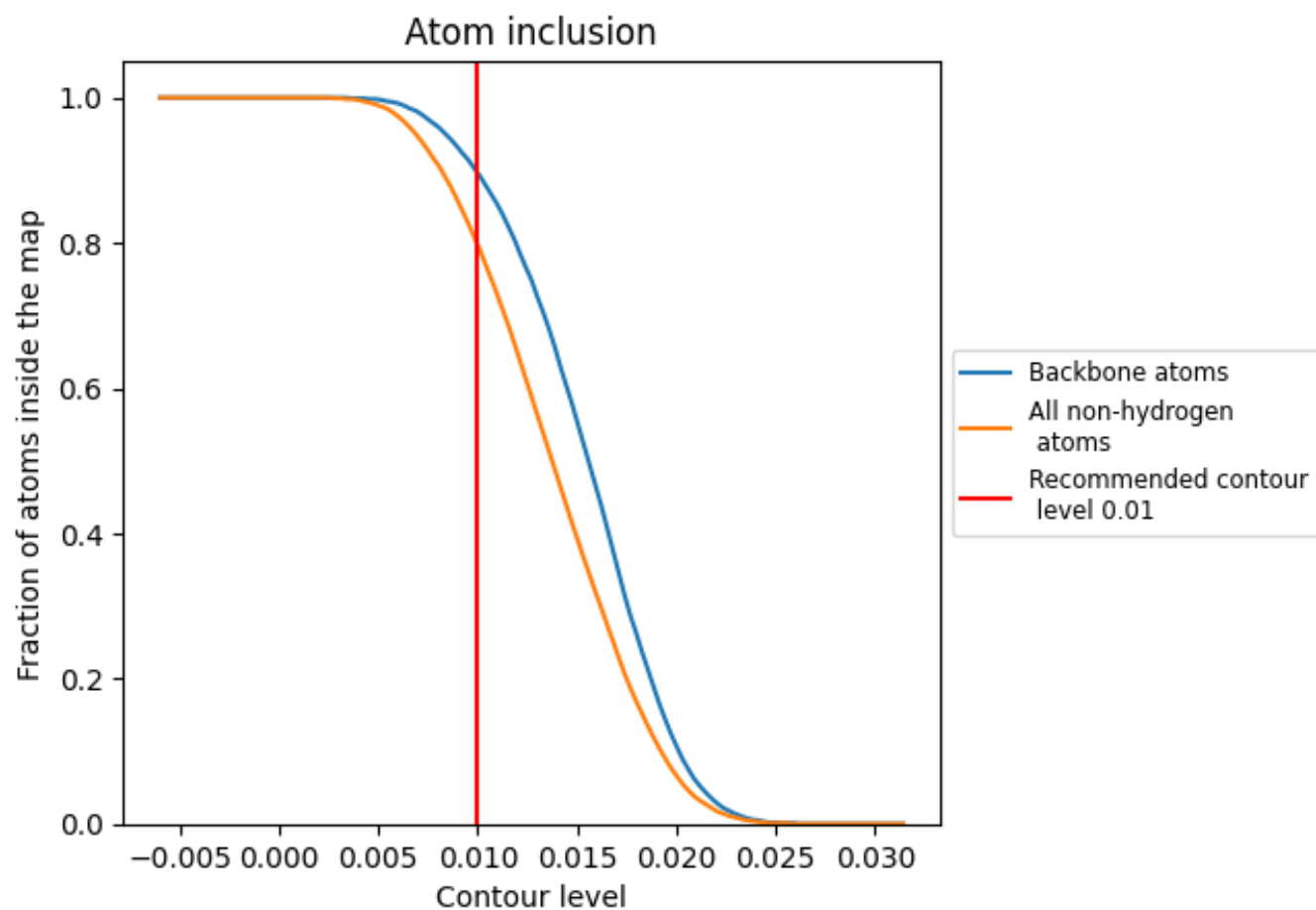
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).











































9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7970	 0.2190
A	 0.8660	 0.2390
B	 0.8500	 0.2250
C	 0.6900	 0.1520
D	 0.8640	 0.2490
E	 0.8460	 0.2250
F	 0.7350	 0.1730
G	 0.8690	 0.2310
H	 0.8490	 0.2390
I	 0.7280	 0.1610
J	 0.8670	 0.2440
K	 0.8460	 0.2420
L	 0.7420	 0.1980
M	 0.4320	 0.1670
N	 0.3160	 0.1630
O	 0.3950	 0.1420
P	 0.3260	 0.1540
Q	 0.2500	 0.1370
R	 0.2240	 0.0880
S	 0.1970	 0.0670
T	 0.1550	 0.0530

