



Full wwPDB EM Validation Report ⓘ

May 5, 2025 – 05:17 AM EDT

PDB ID : 8UA9 / pdb_00008ua9
EMDB ID : EMD-42055
Title : Structure of eastern equine encephalitis virus VLP unliganded quasi-threefold spike protein
Authors : Abraham, J.; Yang, P.; Li, W.; Fan, X.; Pan, J.
Deposited on : 2023-09-20
Resolution : 3.00 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.43.1

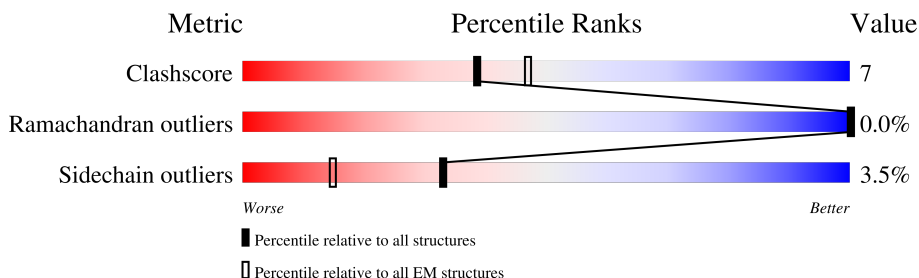
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	
1	E	441	
1	I	441	
1	M	441	
2	B	418	
2	F	418	
2	J	418	
2	N	418	

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Mol	Chain	Length	Quality of chain
3	C	54	<div><div></div><div>6%</div><div>78%</div><div>20%</div><div></div></div>
3	G	54	<div><div></div><div>7%</div><div>85%</div><div>11%</div><div></div></div>
3	K	54	<div><div></div><div>13%</div><div>69%</div><div>30%</div><div></div></div>
3	O	54	<div><div></div><div>11%</div><div>93%</div><div>6%</div><div></div></div>
4	D	260	<div><div></div><div></div><div>41%</div><div>15%</div><div></div><div>42%</div></div>
4	H	260	<div><div></div><div></div><div>40%</div><div>17%</div><div></div><div>42%</div></div>
4	L	260	<div><div></div><div></div><div>40%</div><div>16%</div><div></div><div>42%</div></div>
4	P	260	<div><div></div><div></div><div>40%</div><div>17%</div><div></div><div>42%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 33106 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 Envelope glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		
1	E	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		
1	I	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		
1	M	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		

- Molecule 2 is a protein called Structural polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	418	Total	C	N	O	S	0	0
			3284	2079	594	587	24		
2	F	418	Total	C	N	O	S	0	0
			3284	2079	594	587	24		
2	J	418	Total	C	N	O	S	0	0
			3284	2079	594	587	24		
2	N	418	Total	C	N	O	S	0	0
			3284	2079	594	587	24		

- Molecule 3 is a protein called Structural polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	54	Total	C	N	O	S	0	0
			422	262	68	83	9		
3	G	54	Total	C	N	O	S	0	0
			422	262	68	83	9		
3	K	54	Total	C	N	O	S	0	0
			422	262	68	83	9		
3	O	54	Total	C	N	O	S	0	0
			422	262	68	83	9		

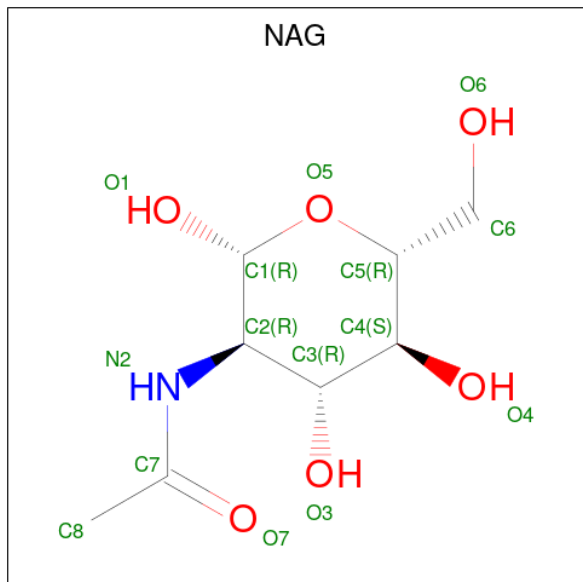
- Molecule 4 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	151	Total 1164	C 734	N 207	O 219	S 4	0	0
4	H	151	Total 1164	C 734	N 207	O 219	S 4	0	0
4	L	151	Total 1164	C 734	N 207	O 219	S 4	0	0
4	P	151	Total 1164	C 734	N 207	O 219	S 4	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	51	ASN	SER	conflict	UNP Q88678
D	?	-	LYS	deletion	UNP Q88678
D	75	SER	PRO	conflict	UNP Q88678
D	76	LEU	LYS	conflict	UNP Q88678
D	77	SER	PRO	conflict	UNP Q88678
D	78	LEU	ALA	conflict	UNP Q88678
D	79	ARG	GLN	conflict	UNP Q88678
D	80	ARG	ALA	conflict	UNP Q88678
H	51	ASN	SER	conflict	UNP Q88678
H	?	-	LYS	deletion	UNP Q88678
H	75	SER	PRO	conflict	UNP Q88678
H	76	LEU	LYS	conflict	UNP Q88678
H	77	SER	PRO	conflict	UNP Q88678
H	78	LEU	ALA	conflict	UNP Q88678
H	79	ARG	GLN	conflict	UNP Q88678
H	80	ARG	ALA	conflict	UNP Q88678
L	51	ASN	SER	conflict	UNP Q88678
L	?	-	LYS	deletion	UNP Q88678
L	75	SER	PRO	conflict	UNP Q88678
L	76	LEU	LYS	conflict	UNP Q88678
L	77	SER	PRO	conflict	UNP Q88678
L	78	LEU	ALA	conflict	UNP Q88678
L	79	ARG	GLN	conflict	UNP Q88678
L	80	ARG	ALA	conflict	UNP Q88678
P	51	ASN	SER	conflict	UNP Q88678
P	?	-	LYS	deletion	UNP Q88678
P	75	SER	PRO	conflict	UNP Q88678
P	76	LEU	LYS	conflict	UNP Q88678
P	77	SER	PRO	conflict	UNP Q88678
P	78	LEU	ALA	conflict	UNP Q88678
P	79	ARG	GLN	conflict	UNP Q88678
P	80	ARG	ALA	conflict	UNP Q88678

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

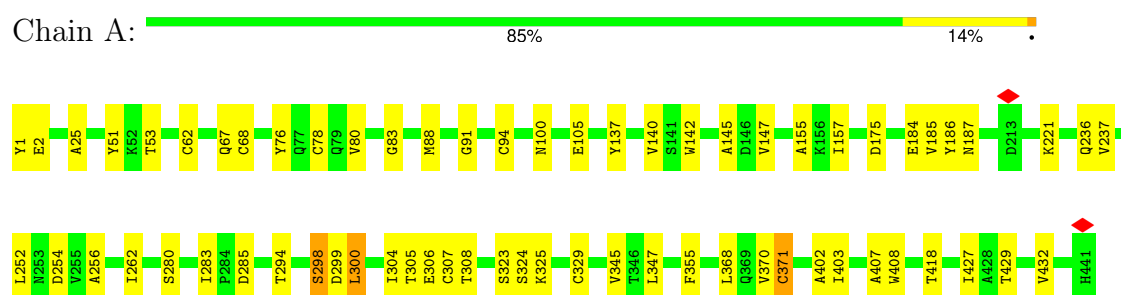


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	M	1	Total	C	N	O	0
			14	8	1	5	
5	N	1	Total	C	N	O	0
			14	8	1	5	

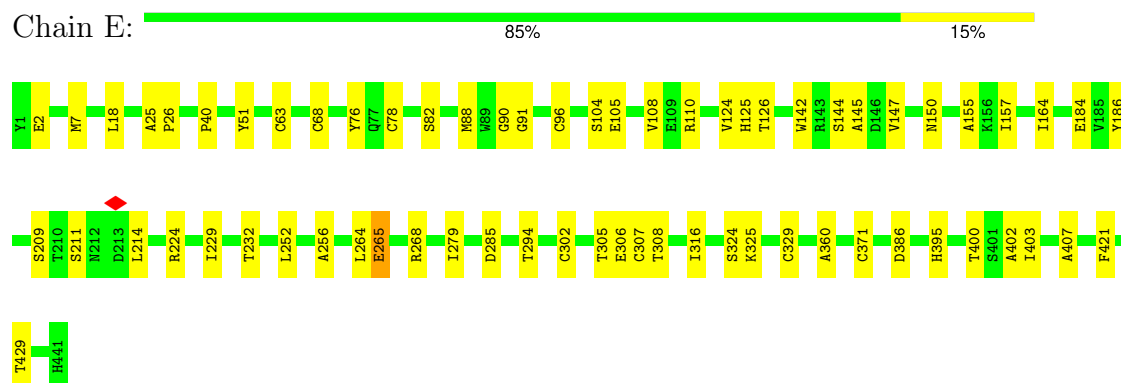
3 Residue-property plots

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.

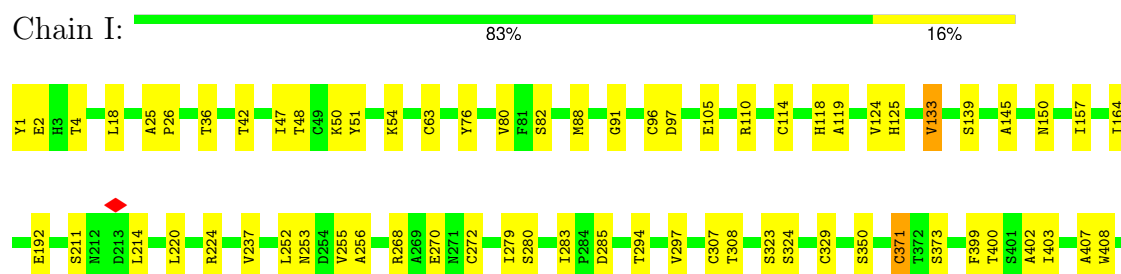
- Molecule 1: Envelope glycoprotein E1

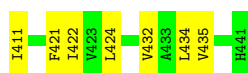


- Molecule 1: Envelope glycoprotein E1



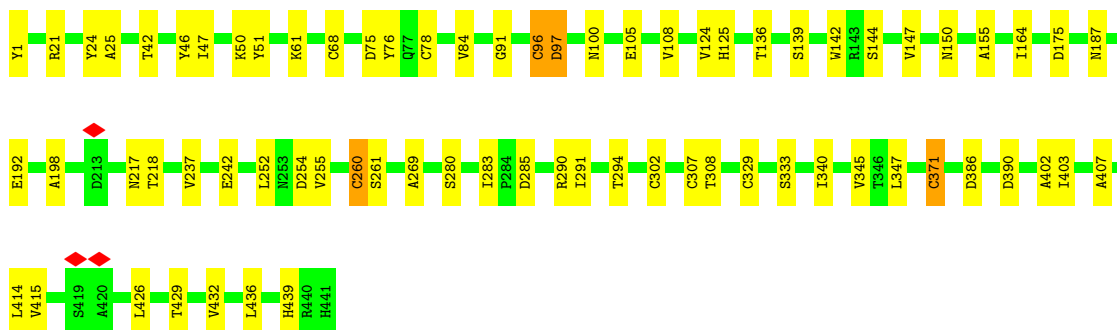
- Molecule 1: Envelope glycoprotein E1





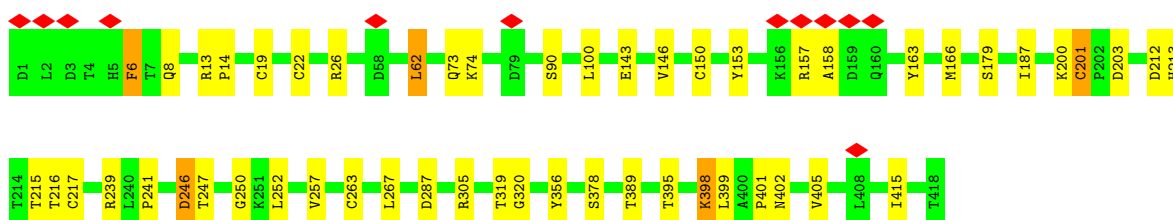
- Molecule 1: Envelope glycoprotein E1

Chain M: 84% 15%



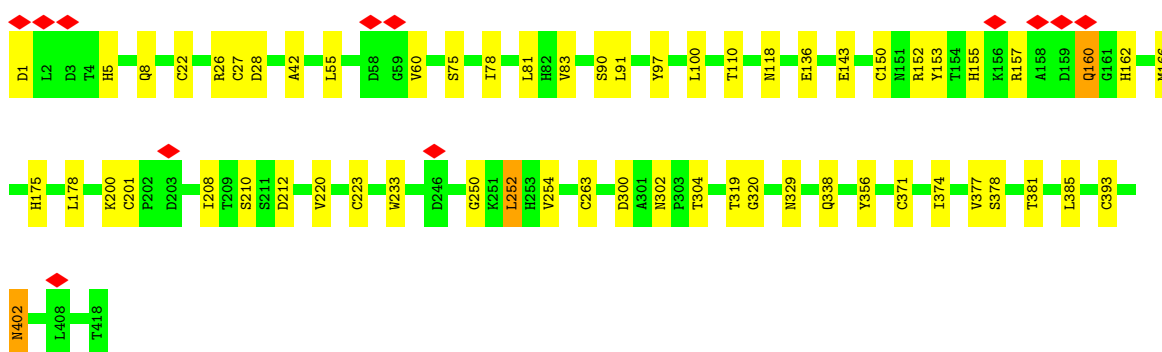
- Molecule 2: Structural polypeptide

Chain B: 87% 11%



- Molecule 2: Structural polypeptide

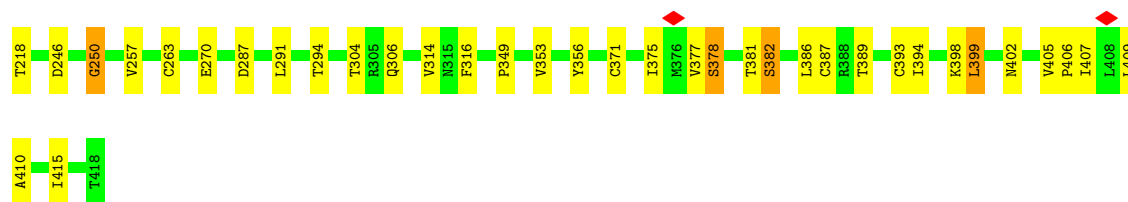
Chain F: 86% 14%



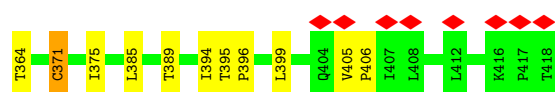
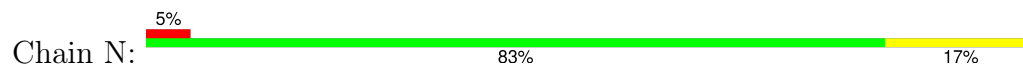
- Molecule 2: Structural polypeptide

Chain J: 84% 14%

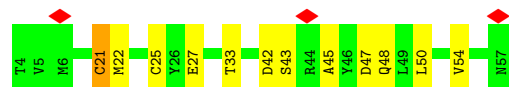
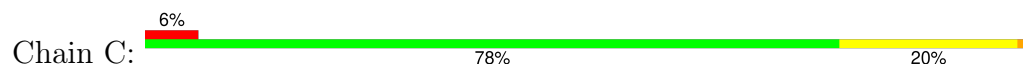




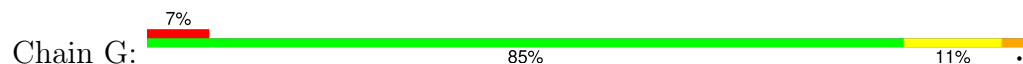
- Molecule 2: Structural polypeptide



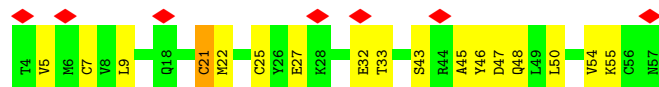
- Molecule 3: Structural polypeptide



- Molecule 3: Structural polypeptide



- Molecule 3: Structural polypeptide

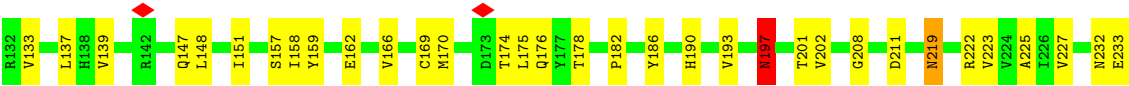
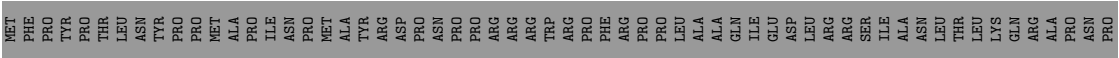


- Molecule 3: Structural polypeptide





● Molecule 4: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.981	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	330.71997, 330.71997, 330.71997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.65	0/3469	0.70	0/4734
1	E	0.64	0/3469	0.69	0/4734
1	I	0.62	0/3469	0.65	0/4734
1	M	0.63	0/3469	0.68	1/4734 (0.0%)
2	B	0.58	0/3379	0.66	2/4609 (0.0%)
2	F	0.57	0/3379	0.68	2/4609 (0.0%)
2	J	0.59	0/3379	0.69	1/4609 (0.0%)
2	N	0.60	0/3379	0.73	0/4609
3	C	0.45	0/431	0.78	0/588
3	G	0.44	0/431	0.82	0/588
3	K	0.47	0/431	0.77	0/588
3	O	0.41	0/431	0.76	0/588
4	D	0.60	0/1191	0.83	1/1615 (0.1%)
4	H	0.53	0/1191	0.79	0/1615
4	L	0.53	0/1191	0.83	2/1615 (0.1%)
4	P	0.60	0/1191	0.88	1/1615 (0.1%)
All	All	0.60	0/33880	0.71	10/46184 (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	E	0	2
1	M	0	1
2	B	0	3
2	F	0	1
2	J	0	3
2	N	0	2
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1
4	D	0	1
4	P	0	1
All	All	0	16

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	255	PRO	CA-N-CD	-10.61	97.15	112.00
2	B	401	PRO	CA-N-CD	-8.30	100.38	112.00
4	D	182	PRO	CA-N-CD	-6.86	102.39	112.00
1	M	260	CYS	CA-CB-SG	6.46	129.25	114.40
4	L	163	TYR	CA-CB-CG	-6.31	102.55	113.90
2	J	250	GLY	N-CA-C	6.01	127.43	113.18
4	P	197	ASN	CA-CB-CG	5.91	118.51	112.60
2	F	201	CYS	N-CA-C	-5.89	101.72	110.20
2	F	160	GLN	N-CA-C	5.61	118.14	110.24
2	B	398	LYS	CA-CB-CG	5.18	124.45	114.10

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	157	ARG	Peptide
2	B	200	LYS	Peptide
2	B	201	CYS	Peptide
3	C	21	CYS	Peptide
4	D	199	ARG	Sidechain
1	E	264	LEU	Peptide
1	E	265	GLU	Peptide
2	F	200	LYS	Peptide
2	J	157	ARG	Peptide
2	J	200	LYS	Peptide
2	J	201	CYS	Peptide
3	K	21	CYS	Peptide
1	M	91	GLY	Peptide
2	N	201	CYS	Peptide
2	N	310	ARG	Sidechain
4	P	236	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3375	0	3286	42	0
1	E	3375	0	3286	41	0
1	I	3375	0	3290	37	0
1	M	3375	0	3288	40	0
2	B	3284	0	3255	31	0
2	F	3284	0	3251	36	0
2	J	3284	0	3255	39	0
2	N	3284	0	3255	37	0
3	C	422	0	397	11	0
3	G	422	0	394	6	0
3	K	422	0	399	14	0
3	O	422	0	399	2	0
4	D	1164	0	1146	33	0
4	H	1164	0	1146	33	0
4	L	1164	0	1146	34	0
4	P	1164	0	1146	40	0
5	A	14	0	13	2	0
5	B	14	0	13	0	0
5	E	14	0	13	2	0
5	F	14	0	13	0	0
5	G	14	0	13	0	0
5	I	14	0	13	1	0
5	J	14	0	13	0	0
5	M	14	0	13	1	0
5	N	14	0	13	1	0
All	All	33106	0	32456	441	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 7.

All (441) 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:I:63:CYS:SG	1:I:96:CYS:HB2	2.09	0.92
4:L:202:VAL:HG13	4:L:239:LEU:HD11	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:197:ASN:O	4:P:197:ASN:ND2	2.08	0.84
1:E:82:SER:O	1:E:224:ARG:NH2	2.11	0.83
3:O:21:CYS:HG	3:O:25:CYS:HG	0.89	0.83
1:E:63:CYS:SG	1:E:96:CYS:HB2	2.19	0.82
3:C:25:CYS:O	3:C:33:THR:OG1	1.98	0.81
2:F:136:GLU:OE1	2:F:329:ASN:ND2	2.14	0.81
3:K:25:CYS:O	3:K:33:THR:OG1	1.98	0.81
3:K:22:MET:SD	3:K:55:LYS:NZ	2.55	0.80
4:P:197:ASN:HD22	4:P:197:ASN:C	1.91	0.79
1:A:329:CYS:SG	1:A:371:CYS:CB	2.71	0.79
1:M:402:ALA:O	2:N:356:TYR:OH	2.00	0.79
1:A:300:LEU:HD21	1:A:370:VAL:HG12	1.64	0.79
1:I:2:GLU:OE2	1:I:280:SER:OG	2.00	0.79
1:I:82:SER:O	1:I:224:ARG:NH2	2.17	0.78
1:M:68:CYS:HG	1:M:78:CYS:HG	0.78	0.77
4:D:252:LYS:NZ	4:D:254:THR:OG1	2.19	0.76
2:N:344:ASN:ND2	2:N:345:PRO:O	2.19	0.76
1:M:75:ASP:OD2	1:M:218:THR:OG1	2.05	0.75
4:H:211:ASP:OD1	4:H:214:ARG:NH1	2.20	0.74
1:I:88:MET:O	1:I:91:GLY:N	2.20	0.74
4:P:116:ILE:HD11	4:P:139:VAL:HG22	1.69	0.74
2:J:38:GLY:O	2:J:131:ARG:NH1	2.21	0.74
4:H:182:PRO:O	4:H:186:TYR:OH	2.04	0.73
1:A:88:MET:O	1:A:91:GLY:N	2.22	0.73
4:D:255:PRO:O	4:D:258:SER:OG	2.07	0.73
2:J:163:TYR:OH	3:K:47:ASP:OD1	2.07	0.72
1:I:150:ASN:ND2	1:M:192:GLU:OE1	2.22	0.72
4:D:225:ALA:HB1	4:D:241:VAL:CG2	2.20	0.72
4:L:178:THR:OG1	4:L:222:ARG:NE	2.22	0.71
2:B:166:MET:HE2	2:B:252:LEU:HD12	1.70	0.71
4:D:225:ALA:HB1	4:D:241:VAL:HG21	1.72	0.71
2:B:399:LEU:HD21	4:D:163:TYR:CE1	2.24	0.71
2:F:143:GLU:O	2:J:26:ARG:NH2	2.23	0.71
4:H:202:VAL:HG13	4:H:239:LEU:HD11	1.71	0.71
1:I:145:ALA:HB3	1:I:157:ILE:HG12	1.73	0.71
3:G:27:GLU:N	3:G:27:GLU:OE1	2.23	0.71
1:E:329:CYS:SG	1:E:371:CYS:HB2	2.30	0.71
2:N:22:CYS:SG	2:N:27:CYS:HB3	2.31	0.70
1:I:192:GLU:OE2	1:M:150:ASN:ND2	2.24	0.70
4:H:255:PRO:O	4:H:258:SER:OG	2.09	0.70
2:J:294:THR:HG1	2:J:304:THR:HG1	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:ALA:HB3	2:F:152:ARG:HH12	1.57	0.70
4:P:158:ILE:HG23	4:P:159:TYR:HD1	1.56	0.70
1:A:137:TYR:O	1:A:140:VAL:HG22	1.92	0.70
4:H:225:ALA:HB1	4:H:241:VAL:CG2	2.23	0.69
3:C:21:CYS:SG	3:C:25:CYS:HB2	2.33	0.69
4:P:129:VAL:HG22	4:P:223:VAL:HG11	1.76	0.68
1:A:175:ASP:OD1	1:A:187:ASN:ND2	2.27	0.68
4:H:121:GLN:OE1	4:H:121:GLN:N	2.25	0.68
1:I:307:CYS:SG	1:I:308:THR:N	2.67	0.68
1:A:307:CYS:SG	1:A:308:THR:N	2.66	0.67
2:J:150:CYS:SG	2:J:263:CYS:N	2.67	0.67
1:I:329:CYS:SG	1:I:371:CYS:CB	2.82	0.67
2:F:160:GLN:NE2	2:F:254:VAL:O	2.27	0.67
2:J:399:LEU:HB3	4:L:250:THR:HG21	1.75	0.67
2:N:395:THR:HG23	2:N:396:PRO:HD3	1.77	0.67
1:A:76:TYR:OH	1:A:105:GLU:OE1	2.12	0.67
3:K:46:TYR:HE2	3:K:50:LEU:HD12	1.59	0.67
1:M:50:LYS:NZ	1:M:242:GLU:OE1	2.26	0.67
4:L:225:ALA:HB1	4:L:241:VAL:CG2	2.24	0.66
4:H:216:ILE:HD13	4:H:227:VAL:HG13	1.78	0.66
1:E:145:ALA:HB3	1:E:157:ILE:HG12	1.77	0.66
4:P:133:VAL:HG13	4:P:166:VAL:HG12	1.76	0.66
2:J:166:MET:O	2:J:250:GLY:N	2.30	0.65
2:B:166:MET:O	2:B:250:GLY:N	2.29	0.65
1:I:323:SER:OG	1:I:324:SER:N	2.29	0.65
1:M:307:CYS:SG	1:M:308:THR:N	2.69	0.65
4:P:202:VAL:O	4:P:237:THR:OG1	2.09	0.65
1:A:300:LEU:HD21	1:A:370:VAL:CG1	2.27	0.65
3:C:27:GLU:OE1	3:C:27:GLU:N	2.30	0.65
2:J:406:PRO:O	2:J:409:LEU:N	2.29	0.65
1:E:307:CYS:SG	1:E:308:THR:N	2.69	0.65
4:L:178:THR:HG22	4:L:180:ASP:H	1.61	0.65
1:E:76:TYR:OH	1:E:105:GLU:OE1	2.14	0.65
2:F:166:MET:O	2:F:250:GLY:N	2.30	0.65
4:P:225:ALA:HB1	4:P:241:VAL:CG1	2.27	0.65
2:B:163:TYR:OH	3:C:47:ASP:OD1	2.10	0.64
4:D:199:ARG:HD2	4:D:238:ALA:HB1	1.79	0.64
2:F:178:LEU:HD21	2:F:223:CYS:O	1.97	0.64
1:I:110:ARG:NH2	1:I:211:SER:O	2.30	0.64
1:A:221:LYS:NZ	2:J:270:GLU:OE2	2.26	0.64
3:G:21:CYS:SG	3:G:22:MET:N	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:10:LYS:NZ	3:K:54:VAL:O	2.31	0.64
1:I:402:ALA:O	2:J:356:TYR:OH	2.13	0.64
4:P:158:ILE:HG23	4:P:159:TYR:CD1	2.33	0.64
2:N:201:CYS:O	2:N:203:ASP:N	2.30	0.64
2:N:219:ASP:OD1	2:N:220:VAL:N	2.30	0.64
1:A:51:TYR:OH	1:A:237:VAL:O	2.16	0.63
2:J:399:LEU:HD11	4:L:163:TYR:CZ	2.33	0.63
1:E:184:GLU:OE1	1:E:186:TYR:OH	2.14	0.63
1:M:76:TYR:OH	1:M:105:GLU:OE1	2.11	0.63
2:J:398:LYS:O	4:L:132:ARG:NH1	2.32	0.63
1:I:76:TYR:OH	1:I:105:GLU:OE1	2.11	0.62
3:C:21:CYS:HB2	3:C:25:CYS:HB3	1.81	0.62
1:M:25:ALA:HB2	1:M:294:THR:HG21	1.82	0.62
4:P:151:ILE:O	4:P:151:ILE:HD12	2.00	0.62
1:E:7:MET:HE2	1:E:279:ILE:HG21	1.81	0.62
3:K:27:GLU:N	3:K:27:GLU:OE1	2.33	0.62
4:L:142:ARG:NH1	4:L:143:ILE:O	2.32	0.62
2:B:399:LEU:HD22	4:D:134:PHE:CZ	2.35	0.62
1:A:329:CYS:SG	1:A:371:CYS:HB2	2.38	0.62
2:B:143:GLU:O	2:F:26:ARG:NH2	2.33	0.62
2:F:162:HIS:O	2:F:254:VAL:HG12	2.00	0.61
2:J:377:VAL:O	2:J:381:THR:HG23	2.00	0.61
2:B:26:ARG:NH2	2:J:143:GLU:O	2.33	0.61
1:M:24:TYR:OH	1:M:290:ARG:NH2	2.34	0.61
1:A:145:ALA:HB3	1:A:157:ILE:HG12	1.83	0.61
2:F:150:CYS:SG	2:F:263:CYS:N	2.74	0.61
1:E:110:ARG:NH2	1:E:211:SER:O	2.33	0.60
1:E:144:SER:O	1:E:144:SER:OG	2.18	0.60
4:H:244:TRP:CD1	4:H:250:THR:HG22	2.36	0.60
2:F:1:ASP:O	2:F:5:HIS:ND1	2.34	0.60
2:N:178:LEU:HD11	2:N:223:CYS:O	2.01	0.60
4:L:204:ARG:NE	4:L:234:GLY:O	2.33	0.60
3:K:9:LEU:HD21	3:K:32:GLU:OE2	2.02	0.60
2:B:399:LEU:HD21	4:D:163:TYR:CD1	2.36	0.60
3:K:46:TYR:CE2	3:K:50:LEU:HD12	2.37	0.60
1:A:147:VAL:HG12	1:A:155:ALA:CB	2.32	0.60
4:P:225:ALA:HB1	4:P:241:VAL:HG13	1.83	0.59
1:I:63:CYS:SG	1:I:96:CYS:CB	2.88	0.59
2:N:3:ASP:O	2:N:7:THR:OG1	2.15	0.59
1:M:329:CYS:SG	1:M:371:CYS:N	2.76	0.59
2:N:152:ARG:HG3	2:N:261:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:CYS:SG	2:B:263:CYS:N	2.75	0.59
1:I:42:THR:HG22	1:I:124:VAL:HG12	1.85	0.59
1:E:403:ILE:O	1:E:407:ALA:HB3	2.03	0.59
1:M:439:HIS:NE2	4:P:249:VAL:HG21	2.18	0.59
4:D:244:TRP:CD1	4:D:250:THR:HG22	2.38	0.58
1:E:25:ALA:HB2	1:E:294:THR:HG21	1.84	0.58
4:H:225:ALA:HB1	4:H:241:VAL:HG21	1.85	0.58
4:P:232:ASN:HA	4:P:237:THR:HG22	1.84	0.58
1:E:18:LEU:HD22	1:E:26:PRO:HB2	1.86	0.58
1:I:403:ILE:O	1:I:407:ALA:HB3	2.03	0.58
4:L:225:ALA:HB1	4:L:241:VAL:HG21	1.85	0.58
3:G:22:MET:HA	3:G:22:MET:HE2	1.86	0.58
1:I:51:TYR:OH	1:I:237:VAL:O	2.20	0.58
4:D:259:GLU:OE1	4:D:259:GLU:N	2.34	0.58
1:M:147:VAL:HG12	1:M:155:ALA:CB	2.34	0.58
1:E:265:GLU:O	1:E:268:ARG:NH1	2.37	0.57
3:K:22:MET:HE2	3:K:22:MET:HA	1.87	0.57
4:P:128:VAL:HG22	4:P:174:THR:HG23	1.86	0.57
4:D:145:ASN:HB3	4:D:148:LEU:HD13	1.86	0.57
1:A:137:TYR:CE2	1:A:140:VAL:HG21	2.40	0.56
4:D:229:GLY:N	4:D:240:SER:OG	2.38	0.56
1:I:18:LEU:HD22	1:I:26:PRO:HB2	1.87	0.56
2:J:349:PRO:O	2:J:353:VAL:HG23	2.05	0.56
1:M:218:THR:O	1:M:237:VAL:HG22	2.05	0.56
4:P:176:GLN:O	4:P:223:VAL:HG12	2.05	0.56
4:D:118:LEU:HD13	4:D:123:ASN:ND2	2.20	0.56
1:M:198:ALA:HB2	1:M:217:ASN:OD1	2.06	0.56
2:N:146:VAL:HG13	2:N:148:LEU:HD13	1.87	0.56
2:N:276:LYS:NZ	5:N:501:NAG:O6	2.38	0.56
2:F:42:ALA:HB3	2:F:152:ARG:NH1	2.21	0.56
4:P:148:LEU:HD21	4:P:170:MET:SD	2.46	0.55
1:M:42:THR:HG22	1:M:124:VAL:HG12	1.89	0.55
1:I:329:CYS:SG	1:I:371:CYS:HB2	2.46	0.55
4:L:182:PRO:O	4:L:186:TYR:OH	2.07	0.55
1:A:402:ALA:O	2:B:356:TYR:OH	2.20	0.55
2:B:158:ALA:HB3	2:B:257:VAL:HG21	1.89	0.55
4:D:245:ASN:O	4:D:248:GLY:N	2.37	0.55
4:D:232:ASN:OD1	4:D:232:ASN:N	2.40	0.55
4:P:116:ILE:HD11	4:P:139:VAL:CG2	2.37	0.55
4:D:204:ARG:NH2	4:D:234:GLY:O	2.38	0.55
3:K:45:ALA:HB1	3:K:48:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:51:TYR:OH	1:M:237:VAL:O	2.23	0.55
2:J:200:LYS:HE3	2:J:204:VAL:HG22	1.88	0.55
4:D:142:ARG:NH1	4:D:143:ILE:O	2.40	0.55
4:P:208:GLY:N	4:P:211:ASP:OD2	2.40	0.55
4:P:133:VAL:CG1	4:P:166:VAL:HG12	2.37	0.54
2:F:233:TRP:NE1	3:G:38:GLU:OE2	2.41	0.54
2:J:394:ILE:HG22	2:J:415:ILE:HD11	1.90	0.54
1:E:402:ALA:O	2:F:356:TYR:OH	2.17	0.54
2:J:201:CYS:O	2:J:203:ASP:N	2.41	0.54
1:M:96:CYS:O	1:M:100:ASN:ND2	2.41	0.54
2:N:9:TYR:CD1	2:N:52:MET:HE1	2.43	0.53
2:N:85:THR:OG1	2:N:103:CYS:SG	2.66	0.53
2:B:319:THR:OG1	2:B:320:GLY:N	2.40	0.53
1:E:142:TRP:CZ2	5:E:501:NAG:H82	2.43	0.53
2:F:166:MET:SD	2:F:252:LEU:HD12	2.49	0.53
1:I:25:ALA:HB2	1:I:294:THR:HG21	1.90	0.53
2:N:405:VAL:HG12	2:N:406:PRO:O	2.08	0.53
4:L:225:ALA:HB1	4:L:241:VAL:HG22	1.89	0.53
2:B:405:VAL:HG11	2:B:415:ILE:HG21	1.89	0.53
4:P:131:GLY:N	4:P:174:THR:HG21	2.24	0.53
1:E:104:SER:HB2	1:E:232:THR:HG23	1.89	0.53
1:M:136:THR:HG23	1:M:142:TRP:CE3	2.43	0.53
1:A:67:GLN:HA	1:A:80:VAL:HG21	1.89	0.53
4:L:158:ILE:HG23	4:L:159:TYR:CD1	2.44	0.53
1:I:164:ILE:HG13	1:I:279:ILE:HG22	1.91	0.52
1:A:252:LEU:O	1:A:256:ALA:HB2	2.09	0.52
4:L:131:GLY:H	4:L:174:THR:HG21	1.75	0.52
1:M:345:VAL:HG23	1:M:347:LEU:HD11	1.91	0.52
4:P:190:HIS:NE2	4:P:211:ASP:OD1	2.41	0.52
4:D:131:GLY:O	4:D:166:VAL:HG22	2.10	0.52
2:F:97:TYR:HE2	2:F:166:MET:HE1	1.75	0.52
2:J:207:GLY:C	2:J:208:ILE:HD13	2.35	0.52
3:C:22:MET:HE2	3:C:22:MET:HA	1.91	0.52
1:E:147:VAL:HG12	1:E:155:ALA:CB	2.40	0.52
2:F:28:ASP:OD1	2:F:28:ASP:N	2.42	0.52
1:I:1:TYR:N	1:I:283:ILE:O	2.42	0.52
4:L:244:TRP:CE3	4:L:250:THR:HG22	2.44	0.52
2:N:189:VAL:HG13	2:N:193:ALA:O	2.10	0.52
2:N:350:HIS:NE2	2:N:351:GLU:OE2	2.43	0.52
1:A:305:THR:HG22	1:A:306:GLU:H	1.74	0.52
1:A:403:ILE:O	1:A:407:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:CYS:SG	1:E:371:CYS:CB	2.98	0.51
4:L:229:GLY:N	4:L:240:SER:OG	2.43	0.51
2:B:187:ILE:HD13	2:B:215:THR:HG23	1.93	0.51
1:M:97:ASP:OD1	1:M:97:ASP:N	2.42	0.51
1:A:254:ASP:OD1	1:A:254:ASP:N	2.44	0.51
1:A:432:VAL:HG11	2:B:389:THR:OG1	2.11	0.51
5:E:501:NAG:O7	5:E:501:NAG:O3	2.25	0.51
4:P:178:THR:HG21	4:P:222:ARG:NH1	2.26	0.51
2:F:78:ILE:HG23	2:F:81:LEU:HB2	1.92	0.51
4:H:158:ILE:HG23	4:H:159:TYR:CD2	2.46	0.50
2:N:6:PHE:CZ	2:N:62:LEU:HD22	2.45	0.50
2:N:199:CYS:SG	2:N:215:THR:HG21	2.51	0.50
4:L:216:ILE:HD13	4:L:227:VAL:HG13	1.93	0.50
4:D:147:GLN:CG	4:D:148:LEU:HD12	2.41	0.50
1:E:40:PRO:HB2	1:E:124:VAL:HG13	1.94	0.50
2:F:300:ASP:OD1	2:F:302:ASN:N	2.45	0.50
2:J:291:LEU:HD12	2:J:306:GLN:O	2.12	0.50
5:I:501:NAG:O7	5:I:501:NAG:O3	2.24	0.49
3:O:22:MET:HA	3:O:22:MET:HE2	1.94	0.49
2:B:100:LEU:HD11	2:B:153:TYR:HB2	1.94	0.49
4:D:219:ASN:OD1	4:D:219:ASN:N	2.42	0.49
4:H:259:GLU:OE1	4:H:259:GLU:N	2.45	0.49
1:M:403:ILE:O	1:M:407:ALA:HB3	2.11	0.49
2:B:395:THR:HA	2:B:398:LYS:HB3	1.94	0.49
2:J:213:HIS:CE1	2:J:215:THR:HG22	2.47	0.49
2:N:319:THR:HG22	2:N:320:GLY:H	1.78	0.49
4:H:170:MET:SD	4:H:170:MET:N	2.85	0.49
1:A:25:ALA:HB2	1:A:294:THR:HG21	1.94	0.49
4:D:123:ASN:N	4:D:123:ASN:OD1	2.46	0.49
2:N:22:CYS:SG	2:N:27:CYS:CB	3.01	0.49
1:I:252:LEU:HA	1:I:255:VAL:HG22	1.95	0.49
1:A:68:CYS:HB3	1:A:78:CYS:SG	2.52	0.49
4:L:228:LEU:HD12	4:L:241:VAL:HA	1.95	0.48
1:I:422:ILE:HD11	2:J:378:SER:OG	2.14	0.48
4:D:133:VAL:HG23	4:D:166:VAL:HG12	1.95	0.48
4:H:116:ILE:HD12	4:H:116:ILE:H	1.78	0.48
1:A:62:CYS:HG	1:A:94:CYS:HG	0.95	0.48
2:F:377:VAL:O	2:F:381:THR:HG23	2.13	0.48
1:M:108:VAL:HG11	1:M:218:THR:HG21	1.96	0.48
1:E:429:THR:OG1	2:F:385:LEU:HD21	2.13	0.48
4:H:116:ILE:HD12	4:H:124:GLY:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:216:ILE:CD1	4:H:227:VAL:HG13	2.42	0.48
2:J:39:ASP:OD1	2:J:39:ASP:N	2.42	0.48
4:L:116:ILE:HD12	4:L:124:GLY:O	2.14	0.48
1:M:21:ARG:NH2	1:M:285:ASP:OD2	2.45	0.48
1:E:252:LEU:O	1:E:256:ALA:HB2	2.13	0.48
1:E:316:ILE:HD12	1:M:291:ILE:HG21	1.95	0.48
3:C:42:ASP:N	3:C:42:ASP:OD1	2.47	0.48
2:B:146:VAL:HG13	2:B:267:LEU:HD13	1.95	0.47
2:B:399:LEU:CB	4:D:250:THR:HG21	2.44	0.47
2:F:83:VAL:HG23	2:F:91:LEU:HD21	1.97	0.47
1:I:54:LYS:NZ	2:J:165:GLU:OE2	2.35	0.47
4:H:147:GLN:NE2	4:H:170:MET:HE2	2.29	0.47
4:L:228:LEU:HD11	4:L:242:VAL:HG23	1.96	0.47
1:A:185:VAL:HG21	1:A:262:ILE:HG21	1.95	0.47
5:A:501:NAG:O7	5:A:501:NAG:O3	2.31	0.47
1:I:252:LEU:O	1:I:256:ALA:HB2	2.12	0.47
1:M:333:SER:HB3	1:M:340:ILE:HD13	1.95	0.47
2:N:284:LEU:HD23	2:N:327:TRP:CZ3	2.49	0.47
1:E:150:ASN:OD1	1:E:150:ASN:N	2.45	0.47
4:L:193:VAL:HG13	4:L:202:VAL:HG12	1.97	0.47
1:M:1:TYR:N	1:M:283:ILE:O	2.46	0.47
4:D:116:ILE:HD12	4:D:124:GLY:O	2.15	0.47
4:H:203:PRO:O	4:H:206:VAL:HG22	2.15	0.47
2:J:382:SER:O	2:J:386:LEU:HD23	2.15	0.47
4:P:124:GLY:HA3	4:P:139:VAL:HG21	1.96	0.47
2:B:100:LEU:HD11	2:B:153:TYR:CB	2.45	0.47
4:H:229:GLY:N	4:H:240:SER:OG	2.47	0.47
2:J:200:LYS:O	2:J:200:LYS:HG3	2.15	0.47
2:J:210:SER:O	2:J:210:SER:OG	2.33	0.47
2:N:371:CYS:O	2:N:375:ILE:HG23	2.14	0.47
2:B:213:HIS:CE1	2:B:215:THR:HG22	2.50	0.47
2:B:399:LEU:HB3	4:D:250:THR:HG21	1.96	0.47
4:L:203:PRO:O	4:L:206:VAL:HG22	2.14	0.47
5:M:501:NAG:O7	5:M:501:NAG:O3	2.31	0.47
2:N:385:LEU:O	2:N:389:THR:HG23	2.15	0.47
4:H:172:SER:OG	4:P:233:GLU:O	2.19	0.47
2:J:407:ILE:HD12	2:J:410:ALA:HB3	1.96	0.47
2:N:166:MET:H	2:N:250:GLY:HA3	1.79	0.47
4:L:123:ASN:OD1	4:L:123:ASN:N	2.48	0.46
1:M:260:CYS:SG	1:M:269:ALA:HB1	2.54	0.46
1:A:1:TYR:N	1:A:283:ILE:O	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:285:ASP:N	1:I:285:ASP:OD2	2.48	0.46
1:A:80:VAL:HG12	1:A:80:VAL:O	2.15	0.46
1:E:68:CYS:HB3	1:E:78:CYS:SG	2.55	0.46
1:M:175:ASP:OD1	1:M:187:ASN:ND2	2.49	0.46
4:L:127:CYS:SG	4:L:226:ILE:HD13	2.55	0.46
4:P:182:PRO:O	4:P:186:TYR:OH	2.23	0.46
4:H:131:GLY:O	4:H:166:VAL:HG22	2.15	0.46
4:P:169:CYS:SG	4:P:170:MET:N	2.88	0.46
1:A:2:GLU:OE2	1:A:280:SER:OG	2.29	0.46
4:D:147:GLN:HG3	4:D:148:LEU:HD12	1.98	0.46
4:P:227:VAL:HA	4:P:241:VAL:HG22	1.97	0.46
1:A:53:THR:OG1	1:A:236:GLN:NE2	2.45	0.46
2:N:65:MET:HE1	2:N:113:PHE:CG	2.51	0.45
1:E:305:THR:HG22	1:E:306:GLU:H	1.81	0.45
4:H:118:LEU:HD23	4:H:140:GLU:OE2	2.16	0.45
4:D:218:ASP:OD1	4:D:224:VAL:HG23	2.17	0.45
1:M:414:LEU:HD23	1:M:415:VAL:N	2.31	0.45
2:B:212:ASP:N	2:B:212:ASP:OD1	2.48	0.45
1:E:285:ASP:N	1:E:285:ASP:OD1	2.46	0.45
1:I:97:ASP:OD1	1:I:97:ASP:N	2.50	0.45
4:L:245:ASN:O	4:L:248:GLY:N	2.42	0.45
2:N:357:TYR:HA	2:N:364:THR:HG21	1.97	0.45
4:H:232:ASN:OD1	4:H:232:ASN:N	2.49	0.45
2:J:212:ASP:N	2:J:212:ASP:OD1	2.48	0.45
1:A:83:GLY:N	1:A:100:ASN:O	2.49	0.45
4:H:240:SER:OG	4:H:240:SER:O	2.30	0.45
3:K:5:VAL:HG21	3:K:45:ALA:HB2	1.97	0.45
4:D:213:GLY:O	4:D:226:ILE:HD11	2.17	0.45
2:J:371:CYS:O	2:J:375:ILE:HG23	2.16	0.45
1:M:386:ASP:O	2:N:338:GLN:NE2	2.50	0.45
4:P:112:LYS:CG	4:P:175:LEU:HD11	2.46	0.45
4:L:244:TRP:HE3	4:L:250:THR:HG22	1.82	0.44
1:A:355:PHE:CE1	1:A:368:LEU:HD22	2.52	0.44
2:F:97:TYR:CE2	2:F:166:MET:HE1	2.52	0.44
4:H:123:ASN:OD1	4:H:123:ASN:N	2.49	0.44
4:H:188:TRP:HB3	4:H:193:VAL:HG23	1.99	0.44
4:H:225:ALA:HB1	4:H:241:VAL:HG22	1.96	0.44
1:I:268:ARG:NE	1:I:270:GLU:OE2	2.45	0.44
2:J:287:ASP:N	2:J:287:ASP:OD1	2.48	0.44
1:A:25:ALA:CB	1:A:294:THR:HG21	2.48	0.44
1:A:345:VAL:HG23	1:A:347:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:OE1	1:A:186:TYR:OH	2.35	0.44
1:E:164:ILE:HG13	1:E:279:ILE:HG22	2.00	0.44
2:F:81:LEU:HD13	2:F:81:LEU:O	2.18	0.44
1:I:18:LEU:HD22	1:I:26:PRO:CB	2.46	0.44
2:J:386:LEU:HA	2:J:389:THR:HG22	2.00	0.44
1:M:144:SER:O	1:M:144:SER:OG	2.20	0.44
1:A:298:SER:OG	1:A:299:ASP:N	2.50	0.44
4:D:216:ILE:HD13	4:D:227:VAL:HG13	1.99	0.44
2:F:100:LEU:HD11	2:F:153:TYR:CB	2.48	0.44
4:L:259:GLU:OE1	4:L:259:GLU:N	2.49	0.44
1:A:329:CYS:SG	1:A:371:CYS:CA	3.06	0.44
2:F:8:GLN:HA	3:G:54:VAL:HG11	2.00	0.44
1:M:252:LEU:HA	1:M:255:VAL:HG22	1.99	0.44
2:B:216:THR:OG1	2:B:217:CYS:N	2.51	0.43
1:E:329:CYS:HG	1:E:371:CYS:HG	1.57	0.43
4:D:118:LEU:HD23	4:D:119:ASN:OD1	2.18	0.43
2:N:9:TYR:HD1	2:N:52:MET:HE1	1.82	0.43
1:A:403:ILE:HG21	1:A:408:TRP:CD2	2.54	0.43
1:E:63:CYS:SG	1:E:96:CYS:CB	3.00	0.43
4:P:137:LEU:HD11	4:P:157:SER:HA	1.99	0.43
4:L:118:LEU:HD23	4:L:123:ASN:HD21	1.83	0.43
1:E:51:TYR:HB2	1:E:108:VAL:HG13	2.00	0.43
1:E:88:MET:O	1:E:91:GLY:N	2.51	0.43
1:E:324:SER:OG	1:E:325:LYS:N	2.51	0.43
1:E:360:ALA:HB2	1:E:395:HIS:CD2	2.54	0.43
1:I:133:VAL:HG23	1:I:157:ILE:HD11	1.99	0.43
4:L:136:PRO:O	4:L:139:VAL:HG22	2.19	0.43
4:L:146:GLU:O	4:L:149:ALA:N	2.51	0.43
2:N:287:ASP:OD1	2:N:287:ASP:N	2.51	0.43
4:P:128:VAL:O	4:P:128:VAL:HG13	2.19	0.43
3:K:50:LEU:O	3:K:54:VAL:HG22	2.18	0.43
2:F:319:THR:OG1	2:F:320:GLY:N	2.52	0.43
4:H:227:VAL:HG12	4:H:241:VAL:HG23	2.01	0.43
1:M:439:HIS:CE1	4:P:249:VAL:HG21	2.53	0.43
2:N:45:ILE:HD11	2:N:103:CYS:SG	2.58	0.43
2:B:287:ASP:OD1	2:B:287:ASP:N	2.50	0.43
1:M:147:VAL:HG21	1:M:164:ILE:HG21	2.00	0.43
4:D:178:THR:HG23	4:D:224:VAL:HG22	2.00	0.42
2:J:189:VAL:HG13	2:J:193:ALA:O	2.19	0.42
2:N:158:ALA:HB3	2:N:257:VAL:HG21	2.00	0.42
1:A:88:MET:HE1	2:B:241:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:402:ASN:OD1	2:F:402:ASN:N	2.52	0.42
4:H:200:PHE:HE2	4:H:216:ILE:HG21	1.84	0.42
2:J:36:VAL:HG22	2:J:47:ILE:HG23	2.00	0.42
4:P:131:GLY:H	4:P:174:THR:HG21	1.83	0.42
1:A:68:CYS:SG	1:A:80:VAL:HG23	2.59	0.42
1:A:285:ASP:N	1:A:285:ASP:OD1	2.52	0.42
2:B:201:CYS:O	2:B:203:ASP:N	2.51	0.42
2:F:371:CYS:HA	2:F:374:ILE:HG22	2.01	0.42
2:N:172:VAL:O	2:N:227:LEU:N	2.52	0.42
1:E:386:ASP:O	2:F:338:GLN:NE2	2.47	0.42
1:M:46:TYR:O	1:M:47:ILE:HD12	2.19	0.42
2:F:22:CYS:CB	2:F:27:CYS:SG	3.06	0.42
1:I:407:ALA:O	1:I:411:ILE:HG13	2.19	0.42
1:M:84:VAL:O	1:M:100:ASN:HB2	2.20	0.42
4:P:193:VAL:HG23	4:P:202:VAL:HG23	2.02	0.42
3:C:45:ALA:HB1	3:C:48:GLN:OE1	2.18	0.42
2:F:100:LEU:HD11	2:F:153:TYR:HB2	2.02	0.42
4:H:132:ARG:NE	4:H:165:ASP:OD1	2.46	0.42
1:I:114:CYS:O	1:I:118:HIS:ND1	2.46	0.42
1:I:297:VAL:HG23	1:I:373:SER:OG	2.19	0.42
4:L:201:THR:HB	4:L:236:ARG:HE	1.85	0.42
3:C:21:CYS:SG	3:C:25:CYS:CB	3.07	0.42
1:I:48:THR:CG2	1:I:119:ALA:HB3	2.49	0.42
4:D:224:VAL:HG12	4:D:224:VAL:O	2.19	0.42
2:F:208:ILE:N	2:F:208:ILE:HD12	2.35	0.42
1:A:324:SER:OG	1:A:325:LYS:N	2.52	0.42
2:B:6:PHE:CE2	2:B:62:LEU:HD22	2.55	0.42
1:E:229:ILE:N	1:E:229:ILE:HD12	2.34	0.42
2:J:405:VAL:O	2:J:407:ILE:N	2.52	0.42
4:P:137:LEU:HD23	4:P:162:GLU:HG3	2.01	0.42
4:D:244:TRP:NE1	4:D:250:THR:HG22	2.35	0.41
1:E:403:ILE:O	2:F:356:TYR:OH	2.38	0.41
2:F:210:SER:O	2:F:210:SER:OG	2.35	0.41
2:F:212:ASP:OD1	2:F:212:ASP:N	2.53	0.41
4:L:255:PRO:HD2	4:L:258:SER:HG	1.84	0.41
2:N:150:CYS:SG	2:N:263:CYS:N	2.93	0.41
4:H:158:ILE:HG23	4:H:159:TYR:CE2	2.55	0.41
1:E:90:GLY:O	2:F:175:HIS:ND1	2.49	0.41
1:M:436:LEU:HD23	4:P:158:ILE:HD11	2.02	0.41
4:P:246:GLN:OE1	4:P:246:GLN:N	2.43	0.41
1:E:125:HIS:O	1:E:126:THR:OG1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:403:ILE:HG21	1:I:408:TRP:CD2	2.55	0.41
3:K:21:CYS:HB3	3:K:25:CYS:HB3	2.03	0.41
1:M:254:ASP:OD1	1:M:254:ASP:N	2.54	0.41
2:B:246:ASP:OD1	2:B:246:ASP:N	2.54	0.41
4:H:215:PRO:C	4:H:216:ILE:HD12	2.46	0.41
3:K:21:CYS:CB	3:K:25:CYS:HB3	2.51	0.41
3:G:50:LEU:O	3:G:54:VAL:HG22	2.20	0.41
4:H:200:PHE:CE2	4:H:216:ILE:HG21	2.55	0.41
4:L:255:PRO:HD2	4:L:255:PRO:O	2.21	0.41
4:P:219:ASN:N	4:P:219:ASN:OD1	2.51	0.41
1:A:142:TRP:CE2	5:A:501:NAG:H82	2.56	0.41
2:B:13:ARG:NH1	2:B:14:PRO:O	2.49	0.41
1:E:214:LEU:HD13	1:E:214:LEU:O	2.21	0.41
1:E:25:ALA:CB	1:E:294:THR:HG21	2.48	0.41
1:I:253:ASN:OD1	1:I:253:ASN:N	2.54	0.41
2:N:39:ASP:OD1	2:N:39:ASP:N	2.43	0.41
2:J:399:LEU:HD11	4:L:163:TYR:CE2	2.55	0.41
2:N:127:LYS:NZ	2:N:129:GLU:OE2	2.54	0.41
2:N:395:THR:HG23	2:N:396:PRO:CD	2.48	0.41
2:B:8:GLN:HA	3:C:54:VAL:HG11	2.03	0.40
4:P:202:VAL:CG2	4:P:239:LEU:HD11	2.52	0.40
3:C:25:CYS:SG	3:C:33:THR:HG23	2.62	0.40
4:H:179:SER:OG	4:H:245:ASN:O	2.35	0.40
4:P:225:ALA:HB1	4:P:241:VAL:HG11	2.03	0.40
2:J:405:VAL:HG12	2:J:406:PRO:HD2	2.02	0.40
1:M:175:ASP:OD1	1:M:175:ASP:N	2.55	0.40
2:N:12:ALA:HB2	2:N:166:MET:HE2	2.04	0.40
4:P:147:GLN:O	4:P:148:LEU:HD23	2.22	0.40
2:J:314:VAL:HG11	2:J:316:PHE:CZ	2.56	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%)	435 (99%)	4 (1%)	0	100	100
1	E	439/441 (100%)	436 (99%)	3 (1%)	0	100	100
1	I	439/441 (100%)	435 (99%)	4 (1%)	0	100	100
1	M	439/441 (100%)	436 (99%)	2 (0%)	1 (0%)	44	77
2	B	416/418 (100%)	411 (99%)	5 (1%)	0	100	100
2	F	416/418 (100%)	411 (99%)	5 (1%)	0	100	100
2	J	416/418 (100%)	409 (98%)	7 (2%)	0	100	100
2	N	416/418 (100%)	412 (99%)	4 (1%)	0	100	100
3	C	52/54 (96%)	49 (94%)	3 (6%)	0	100	100
3	G	52/54 (96%)	50 (96%)	1 (2%)	1 (2%)	6	31
3	K	52/54 (96%)	49 (94%)	3 (6%)	0	100	100
3	O	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	D	149/260 (57%)	149 (100%)	0	0	100	100
4	H	149/260 (57%)	149 (100%)	0	0	100	100
4	L	149/260 (57%)	149 (100%)	0	0	100	100
4	P	149/260 (57%)	149 (100%)	0	0	100	100
All	All	4224/4692 (90%)	4179 (99%)	43 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	22	MET
1	M	371	CYS

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%)	363 (98%)	8 (2%)	47	76
1	E	371/371 (100%)	366 (99%)	5 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	371/371 (100%)	351 (95%)	20 (5%)	18	50
1	M	371/371 (100%)	359 (97%)	12 (3%)	34	67
2	B	366/366 (100%)	352 (96%)	14 (4%)	28	62
2	F	366/366 (100%)	352 (96%)	14 (4%)	28	62
2	J	366/366 (100%)	351 (96%)	15 (4%)	26	60
2	N	366/366 (100%)	356 (97%)	10 (3%)	40	71
3	C	50/50 (100%)	48 (96%)	2 (4%)	27	61
3	G	50/50 (100%)	47 (94%)	3 (6%)	16	47
3	K	50/50 (100%)	48 (96%)	2 (4%)	27	61
3	O	50/50 (100%)	48 (96%)	2 (4%)	27	61
4	D	125/222 (56%)	119 (95%)	6 (5%)	21	55
4	H	125/222 (56%)	118 (94%)	7 (6%)	17	49
4	L	125/222 (56%)	120 (96%)	5 (4%)	27	61
4	P	125/222 (56%)	121 (97%)	4 (3%)	34	67
All	All	3648/4036 (90%)	3519 (96%)	129 (4%)	33	65

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	SER
1	A	300	LEU
1	A	304	ILE
1	A	323	SER
1	A	371	CYS
1	A	418	THR
1	A	427	ILE
1	A	429	THR
2	B	6	PHE
2	B	19	CYS
2	B	22	CYS
2	B	62	LEU
2	B	73	GLN
2	B	74	LYS
2	B	90	SER
2	B	179	SER
2	B	239	ARG
2	B	246	ASP

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Mol	Chain	Res	Type
2	B	247	THR
2	B	305	ARG
2	B	378	SER
2	B	402	ASN
3	C	43	SER
3	C	50	LEU
4	D	155	LYS
4	D	190	HIS
4	D	232	ASN
4	D	252	LYS
4	D	258	SER
4	D	259	GLU
1	E	2	GLU
1	E	209	SER
1	E	302	CYS
1	E	400	THR
1	E	421	PHE
2	F	55	LEU
2	F	60	VAL
2	F	75	SER
2	F	90	SER
2	F	110	THR
2	F	118	ASN
2	F	155	HIS
2	F	157	ARG
2	F	220	VAL
2	F	252	LEU
2	F	304	THR
2	F	378	SER
2	F	393	CYS
2	F	402	ASN
3	G	27	GLU
3	G	35	THR
3	G	43	SER
4	H	119	ASN
4	H	123	ASN
4	H	178	THR
4	H	194	GLN
4	H	228	LEU
4	H	256	GLU
4	H	258	SER
1	I	4	THR

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Mol	Chain	Res	Type
1	I	36	THR
1	I	47	ILE
1	I	50	LYS
1	I	80	VAL
1	I	125	HIS
1	I	133	VAL
1	I	139	SER
1	I	214	LEU
1	I	220	LEU
1	I	272	CYS
1	I	350	SER
1	I	371	CYS
1	I	399	PHE
1	I	400	THR
1	I	421	PHE
1	I	424	LEU
1	I	432	VAL
1	I	434	LEU
1	I	435	VAL
2	J	6	PHE
2	J	19	CYS
2	J	22	CYS
2	J	188	THR
2	J	203	ASP
2	J	208	ILE
2	J	218	THR
2	J	246	ASP
2	J	257	VAL
2	J	378	SER
2	J	382	SER
2	J	387	CYS
2	J	393	CYS
2	J	399	LEU
2	J	402	ASN
3	K	7	CYS
3	K	43	SER
4	L	123	ASN
4	L	228	LEU
4	L	244	TRP
4	L	254	THR
4	L	258	SER
1	M	61	LYS

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Mol	Chain	Res	Type
1	M	96	CYS
1	M	97	ASP
1	M	125	HIS
1	M	139	SER
1	M	261	SER
1	M	280	SER
1	M	302	CYS
1	M	390	ASP
1	M	426	LEU
1	M	429	THR
1	M	432	VAL
2	N	8	GLN
2	N	86	SER
2	N	90	SER
2	N	123	THR
2	N	210	SER
2	N	228	ILE
2	N	305	ARG
2	N	371	CYS
2	N	394	ILE
2	N	399	LEU
3	O	21	CYS
3	O	36	MET
4	P	197	ASN
4	P	201	THR
4	P	219	ASN
4	P	240	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	441	HIS
2	B	114	HIS
2	B	140	HIS
2	B	222	GLN
1	E	43	ASN
1	E	223	GLN
2	F	8	GLN
2	F	162	HIS
2	F	302	ASN
4	H	168	GLN

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Mol	Chain	Res	Type
1	I	219	ASN
2	J	126	HIS
2	J	168	GLN
2	J	275	HIS
2	J	285	HIS
1	M	187	ASN
1	M	328	ASN
2	N	73	GLN
2	N	181	HIS
2	N	230	ASN
2	N	277	HIS
2	N	285	HIS
2	N	344	ASN
4	P	197	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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	501	1	14,14,15	0.62	1 (7%)	17,19,21	0.46	0
5	NAG	I	501	1	14,14,15	0.63	1 (7%)	17,19,21	0.53	0
5	NAG	E	501	1	14,14,15	1.04	1 (7%)	17,19,21	0.55	0
5	NAG	F	501	2	14,14,15	0.40	0	17,19,21	0.43	0
5	NAG	B	501	2	14,14,15	0.38	0	17,19,21	0.42	0
5	NAG	J	501	2	14,14,15	0.48	0	17,19,21	0.40	0
5	NAG	G	101	3	14,14,15	0.27	0	17,19,21	0.37	0
5	NAG	M	501	1	14,14,15	0.89	1 (7%)	17,19,21	0.42	0
5	NAG	N	501	2	14,14,15	0.37	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	I	501	1	-	2/6/23/26	0/1/1/1
5	NAG	E	501	1	-	2/6/23/26	0/1/1/1
5	NAG	F	501	2	-	2/6/23/26	0/1/1/1
5	NAG	B	501	2	-	2/6/23/26	0/1/1/1
5	NAG	J	501	2	-	2/6/23/26	0/1/1/1
5	NAG	G	101	3	-	0/6/23/26	0/1/1/1
5	NAG	M	501	1	-	2/6/23/26	0/1/1/1
5	NAG	N	501	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	501	NAG	O5-C1	-3.74	1.37	1.43
5	M	501	NAG	O5-C1	-3.14	1.38	1.43
5	A	501	NAG	O5-C1	-2.07	1.40	1.43
5	I	501	NAG	O5-C1	-2.07	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	501	NAG	O5-C5-C6-O6
5	J	501	NAG	C4-C5-C6-O6
5	F	501	NAG	O5-C5-C6-O6
5	F	501	NAG	C4-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
5	I	501	NAG	C1-C2-N2-C7
5	M	501	NAG	O5-C5-C6-O6
5	E	501	NAG	C3-C2-N2-C7
5	I	501	NAG	C3-C2-N2-C7
5	A	501	NAG	O5-C5-C6-O6
5	E	501	NAG	C1-C2-N2-C7
5	A	501	NAG	C3-C2-N2-C7
5	M	501	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	NAG	2	0
5	I	501	NAG	1	0
5	E	501	NAG	2	0
5	M	501	NAG	1	0
5	N	501	NAG	1	0

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.

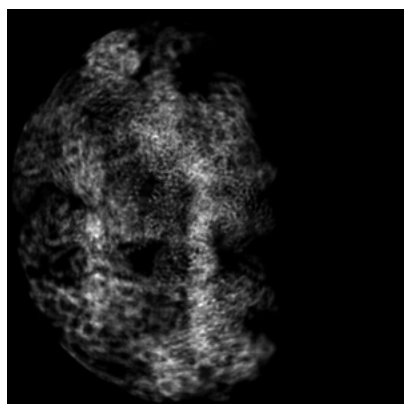
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42055. These allow visual inspection of the internal detail of the map and identification of artifacts.

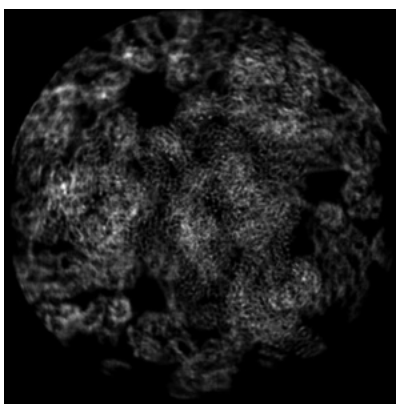
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

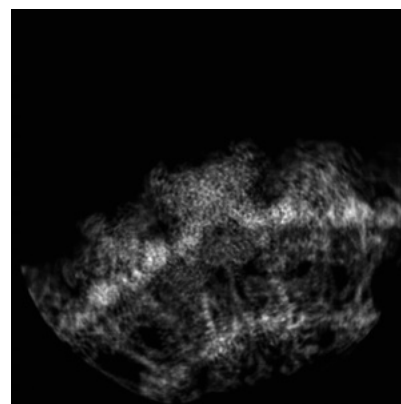
6.1.1 Primary map



X

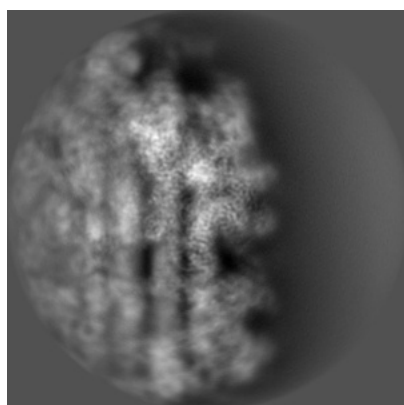


Y

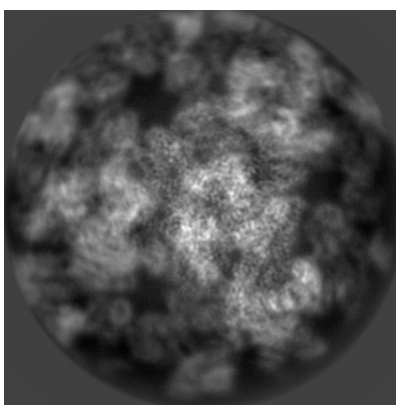


Z

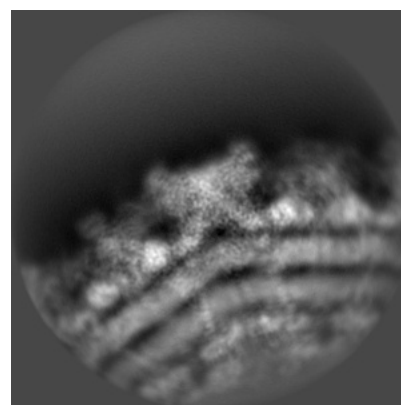
6.1.2 Raw map



X



Y

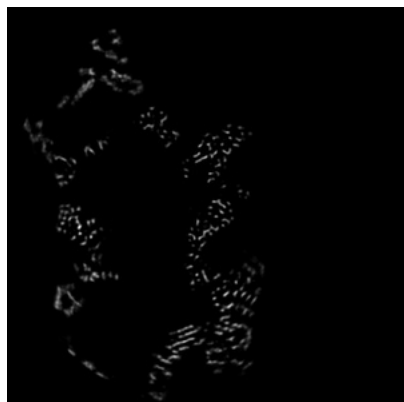


Z

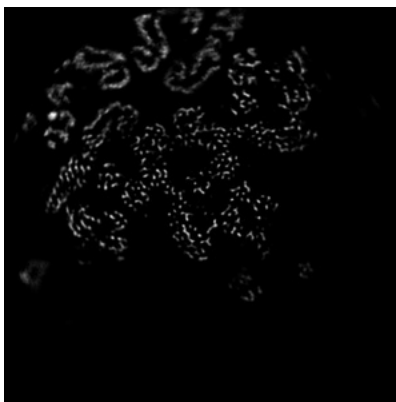
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 156

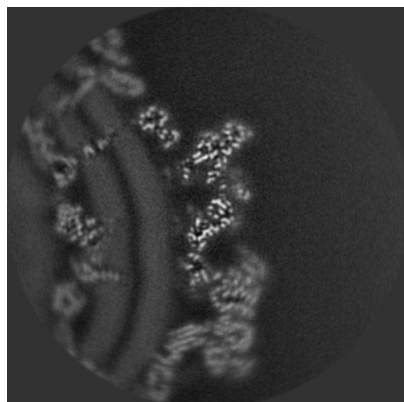


Y Index: 156

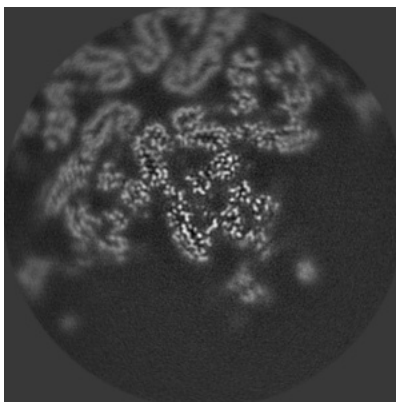


Z Index: 156

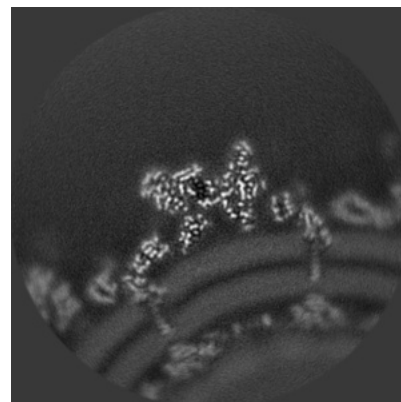
6.2.2 Raw map



X Index: 156



Y Index: 156



Z Index: 156

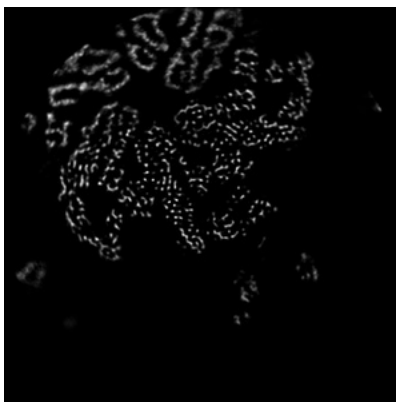
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

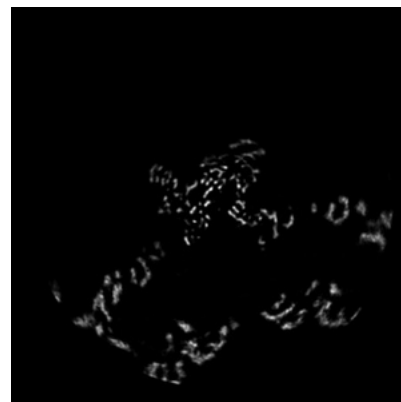
6.3.1 Primary map



X Index: 153

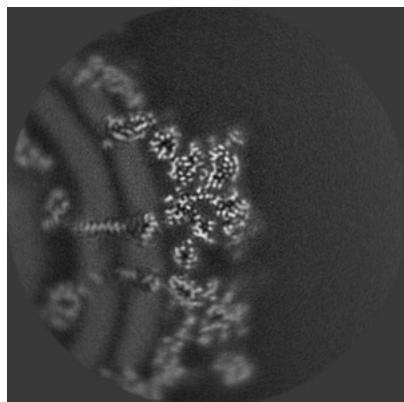


Y Index: 152

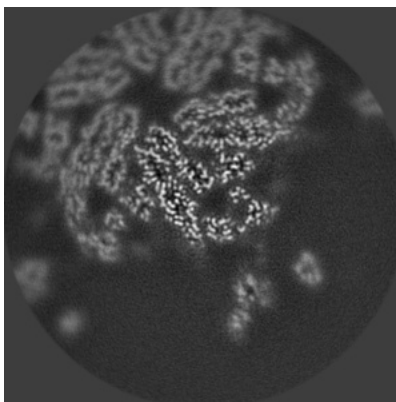


Z Index: 87

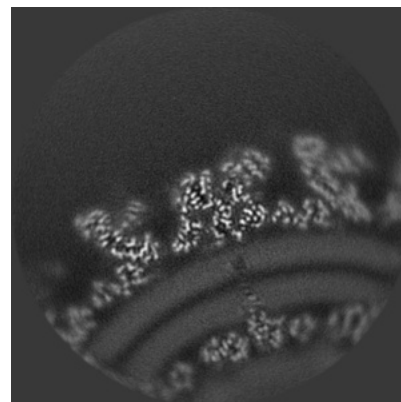
6.3.2 Raw map



X Index: 143



Y Index: 150

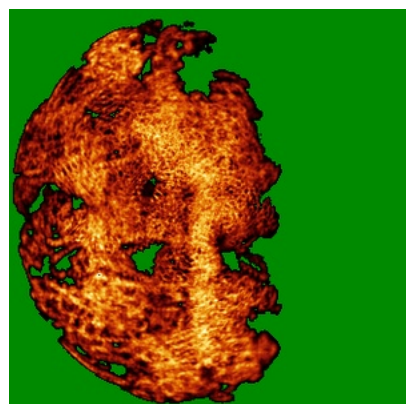


Z Index: 181

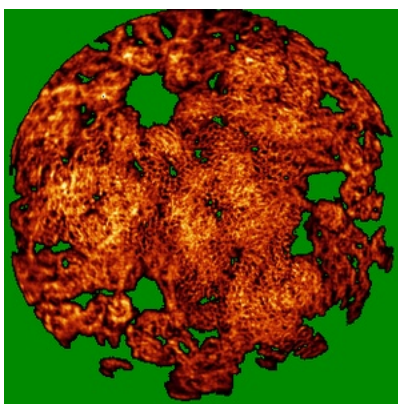
The images above show the largest variance slices of the map in three orthogonal directions.

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

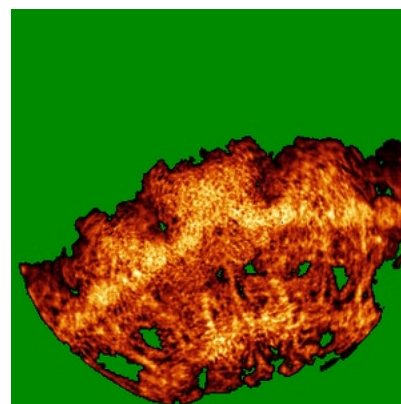
6.4.1 Primary map



X

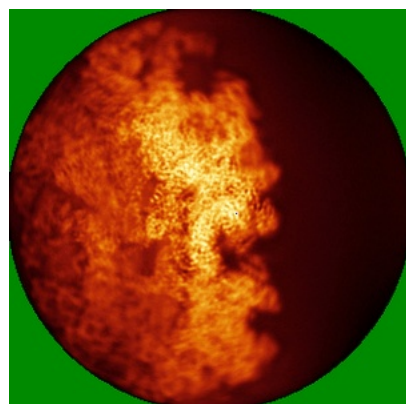


Y

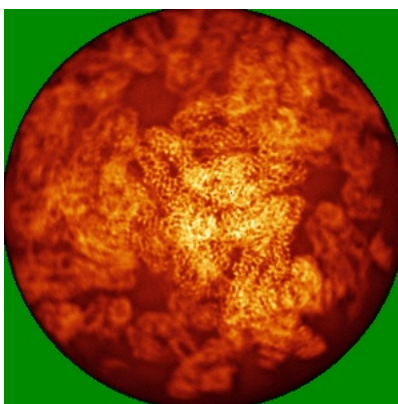


Z

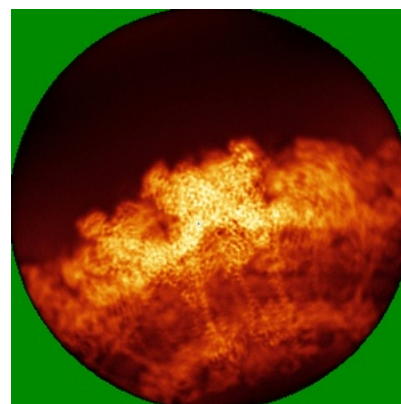
6.4.2 Raw map



X



Y

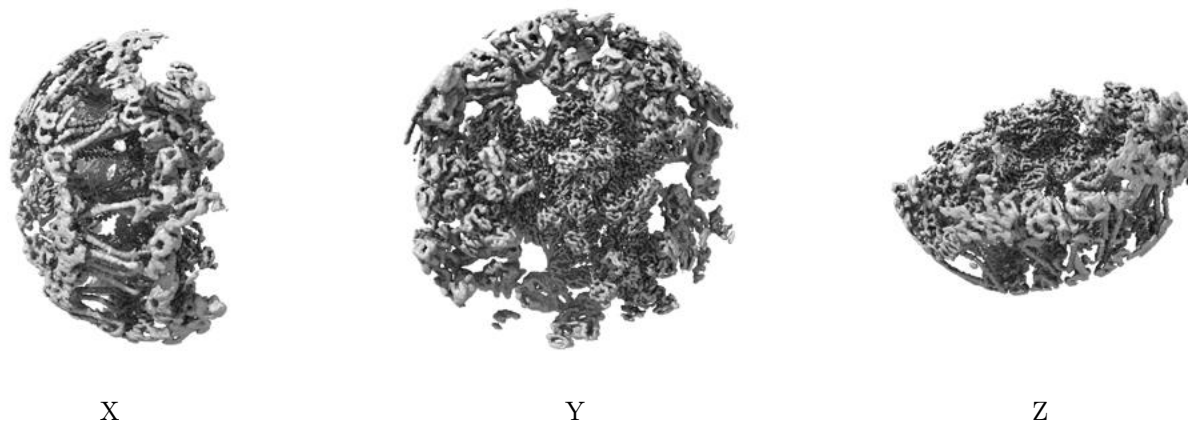


Z

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.

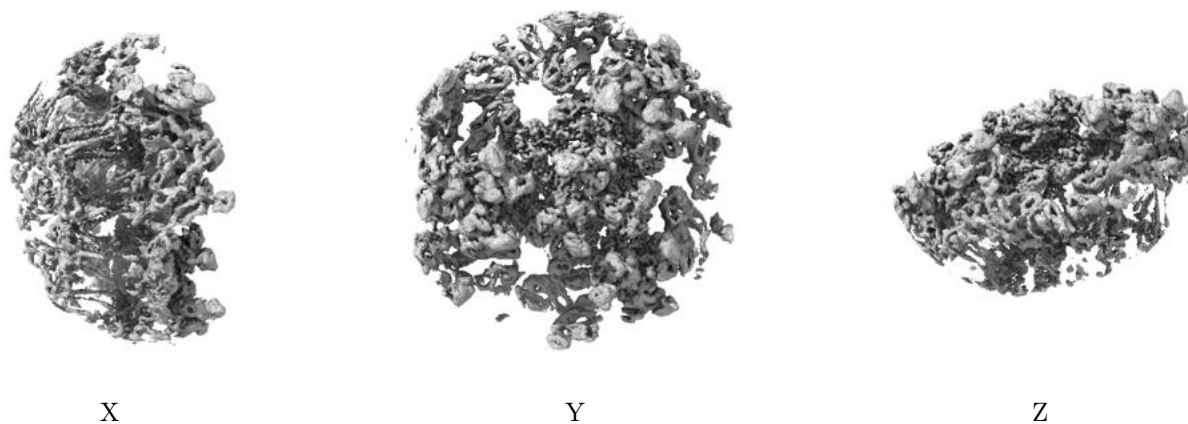
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

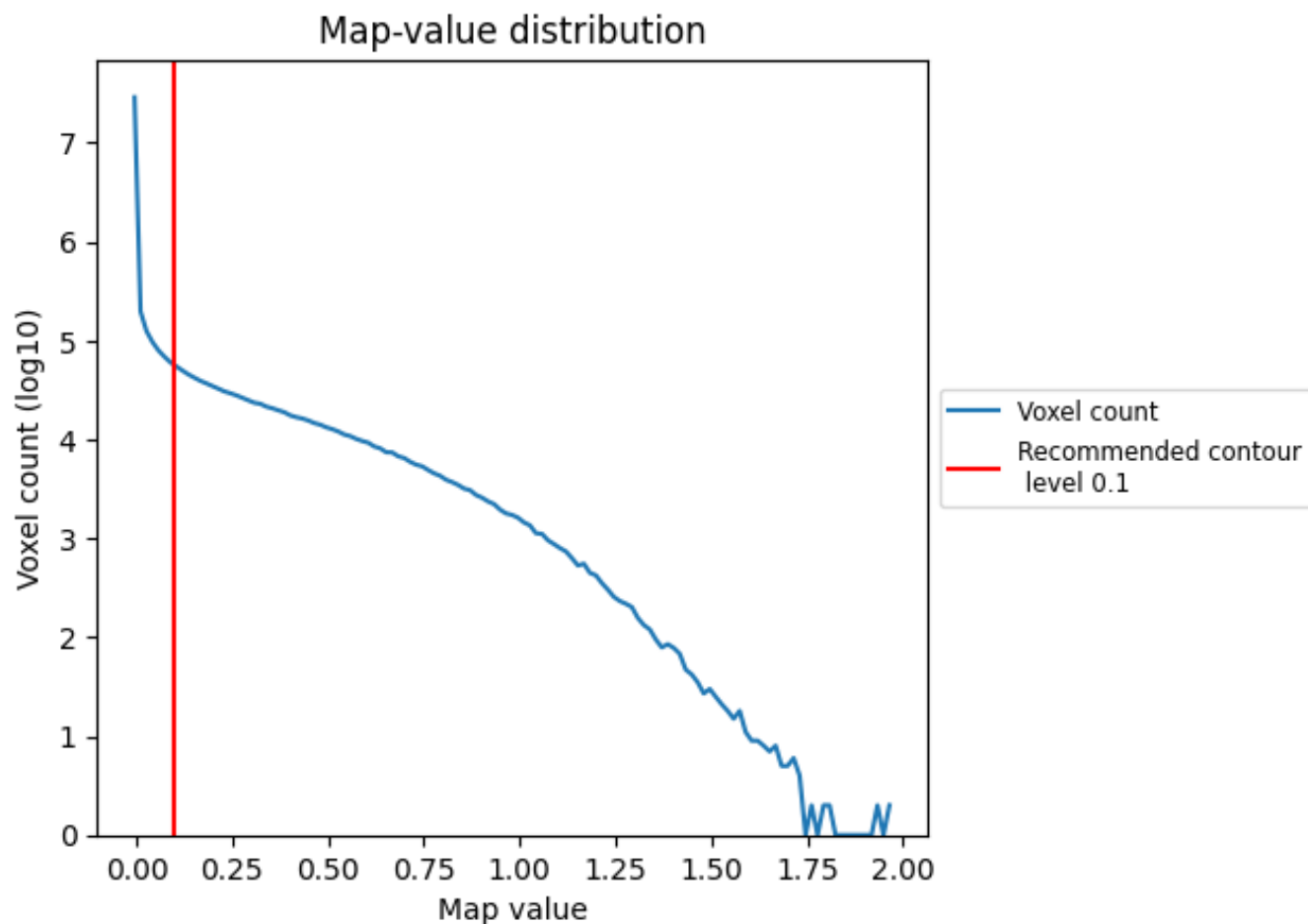
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

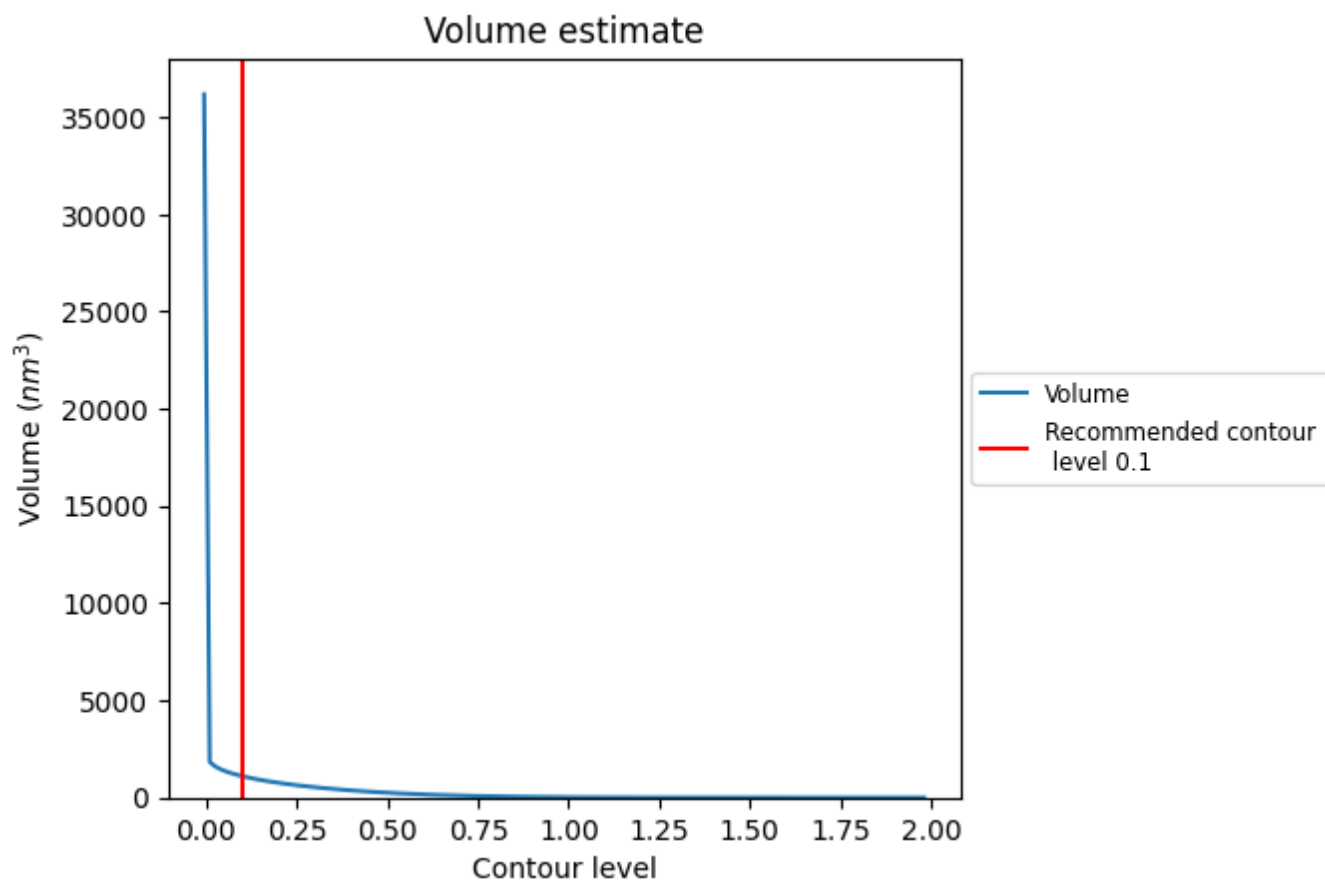
This section contains the results of statistical analysis of the map.

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.

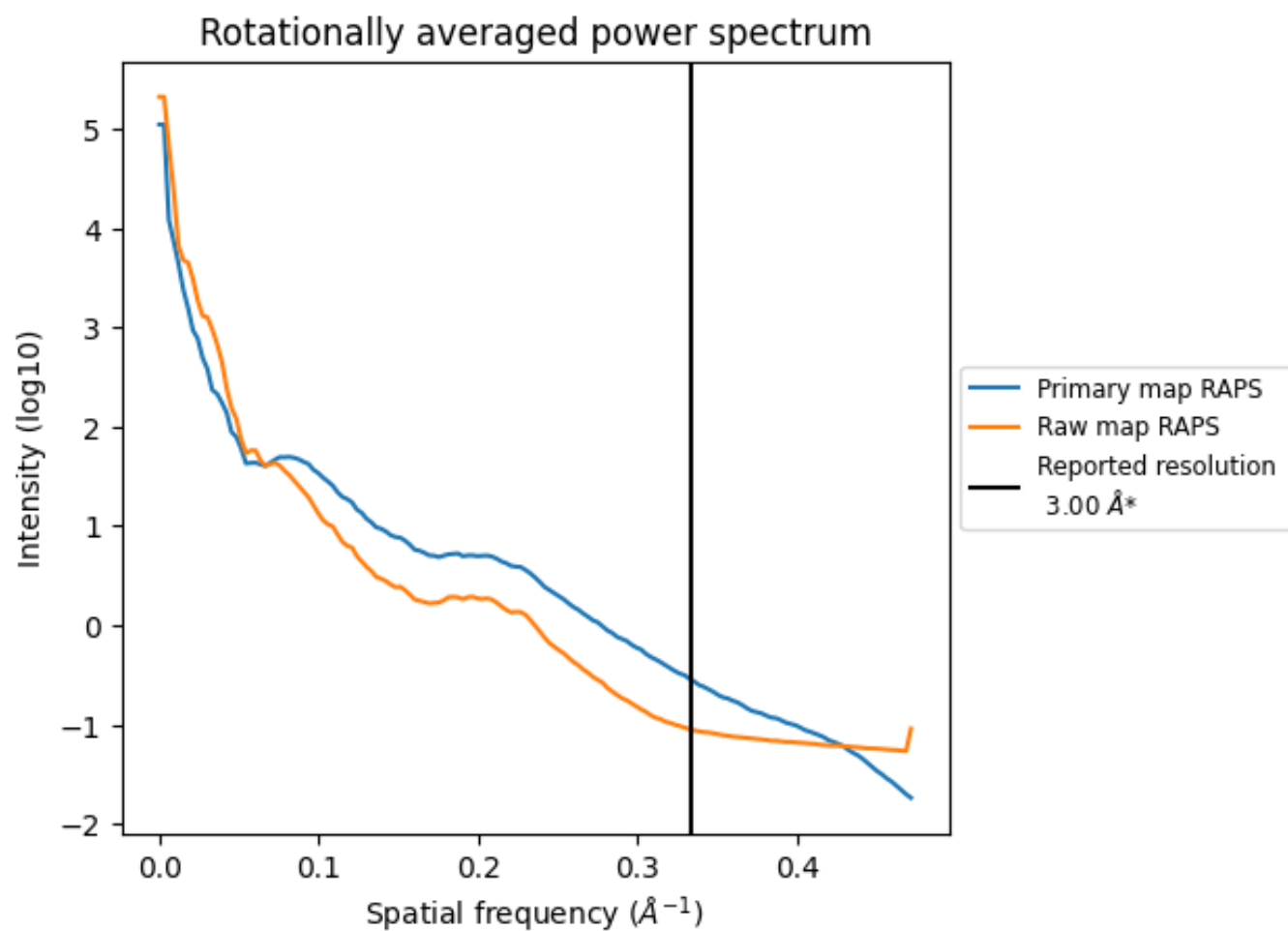
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1101 nm^3 ; this corresponds to an approximate mass of 994 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 ⓘ

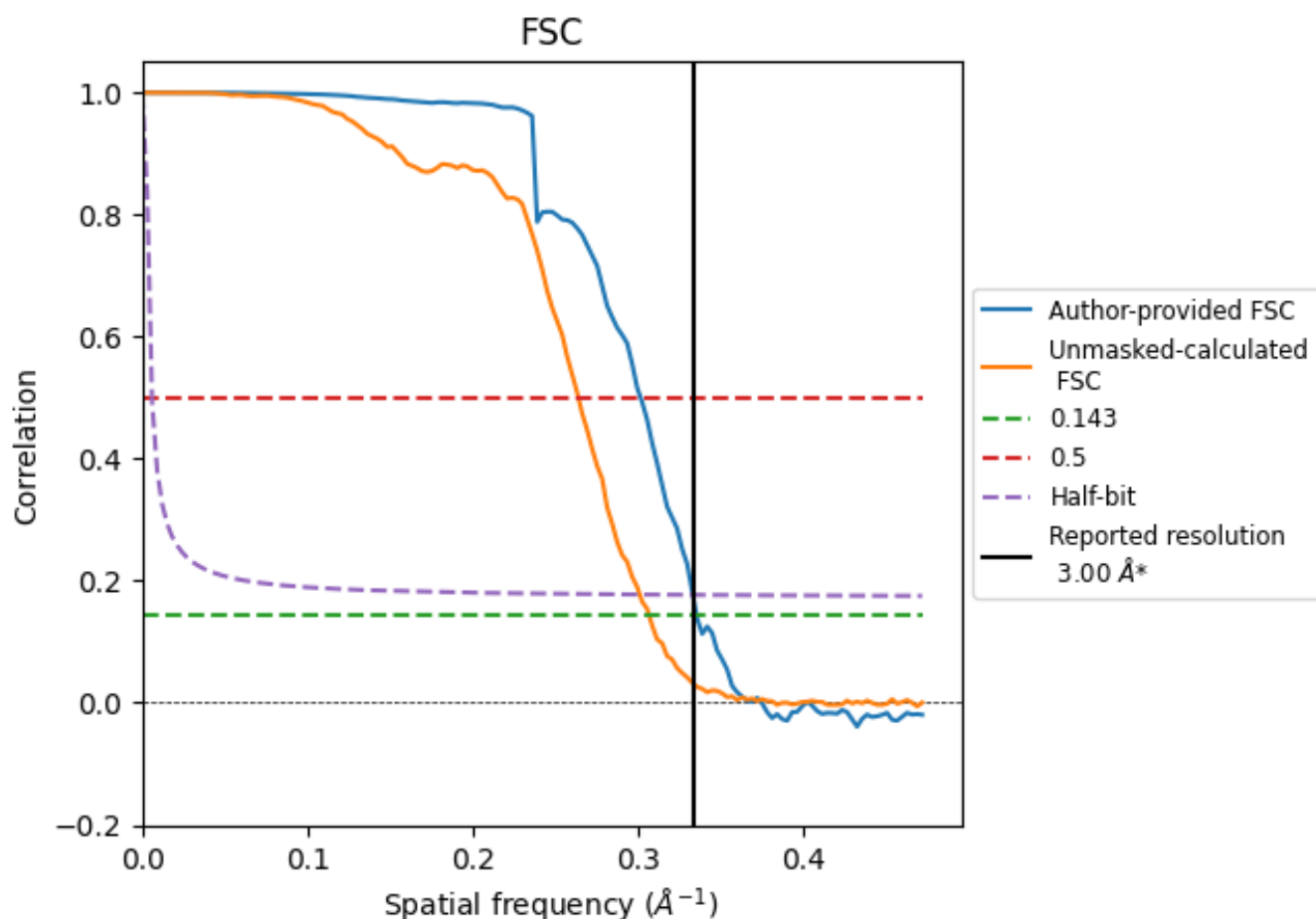


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

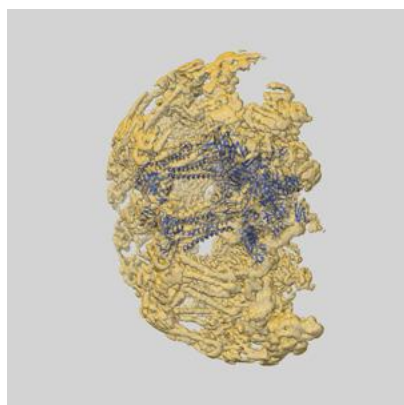
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.32	3.00
Unmasked-calculated*	3.26	3.79	3.32

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

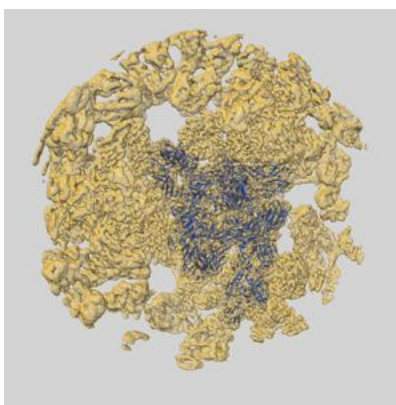
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42055 and PDB model 8UA9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

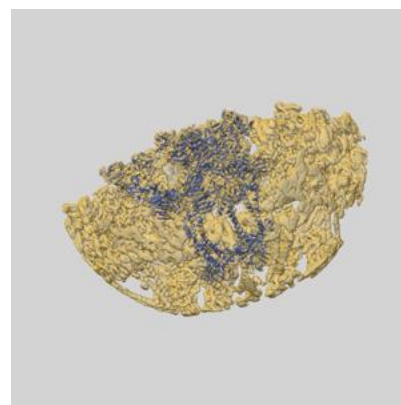
9.1 Map-model overlay [i](#)



X



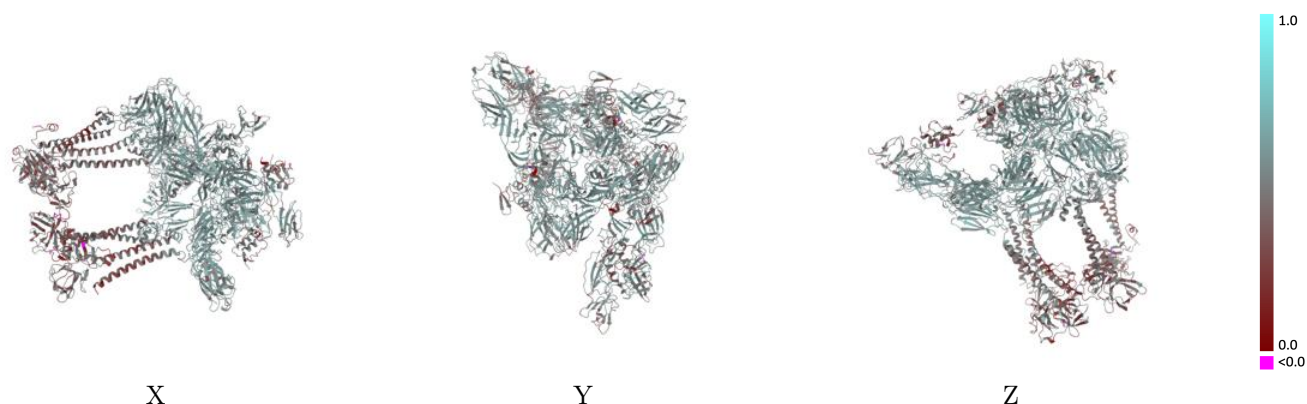
Y



Z

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



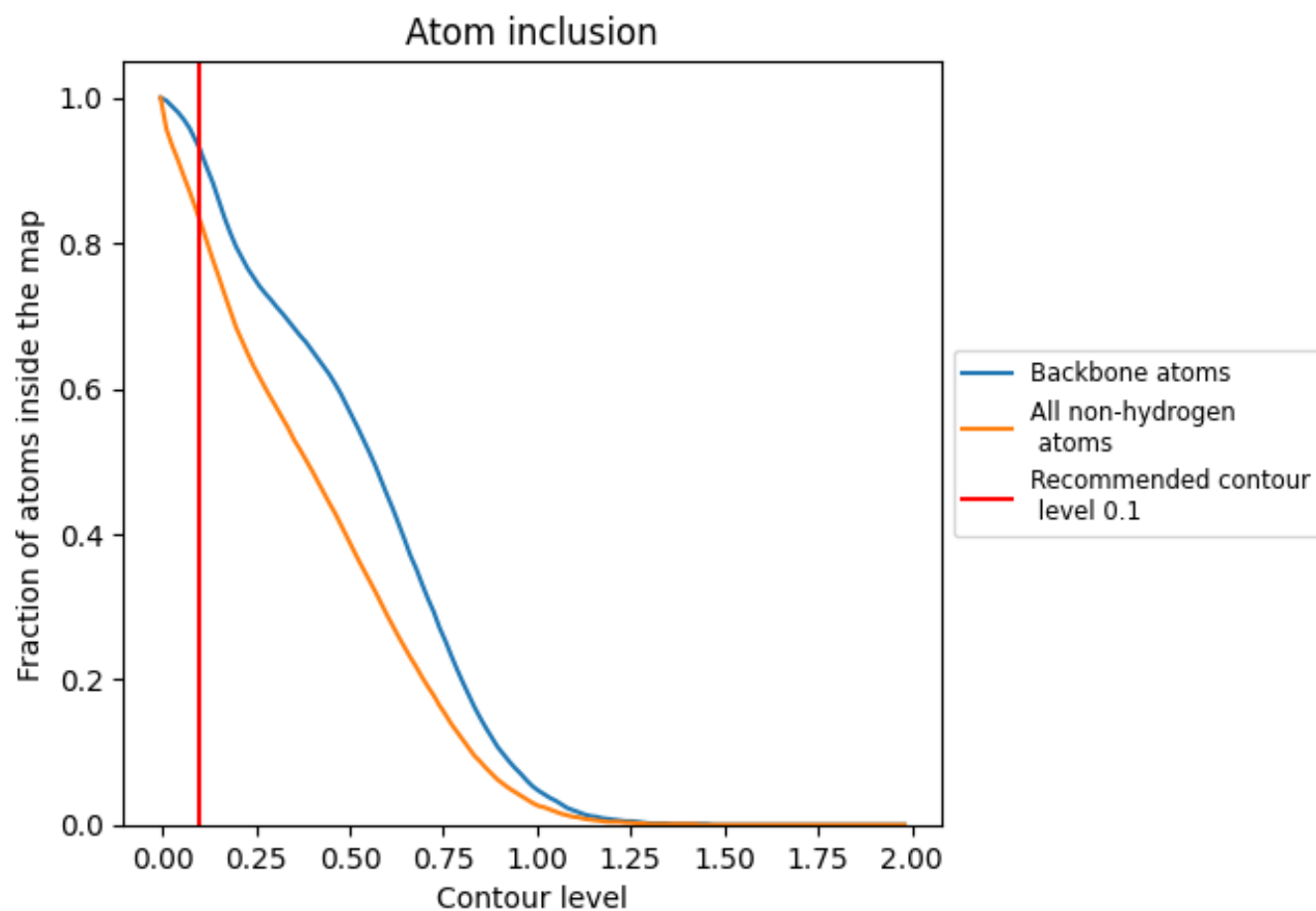
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 83% 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	<div></div> 0.8300	<div></div> 0.5000
A	<div></div> 0.8710	<div></div> 0.5360
B	<div></div> 0.8350	<div></div> 0.5180
C	<div></div> 0.7150	<div></div> 0.4420
D	<div></div> 0.7760	<div></div> 0.3800
E	<div></div> 0.8720	<div></div> 0.5440
F	<div></div> 0.8260	<div></div> 0.5160
G	<div></div> 0.6540	<div></div> 0.4140
H	<div></div> 0.7900	<div></div> 0.3870
I	<div></div> 0.8760	<div></div> 0.5450
J	<div></div> 0.8320	<div></div> 0.5200
K	<div></div> 0.6550	<div></div> 0.4160
L	<div></div> 0.7570	<div></div> 0.3670
M	<div></div> 0.8630	<div></div> 0.5240
N	<div></div> 0.8260	<div></div> 0.5000
O	<div></div> 0.6260	<div></div> 0.3840
P	<div></div> 0.7860	<div></div> 0.3980

