Full wwPDB EM Validation Report (i)

Apr 29, 2024 – 10:38 am BST

PDB ID	:	2XVR
EMDB ID	:	EMD-1810
Title	:	Phage T7 empty mature head shell
Authors	:	Ionel, A.; Velazquez-Muriel, J.A.; Luque, D.; Cuervo, A.; Caston, J.R.; Valpuesta, J.M.; Martin-Benito, J.; Carrascosa, J.L.
Deposited on	:	2010-10-28
Resolution	:	10.80 Å(reported)
Based on initial model	:	1OHG

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 (i) 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 (i)) were used in the production of this report:

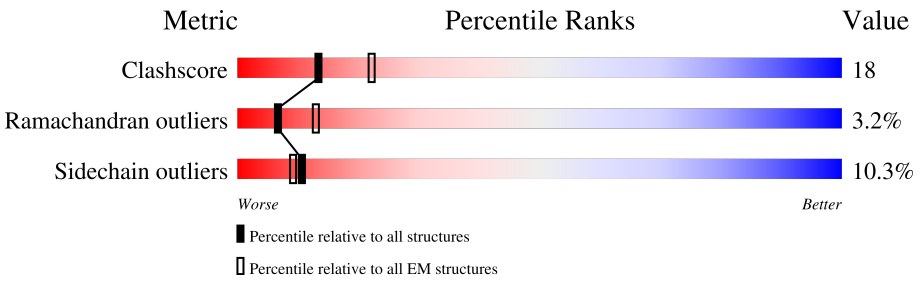
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 10.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	345	11% 46% 20% • • 29%
1	B	345	9% 44% 21% 5% • 29%
1	C	345	10% 45% 22% • • 29%
1	D	345	10% 44% 23% • • 29%
1	E	345	11% 46% 20% • • 29%
1	F	345	9% 47% 20% • • 29%
1	G	345	12% 49% 18% • • 29%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MAJOR CAPSID PROTEIN 10A.

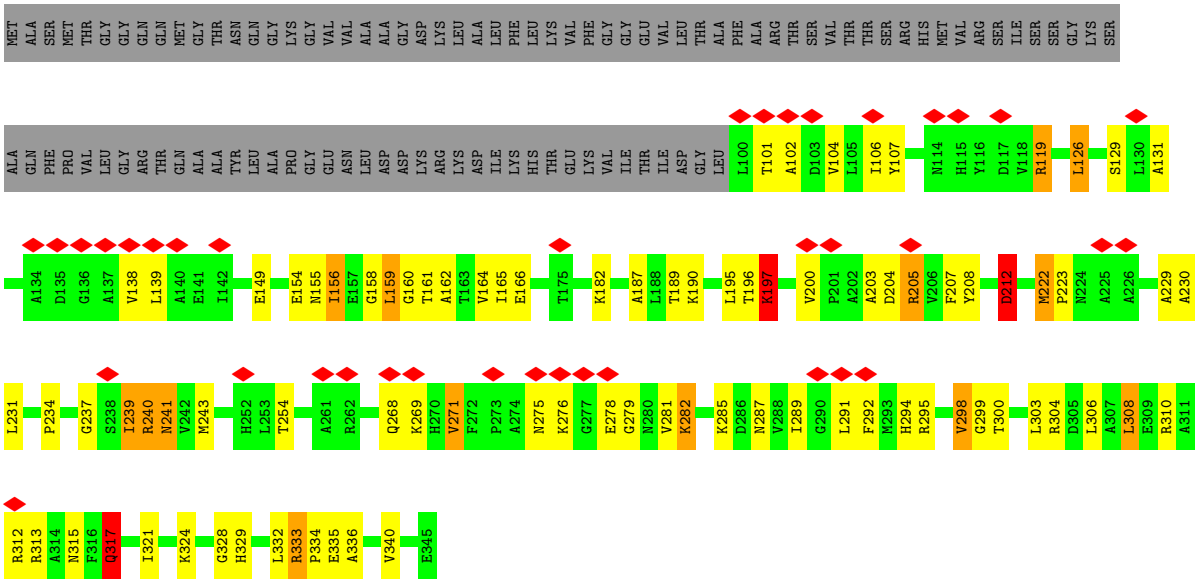
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	246	1833	1147	321	357	8	0	0
1	B	246	1833	1147	321	357	8	0	0
1	C	246	1833	1147	321	357	8	0	0
1	D	246	1833	1147	321	357	8	0	0
1	E	246	1833	1147	321	357	8	0	0
1	F	246	1833	1147	321	357	8	0	0
1	G	246	1833	1147	321	357	8	0	0

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.

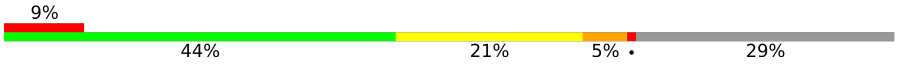
• Molecule 1: MAJOR CAPSID PROTEIN 10A

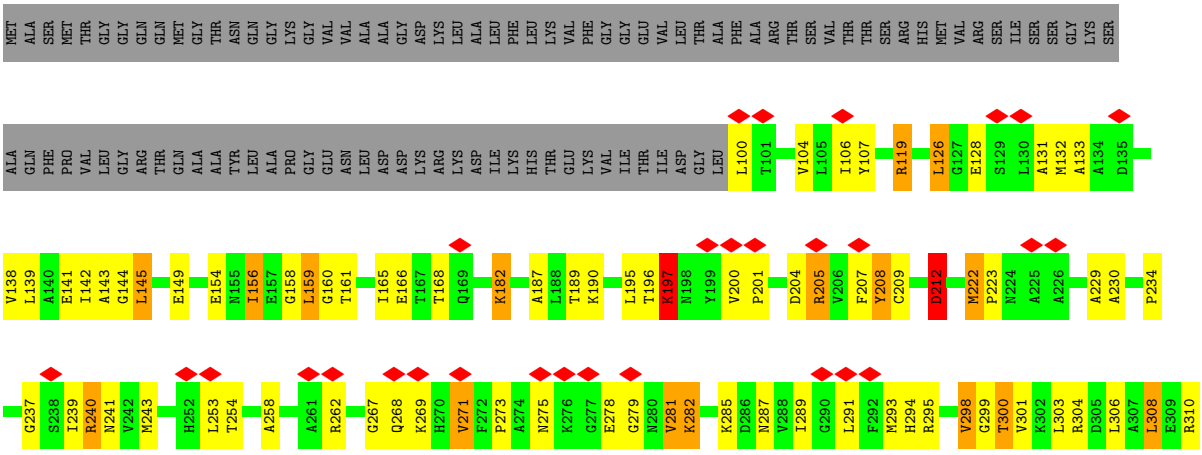
Chain A:

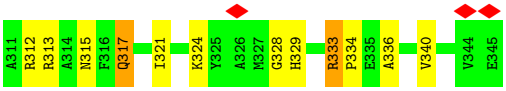


• Molecule 1: MAJOR CAPSID PROTEIN 10A

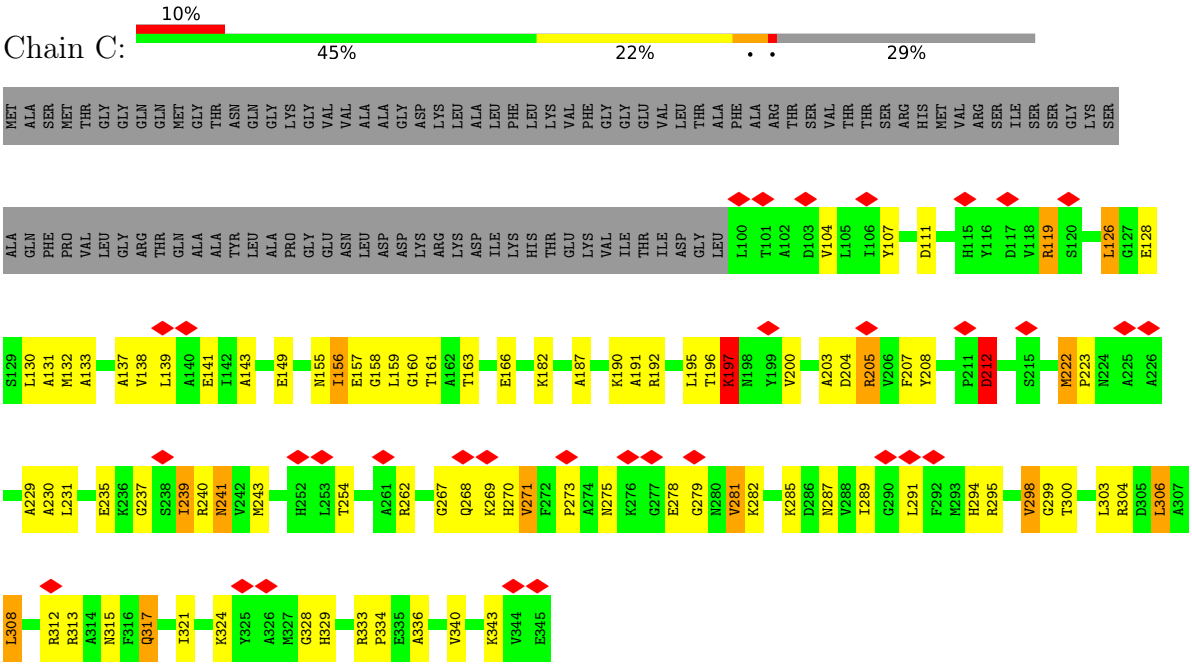
Chain B:



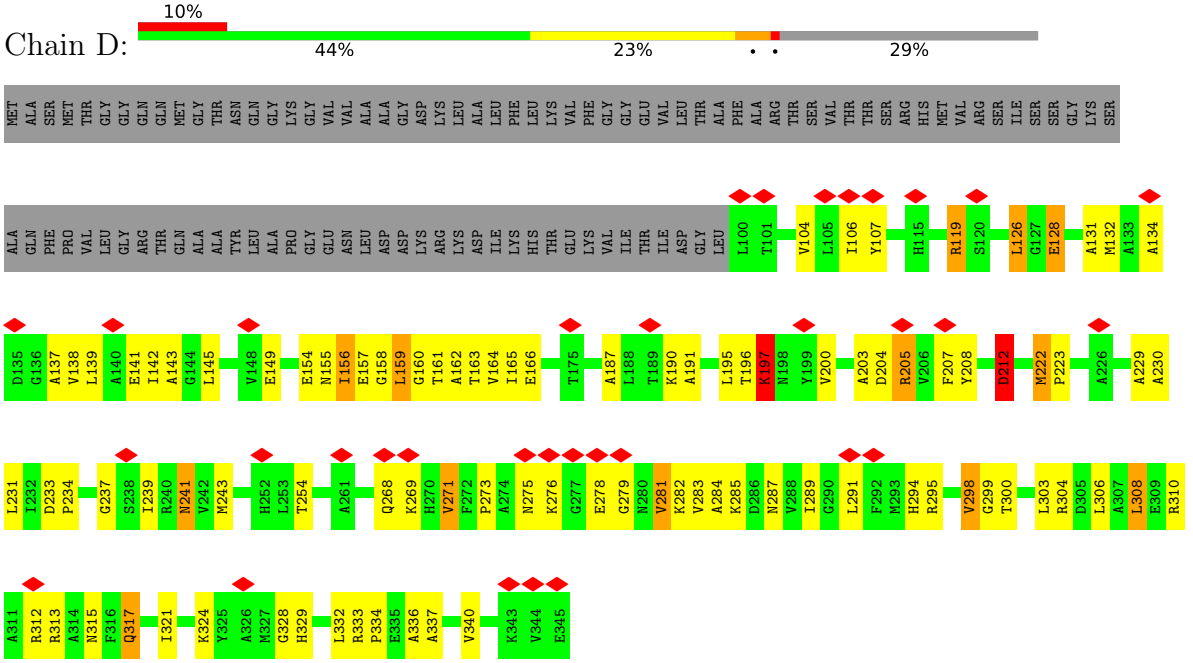




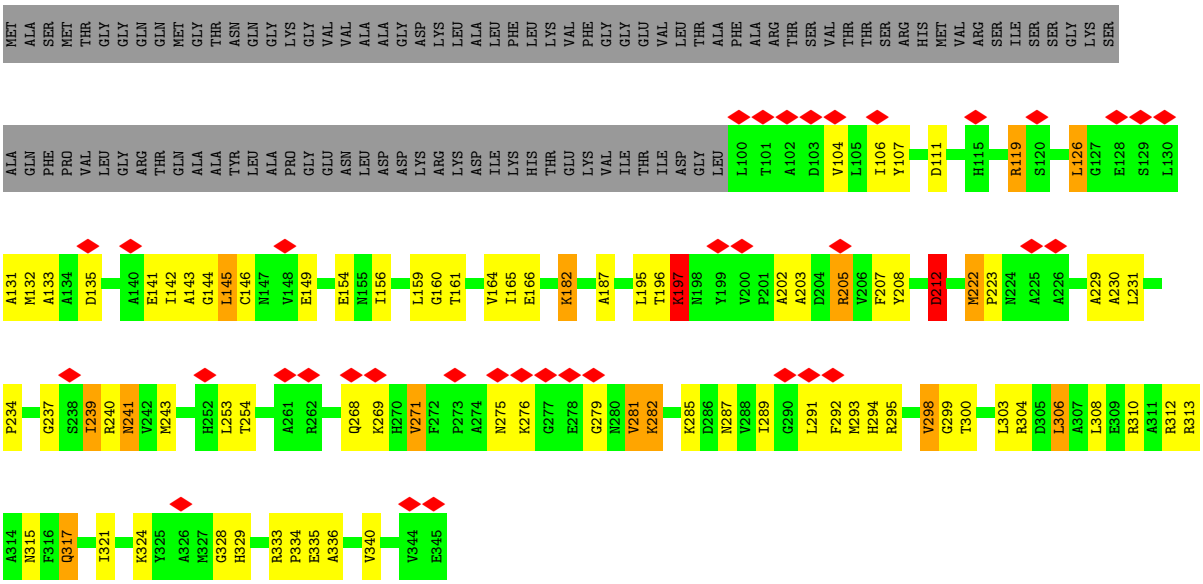
• Molecule 1: MAJOR CAPSID PROTEIN 10A



• Molecule 1: MAJOR CAPSID PROTEIN 10A

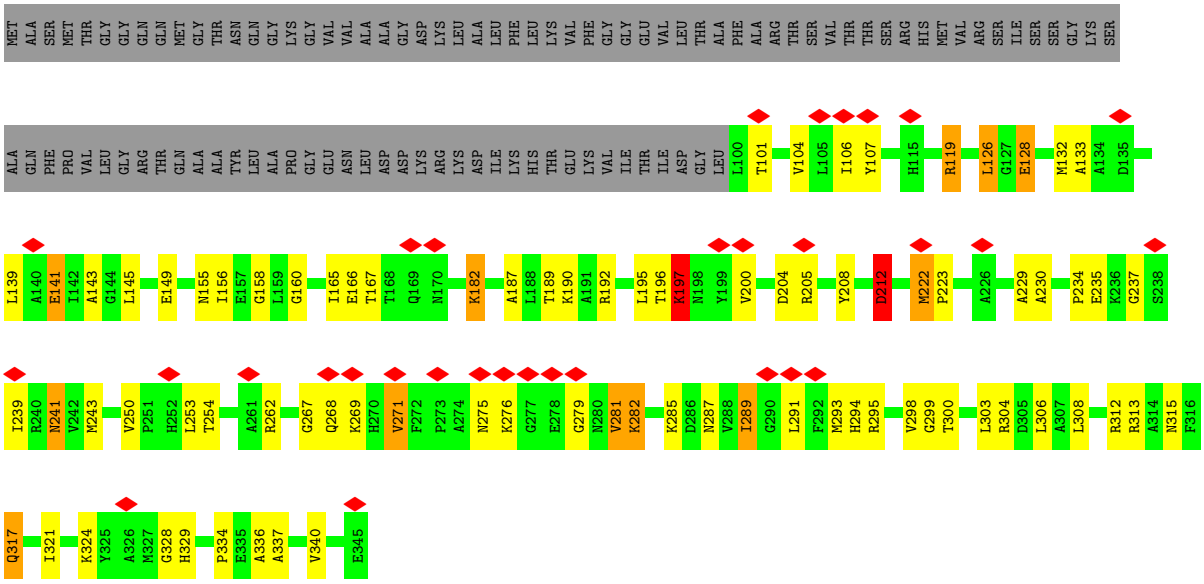


• Molecule 1: MAJOR CAPSID PROTEIN 10A



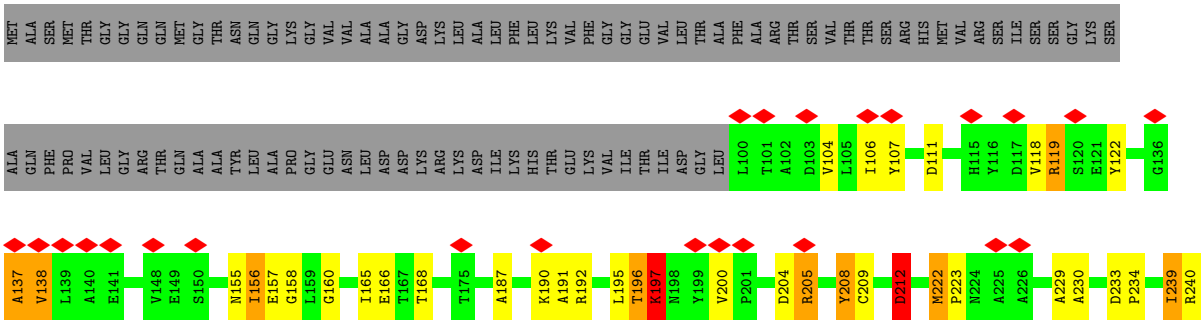
• Molecule 1: MAJOR CAPSID PROTEIN 10A

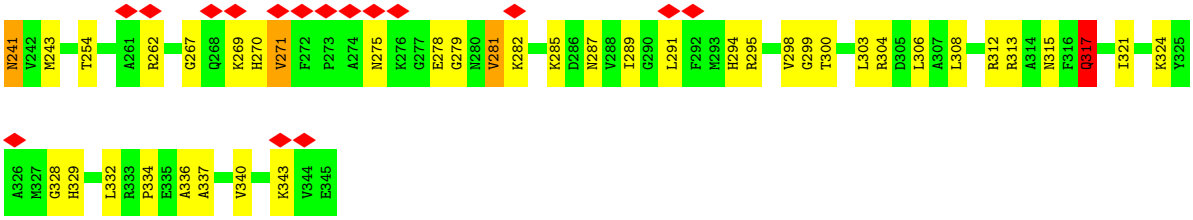
Chain F: 9% 47% 20% • • 29%



• Molecule 1: MAJOR CAPSID PROTEIN 10A

Chain G: 12% 49% 18% • • 29%




N241
V242
M243
T254
A261
R262
G267
Q268
K269
H270
V271
F272
P273
A274
N275
K276
G277
E278
G279
N280
V281
K282
K285
D286
N287
V288
I289
G290
L291
F292
M293
H294
R295
V298
G299
T300
L303
R304
D305
L306
A307
L308
R312
R313
A314
N315
E316
Q317
I321
K324
Y325

A326
M327
G328
H329
L332
R333
P334
E335
A336
A337
V340
K343
V344
E345

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5100	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	772.8, 772.8, 772.8	wwPDB
Map dimensions	552, 552, 552	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.32	0/1859	0.72	3/2518 (0.1%)
1	B	0.34	0/1859	0.58	2/2518 (0.1%)
1	C	0.36	1/1859 (0.1%)	0.53	1/2518 (0.0%)
1	D	0.32	0/1859	0.65	3/2518 (0.1%)
1	E	0.33	0/1859	0.69	2/2518 (0.1%)
1	F	0.35	0/1859	0.57	1/2518 (0.0%)
1	G	0.32	0/1859	0.84	3/2518 (0.1%)
All	All	0.34	1/13013 (0.0%)	0.66	15/17626 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	317	GLN	CD-OE1	6.77	1.38	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	317	GLN	CG-CD-OE1	-28.75	64.11	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	GLN	CG-CD-OE1	-21.72	78.15	121.60
1	E	317	GLN	CG-CD-OE1	-18.80	83.99	121.60
1	D	317	GLN	CG-CD-OE1	-16.15	89.29	121.60
1	G	317	GLN	CG-CD-NE2	-13.21	85.00	116.70
1	A	317	GLN	CG-CD-NE2	-9.71	93.40	116.70
1	F	317	GLN	CG-CD-OE1	-9.13	103.33	121.60
1	B	317	GLN	CG-CD-OE1	-8.84	103.92	121.60
1	E	317	GLN	CG-CD-NE2	-8.26	96.88	116.70
1	D	317	GLN	CG-CD-NE2	-6.94	100.04	116.70
1	G	317	GLN	OE1-CD-NE2	6.54	136.95	121.90
1	D	308	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	308	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	308	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	308	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	GLN	Sidechain
1	B	317	GLN	Sidechain
1	C	317	GLN	Sidechain
1	D	317	GLN	Sidechain
1	E	317	GLN	Sidechain
1	F	317	GLN	Sidechain
1	G	137	ALA	Peptide
1	G	317	GLN	Sidechain

5.2 Too-close contacts (i)

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	1833	0	1832	81	0
1	B	1833	0	1832	90	0
1	C	1833	0	1832	73	0
1	D	1833	0	1832	80	0
1	E	1833	0	1832	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1833	0	1832	71	0
1	G	1833	0	1832	55	0
All	All	12831	0	12824	463	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 18.

All (463) 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:G:137:ALA:HB3	1:G:138:VAL:CB	1.84	1.06
1:G:137:ALA:CB	1:G:138:VAL:HB	1.91	1.01
1:A:333:ARG:HH22	1:B:141:GLU:HB3	1.23	1.00
1:C:254:THR:HG21	1:C:287:ASN:HD21	1.26	0.99
1:D:254:THR:HG21	1:D:287:ASN:HD21	1.26	0.99
1:B:254:THR:HG21	1:B:287:ASN:HD21	1.25	0.98
1:B:239:ILE:HG13	1:B:240:ARG:H	1.29	0.96
1:B:273:PRO:HB3	1:C:231:LEU:HD21	1.49	0.95
1:A:254:THR:HG21	1:A:287:ASN:HD21	1.30	0.94
1:G:254:THR:HG21	1:G:287:ASN:HD21	1.31	0.94
1:F:254:THR:HG21	1:F:287:ASN:HD21	1.32	0.92
1:G:137:ALA:HB3	1:G:138:VAL:HB	0.94	0.92
1:B:159:LEU:HB2	1:C:133:ALA:HB3	1.53	0.90
1:D:241:ASN:HD22	1:D:241:ASN:H	1.20	0.88
1:E:254:THR:HG21	1:E:287:ASN:HD21	1.39	0.88
1:E:333:ARG:HH21	1:F:141:GLU:HB2	1.37	0.86
1:C:299:GLY:HA3	1:C:303:LEU:HD23	1.58	0.84
1:A:162:ALA:HA	1:B:144:GLY:H	1.41	0.84
1:D:333:ARG:HH22	1:E:141:GLU:HB2	1.44	0.83
1:E:156:ILE:HG22	1:E:205:ARG:HD3	1.59	0.82
1:B:299:GLY:HA3	1:B:303:LEU:HD23	1.60	0.81
1:E:299:GLY:HA3	1:E:303:LEU:HD23	1.63	0.81
1:A:156:ILE:HG22	1:A:205:ARG:HD3	1.61	0.80
1:E:159:LEU:H	1:F:133:ALA:CB	1.96	0.79
1:D:299:GLY:HA3	1:D:303:LEU:HD23	1.64	0.78
1:A:333:ARG:NH2	1:B:141:GLU:HB3	2.00	0.77
1:B:275:ASN:H	1:B:287:ASN:HD22	1.32	0.77
1:E:159:LEU:O	1:F:132:MET:N	2.18	0.77
1:E:159:LEU:H	1:F:133:ALA:HB3	1.49	0.77
1:E:196:THR:HB	1:E:291:LEU:HD21	1.65	0.76
1:D:160:GLY:HA3	1:E:132:MET:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:THR:HB	1:G:291:LEU:HD21	1.68	0.76
1:D:241:ASN:H	1:D:241:ASN:ND2	1.83	0.76
1:B:196:THR:HB	1:B:291:LEU:HD21	1.67	0.76
1:A:299:GLY:HA3	1:A:303:LEU:HD23	1.66	0.75
1:D:196:THR:HB	1:D:291:LEU:HD21	1.68	0.75
1:C:275:ASN:H	1:C:287:ASN:HD22	1.34	0.75
1:C:196:THR:HB	1:C:291:LEU:HD21	1.67	0.75
1:F:196:THR:HB	1:F:291:LEU:HD21	1.69	0.75
1:C:273:PRO:HB3	1:D:231:LEU:HD21	1.67	0.75
1:E:212:ASP:HB3	1:E:298:VAL:HG12	1.69	0.75
1:B:156:ILE:HG22	1:B:205:ARG:HD3	1.69	0.74
1:A:196:THR:HB	1:A:291:LEU:HD21	1.69	0.74
1:B:212:ASP:HB3	1:B:298:VAL:HG12	1.69	0.74
1:D:161:THR:HG23	1:E:143:ALA:HB2	1.70	0.74
1:G:299:GLY:HA3	1:G:303:LEU:HD23	1.71	0.73
1:B:239:ILE:HG13	1:B:240:ARG:N	2.03	0.73
1:G:212:ASP:HB3	1:G:298:VAL:HG12	1.70	0.73
1:F:212:ASP:HB3	1:F:298:VAL:HG12	1.69	0.73
1:F:166:GLU:HB2	1:F:328:GLY:HA3	1.70	0.73
1:D:212:ASP:HB3	1:D:298:VAL:HG12	1.71	0.73
1:A:166:GLU:HB2	1:A:328:GLY:HA3	1.69	0.73
1:A:212:ASP:HB3	1:A:298:VAL:HG12	1.69	0.73
1:B:166:GLU:HB2	1:B:328:GLY:HA3	1.72	0.72
1:C:212:ASP:HB3	1:C:298:VAL:HG12	1.70	0.72
1:F:229:ALA:HB1	1:F:295:ARG:HG3	1.73	0.71
1:A:159:LEU:O	1:B:131:ALA:HB1	1.90	0.71
1:F:299:GLY:HA3	1:F:303:LEU:HD23	1.72	0.71
1:F:165:ILE:HB	1:F:329:HIS:HD2	1.54	0.70
1:C:237:GLY:HA2	1:C:241:ASN:HB2	1.74	0.70
1:G:166:GLU:HB2	1:G:328:GLY:HA3	1.73	0.70
1:D:126:LEU:HD11	1:D:149:GLU:HB3	1.74	0.69
1:F:200:VAL:HG11	1:F:204:ASP:HB2	1.75	0.69
1:B:275:ASN:HB2	1:C:235:GLU:HG3	1.74	0.69
1:D:166:GLU:HB2	1:D:328:GLY:HA3	1.73	0.69
1:B:254:THR:HG21	1:B:287:ASN:ND2	2.04	0.69
1:D:275:ASN:H	1:D:287:ASN:HD22	1.40	0.69
1:E:275:ASN:H	1:E:287:ASN:HD22	1.40	0.69
1:C:195:LEU:HD23	1:C:340:VAL:HB	1.75	0.69
1:C:166:GLU:HB2	1:C:328:GLY:HA3	1.75	0.69
1:D:156:ILE:HG22	1:D:205:ARG:HD3	1.75	0.69
1:E:166:GLU:HB2	1:E:328:GLY:HA3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ALA:HB1	1:A:295:ARG:HG3	1.73	0.68
1:A:160:GLY:H	1:A:333:ARG:HE	1.40	0.68
1:E:182:LYS:HE3	1:F:128:GLU:HB2	1.74	0.68
1:F:313:ARG:HD2	1:F:334:PRO:HB3	1.74	0.68
1:E:119:ARG:HD3	1:E:154:GLU:HA	1.75	0.68
1:A:129:SER:H	1:F:182:LYS:HE3	1.59	0.68
1:E:159:LEU:HG	1:E:335:GLU:HG2	1.75	0.68
1:G:313:ARG:HD2	1:G:334:PRO:HB3	1.76	0.68
1:E:126:LEU:HD11	1:E:149:GLU:HB3	1.75	0.67
1:F:275:ASN:H	1:F:287:ASN:HD22	1.40	0.67
1:A:126:LEU:HD11	1:A:149:GLU:HB3	1.77	0.67
1:C:158:GLY:H	1:C:336:ALA:HB3	1.58	0.67
1:A:119:ARG:HD3	1:A:154:GLU:HA	1.76	0.67
1:E:275:ASN:HB2	1:F:235:GLU:HG3	1.77	0.67
1:E:313:ARG:HH12	1:E:315:ASN:HB3	1.59	0.67
1:B:333:ARG:HH22	1:C:141:GLU:HB3	1.60	0.66
1:E:142:ILE:HG13	1:E:143:ALA:H	1.59	0.66
1:B:313:ARG:HH12	1:B:315:ASN:HB3	1.61	0.66
1:D:195:LEU:HD23	1:D:340:VAL:HB	1.78	0.66
1:C:254:THR:HG21	1:C:287:ASN:ND2	2.07	0.66
1:D:313:ARG:HH12	1:D:315:ASN:HB3	1.61	0.66
1:E:313:ARG:HD2	1:E:334:PRO:HB3	1.78	0.66
1:E:333:ARG:NH2	1:F:141:GLU:HB2	2.09	0.65
1:C:313:ARG:HH12	1:C:315:ASN:HB3	1.62	0.65
1:B:119:ARG:HD3	1:B:154:GLU:HA	1.77	0.65
1:C:182:LYS:HE2	1:D:128:GLU:HB2	1.77	0.65
1:A:160:GLY:HA3	1:B:131:ALA:HA	1.78	0.64
1:E:197:LYS:HG3	1:E:197:LYS:O	1.96	0.64
1:B:229:ALA:HB1	1:B:295:ARG:HG3	1.80	0.64
1:D:197:LYS:O	1:D:197:LYS:HG3	1.96	0.64
1:B:126:LEU:HD11	1:B:149:GLU:HB3	1.78	0.64
1:E:229:ALA:HB1	1:E:295:ARG:HG3	1.80	0.64
1:F:241:ASN:HD22	1:F:241:ASN:H	1.45	0.64
1:A:160:GLY:HA3	1:B:132:MET:H	1.63	0.63
1:C:126:LEU:HD11	1:C:149:GLU:HB3	1.78	0.63
1:C:313:ARG:HD2	1:C:334:PRO:HB3	1.80	0.63
1:A:234:PRO:HG2	1:A:282:LYS:HZ3	1.64	0.63
1:B:313:ARG:HD2	1:B:334:PRO:HB3	1.79	0.63
1:B:160:GLY:HA3	1:C:131:ALA:HB1	1.81	0.62
1:C:269:LYS:HD3	1:C:281:VAL:HG22	1.81	0.62
1:A:313:ARG:HD2	1:A:334:PRO:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ALA:HB1	1:C:295:ARG:HG3	1.80	0.62
1:D:254:THR:HG21	1:D:287:ASN:ND2	2.07	0.62
1:G:197:LYS:HG3	1:G:197:LYS:O	2.00	0.62
1:C:197:LYS:O	1:C:197:LYS:HG3	1.99	0.62
1:F:197:LYS:O	1:F:197:LYS:HG3	1.98	0.62
1:D:229:ALA:HB1	1:D:295:ARG:HG3	1.82	0.62
1:B:158:GLY:H	1:B:336:ALA:HB3	1.65	0.62
1:A:275:ASN:H	1:A:287:ASN:HD22	1.47	0.61
1:F:126:LEU:HD11	1:F:149:GLU:HB3	1.81	0.61
1:E:159:LEU:HA	1:E:334:PRO:O	2.00	0.61
1:E:195:LEU:HA	1:E:340:VAL:HG21	1.82	0.61
1:F:165:ILE:HB	1:F:329:HIS:CD2	2.35	0.61
1:F:187:ALA:HB3	1:F:313:ARG:HD3	1.81	0.61
1:G:313:ARG:HH12	1:G:315:ASN:HB3	1.66	0.61
1:D:313:ARG:HD2	1:D:334:PRO:HB3	1.82	0.61
1:B:161:THR:HG23	1:C:143:ALA:HB2	1.83	0.60
1:A:239:ILE:HG13	1:A:240:ARG:H	1.65	0.60
1:F:313:ARG:HH12	1:F:315:ASN:HB3	1.66	0.60
1:C:195:LEU:HA	1:C:340:VAL:HG21	1.83	0.60
1:F:321:ILE:HB	1:F:324:LYS:HB2	1.84	0.60
1:A:197:LYS:O	1:A:197:LYS:HG3	2.01	0.60
1:D:119:ARG:HD3	1:D:154:GLU:HA	1.82	0.60
1:A:237:GLY:HA2	1:A:241:ASN:HB2	1.84	0.60
1:A:241:ASN:N	1:A:241:ASN:HD22	2.00	0.59
1:C:187:ALA:HA	1:C:190:LYS:HB2	1.84	0.59
1:A:254:THR:HG21	1:A:287:ASN:ND2	2.11	0.59
1:G:187:ALA:HB3	1:G:313:ARG:HD3	1.84	0.59
1:A:333:ARG:HH22	1:B:141:GLU:CB	2.08	0.59
1:G:200:VAL:HG11	1:G:204:ASP:HB2	1.83	0.59
1:D:187:ALA:HA	1:D:190:LYS:HB2	1.85	0.59
1:D:195:LEU:HA	1:D:340:VAL:HG21	1.85	0.58
1:E:145:LEU:HD22	1:E:146:CYS:H	1.67	0.58
1:A:159:LEU:H	1:B:133:ALA:HB3	1.67	0.58
1:B:138:VAL:HG22	1:B:139:LEU:H	1.68	0.58
1:F:195:LEU:HA	1:F:340:VAL:HG21	1.85	0.58
1:B:197:LYS:HG3	1:B:197:LYS:O	2.03	0.58
1:D:321:ILE:HB	1:D:324:LYS:HB2	1.86	0.57
1:A:195:LEU:HA	1:A:340:VAL:HG21	1.85	0.57
1:C:241:ASN:H	1:C:241:ASN:HD22	1.52	0.57
1:B:195:LEU:HA	1:B:340:VAL:HG21	1.86	0.57
1:C:203:ALA:HB3	1:D:134:ALA:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:ILE:HA	1:F:329:HIS:HA	1.87	0.57
1:A:313:ARG:HH12	1:A:315:ASN:HB3	1.69	0.57
1:G:195:LEU:HD23	1:G:340:VAL:HB	1.85	0.57
1:A:159:LEU:HG	1:A:335:GLU:HG2	1.86	0.57
1:D:119:ARG:HH22	1:D:310:ARG:HB2	1.69	0.57
1:F:230:ALA:HB3	1:F:269:LYS:HE2	1.87	0.57
1:F:158:GLY:H	1:F:336:ALA:HB3	1.68	0.57
1:D:158:GLY:H	1:D:336:ALA:HB3	1.68	0.56
1:G:275:ASN:H	1:G:287:ASN:HD22	1.52	0.56
1:B:240:ARG:HG2	1:B:240:ARG:HH11	1.70	0.56
1:F:254:THR:HG21	1:F:287:ASN:ND2	2.13	0.56
1:C:313:ARG:HA	1:C:336:ALA:HA	1.87	0.56
1:B:187:ALA:HB3	1:B:313:ARG:HD3	1.87	0.56
1:G:254:THR:HG21	1:G:287:ASN:ND2	2.13	0.56
1:B:165:ILE:HB	1:B:329:HIS:HD2	1.70	0.55
1:G:158:GLY:H	1:G:336:ALA:HB3	1.72	0.55
1:G:321:ILE:HB	1:G:324:LYS:HB2	1.87	0.55
1:C:279:GLY:HA2	1:C:285:LYS:H	1.71	0.55
1:A:159:LEU:O	1:B:132:MET:N	2.40	0.55
1:C:187:ALA:HB3	1:C:313:ARG:HD3	1.88	0.55
1:D:187:ALA:HB3	1:D:313:ARG:HD3	1.89	0.55
1:A:222:MET:HB3	1:A:223:PRO:HD3	1.89	0.55
1:B:237:GLY:HA2	1:B:241:ASN:HB3	1.87	0.55
1:A:159:LEU:HB2	1:B:133:ALA:CB	2.37	0.55
1:B:275:ASN:HB2	1:C:235:GLU:CG	2.36	0.55
1:C:159:LEU:HD22	1:C:333:ARG:HH21	1.71	0.55
1:C:161:THR:HG23	1:D:143:ALA:HB2	1.88	0.55
1:A:164:VAL:HG22	1:B:145:LEU:HG	1.88	0.55
1:E:279:GLY:HA2	1:E:285:LYS:H	1.72	0.55
1:D:200:VAL:HG11	1:D:204:ASP:HB2	1.89	0.55
1:B:182:LYS:HE3	1:C:128:GLU:HB2	1.89	0.54
1:B:279:GLY:HA2	1:B:285:LYS:H	1.72	0.54
1:A:119:ARG:HH22	1:A:310:ARG:HB2	1.72	0.54
1:D:165:ILE:HB	1:D:329:HIS:HD2	1.73	0.54
1:G:317:GLN:HE22	1:G:332:LEU:HB2	1.72	0.54
1:D:222:MET:HB3	1:D:223:PRO:HD3	1.89	0.54
1:G:119:ARG:H	1:G:119:ARG:HD3	1.73	0.54
1:B:200:VAL:HG11	1:B:204:ASP:HB2	1.89	0.54
1:A:200:VAL:HG11	1:A:204:ASP:HB2	1.89	0.54
1:B:313:ARG:HA	1:B:336:ALA:HA	1.88	0.54
1:C:119:ARG:HA	1:C:119:ARG:NE	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ILE:HG13	1:E:143:ALA:N	2.21	0.54
1:C:191:ALA:O	1:C:195:LEU:HG	2.08	0.54
1:E:187:ALA:HB3	1:E:313:ARG:HD3	1.90	0.54
1:G:165:ILE:HB	1:G:329:HIS:HD2	1.72	0.54
1:F:269:LYS:HD3	1:F:281:VAL:HG22	1.90	0.54
1:C:107:TYR:HB2	1:C:195:LEU:HD13	1.89	0.54
1:A:230:ALA:HB3	1:A:269:LYS:HE2	1.90	0.54
1:D:233:ASP:HB2	1:D:234:PRO:HD3	1.89	0.54
1:E:165:ILE:HB	1:E:329:HIS:HD2	1.73	0.53
1:C:130:LEU:HG	1:C:131:ALA:H	1.73	0.53
1:D:107:TYR:HB2	1:D:195:LEU:HD13	1.90	0.53
1:B:142:ILE:HG13	1:B:143:ALA:H	1.74	0.53
1:B:165:ILE:HA	1:B:329:HIS:HA	1.91	0.53
1:B:160:GLY:H	1:B:333:ARG:HH21	1.54	0.53
1:B:269:LYS:HD3	1:B:281:VAL:HG22	1.90	0.53
1:C:321:ILE:HB	1:C:324:LYS:HB2	1.91	0.53
1:E:321:ILE:HB	1:E:324:LYS:HB2	1.91	0.53
1:A:279:GLY:HA2	1:A:285:LYS:H	1.74	0.53
1:B:187:ALA:HA	1:B:190:LYS:HB2	1.90	0.53
1:A:241:ASN:HD22	1:A:241:ASN:H	1.57	0.53
1:D:279:GLY:HA2	1:D:285:LYS:H	1.74	0.52
1:G:222:MET:HB3	1:G:223:PRO:HD3	1.91	0.52
1:B:321:ILE:HB	1:B:324:LYS:HB2	1.91	0.52
1:D:205:ARG:HB3	1:D:207:PHE:CE2	2.45	0.52
1:E:254:THR:HG21	1:E:287:ASN:ND2	2.17	0.52
1:G:229:ALA:HB1	1:G:295:ARG:HG3	1.90	0.52
1:G:233:ASP:HB2	1:G:234:PRO:HD3	1.91	0.52
1:E:269:LYS:HD3	1:E:281:VAL:HG22	1.91	0.52
1:G:187:ALA:HA	1:G:190:LYS:HB2	1.91	0.52
1:C:222:MET:HB3	1:C:223:PRO:HD3	1.92	0.52
1:G:279:GLY:HA2	1:G:285:LYS:H	1.75	0.52
1:E:222:MET:HB3	1:E:223:PRO:HD3	1.92	0.51
1:A:161:THR:HG23	1:B:143:ALA:HB2	1.93	0.51
1:D:269:LYS:HD3	1:D:281:VAL:HG22	1.91	0.51
1:A:203:ALA:HB3	1:B:133:ALA:O	2.11	0.51
1:F:268:GLN:HE21	1:F:285:LYS:HE2	1.76	0.51
1:G:138:VAL:O	1:G:138:VAL:HG13	2.11	0.51
1:G:165:ILE:HA	1:G:329:HIS:HA	1.91	0.51
1:G:269:LYS:HD3	1:G:281:VAL:HG22	1.92	0.51
1:F:222:MET:HB3	1:F:223:PRO:HD3	1.92	0.50
1:E:230:ALA:HB3	1:E:269:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ARG:HA	1:E:336:ALA:HA	1.93	0.50
1:A:234:PRO:HG2	1:A:282:LYS:NZ	2.25	0.50
1:E:268:GLN:HE21	1:E:285:LYS:HE2	1.76	0.50
1:F:167:THR:HB	1:G:118:VAL:HG21	1.93	0.50
1:A:131:ALA:HB3	1:F:160:GLY:HA3	1.93	0.50
1:A:187:ALA:HA	1:A:190:LYS:HB2	1.94	0.50
1:B:119:ARG:HH22	1:B:310:ARG:HB2	1.76	0.50
1:F:119:ARG:HA	1:F:119:ARG:NE	2.25	0.50
1:F:160:GLY:O	1:F:334:PRO:HD2	2.12	0.50
1:A:187:ALA:HB3	1:A:313:ARG:HD3	1.94	0.50
1:D:333:ARG:NH2	1:E:141:GLU:HB2	2.20	0.50
1:B:182:LYS:CE	1:C:128:GLU:HB2	2.42	0.49
1:G:107:TYR:HB2	1:G:195:LEU:HD13	1.94	0.49
1:E:165:ILE:HB	1:E:329:HIS:CD2	2.47	0.49
1:C:230:ALA:HB3	1:C:269:LYS:HE2	1.94	0.49
1:D:191:ALA:O	1:D:195:LEU:HG	2.12	0.49
1:F:279:GLY:HA2	1:F:285:LYS:H	1.77	0.49
1:B:222:MET:HB3	1:B:223:PRO:HD3	1.94	0.49
1:D:237:GLY:HA2	1:D:241:ASN:HB2	1.94	0.49
1:E:205:ARG:HB3	1:E:207:PHE:CE2	2.47	0.49
1:A:205:ARG:HB3	1:A:207:PHE:CE2	2.48	0.49
1:E:202:ALA:HA	1:F:132:MET:CB	2.42	0.49
1:D:159:LEU:H	1:E:133:ALA:HB3	1.77	0.49
1:D:165:ILE:HB	1:D:329:HIS:CD2	2.48	0.49
1:E:276:LYS:HD2	1:F:282:LYS:HD3	1.94	0.49
1:F:196:THR:O	1:F:197:LYS:HB3	2.12	0.49
1:E:107:TYR:HB2	1:E:195:LEU:HD13	1.95	0.49
1:C:138:VAL:HG22	1:C:139:LEU:H	1.77	0.48
1:E:159:LEU:H	1:F:133:ALA:HB2	1.73	0.48
1:B:160:GLY:HA3	1:C:132:MET:H	1.76	0.48
1:F:294:HIS:CG	1:F:295:ARG:N	2.81	0.48
1:B:160:GLY:HA3	1:C:132:MET:N	2.28	0.48
1:F:275:ASN:H	1:F:287:ASN:ND2	2.10	0.48
1:C:324:LYS:HG3	1:C:329:HIS:O	2.13	0.48
1:F:107:TYR:HB2	1:F:195:LEU:HD13	1.96	0.48
1:E:196:THR:O	1:E:197:LYS:HB3	2.13	0.48
1:G:155:ASN:HD21	1:G:337:ALA:HA	1.78	0.48
1:C:200:VAL:HG11	1:C:204:ASP:HB2	1.94	0.48
1:B:205:ARG:HB3	1:B:207:PHE:CE2	2.49	0.48
1:E:237:GLY:HA2	1:E:241:ASN:HB2	1.95	0.48
1:F:187:ALA:HA	1:F:190:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:HIS:CG	1:A:295:ARG:N	2.82	0.48
1:C:237:GLY:CA	1:C:241:ASN:HB2	2.42	0.48
1:A:104:VAL:HG12	1:A:107:TYR:HB3	1.96	0.48
1:B:237:GLY:HA2	1:B:241:ASN:CB	2.44	0.47
1:C:294:HIS:CG	1:C:295:ARG:N	2.82	0.47
1:D:273:PRO:HB3	1:E:231:LEU:HD21	1.95	0.47
1:C:156:ILE:HD13	1:C:157:GLU:N	2.29	0.47
1:D:230:ALA:HB3	1:D:269:LYS:HE2	1.95	0.47
1:E:241:ASN:H	1:E:241:ASN:HD22	1.63	0.47
1:D:294:HIS:CG	1:D:295:ARG:N	2.83	0.47
1:G:122:TYR:CZ	1:G:343:LYS:HE2	2.49	0.47
1:D:196:THR:O	1:D:197:LYS:HB3	2.14	0.47
1:D:324:LYS:HG3	1:D:329:HIS:O	2.15	0.47
1:D:156:ILE:HG21	1:D:204:ASP:HA	1.96	0.47
1:A:107:TYR:HB2	1:A:195:LEU:HD13	1.95	0.47
1:A:161:THR:OG1	1:A:162:ALA:N	2.48	0.47
1:E:161:THR:O	1:F:143:ALA:HB3	2.15	0.47
1:A:158:GLY:H	1:A:336:ALA:HB3	1.80	0.47
1:D:156:ILE:HD13	1:D:157:GLU:H	1.80	0.47
1:A:321:ILE:HB	1:A:324:LYS:HB2	1.96	0.47
1:B:230:ALA:HB3	1:B:269:LYS:HE2	1.96	0.47
1:B:278:GLU:HG2	1:B:287:ASN:ND2	2.30	0.47
1:D:313:ARG:HA	1:D:336:ALA:HA	1.97	0.47
1:A:324:LYS:HG3	1:A:329:HIS:O	2.15	0.46
1:D:269:LYS:HD3	1:D:281:VAL:H	1.78	0.46
1:A:268:GLN:HE21	1:A:285:LYS:HE2	1.81	0.46
1:B:294:HIS:CG	1:B:295:ARG:N	2.83	0.46
1:F:237:GLY:HA2	1:F:241:ASN:HB2	1.97	0.46
1:B:165:ILE:HB	1:B:329:HIS:CD2	2.49	0.46
1:E:104:VAL:HG12	1:E:107:TYR:HB3	1.96	0.46
1:B:107:TYR:HB2	1:B:195:LEU:HD13	1.97	0.46
1:C:270:HIS:HD2	1:C:279:GLY:HA3	1.81	0.46
1:F:195:LEU:HD23	1:F:340:VAL:HB	1.98	0.46
1:G:137:ALA:HB3	1:G:138:VAL:CA	2.44	0.46
1:G:191:ALA:O	1:G:195:LEU:HG	2.16	0.46
1:E:294:HIS:CG	1:E:295:ARG:N	2.83	0.46
1:F:269:LYS:HD3	1:F:281:VAL:H	1.80	0.46
1:G:195:LEU:HA	1:G:340:VAL:HG21	1.98	0.46
1:C:196:THR:O	1:C:197:LYS:HB3	2.16	0.46
1:G:156:ILE:HD13	1:G:157:GLU:H	1.81	0.46
1:G:294:HIS:CG	1:G:295:ARG:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:HG12	1:B:107:TYR:HB3	1.98	0.46
1:D:142:ILE:HG13	1:D:143:ALA:H	1.81	0.46
1:G:239:ILE:HG13	1:G:240:ARG:H	1.81	0.46
1:A:276:LYS:HD2	1:B:282:LYS:HD3	1.98	0.45
1:D:276:LYS:HD2	1:E:282:LYS:HD3	1.97	0.45
1:E:119:ARG:HH22	1:E:310:ARG:HB2	1.80	0.45
1:D:157:GLU:HB3	1:D:159:LEU:CD1	2.46	0.45
1:D:160:GLY:HA3	1:E:132:MET:N	2.25	0.45
1:D:278:GLU:HG2	1:D:287:ASN:ND2	2.31	0.45
1:C:268:GLN:HE21	1:C:285:LYS:HE2	1.82	0.45
1:C:241:ASN:H	1:C:241:ASN:ND2	2.15	0.45
1:F:234:PRO:HG2	1:F:282:LYS:NZ	2.32	0.45
1:G:230:ALA:HB3	1:G:269:LYS:HE2	1.97	0.45
1:A:241:ASN:N	1:A:241:ASN:ND2	2.63	0.45
1:D:163:THR:N	1:E:143:ALA:HB1	2.32	0.44
1:B:160:GLY:N	1:B:333:ARG:HH21	2.14	0.44
1:C:119:ARG:HD3	1:C:155:ASN:N	2.32	0.44
1:F:313:ARG:HA	1:F:336:ALA:HA	1.99	0.44
1:A:165:ILE:HB	1:A:329:HIS:CD2	2.52	0.44
1:C:278:GLU:HG2	1:C:287:ASN:ND2	2.32	0.44
1:G:269:LYS:HD3	1:G:281:VAL:H	1.81	0.44
1:A:269:LYS:HD3	1:A:281:VAL:H	1.82	0.44
1:B:106:ILE:HG13	1:B:196:THR:HG22	1.99	0.44
1:D:268:GLN:HE21	1:D:285:LYS:HE2	1.83	0.44
1:A:102:ALA:HA	1:B:239:ILE:HB	1.98	0.44
1:E:239:ILE:HG13	1:E:240:ARG:H	1.83	0.44
1:D:162:ALA:HA	1:E:144:GLY:H	1.82	0.44
1:B:195:LEU:HD23	1:B:340:VAL:HB	1.99	0.44
1:B:269:LYS:HD3	1:B:281:VAL:H	1.83	0.44
1:C:279:GLY:HA2	1:C:285:LYS:N	2.32	0.44
1:E:269:LYS:HD3	1:E:281:VAL:H	1.83	0.44
1:A:237:GLY:CA	1:A:241:ASN:HB2	2.46	0.44
1:B:208:TYR:HB2	1:B:209:CYS:H	1.65	0.44
1:D:137:ALA:HA	1:D:138:VAL:HA	1.80	0.44
1:E:202:ALA:HA	1:F:132:MET:HB3	1.99	0.44
1:A:161:THR:HA	1:A:333:ARG:HA	2.00	0.44
1:B:279:GLY:HA2	1:B:285:LYS:N	2.33	0.44
1:F:324:LYS:HG3	1:F:329:HIS:O	2.18	0.44
1:D:156:ILE:HG22	1:D:205:ARG:HH11	1.83	0.43
1:E:275:ASN:H	1:E:287:ASN:ND2	2.13	0.43
1:B:165:ILE:HG23	1:B:168:THR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:ILE:HG23	1:G:168:THR:H	1.83	0.43
1:D:159:LEU:HD23	1:D:333:ARG:HD3	2.00	0.43
1:A:269:LYS:HD3	1:A:281:VAL:HG22	2.00	0.43
1:B:100:LEU:O	1:B:189:THR:HB	2.18	0.43
1:B:268:GLN:HE21	1:B:285:LYS:HE2	1.83	0.43
1:C:160:GLY:HA3	1:D:131:ALA:HB1	2.01	0.43
1:A:106:ILE:HG13	1:A:196:THR:HG22	2.00	0.43
1:A:313:ARG:HA	1:A:336:ALA:HA	2.00	0.43
1:C:269:LYS:HD3	1:C:281:VAL:H	1.83	0.43
1:D:104:VAL:HG12	1:D:107:TYR:HB3	2.00	0.43
1:E:268:GLN:HB3	1:E:269:LYS:H	1.69	0.43
1:F:262:ARG:HG3	1:F:267:GLY:O	2.19	0.43
1:A:278:GLU:HG2	1:A:287:ASN:ND2	2.33	0.43
1:E:164:VAL:HA	1:F:145:LEU:HD11	2.00	0.43
1:F:106:ILE:HG13	1:F:196:THR:HG22	2.00	0.43
1:G:196:THR:O	1:G:197:LYS:HB3	2.19	0.43
1:A:138:VAL:HG22	1:A:139:LEU:H	1.83	0.43
1:A:196:THR:O	1:A:197:LYS:HB3	2.18	0.43
1:C:306:LEU:HD22	1:C:343:LYS:NZ	2.33	0.43
1:D:159:LEU:O	1:E:131:ALA:HB1	2.19	0.43
1:G:241:ASN:ND2	1:G:241:ASN:H	2.16	0.43
1:E:164:VAL:HG22	1:F:145:LEU:HD21	2.01	0.43
1:B:165:ILE:CB	1:B:329:HIS:HD2	2.31	0.42
1:C:262:ARG:HG3	1:C:267:GLY:O	2.19	0.42
1:E:182:LYS:HE3	1:F:128:GLU:CB	2.44	0.42
1:G:313:ARG:HA	1:G:336:ALA:HA	2.01	0.42
1:A:159:LEU:HB2	1:B:133:ALA:HB2	2.01	0.42
1:A:165:ILE:HB	1:A:329:HIS:HD2	1.84	0.42
1:E:159:LEU:HD23	1:E:333:ARG:HD3	2.01	0.42
1:F:155:ASN:HD21	1:F:337:ALA:HA	1.85	0.42
1:A:160:GLY:CA	1:B:132:MET:H	2.32	0.42
1:C:104:VAL:HG12	1:C:107:TYR:HB3	2.02	0.42
1:E:234:PRO:HG2	1:E:282:LYS:HZ2	1.84	0.42
1:E:253:LEU:HD11	1:E:293:MET:HG2	2.01	0.42
1:A:317:GLN:HE22	1:A:332:LEU:HB2	1.85	0.42
1:C:163:THR:N	1:D:143:ALA:HB1	2.34	0.42
1:C:239:ILE:HG13	1:C:240:ARG:H	1.85	0.42
1:F:101:THR:HG23	1:F:189:THR:HG21	2.00	0.42
1:A:119:ARG:HD3	1:A:155:ASN:N	2.34	0.42
1:A:159:LEU:HB3	1:A:160:GLY:H	1.68	0.42
1:B:333:ARG:HH22	1:C:141:GLU:CB	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:HIS:CG	1:C:295:ARG:H	2.37	0.42
1:G:208:TYR:HB2	1:G:209:CYS:H	1.65	0.42
1:D:268:GLN:HB3	1:D:269:LYS:H	1.71	0.42
1:A:282:LYS:HD3	1:F:276:LYS:HD2	2.01	0.42
1:G:104:VAL:HG22	1:G:192:ARG:HD2	2.02	0.42
1:B:196:THR:O	1:B:197:LYS:HB3	2.20	0.42
1:B:200:VAL:HA	1:B:201:PRO:HD3	1.97	0.42
1:D:283:VAL:HG22	1:D:284:ALA:H	1.85	0.42
1:G:279:GLY:HA2	1:G:285:LYS:N	2.34	0.42
1:A:268:GLN:HB3	1:A:269:LYS:H	1.71	0.42
1:F:104:VAL:HG12	1:F:107:TYR:HB3	2.01	0.42
1:G:165:ILE:HB	1:G:329:HIS:CD2	2.52	0.42
1:C:111:ASP:HB3	1:C:306:LEU:HD12	2.02	0.41
1:C:137:ALA:HA	1:C:138:VAL:HA	1.75	0.41
1:E:160:GLY:O	1:E:334:PRO:HD2	2.19	0.41
1:C:104:VAL:HG22	1:C:192:ARG:HD2	2.02	0.41
1:D:162:ALA:N	1:D:332:LEU:O	2.50	0.41
1:D:279:GLY:HA2	1:D:285:LYS:N	2.35	0.41
1:E:106:ILE:HG13	1:E:196:THR:HG22	2.02	0.41
1:E:202:ALA:HA	1:F:132:MET:HA	2.01	0.41
1:B:156:ILE:HG22	1:B:205:ARG:CD	2.44	0.41
1:G:156:ILE:HG22	1:G:205:ARG:HD3	2.03	0.41
1:E:324:LYS:HG3	1:E:329:HIS:O	2.20	0.41
1:F:165:ILE:CB	1:F:329:HIS:HD2	2.28	0.41
1:D:132:MET:O	1:D:141:GLU:HG2	2.20	0.41
1:F:253:LEU:HD11	1:F:293:MET:HG2	2.03	0.41
1:G:111:ASP:HB3	1:G:306:LEU:HD12	2.03	0.41
1:B:234:PRO:HG2	1:B:282:LYS:NZ	2.35	0.41
1:D:160:GLY:O	1:D:334:PRO:HD2	2.20	0.41
1:G:106:ILE:HG13	1:G:196:THR:HG22	2.03	0.41
1:G:278:GLU:HG2	1:G:287:ASN:ND2	2.35	0.41
1:D:157:GLU:HB3	1:D:159:LEU:HD11	2.03	0.41
1:D:164:VAL:HA	1:E:145:LEU:HG	2.01	0.41
1:E:145:LEU:HD22	1:E:146:CYS:N	2.35	0.41
1:A:101:THR:HA	1:A:189:THR:HB	2.03	0.41
1:A:119:ARG:HD3	1:A:155:ASN:H	1.85	0.41
1:A:279:GLY:HA2	1:A:285:LYS:N	2.35	0.41
1:E:165:ILE:HA	1:E:329:HIS:HA	2.02	0.41
1:B:258:ALA:HA	1:B:267:GLY:O	2.21	0.41
1:B:300:THR:HG22	1:B:301:VAL:H	1.86	0.41
1:E:111:ASP:HB3	1:E:306:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:ASN:HD22	1:F:241:ASN:N	2.16	0.41
1:A:160:GLY:O	1:A:334:PRO:HD2	2.21	0.41
1:B:253:LEU:HD11	1:B:293:MET:HG2	2.03	0.41
1:C:205:ARG:HB3	1:C:207:PHE:CE2	2.56	0.41
1:C:275:ASN:H	1:C:287:ASN:ND2	2.11	0.41
1:D:156:ILE:CG2	1:D:205:ARG:HD3	2.47	0.41
1:G:270:HIS:HD2	1:G:279:GLY:HA3	1.85	0.41
1:A:237:GLY:HA2	1:A:241:ASN:CB	2.50	0.40
1:C:241:ASN:ND2	1:C:241:ASN:N	2.69	0.40
1:D:155:ASN:HD21	1:D:337:ALA:HA	1.86	0.40
1:A:294:HIS:CG	1:A:295:ARG:H	2.39	0.40
1:D:106:ILE:HG13	1:D:196:THR:HG22	2.04	0.40
1:F:104:VAL:HG22	1:F:192:ARG:HD2	2.03	0.40
1:F:268:GLN:HB3	1:F:269:LYS:H	1.71	0.40
1:B:268:GLN:HB3	1:B:269:LYS:H	1.69	0.40
1:D:165:ILE:CB	1:D:329:HIS:HD2	2.34	0.40
1:E:279:GLY:HA2	1:E:285:LYS:N	2.34	0.40
1:B:262:ARG:HG3	1:B:267:GLY:O	2.22	0.40
1:D:294:HIS:CG	1:D:295:ARG:H	2.39	0.40
1:E:203:ALA:HB3	1:F:133:ALA:O	2.22	0.40
1:F:250:VAL:HG13	1:F:289:ILE:HA	2.04	0.40
1:G:262:ARG:HG3	1:G:267:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	244/345 (71%)	207 (85%)	29 (12%)	8 (3%)	4 26
1	B	244/345 (71%)	202 (83%)	35 (14%)	7 (3%)	4 29
1	C	244/345 (71%)	204 (84%)	33 (14%)	7 (3%)	4 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	244/345 (71%)	204 (84%)	31 (13%)	9 (4%)	3	24
1	E	244/345 (71%)	206 (84%)	31 (13%)	7 (3%)	4	29
1	F	244/345 (71%)	206 (84%)	31 (13%)	7 (3%)	4	29
1	G	244/345 (71%)	206 (84%)	28 (12%)	10 (4%)	3	23
All	All	1708/2415 (71%)	1435 (84%)	218 (13%)	55 (3%)	7	26

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	B	197	LYS
1	C	197	LYS
1	D	197	LYS
1	E	197	LYS
1	E	282	LYS
1	F	197	LYS
1	F	239	ILE
1	G	138	VAL
1	G	197	LYS
1	A	212	ASP
1	A	282	LYS
1	A	304	ARG
1	B	282	LYS
1	B	304	ARG
1	C	212	ASP
1	C	239	ILE
1	C	282	LYS
1	C	304	ARG
1	D	203	ALA
1	D	212	ASP
1	D	239	ILE
1	D	304	ARG
1	E	239	ILE
1	F	282	LYS
1	G	212	ASP
1	G	282	LYS
1	A	159	LEU
1	A	243	MET
1	B	159	LEU
1	B	212	ASP
1	D	159	LEU

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Mol	Chain	Res	Type
1	D	243	MET
1	D	282	LYS
1	E	212	ASP
1	E	243	MET
1	E	304	ARG
1	F	212	ASP
1	F	304	ARG
1	G	243	MET
1	B	243	MET
1	C	243	MET
1	F	243	MET
1	G	239	ILE
1	G	304	ARG
1	G	196	THR
1	A	271	VAL
1	G	160	GLY
1	D	271	VAL
1	E	271	VAL
1	A	239	ILE
1	B	271	VAL
1	C	271	VAL
1	G	271	VAL
1	F	271	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/261 (70%)	163 (89%)	21 (11%)	5	21
1	B	184/261 (70%)	163 (89%)	21 (11%)	5	21
1	C	184/261 (70%)	167 (91%)	17 (9%)	9	29
1	D	184/261 (70%)	164 (89%)	20 (11%)	6	23
1	E	184/261 (70%)	164 (89%)	20 (11%)	6	23
1	F	184/261 (70%)	164 (89%)	20 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	184/261 (70%)	170 (92%)	14 (8%)	13	37
All	All	1288/1827 (70%)	1155 (90%)	133 (10%)	11	25

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ARG
1	A	126	LEU
1	A	156	ILE
1	A	182	LYS
1	A	197	LYS
1	A	205	ARG
1	A	208	TYR
1	A	212	ASP
1	A	222	MET
1	A	231	LEU
1	A	240	ARG
1	A	241	ASN
1	A	271	VAL
1	A	289	ILE
1	A	292	PHE
1	A	298	VAL
1	A	300	THR
1	A	306	LEU
1	A	308	LEU
1	A	312	ARG
1	A	333	ARG
1	B	119	ARG
1	B	126	LEU
1	B	128	GLU
1	B	145	LEU
1	B	156	ILE
1	B	182	LYS
1	B	197	LYS
1	B	205	ARG
1	B	208	TYR
1	B	212	ASP
1	B	222	MET
1	B	240	ARG
1	B	271	VAL
1	B	281	VAL
1	B	289	ILE

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Mol	Chain	Res	Type
1	B	298	VAL
1	B	300	THR
1	B	306	LEU
1	B	308	LEU
1	B	312	ARG
1	B	333	ARG
1	C	119	ARG
1	C	126	LEU
1	C	156	ILE
1	C	197	LYS
1	C	205	ARG
1	C	208	TYR
1	C	212	ASP
1	C	222	MET
1	C	241	ASN
1	C	271	VAL
1	C	281	VAL
1	C	289	ILE
1	C	298	VAL
1	C	300	THR
1	C	306	LEU
1	C	308	LEU
1	C	312	ARG
1	D	119	ARG
1	D	126	LEU
1	D	128	GLU
1	D	139	LEU
1	D	145	LEU
1	D	156	ILE
1	D	197	LYS
1	D	205	ARG
1	D	208	TYR
1	D	212	ASP
1	D	222	MET
1	D	241	ASN
1	D	271	VAL
1	D	281	VAL
1	D	289	ILE
1	D	298	VAL
1	D	300	THR
1	D	306	LEU
1	D	308	LEU

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Mol	Chain	Res	Type
1	D	312	ARG
1	E	119	ARG
1	E	126	LEU
1	E	135	ASP
1	E	145	LEU
1	E	182	LYS
1	E	197	LYS
1	E	205	ARG
1	E	208	TYR
1	E	212	ASP
1	E	222	MET
1	E	241	ASN
1	E	271	VAL
1	E	281	VAL
1	E	289	ILE
1	E	292	PHE
1	E	298	VAL
1	E	300	THR
1	E	306	LEU
1	E	308	LEU
1	E	312	ARG
1	F	119	ARG
1	F	126	LEU
1	F	128	GLU
1	F	139	LEU
1	F	141	GLU
1	F	156	ILE
1	F	182	LYS
1	F	197	LYS
1	F	205	ARG
1	F	208	TYR
1	F	212	ASP
1	F	222	MET
1	F	241	ASN
1	F	271	VAL
1	F	281	VAL
1	F	289	ILE
1	F	300	THR
1	F	306	LEU
1	F	308	LEU
1	F	312	ARG
1	G	119	ARG

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Mol	Chain	Res	Type
1	G	156	ILE
1	G	197	LYS
1	G	205	ARG
1	G	208	TYR
1	G	212	ASP
1	G	222	MET
1	G	241	ASN
1	G	271	VAL
1	G	281	VAL
1	G	289	ILE
1	G	300	THR
1	G	308	LEU
1	G	312	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	198	ASN
1	A	241	ASN
1	A	270	HIS
1	A	280	ASN
1	A	287	ASN
1	A	315	ASN
1	A	317	GLN
1	B	155	ASN
1	B	198	ASN
1	B	241	ASN
1	B	270	HIS
1	B	287	ASN
1	B	315	ASN
1	B	317	GLN
1	C	155	ASN
1	C	198	ASN
1	C	241	ASN
1	C	270	HIS
1	C	280	ASN
1	C	287	ASN
1	C	315	ASN
1	C	317	GLN
1	D	155	ASN
1	D	198	ASN

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Mol	Chain	Res	Type
1	D	241	ASN
1	D	270	HIS
1	D	287	ASN
1	D	315	ASN
1	D	329	HIS
1	E	198	ASN
1	E	241	ASN
1	E	270	HIS
1	E	287	ASN
1	E	315	ASN
1	E	317	GLN
1	E	329	HIS
1	F	155	ASN
1	F	198	ASN
1	F	241	ASN
1	F	270	HIS
1	F	280	ASN
1	F	287	ASN
1	F	315	ASN
1	F	317	GLN
1	G	153	ASN
1	G	155	ASN
1	G	198	ASN
1	G	241	ASN
1	G	270	HIS
1	G	287	ASN
1	G	315	ASN
1	G	317	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

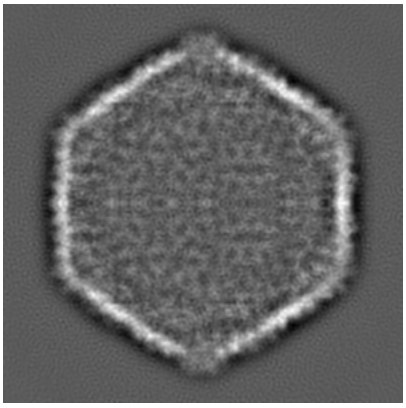
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1810. These allow visual inspection of the internal detail of the map and identification of artifacts.

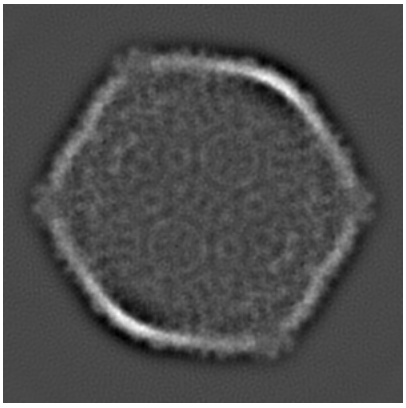
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

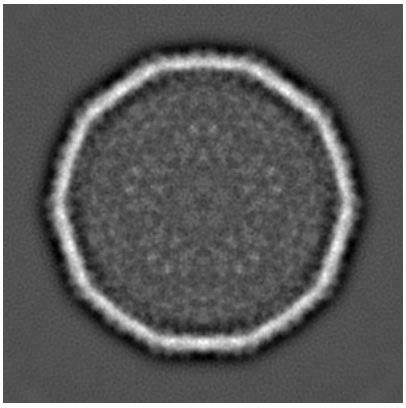
6.1.1 Primary map



X



Y

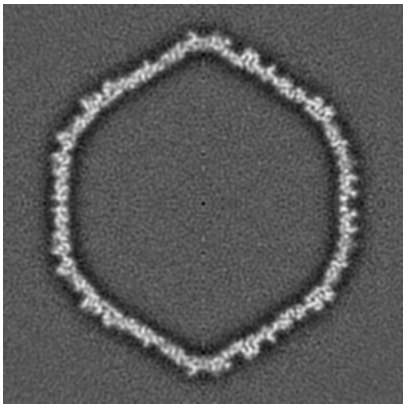


Z

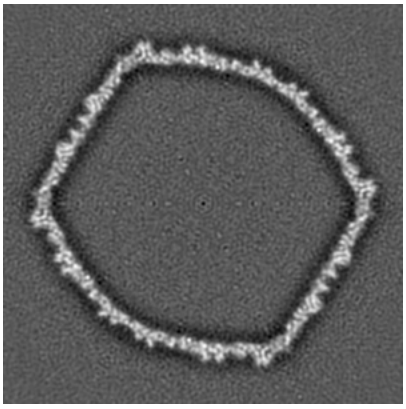
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

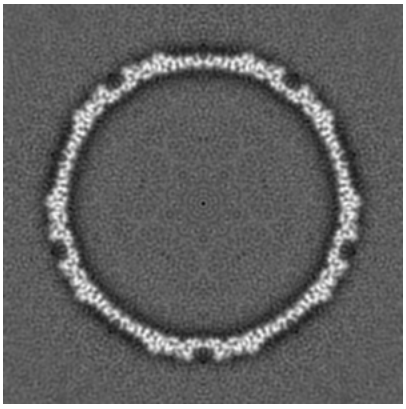
6.2.1 Primary map



X Index: 276



Y Index: 276

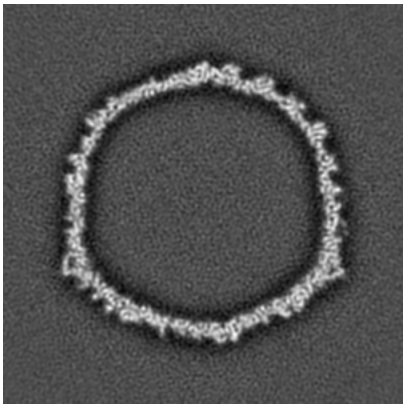


Z Index: 276

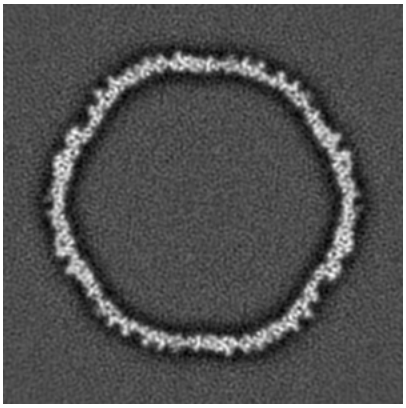
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

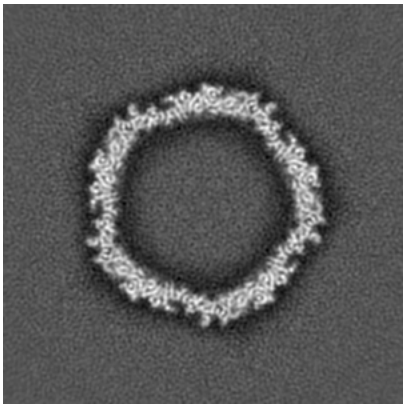
6.3.1 Primary map



X Index: 367



Y Index: 321

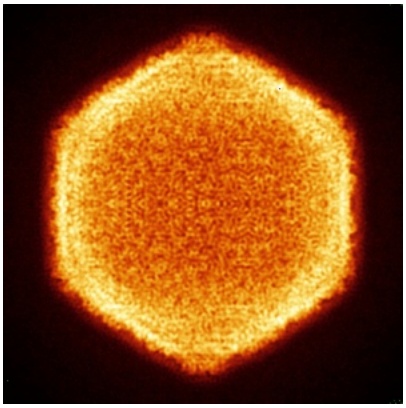


Z Index: 134

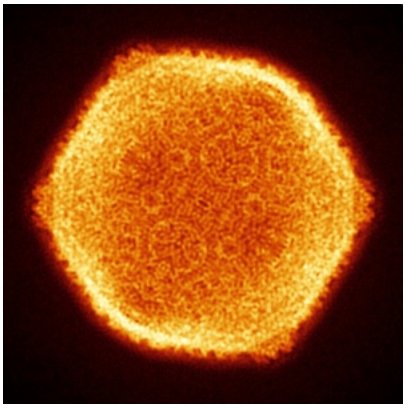
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

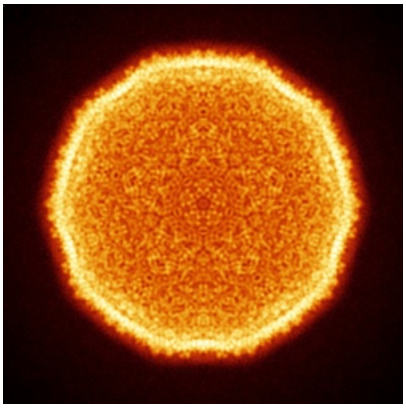
6.4.1 Primary map



X



Y

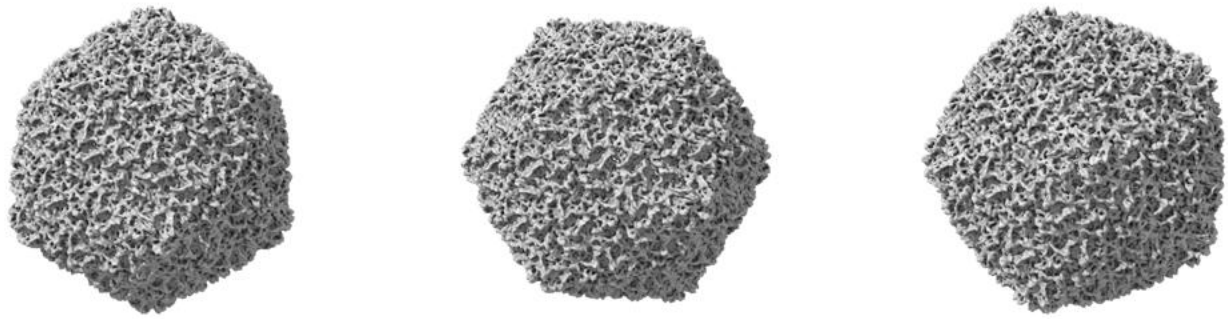


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

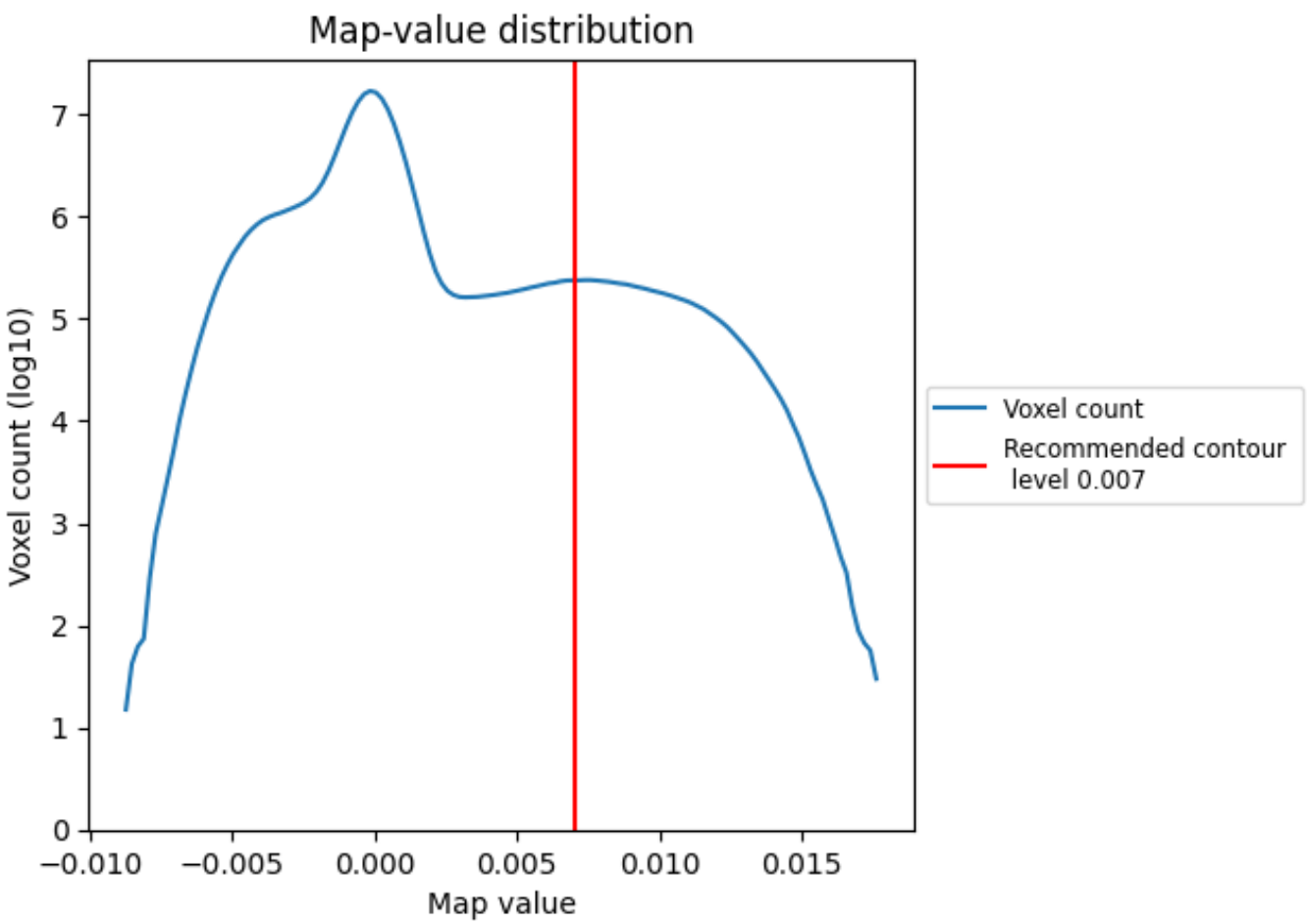
6.6 Mask visualisation (i)

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

7 Map analysis (i)

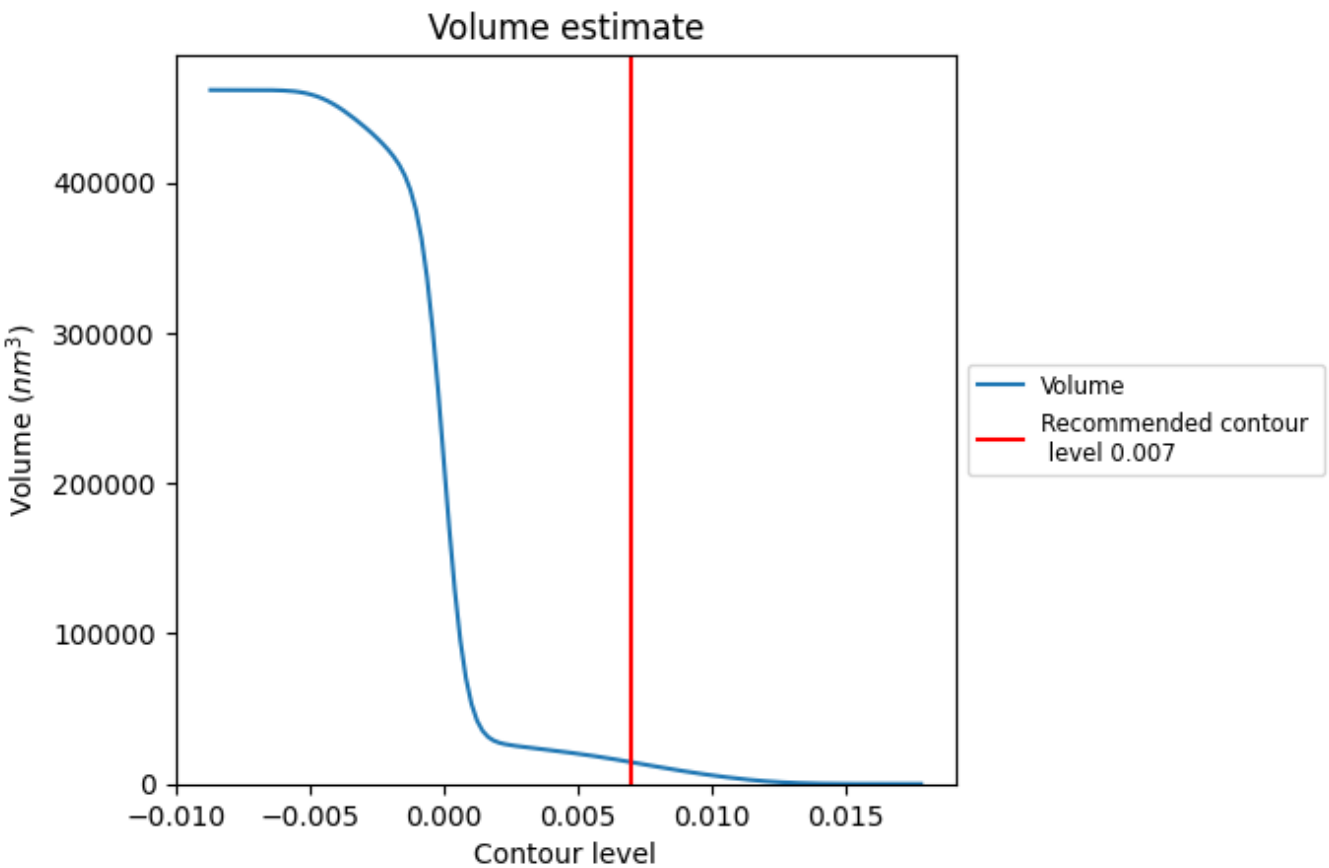
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

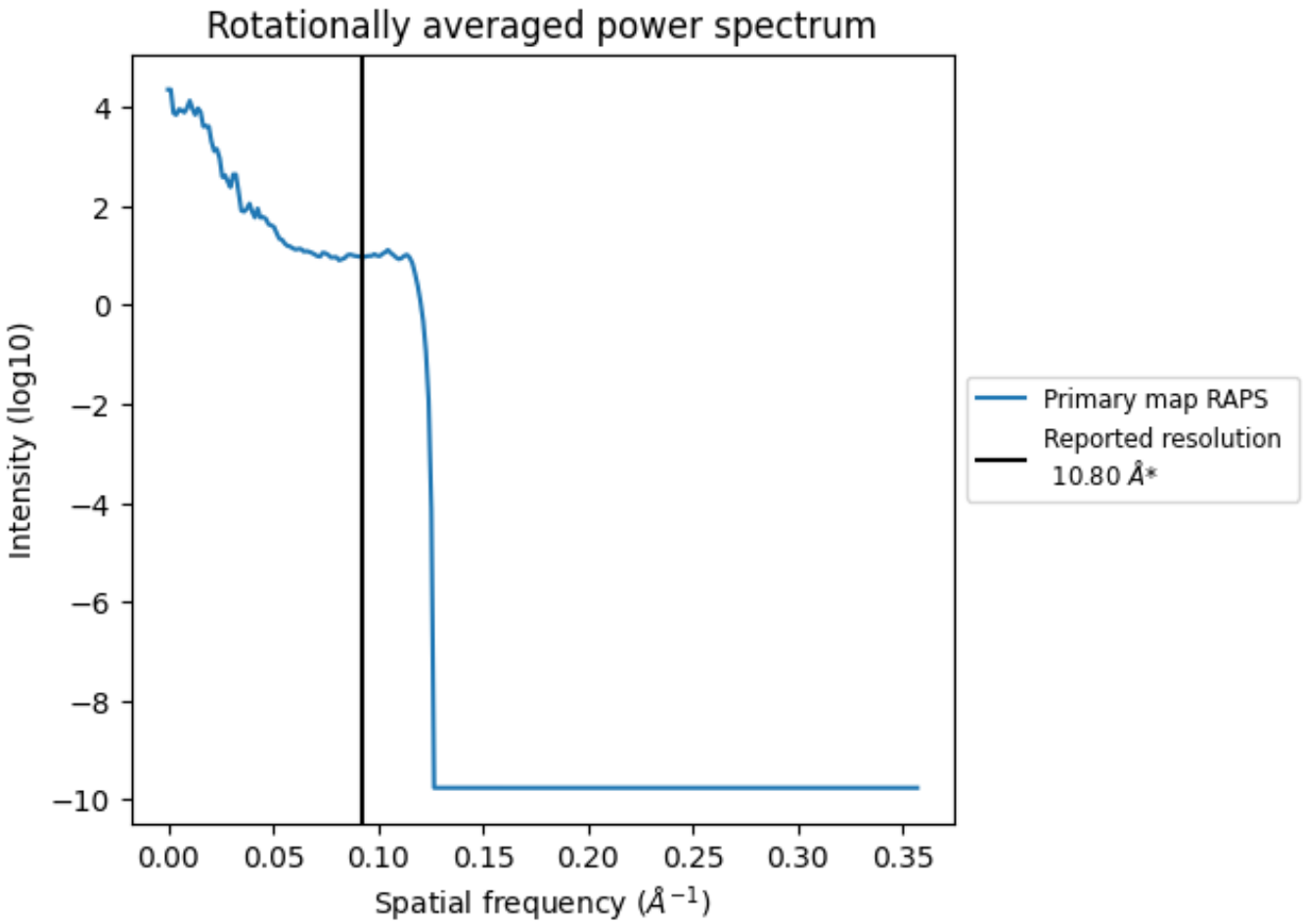
7.2 Volume estimate (i)



The volume at the recommended contour level is 14487 nm^3; this corresponds to an approximate mass of 13086 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 (i)



*Reported resolution corresponds to spatial frequency of 0.093 Å^{-1}

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

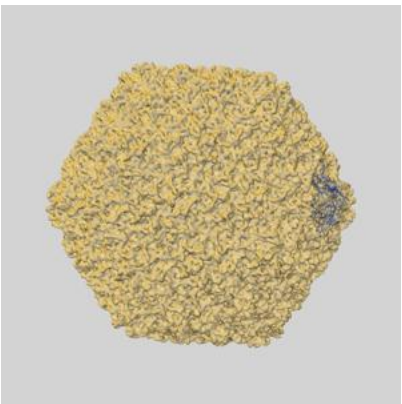
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1810 and PDB model 2XVR. Per-residue inclusion information can be found in section 3 on page 4.

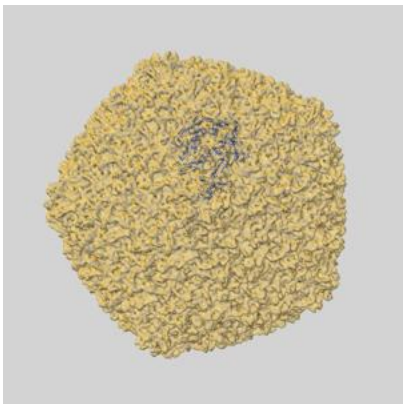
9.1 Map-model overlays

9.1.1 Map-model overlay (i)

X

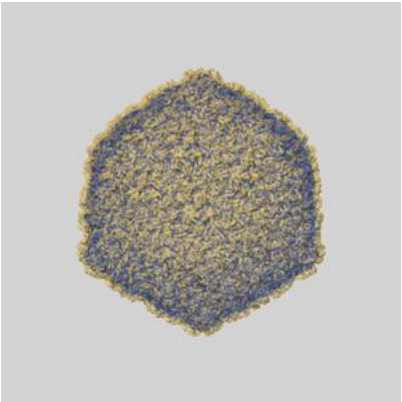


Y

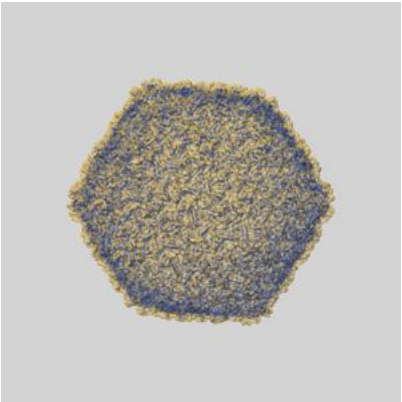


Z

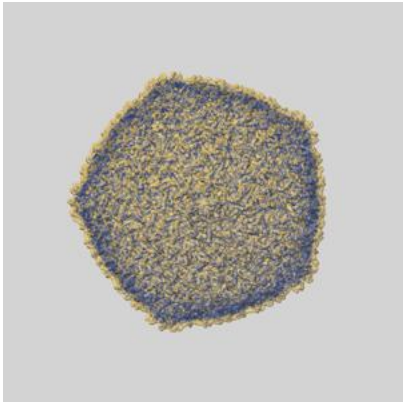
9.1.2 Map-model assembly overlay (i)



X



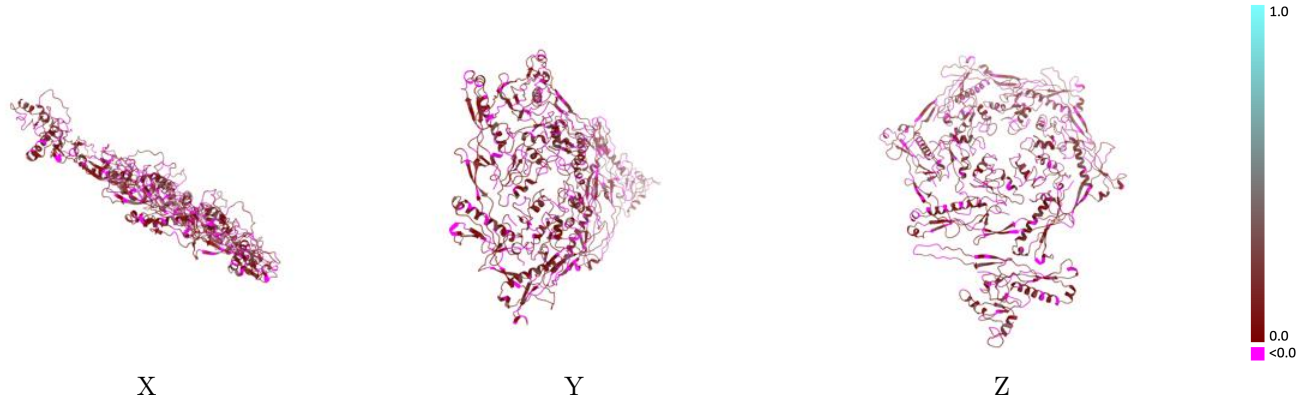
Y



Z

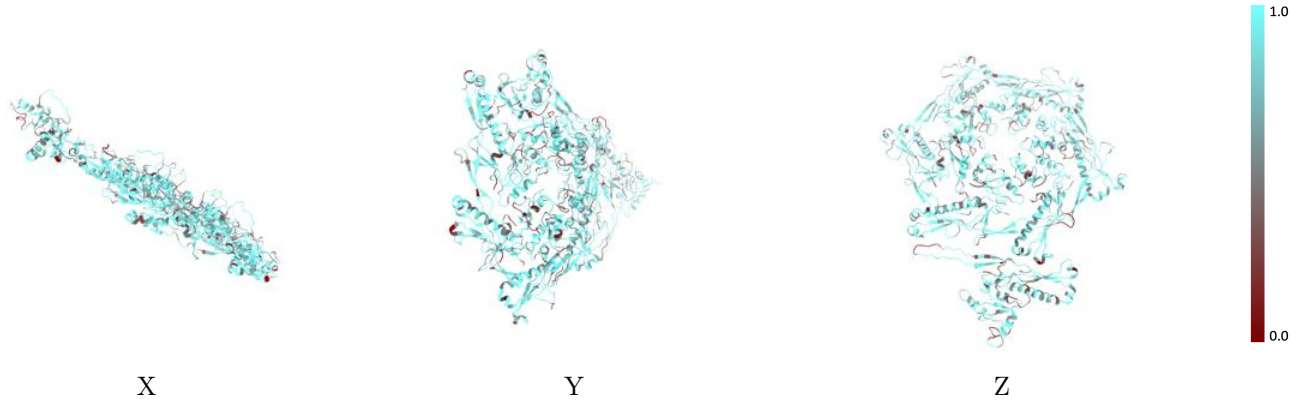
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



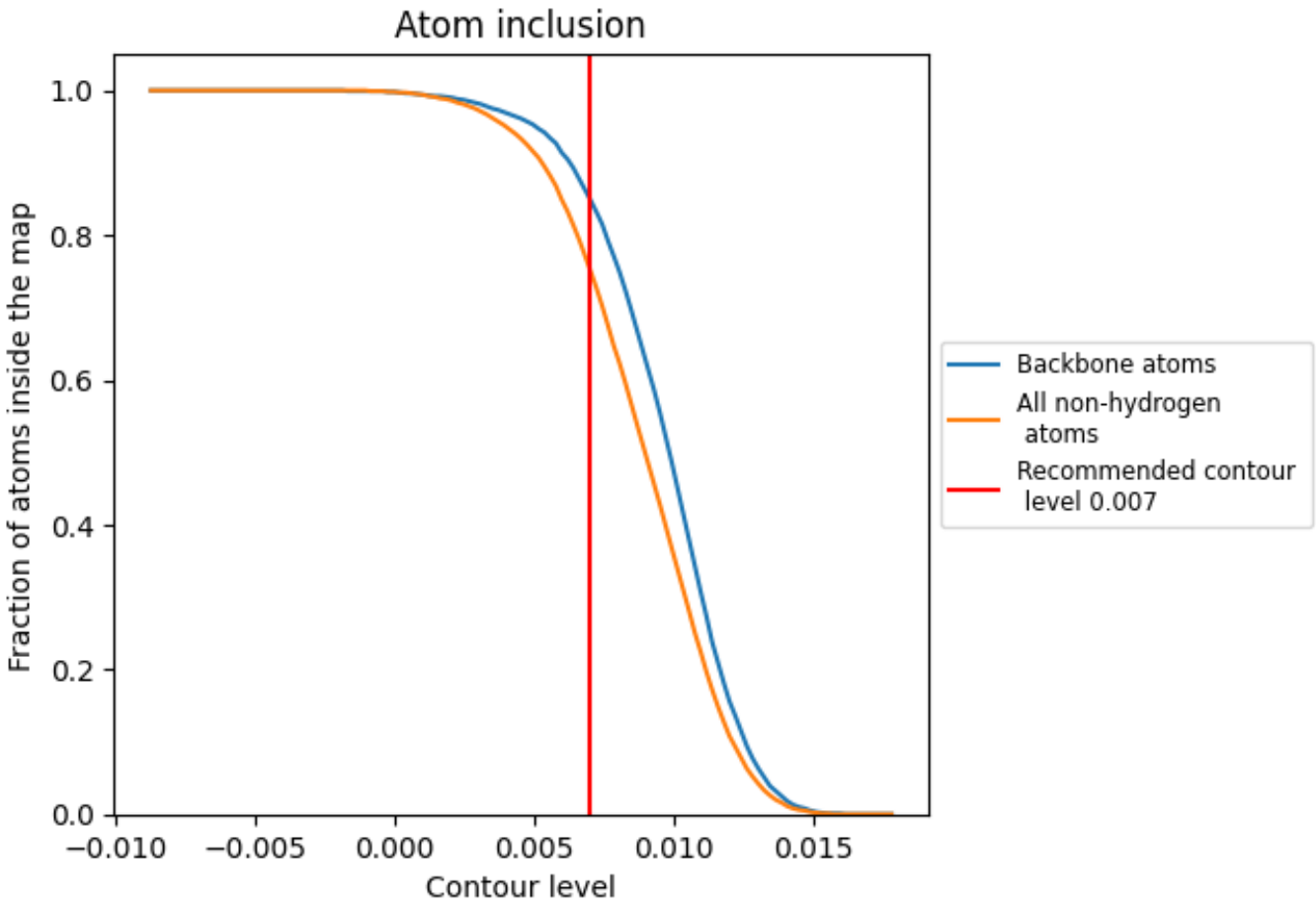
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7540	0.0900
A	0.7570	0.0790
B	0.7660	0.0900
C	0.7750	0.0920
D	0.7580	0.0910
E	0.7540	0.0880
F	0.7710	0.0950
G	0.6980	0.0910