Full wwPDB EM Validation Report (i)

Feb 12, 2024 – 08:29 PM EST

PDB ID	:	3J7X
EMDB ID	:	EMD-6037
Title	:	Capsid Expansion Mechanism Of Bacteriophage T7 Revealed By Multi-State Atomic Models Derived From Cryo-EM Reconstructions
Authors	:	Guo, F.; Liu, Z.; Fang, P.A.; Zhang, Q.; Wright, E.T.; Wu, W.; Zhang, C.; Vago, F.; Ren, Y.; Jakata, J.; Chiu, W.; Serwer, P.; Jiang, W.
Deposited on	:	2014-08-12
Resolution	:	3.60 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 (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:

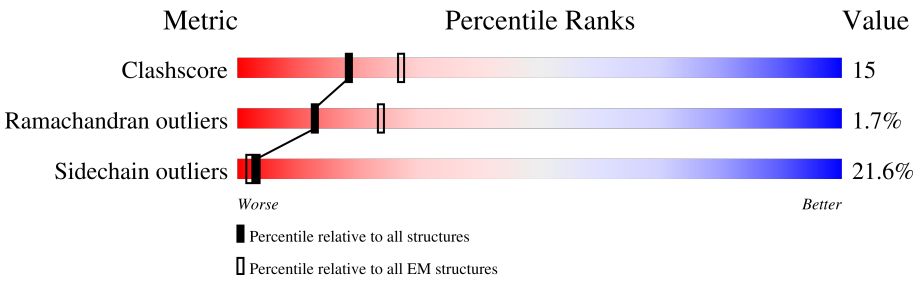
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	15% 59% 32% 8% •
1	B	345	14% 57% 34% 9% •
1	C	345	15% 57% 33% 9% ••
1	D	345	13% 62% 29% 8% ••
1	E	345	16% 60% 31% 8% •
1	F	345	16% 60% 31% 8% ••
1	G	345	33% 61% 31% 8% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17829 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.

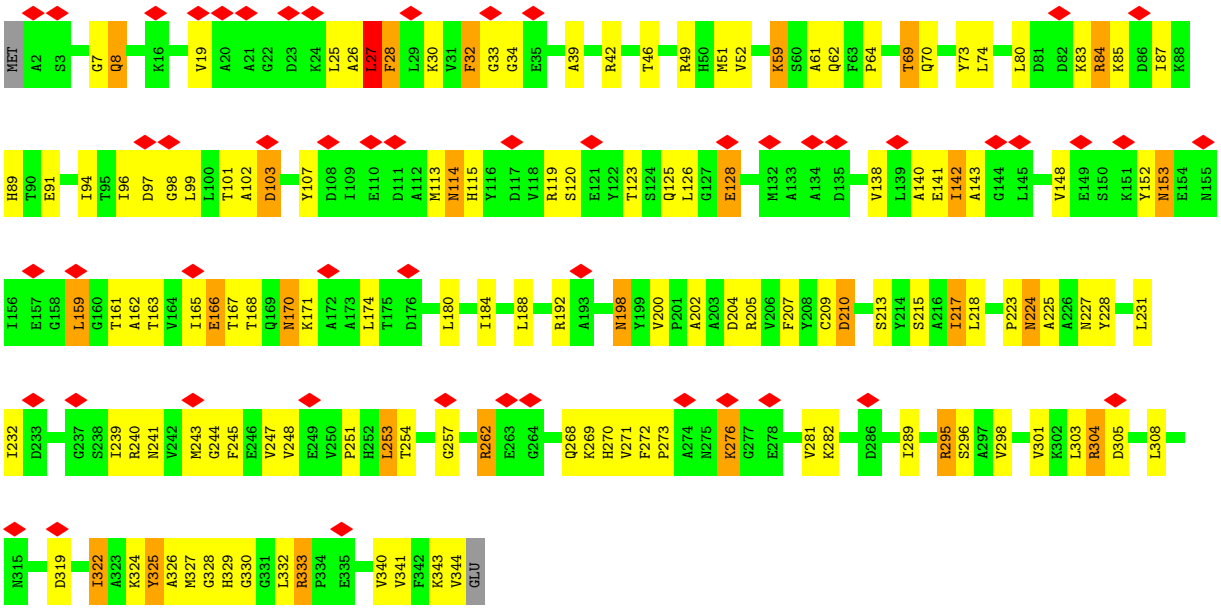
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	343	2547	1593	452	491	11	0	0
1	B	343	2547	1593	452	491	11	0	0
1	C	343	2547	1593	452	491	11	0	0
1	D	343	2547	1593	452	491	11	0	0
1	E	343	2547	1593	452	491	11	0	0
1	F	343	2547	1593	452	491	11	0	0
1	G	343	2547	1593	452	491	11	0	0

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.

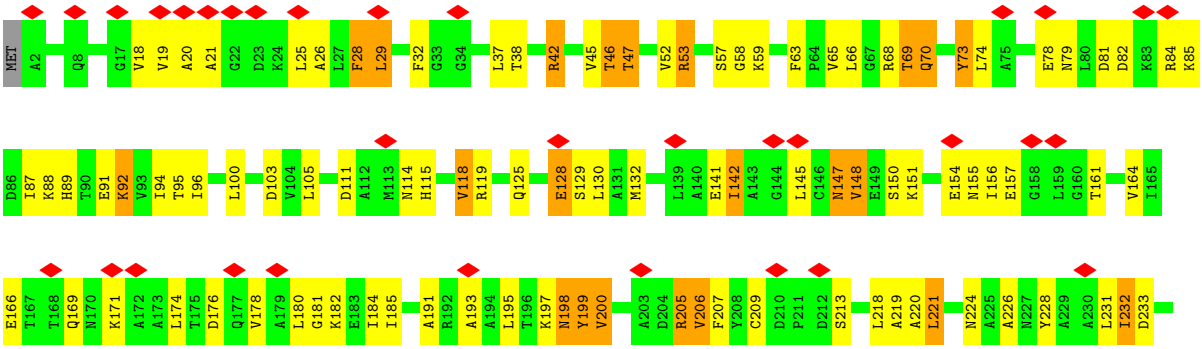
- Molecule 1: Major capsid protein 10A

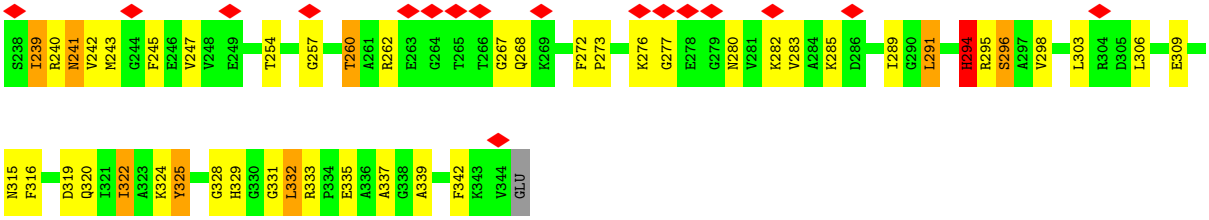
Chain A:



- Molecule 1: Major capsid protein 10A

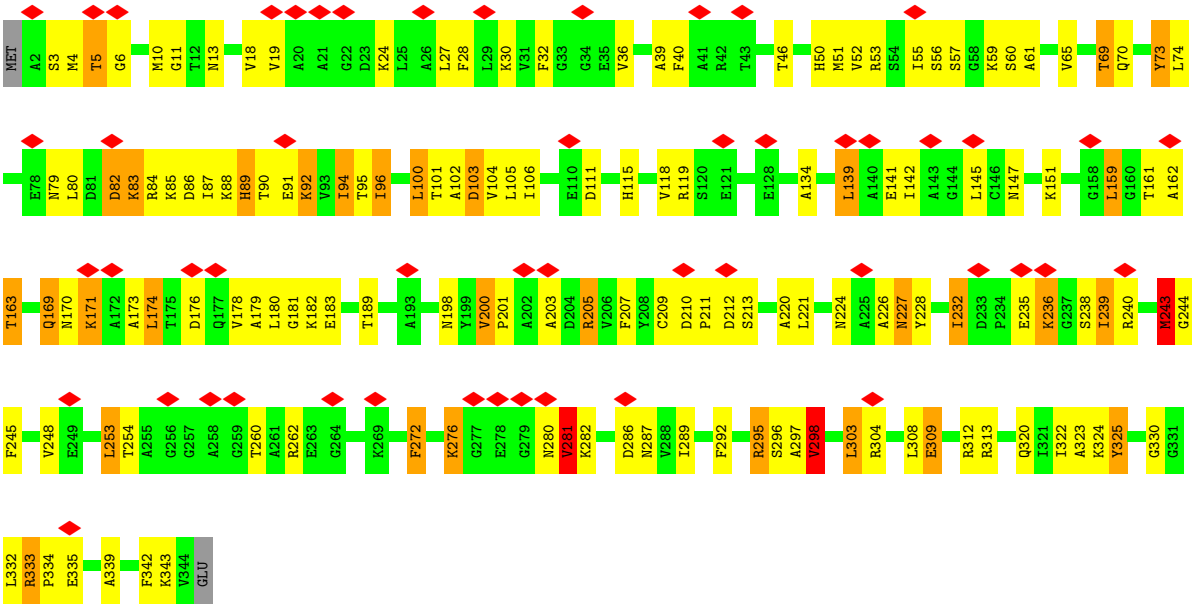
Chain B:





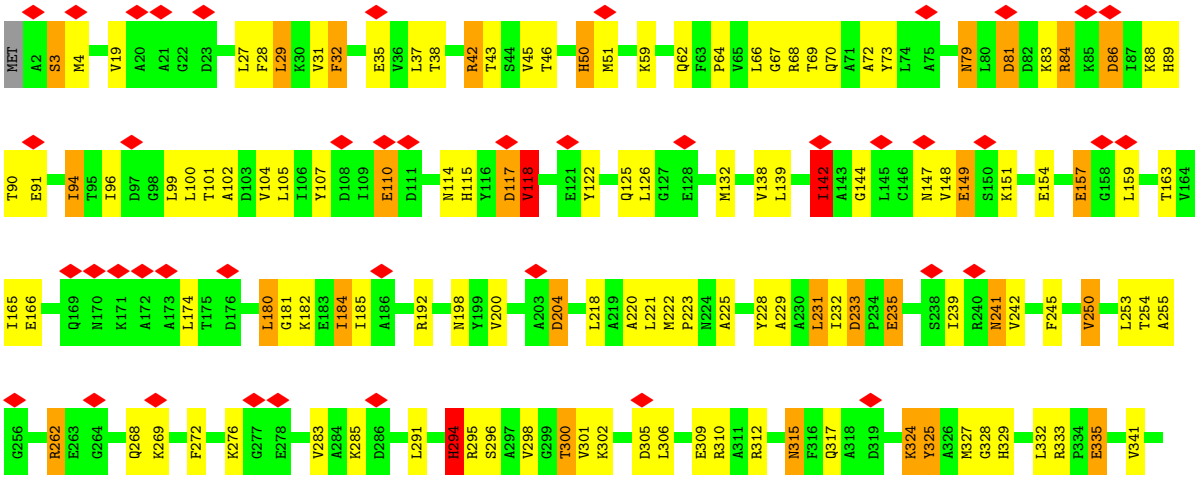
• Molecule 1: Major capsid protein 10A

Chain C:



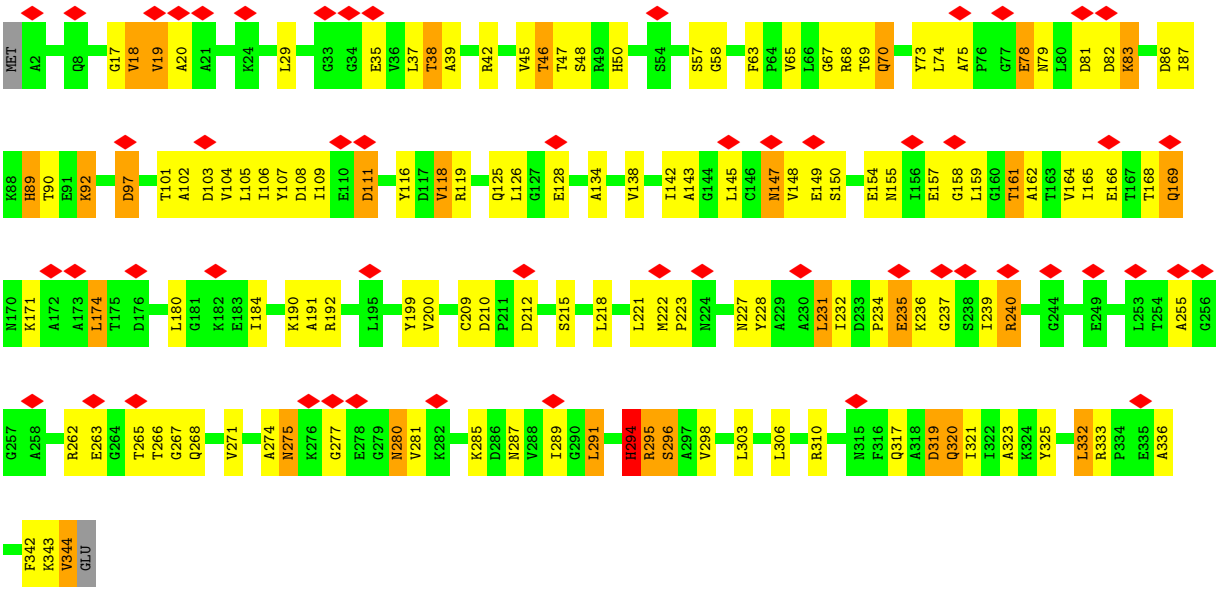
• Molecule 1: Major capsid protein 10A

Chain D:



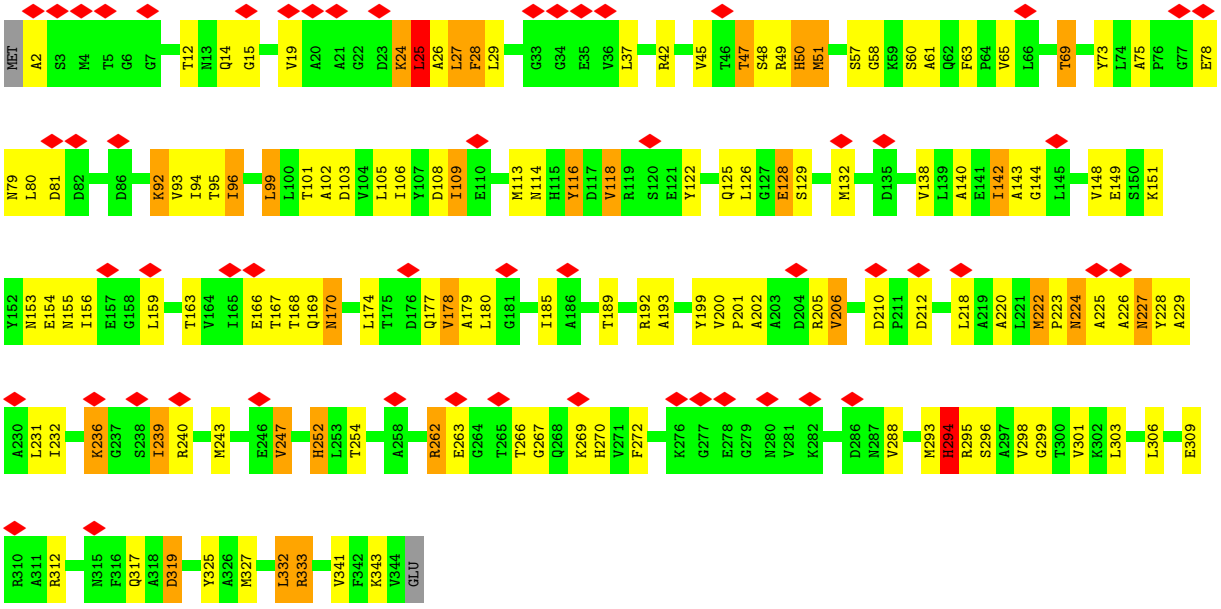
• Molecule 1: Major capsid protein 10A

Chain E:



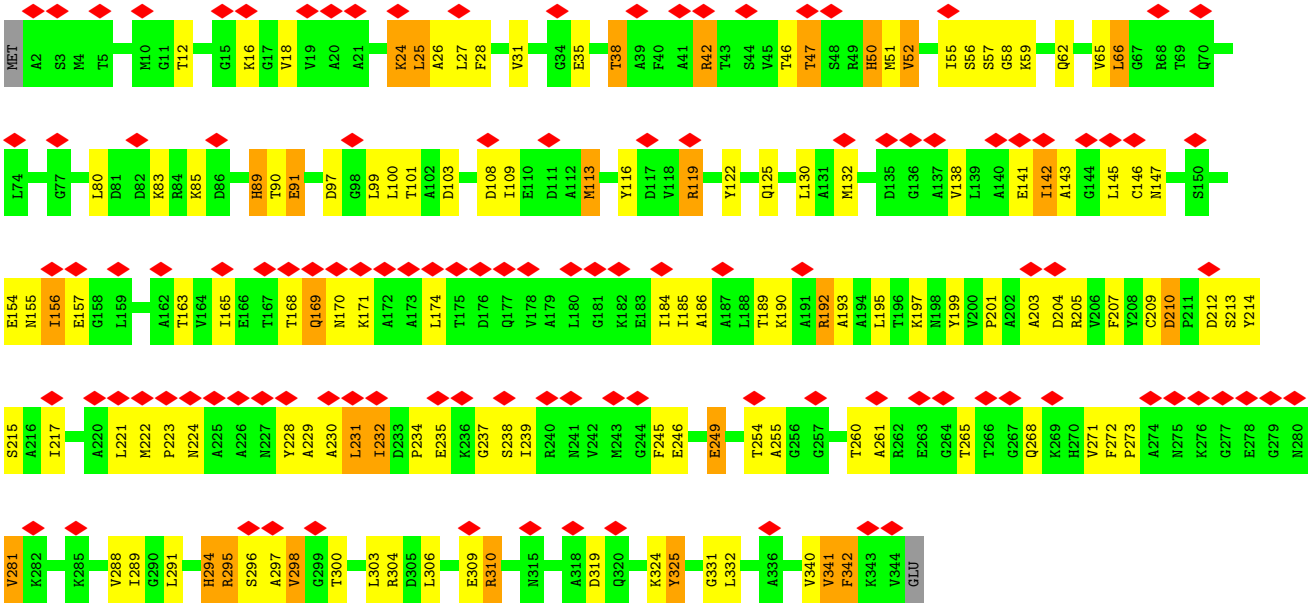
• Molecule 1: Major capsid protein 10A

Chain F:



• Molecule 1: Major capsid protein 10A

Chain G:


MET A2 S3 M4 T5 M10 G11 T12 G15 K16 G17 V18 V19 A20 A21 K24 L25 A26 L27 F28 V31 G34 E35 T38 A39 F40 A41 R42 T43 S44 V45 T46 T47 S48 R49 H50 M51 V52 I55 S56 S57 G58 K59 Q62 V65 L66 G67 R68 T69 Q70
L74 G77 L80 D81 D82 K83 R84 K85 D86 H89 T90 E91 D97 G98 L99 L100 T101 A102 D103 D108 I109 E110 D111 A112 M113 Y116 D117 V118 R119 Y122 Q125 L130 A131 M132 D135 G136 A137 V138 L139 A140 E141 I142 A143 G144 L145 C146 N147 S150
E154 N155 I156 E157 G158 L159 A162 T163 V164 I165 E166 T167 T168 Q169 N170 K171 A172 A173 L174 T175 D176 Q177 V178 A179 L180 G181 K182 E183 I184 I185 A186 A187 L188 T189 K190 A191 R192 A193 A194 L195 T196 K197 N198 Y199 V200 P201 A202 A203 D204 R205 V206 F207 Y208 C209 D210 P211 D212 S213 Y214
S215 A216 I217 A220 L221 M222 P223 N224 A225 A226 N227 Y228 A229 A230 L231 I232 D233 P234 E235 K236 G237 S238 I239 R240 N241 V242 M243 G244 F245 E246 E249 T254 A255 G256 G257 T260 A261 R262 E263 G264 T265 T266 G267 Q268 K269 H270 V271 F272 P273 A274 N275 K276 G277 E278 G279 N280
V281 K282 K285 V288 I289 G290 L291 H294 R295 S296 A297 V298 G299 T300 L303 R304 D305 L306 E309 R310 N315 A318 D319 Q320 K324 Y325 G331 L332 A336 V340 V341 F342 K343 V344 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	33952	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	57727	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	28.700	Depositor
Minimum map value	-18.852	Depositor
Average map value	0.120	Depositor
Map value standard deviation	1.198	Depositor
Recommended contour level	4.6	Depositor
Map size (Å)	880.0, 880.0, 880.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.27	0/2582	0.57	1/3491 (0.0%)
1	B	0.27	0/2582	0.58	0/3491
1	C	0.27	0/2582	0.61	1/3491 (0.0%)
1	D	0.28	0/2582	0.60	0/3491
1	E	0.28	0/2582	0.56	0/3491
1	F	0.28	0/2582	0.59	1/3491 (0.0%)
1	G	0.27	0/2582	0.59	0/3491
All	All	0.27	0/18074	0.58	3/24437 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	2
All	All	0	9

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	25	LEU	CA-CB-CG	6.44	130.11	115.30
1	A	27	LEU	CA-CB-CG	5.28	127.44	115.30
1	C	100	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	GLN	Peptide
1	B	294	HIS	Peptide
1	C	238	SER	Peptide
1	C	243	MET	Peptide
1	D	294	HIS	Peptide
1	E	294	HIS	Peptide
1	F	294	HIS	Peptide
1	G	116	TYR	Peptide
1	G	294	HIS	Peptide

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	2547	0	2573	89	0
1	B	2547	0	2573	92	0
1	C	2547	0	2573	89	0
1	D	2547	0	2573	77	0
1	E	2547	0	2573	83	0
1	F	2547	0	2573	90	0
1	G	2547	0	2573	77	0
All	All	17829	0	18011	523	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 15.

All (523) 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:C:296:SER:HA	1:C:298:VAL:H	1.46	0.80
1:C:32:PHE:HA	1:D:62:GLN:H	1.45	0.79
1:C:147:ASN:HD21	1:C:282:LYS:HB2	1.49	0.77
1:C:163:THR:HB	1:C:339:ALA:H	1.49	0.77
1:A:184:ILE:HD11	1:A:289:ILE:HG21	1.66	0.76
1:E:67:GLY:H	1:E:87:ILE:HG22	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HA	1:C:73:TYR:HB3	1.69	0.74
1:G:205:ARG:HB2	1:G:245:PHE:HB3	1.70	0.73
1:C:170:ASN:HB3	1:C:173:ALA:HB2	1.69	0.73
1:E:75:ALA:HB3	1:E:78:GLU:HG2	1.71	0.73
1:G:154:GLU:HG3	1:G:155:ASN:HD22	1.54	0.72
1:E:158:GLY:HA2	1:E:159:LEU:HB2	1.72	0.71
1:F:239:ILE:HD12	1:F:247:VAL:HG21	1.73	0.71
1:C:276:LYS:HG3	1:C:287:ASN:HD21	1.55	0.71
1:B:205:ARG:HA	1:B:294:HIS:HA	1.73	0.70
1:D:233:ASP:OD1	1:D:233:ASP:N	2.25	0.70
1:F:42:ARG:NH2	1:F:132:MET:SD	2.65	0.69
1:B:231:LEU:HG	1:B:232:ILE:HG23	1.74	0.69
1:E:227:ASN:H	1:F:227:ASN:HD22	1.39	0.69
1:C:198:ASN:ND2	1:C:335:GLU:O	2.25	0.69
1:G:42:ARG:NH2	1:G:132:MET:SD	2.61	0.69
1:A:244:GLY:H	1:F:236:LYS:H	1.41	0.68
1:G:42:ARG:HH11	1:G:42:ARG:H	1.40	0.68
1:A:99:LEU:HD11	1:A:324:LYS:HB2	1.75	0.68
1:G:119:ARG:H	1:G:119:ARG:HH11	1.42	0.68
1:E:102:ALA:HB1	1:E:126:LEU:HD22	1.75	0.67
1:E:215:SER:HB3	1:F:193:ALA:HB2	1.75	0.67
1:D:45:VAL:HG13	1:D:46:THR:HG23	1.77	0.67
1:F:47:THR:OG1	1:F:48:SER:N	2.27	0.67
1:A:119:ARG:NH2	1:A:319:ASP:OD1	2.27	0.67
1:E:274:ALA:HA	1:E:285:LYS:HB3	1.77	0.67
1:E:221:LEU:HD23	1:E:232:ILE:HB	1.77	0.66
1:C:103:ASP:OD1	1:D:84:ARG:NH2	2.28	0.66
1:E:275:ASN:ND2	1:E:277:GLY:O	2.28	0.66
1:F:96:ILE:HG22	1:F:301:VAL:HG21	1.76	0.66
1:G:295:ARG:C	1:G:297:ALA:HA	2.16	0.66
1:B:141:GLU:OE2	1:B:331:GLY:N	2.29	0.65
1:C:88:LYS:O	1:C:89:HIS:ND1	2.30	0.65
1:A:224:ASN:N	1:A:224:ASN:OD1	2.29	0.65
1:D:253:LEU:O	1:D:285:LYS:NZ	2.29	0.64
1:G:209:CYS:SG	1:G:213:SER:OG	2.55	0.64
1:G:51:MET:HB2	1:G:297:ALA:HB3	1.78	0.64
1:B:57:SER:OG	1:B:58:GLY:N	2.31	0.64
1:E:79:ASN:HD21	1:E:81:ASP:HB3	1.63	0.64
1:A:159:LEU:HD13	1:A:198:ASN:HA	1.78	0.63
1:A:241:ASN:ND2	1:A:245:PHE:O	2.30	0.63
1:E:171:LYS:HA	1:E:174:LEU:HD22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASN:N	1:F:224:ASN:OD1	2.31	0.63
1:A:171:LYS:HA	1:A:174:LEU:HB2	1.81	0.63
1:C:254:THR:HA	1:C:272:PHE:HD2	1.64	0.63
1:C:169:GLN:HB3	1:C:343:LYS:HE2	1.80	0.63
1:D:42:ARG:NE	1:E:199:TYR:OH	2.25	0.63
1:B:37:LEU:HB2	1:C:65:VAL:HG12	1.81	0.63
1:G:209:CYS:SG	1:G:210:ASP:N	2.71	0.63
1:E:102:ALA:HB3	1:E:323:ALA:HB3	1.81	0.62
1:A:209:CYS:SG	1:A:210:ASP:N	2.72	0.62
1:C:39:ALA:HB2	1:D:67:GLY:HA2	1.80	0.62
1:C:181:GLY:HA3	1:C:220:ALA:HB2	1.81	0.62
1:D:250:VAL:HG23	1:D:253:LEU:HD23	1.82	0.62
1:A:227:ASN:ND2	1:F:223:PRO:O	2.31	0.62
1:C:243:MET:O	1:C:245:PHE:N	2.32	0.62
1:C:161:THR:OG1	1:C:162:ALA:N	2.25	0.62
1:A:223:PRO:HA	1:B:228:TYR:HE2	1.65	0.61
1:F:178:VAL:HG23	1:F:220:ALA:HA	1.82	0.61
1:A:113:MET:O	1:A:114:ASN:ND2	2.32	0.61
1:B:69:THR:OG1	1:B:70:GLN:N	2.33	0.61
1:F:114:ASN:HD22	1:F:116:TYR:H	1.48	0.61
1:A:103:ASP:HB2	1:A:322:ILE:HG22	1.82	0.60
1:D:253:LEU:C	1:D:254:THR:HG1	2.02	0.60
1:E:296:SER:OG	1:E:333:ARG:NH2	2.34	0.60
1:A:96:ILE:HA	1:A:328:GLY:HA3	1.83	0.60
1:D:302:LYS:NZ	1:D:305:ASP:OD2	2.34	0.60
1:E:125:GLN:OE1	1:F:69:THR:OG1	2.19	0.60
1:D:117:ASP:OD2	1:D:117:ASP:N	2.34	0.60
1:C:203:ALA:HA	1:C:205:ARG:HD2	1.82	0.60
1:B:294:HIS:O	1:B:295:ARG:HG2	2.02	0.60
1:C:51:MET:HG2	1:C:296:SER:HB3	1.83	0.60
1:G:38:THR:OG1	1:G:125:GLN:NE2	2.35	0.59
1:D:88:LYS:O	1:D:89:HIS:ND1	2.35	0.59
1:F:201:PRO:O	1:F:205:ARG:NH1	2.35	0.59
1:D:235:GLU:OE2	1:E:240:ARG:NH1	2.36	0.59
1:B:18:VAL:HB	1:B:21:ALA:HB2	1.84	0.59
1:F:178:VAL:O	1:F:180:LEU:N	2.35	0.59
1:G:232:ILE:HA	1:G:239:ILE:H	1.66	0.59
1:A:125:GLN:HG3	1:B:69:THR:HG22	1.83	0.59
1:A:184:ILE:HG21	1:A:217:ILE:HG12	1.83	0.59
1:D:229:ALA:HB2	1:E:228:TYR:CZ	2.38	0.59
1:E:103:ASP:OD1	1:E:262:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLN:NE2	1:B:128:GLU:OE1	2.35	0.59
1:C:295:ARG:C	1:C:297:ALA:HB3	2.24	0.58
1:D:37:LEU:HD12	1:E:65:VAL:HG12	1.85	0.58
1:G:25:LEU:HD13	1:G:25:LEU:H	1.68	0.58
1:D:117:ASP:HA	1:D:118:VAL:HG12	1.85	0.58
1:E:148:VAL:HG22	1:E:281:VAL:HG23	1.85	0.58
1:G:42:ARG:H	1:G:42:ARG:NH1	2.02	0.58
1:D:181:GLY:O	1:D:185:ILE:HG12	2.04	0.58
1:B:161:THR:OG1	1:B:337:ALA:O	2.21	0.57
1:E:143:ALA:O	1:E:147:ASN:ND2	2.38	0.57
1:B:309:GLU:HG2	1:B:322:ILE:HG12	1.87	0.57
1:C:289:ILE:HD11	1:C:342:PHE:CZ	2.39	0.57
1:A:153:ASN:N	1:A:153:ASN:OD1	2.37	0.57
1:D:181:GLY:HA3	1:D:220:ALA:HB2	1.86	0.57
1:F:202:ALA:O	1:F:205:ARG:NH1	2.38	0.57
1:A:39:ALA:HB1	1:B:68:ARG:HH21	1.67	0.56
1:B:142:ILE:HD12	1:B:291:LEU:HD13	1.88	0.56
1:B:218:LEU:HD11	1:B:232:ILE:HD13	1.88	0.56
1:D:144:GLY:O	1:D:148:VAL:HG23	2.06	0.56
1:F:92:LYS:NZ	1:F:93:VAL:O	2.38	0.56
1:E:319:ASP:OD2	1:E:319:ASP:N	2.38	0.56
1:F:294:HIS:O	1:F:294:HIS:ND1	2.39	0.56
1:B:81:ASP:OD1	1:B:82:ASP:N	2.39	0.56
1:E:266:THR:OG1	1:E:267:GLY:N	2.38	0.56
1:F:288:VAL:HA	1:F:341:VAL:HG12	1.88	0.56
1:E:42:ARG:HG2	1:F:199:TYR:CZ	2.41	0.56
1:A:168:THR:O	1:A:343:LYS:NZ	2.35	0.55
1:B:276:LYS:NZ	1:B:277:GLY:O	2.38	0.55
1:D:165:ILE:HG12	1:D:166:GLU:H	1.71	0.55
1:E:150:SER:OG	1:E:280:ASN:ND2	2.40	0.55
1:F:102:ALA:HB1	1:F:126:LEU:HD22	1.88	0.55
1:G:46:THR:HB	1:G:47:THR:HA	1.87	0.55
1:G:50:HIS:O	1:G:50:HIS:ND1	2.39	0.55
1:C:86:ASP:OD1	1:C:87:ILE:N	2.40	0.55
1:A:273:PRO:HG2	1:A:281:VAL:HG21	1.89	0.55
1:G:119:ARG:HA	1:G:122:TYR:HB2	1.89	0.55
1:E:104:VAL:O	1:E:320:GLN:HB2	2.07	0.54
1:G:25:LEU:HB2	1:G:26:ALA:HA	1.89	0.54
1:G:342:PHE:HD1	1:G:342:PHE:H	1.53	0.54
1:D:45:VAL:HG22	1:D:46:THR:H	1.73	0.54
1:E:235:GLU:O	1:E:237:GLY:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:PHE:CD2	1:C:59:LYS:HB2	2.42	0.54
1:D:147:ASN:HB2	1:D:283:VAL:HG11	1.90	0.54
1:B:125:GLN:HG3	1:C:87:ILE:HD11	1.90	0.54
1:C:171:LYS:NZ	1:C:286:ASP:O	2.40	0.54
1:E:143:ALA:HB2	1:E:291:LEU:HD13	1.88	0.54
1:G:138:VAL:O	1:G:142:ILE:HG22	2.07	0.54
1:G:169:GLN:OE1	1:G:170:ASN:N	2.39	0.54
1:C:69:THR:OG1	1:C:70:GLN:N	2.41	0.54
1:G:203:ALA:O	1:G:205:ARG:N	2.41	0.53
1:B:129:SER:HB3	1:C:69:THR:HG23	1.91	0.53
1:C:235:GLU:N	1:D:242:VAL:O	2.36	0.53
1:A:223:PRO:HB3	1:B:226:ALA:HB1	1.91	0.53
1:B:180:LEU:O	1:B:184:ILE:HG12	2.08	0.53
1:G:273:PRO:HG2	1:G:281:VAL:HG21	1.91	0.53
1:C:297:ALA:H	1:C:333:ARG:HG3	1.74	0.53
1:C:111:ASP:OD1	1:C:119:ARG:NH2	2.41	0.53
1:D:333:ARG:O	1:D:335:GLU:N	2.37	0.53
1:B:65:VAL:HG22	1:B:91:GLU:HA	1.91	0.53
1:D:79:ASN:N	1:D:79:ASN:OD1	2.43	0.52
1:G:56:SER:OG	1:G:57:SER:N	2.42	0.52
1:A:215:SER:HB2	1:B:193:ALA:HB2	1.91	0.52
1:C:226:ALA:O	1:C:227:ASN:ND2	2.42	0.52
1:B:262:ARG:HD3	1:C:85:LYS:HB2	1.91	0.52
1:B:79:ASN:ND2	1:F:2:ALA:O	2.43	0.52
1:D:159:LEU:HB3	1:D:335:GLU:HB2	1.92	0.52
1:E:78:GLU:OE2	1:E:83:LYS:NZ	2.43	0.52
1:C:262:ARG:O	1:D:70:GLN:NE2	2.43	0.52
1:D:101:THR:OG1	1:D:102:ALA:N	2.43	0.52
1:F:168:THR:OG1	1:F:169:GLN:N	2.42	0.52
1:A:273:PRO:HG2	1:A:281:VAL:HG11	1.92	0.52
1:E:174:LEU:HD21	1:E:180:LEU:HD13	1.92	0.52
1:F:178:VAL:C	1:F:180:LEU:H	2.13	0.52
1:A:61:ALA:HB3	1:A:301:VAL:HG21	1.90	0.52
1:D:231:LEU:HG	1:D:232:ILE:HG23	1.92	0.52
1:E:143:ALA:HB1	1:E:291:LEU:HD22	1.92	0.52
1:G:214:TYR:CG	1:G:249:GLU:HG2	2.44	0.52
1:A:205:ARG:HD2	1:A:244:GLY:O	2.10	0.51
1:C:296:SER:HA	1:C:298:VAL:N	2.21	0.51
1:D:327:MET:SD	1:D:329:HIS:NE2	2.83	0.51
1:F:252:HIS:H	1:F:252:HIS:CD2	2.28	0.51
1:A:174:LEU:HD13	1:A:180:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:HIS:HE1	1:F:298:VAL:HG22	1.75	0.51
1:G:201:PRO:HG2	1:G:294:HIS:NE2	2.26	0.51
1:A:202:ALA:HA	1:A:205:ARG:NH2	2.25	0.51
1:A:207:PHE:HD2	1:A:247:VAL:HG22	1.74	0.51
1:F:170:ASN:OD1	1:F:170:ASN:N	2.40	0.51
1:E:180:LEU:O	1:E:184:ILE:HG12	2.10	0.51
1:A:240:ARG:HA	1:A:240:ARG:HH11	1.75	0.51
1:D:100:LEU:HD23	1:D:325:TYR:HE2	1.75	0.51
1:F:79:ASN:OD1	1:F:80:LEU:N	2.44	0.51
1:F:103:ASP:OD2	1:F:103:ASP:N	2.44	0.51
1:B:155:ASN:ND2	1:B:156:ILE:H	2.09	0.51
1:E:287:ASN:HB2	1:E:342:PHE:HB2	1.91	0.51
1:F:294:HIS:O	1:F:295:ARG:HG2	2.11	0.50
1:B:156:ILE:HG23	1:B:157:GLU:H	1.75	0.50
1:D:305:ASP:O	1:D:325:TYR:HB2	2.10	0.50
1:F:101:THR:OG1	1:F:102:ALA:N	2.44	0.50
1:A:170:ASN:OD1	1:A:170:ASN:N	2.43	0.50
1:A:305:ASP:O	1:A:325:TYR:HB2	2.11	0.50
1:D:174:LEU:HD21	1:D:180:LEU:HD12	1.93	0.50
1:E:108:ASP:HA	1:E:111:ASP:HB3	1.93	0.50
1:A:28:PHE:HB3	1:B:59:LYS:HB2	1.94	0.50
1:B:130:LEU:HD23	1:B:306:LEU:HD11	1.92	0.50
1:C:36:VAL:HG23	1:D:64:PRO:HG2	1.93	0.50
1:C:212:ASP:OD2	1:C:213:SER:N	2.44	0.50
1:E:343:LYS:HD3	1:E:344:VAL:HB	1.93	0.50
1:F:174:LEU:HD13	1:F:180:LEU:HB2	1.94	0.50
1:F:227:ASN:OD1	1:F:227:ASN:N	2.45	0.50
1:F:293:MET:HG3	1:F:295:ARG:H	1.77	0.50
1:F:319:ASP:OD2	1:F:319:ASP:N	2.43	0.50
1:F:27:LEU:HD12	1:G:91:GLU:HB3	1.94	0.50
1:B:114:ASN:O	1:B:115:HIS:ND1	2.44	0.50
1:D:315:ASN:OD1	1:D:315:ASN:N	2.41	0.50
1:G:25:LEU:HB2	1:G:26:ALA:CA	2.42	0.50
1:F:199:TYR:O	1:F:200:VAL:HB	2.11	0.50
1:E:166:GLU:HB3	1:E:343:LYS:HB2	1.93	0.49
1:A:74:LEU:HD11	1:F:99:LEU:HG	1.93	0.49
1:A:138:VAL:O	1:A:142:ILE:HG22	2.13	0.49
1:B:241:ASN:OD1	1:B:241:ASN:N	2.45	0.49
1:E:134:ALA:O	1:E:138:VAL:HG23	2.13	0.49
1:G:306:LEU:HA	1:G:325:TYR:HB2	1.95	0.49
1:C:61:ALA:HB3	1:C:94:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:LEU:HD23	1:G:89:HIS:HE1	1.77	0.49
1:G:296:SER:N	1:G:297:ALA:HA	2.28	0.49
1:B:119:ARG:NH2	1:B:319:ASP:OD2	2.45	0.49
1:B:262:ARG:O	1:C:70:GLN:NE2	2.45	0.49
1:E:97:ASP:N	1:E:97:ASP:OD1	2.46	0.49
1:A:120:SER:O	1:A:123:THR:OG1	2.23	0.49
1:D:3:SER:OG	1:D:4:MET:N	2.44	0.49
1:E:234:PRO:O	1:E:235:GLU:HG3	2.13	0.49
1:E:165:ILE:HG12	1:E:166:GLU:H	1.78	0.49
1:C:3:SER:OG	1:C:4:MET:N	2.46	0.48
1:F:60:SER:OG	1:F:61:ALA:N	2.46	0.48
1:B:29:LEU:HD13	1:B:29:LEU:H	1.78	0.48
1:E:294:HIS:CE1	1:E:296:SER:HB3	2.48	0.48
1:G:24:LYS:HE3	1:G:24:LYS:H	1.77	0.48
1:G:51:MET:O	1:G:52:VAL:HG22	2.13	0.48
1:A:327:MET:SD	1:A:329:HIS:NE2	2.75	0.48
1:A:224:ASN:HD22	1:B:182:LYS:NZ	2.11	0.48
1:G:12:THR:O	1:G:27:LEU:HB2	2.14	0.48
1:C:253:LEU:HD13	1:C:254:THR:H	1.79	0.48
1:C:60:SER:OG	1:C:94:ILE:O	2.25	0.48
1:E:223:PRO:HA	1:F:228:TYR:HE1	1.78	0.48
1:F:206:VAL:HG12	1:F:293:MET:H	1.78	0.48
1:G:143:ALA:O	1:G:147:ASN:HB3	2.14	0.48
1:G:203:ALA:O	1:G:205:ARG:HG3	2.13	0.48
1:A:97:ASP:OD1	1:A:98:GLY:N	2.41	0.48
1:D:99:LEU:HD23	1:E:74:LEU:HD23	1.96	0.48
1:F:15:GLY:N	1:G:90:THR:OG1	2.46	0.48
1:G:186:ALA:O	1:G:189:THR:OG1	2.24	0.48
1:F:205:ARG:HA	1:F:294:HIS:HA	1.96	0.48
1:F:149:GLU:OE1	1:F:149:GLU:N	2.44	0.48
1:F:166:GLU:HB2	1:F:341:VAL:O	2.14	0.48
1:B:219:ALA:HB2	1:C:189:THR:HG21	1.96	0.47
1:A:142:ILE:HG23	1:A:143:ALA:H	1.78	0.47
1:D:86:ASP:O	1:D:88:LYS:N	2.47	0.47
1:D:262:ARG:O	1:E:70:GLN:NE2	2.34	0.47
1:G:51:MET:HB3	1:G:300:THR:OG1	2.14	0.47
1:G:309:GLU:OE2	1:G:310:ARG:N	2.45	0.47
1:A:244:GLY:H	1:F:236:LYS:N	2.09	0.47
1:A:253:LEU:HD22	1:A:254:THR:H	1.80	0.47
1:C:50:HIS:H	1:C:295:ARG:NH2	2.13	0.47
1:D:232:ILE:HG22	1:D:239:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:VAL:HG22	1:E:46:THR:H	1.79	0.47
1:E:231:LEU:HD13	1:E:232:ILE:H	1.80	0.47
1:A:167:THR:HG23	1:A:168:THR:HG23	1.96	0.47
1:A:101:THR:OG1	1:A:102:ALA:N	2.48	0.47
1:A:257:GLY:HA2	1:A:268:GLN:HB3	1.96	0.47
1:B:233:ASP:OD2	1:B:233:ASP:N	2.48	0.47
1:C:56:SER:OG	1:C:57:SER:N	2.47	0.47
1:F:205:ARG:HB3	1:F:206:VAL:H	1.54	0.47
1:A:119:ARG:O	1:A:123:THR:HG23	2.14	0.47
1:B:181:GLY:O	1:B:185:ILE:HG12	2.15	0.47
1:C:224:ASN:HD21	1:D:182:LYS:HE2	1.80	0.47
1:E:310:ARG:HB3	1:E:321:ILE:HG13	1.96	0.47
1:A:7:GLY:O	1:A:8:GLN:HB3	2.15	0.47
1:A:204:ASP:OD2	1:A:295:ARG:HB3	2.15	0.47
1:D:89:HIS:O	1:D:90:THR:OG1	2.32	0.47
1:E:89:HIS:CD2	1:E:89:HIS:H	2.32	0.47
1:A:333:ARG:HH11	1:A:333:ARG:HB2	1.78	0.47
1:E:38:THR:OG1	1:E:39:ALA:N	2.48	0.47
1:F:210:ASP:OD1	1:F:210:ASP:N	2.46	0.47
1:G:141:GLU:O	1:G:145:LEU:HB2	2.15	0.47
1:C:239:ILE:HG22	1:C:240:ARG:H	1.79	0.46
1:B:147:ASN:OD1	1:B:147:ASN:N	2.47	0.46
1:E:97:ASP:HB3	1:F:73:TYR:CE2	2.50	0.46
1:G:156:ILE:HG13	1:G:157:GLU:H	1.79	0.46
1:B:150:SER:O	1:B:151:LYS:HG3	2.16	0.46
1:B:213:SER:HB2	1:B:289:ILE:HG23	1.97	0.46
1:C:235:GLU:HG3	1:D:241:ASN:HB2	1.96	0.46
1:B:25:LEU:HA	1:B:26:ALA:HA	1.78	0.46
1:C:308:LEU:HA	1:C:323:ALA:HA	1.96	0.46
1:D:294:HIS:O	1:D:294:HIS:ND1	2.49	0.46
1:E:106:ILE:HG22	1:E:111:ASP:HB2	1.97	0.46
1:G:165:ILE:HD12	1:G:341:VAL:HG13	1.96	0.46
1:A:276:LYS:HA	1:A:281:VAL:HG23	1.98	0.46
1:C:159:LEU:HD22	1:C:159:LEU:H	1.81	0.46
1:E:228:TYR:HA	1:F:228:TYR:HB3	1.96	0.46
1:E:294:HIS:HE1	1:E:296:SER:HB3	1.81	0.46
1:A:59:LYS:HD2	1:F:28:PHE:HB3	1.98	0.46
1:F:24:LYS:O	1:F:25:LEU:HD22	2.16	0.46
1:G:254:THR:HG22	1:G:272:PHE:CE2	2.51	0.46
1:B:42:ARG:HH21	1:B:132:MET:HG2	1.81	0.46
1:C:141:GLU:HG3	1:C:145:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:PRO:HA	1:G:224:ASN:C	2.36	0.46
1:E:184:ILE:HD11	1:E:289:ILE:HG12	1.98	0.46
1:A:69:THR:OG1	1:A:70:GLN:N	2.48	0.45
1:A:223:PRO:HG2	1:B:221:LEU:HD12	1.97	0.45
1:B:291:LEU:HA	1:B:339:ALA:HA	1.99	0.45
1:C:161:THR:HG22	1:C:334:PRO:O	2.16	0.45
1:D:229:ALA:HB2	1:E:228:TYR:CE1	2.51	0.45
1:E:289:ILE:HD11	1:E:342:PHE:CD2	2.51	0.45
1:G:221:LEU:O	1:G:222:MET:HB2	2.15	0.45
1:A:209:CYS:SG	1:A:213:SER:HB2	2.56	0.45
1:A:224:ASN:ND2	1:B:182:LYS:HG2	2.32	0.45
1:A:251:PRO:HG3	1:B:199:TYR:CE1	2.51	0.45
1:E:47:THR:HA	1:E:48:SER:HA	1.56	0.45
1:D:253:LEU:O	1:D:254:THR:OG1	2.23	0.45
1:D:269:LYS:HG3	1:E:73:TYR:CE2	2.50	0.45
1:G:100:LEU:HD21	1:G:325:TYR:CE1	2.51	0.45
1:G:192:ARG:HH11	1:G:193:ALA:HA	1.81	0.45
1:B:176:ASP:OD2	1:B:178:VAL:N	2.48	0.45
1:C:210:ASP:HB2	1:C:211:PRO:HD2	1.98	0.45
1:E:218:LEU:O	1:E:222:MET:HG3	2.16	0.45
1:F:301:VAL:O	1:F:327:MET:HB2	2.16	0.45
1:B:205:ARG:HB3	1:B:206:VAL:H	1.58	0.45
1:C:207:PHE:HD1	1:C:292:PHE:HB3	1.81	0.45
1:F:12:THR:O	1:F:27:LEU:HD22	2.16	0.45
1:F:269:LYS:HB3	1:F:270:HIS:CE1	2.52	0.45
1:C:174:LEU:H	1:C:174:LEU:HD22	1.81	0.45
1:C:94:ILE:HG22	1:C:330:GLY:HA3	1.98	0.45
1:C:309:GLU:HG3	1:C:322:ILE:HG23	1.99	0.45
1:D:100:LEU:HD13	1:E:73:TYR:HD1	1.82	0.45
1:D:138:VAL:O	1:D:142:ILE:HG22	2.16	0.45
1:G:50:HIS:CD2	1:G:138:VAL:HG11	2.52	0.45
1:A:126:LEU:HA	1:B:69:THR:HG21	1.98	0.45
1:C:96:ILE:HG13	1:C:303:LEU:HD11	1.98	0.45
1:B:52:VAL:O	1:B:53:ARG:HD2	2.17	0.45
1:E:154:GLU:OE1	1:E:155:ASN:N	2.47	0.45
1:B:315:ASN:OD1	1:B:316:PHE:N	2.48	0.45
1:C:262:ARG:HD2	1:D:72:ALA:HB2	1.99	0.45
1:D:198:ASN:HD22	1:D:335:GLU:HG3	1.82	0.45
1:E:164:VAL:HG21	1:E:191:ALA:HB2	1.99	0.45
1:A:224:ASN:HA	1:A:225:ALA:HA	1.54	0.44
1:B:295:ARG:HG3	1:B:296:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:GLU:H	1:F:63:PHE:HE1	1.64	0.44
1:G:245:PHE:HB2	1:G:246:GLU:H	1.53	0.44
1:F:144:GLY:O	1:F:148:VAL:HB	2.16	0.44
1:F:225:ALA:HA	1:F:226:ALA:HA	1.62	0.44
1:C:209:CYS:SG	1:C:213:SER:HB2	2.57	0.44
1:D:117:ASP:HA	1:D:118:VAL:CB	2.48	0.44
1:F:154:GLU:OE2	1:F:155:ASN:N	2.51	0.44
1:F:200:VAL:HG13	1:F:294:HIS:CD2	2.52	0.44
1:A:184:ILE:O	1:A:188:LEU:HB2	2.18	0.44
1:B:224:ASN:HB3	1:C:182:LYS:HE2	1.98	0.44
1:C:134:ALA:HB2	1:C:325:TYR:OH	2.17	0.44
1:F:25:LEU:N	1:F:26:ALA:HB3	2.32	0.44
1:G:230:ALA:HA	1:G:231:LEU:HA	1.63	0.44
1:G:254:THR:OG1	1:G:255:ALA:N	2.50	0.44
1:A:103:ASP:OD1	1:B:84:ARG:NH1	2.39	0.44
1:B:257:GLY:HA3	1:B:268:GLN:HB3	2.00	0.44
1:F:201:PRO:HD2	1:F:294:HIS:CD2	2.52	0.44
1:A:99:LEU:HA	1:A:326:ALA:HB2	2.00	0.44
1:C:50:HIS:HB3	1:C:52:VAL:HG23	1.98	0.44
1:E:184:ILE:CD1	1:E:289:ILE:HG12	2.48	0.44
1:E:200:VAL:HG21	1:E:336:ALA:HB2	2.00	0.44
1:G:207:PHE:HB2	1:G:245:PHE:CE1	2.53	0.44
1:G:212:ASP:O	1:G:215:SER:OG	2.27	0.44
1:G:222:MET:HB3	1:G:223:PRO:CD	2.47	0.44
1:C:228:TYR:HA	1:D:228:TYR:HB3	1.99	0.44
1:D:104:VAL:HG11	1:D:122:TYR:HD2	1.83	0.44
1:G:294:HIS:O	1:G:294:HIS:CG	2.70	0.44
1:G:296:SER:O	1:G:296:SER:OG	2.33	0.44
1:A:34:GLY:HA3	1:B:63:PHE:HE1	1.83	0.44
1:A:42:ARG:HE	1:A:128:GLU:CD	2.20	0.44
1:B:164:VAL:HG21	1:B:191:ALA:HB2	2.00	0.44
1:F:125:GLN:O	1:F:128:GLU:HG3	2.17	0.44
1:G:185:ILE:O	1:G:189:THR:HG23	2.17	0.44
1:G:265:THR:O	1:G:268:GLN:HG3	2.18	0.44
1:A:166:GLU:OE2	1:A:167:THR:N	2.51	0.43
1:D:29:LEU:HD12	1:D:29:LEU:H	1.83	0.43
1:G:174:LEU:HD23	1:G:174:LEU:HA	1.86	0.43
1:A:289:ILE:HD12	1:A:340:VAL:HG22	2.00	0.43
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.82	0.43
1:B:89:HIS:O	1:B:89:HIS:ND1	2.50	0.43
1:B:171:LYS:HB3	1:B:342:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ILE:HG23	1:B:240:ARG:H	1.83	0.43
1:C:221:LEU:HG	1:C:232:ILE:HD11	2.00	0.43
1:E:161:THR:OG1	1:E:162:ALA:N	2.51	0.43
1:B:19:VAL:HA	1:B:20:ALA:HA	1.56	0.43
1:B:81:ASP:O	1:B:84:ARG:HG2	2.18	0.43
1:C:92:LYS:HD3	1:C:92:LYS:HA	1.81	0.43
1:D:50:HIS:HE1	1:D:300:THR:HG23	1.84	0.43
1:D:204:ASP:N	1:D:204:ASP:OD1	2.51	0.43
1:F:109:ILE:HG12	1:G:99:LEU:HG	1.99	0.43
1:B:70:GLN:HE21	1:B:70:GLN:HB3	1.60	0.43
1:B:92:LYS:HD3	1:B:332:LEU:HB3	2.00	0.43
1:A:148:VAL:HG11	1:A:281:VAL:HA	2.00	0.43
1:C:101:THR:OG1	1:C:102:ALA:N	2.52	0.43
1:E:57:SER:OG	1:E:58:GLY:N	2.48	0.43
1:A:51:MET:HG2	1:A:296:SER:HA	2.01	0.43
1:B:181:GLY:HA3	1:B:220:ALA:HB2	2.00	0.43
1:C:101:THR:OG1	1:C:323:ALA:O	2.19	0.43
1:C:178:VAL:C	1:C:180:LEU:H	2.21	0.43
1:F:113:MET:SD	1:G:59:LYS:HA	2.59	0.43
1:F:185:ILE:O	1:F:189:THR:HG23	2.19	0.43
1:G:57:SER:OG	1:G:58:GLY:N	2.51	0.43
1:G:289:ILE:HB	1:G:340:VAL:HG23	2.01	0.43
1:A:141:GLU:HG2	1:A:330:GLY:HA2	2.01	0.43
1:A:165:ILE:HG12	1:A:166:GLU:H	1.83	0.43
1:B:273:PRO:O	1:B:285:LYS:HB3	2.19	0.43
1:D:35:GLU:HB2	1:E:63:PHE:CD1	2.53	0.43
1:E:17:GLY:C	1:E:19:VAL:H	2.22	0.43
1:E:69:THR:OG1	1:E:70:GLN:N	2.52	0.43
1:E:280:ASN:ND2	1:E:280:ASN:O	2.52	0.43
1:A:69:THR:HG23	1:F:129:SER:HB2	2.00	0.43
1:A:244:GLY:HA2	1:F:236:LYS:HB3	2.00	0.43
1:B:254:THR:HG21	1:B:285:LYS:HB2	2.01	0.43
1:C:200:VAL:HA	1:C:201:PRO:HD3	1.75	0.43
1:E:19:VAL:HB	1:E:20:ALA:H	1.60	0.43
1:F:151:LYS:HE3	1:F:151:LYS:HB3	1.77	0.43
1:B:328:GLY:O	1:B:329:HIS:ND1	2.52	0.43
1:E:255:ALA:HB1	1:E:268:GLN:HE22	1.84	0.43
1:F:122:TYR:O	1:F:126:LEU:HG	2.19	0.43
1:G:109:ILE:O	1:G:113:MET:HB2	2.19	0.43
1:B:207:PHE:HD1	1:B:247:VAL:HG22	1.84	0.43
1:B:294:HIS:O	1:B:294:HIS:CG	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LEU:HD12	1:B:325:TYR:CG	2.54	0.43
1:C:236:LYS:H	1:C:236:LYS:HG3	1.47	0.43
1:D:223:PRO:O	1:D:225:ALA:N	2.51	0.43
1:A:25:LEU:HA	1:A:26:ALA:HA	1.85	0.42
1:G:103:ASP:OD2	1:G:103:ASP:N	2.51	0.42
1:A:148:VAL:HG22	1:A:282:LYS:H	1.85	0.42
1:E:109:ILE:HD13	1:E:109:ILE:HA	1.88	0.42
1:F:51:MET:HB3	1:F:299:GLY:HA2	2.01	0.42
1:G:260:THR:OG1	1:G:261:ALA:N	2.51	0.42
1:C:106:ILE:HG21	1:C:119:ARG:HH21	1.82	0.42
1:D:149:GLU:HB2	1:D:151:LYS:O	2.19	0.42
1:D:255:ALA:HB1	1:D:268:GLN:OE1	2.20	0.42
1:G:154:GLU:O	1:G:155:ASN:ND2	2.52	0.42
1:B:28:PHE:CE2	1:C:59:LYS:HB2	2.54	0.42
1:C:51:MET:SD	1:C:53:ARG:NH2	2.93	0.42
1:F:75:ALA:HB3	1:F:78:GLU:HG3	2.00	0.42
1:B:232:ILE:HG13	1:B:233:ASP:N	2.35	0.42
1:G:222:MET:SD	1:G:229:ALA:HA	2.59	0.42
1:C:83:LYS:NZ	1:C:83:LYS:H	2.17	0.42
1:D:81:ASP:HA	1:D:84:ARG:NH1	2.33	0.42
1:G:142:ILE:HB	1:G:298:VAL:HG21	2.02	0.42
1:B:322:ILE:HD11	1:B:324:LYS:HE3	2.02	0.42
1:D:96:ILE:HA	1:D:328:GLY:HA3	2.01	0.42
1:A:84:ARG:HA	1:F:262:ARG:HD3	2.01	0.42
1:B:103:ASP:N	1:B:103:ASP:OD1	2.53	0.42
1:C:5:THR:HG22	1:C:6:GLY:H	1.85	0.42
1:G:146:CYS:HB2	1:G:331:GLY:HA3	2.02	0.42
1:E:103:ASP:OD1	1:E:103:ASP:N	2.53	0.42
1:F:266:THR:OG1	1:F:267:GLY:N	2.53	0.42
1:C:232:ILE:H	1:C:232:ILE:HG12	1.62	0.41
1:D:294:HIS:O	1:D:294:HIS:CG	2.72	0.41
1:C:86:ASP:C	1:C:88:LYS:H	2.23	0.41
1:C:104:VAL:HG22	1:C:105:LEU:H	1.84	0.41
1:E:92:LYS:HE2	1:E:332:LEU:HA	2.02	0.41
1:F:14:GLN:HB2	1:G:89:HIS:O	2.20	0.41
1:F:24:LYS:HE3	1:F:24:LYS:HB3	1.89	0.41
1:F:239:ILE:HG22	1:F:240:ARG:H	1.85	0.41
1:A:27:LEU:HD13	1:A:27:LEU:O	2.19	0.41
1:F:138:VAL:O	1:F:142:ILE:HG22	2.20	0.41
1:F:333:ARG:HH11	1:F:333:ARG:HB2	1.85	0.41
1:A:207:PHE:CD2	1:A:247:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:THR:OG1	1:B:47:THR:N	2.53	0.41
1:B:174:LEU:HD11	1:B:180:LEU:HD13	2.02	0.41
1:B:198:ASN:N	1:B:198:ASN:OD1	2.51	0.41
1:B:260:THR:OG1	1:B:267:GLY:O	2.34	0.41
1:E:295:ARG:HD2	1:E:296:SER:H	1.86	0.41
1:A:140:ALA:HA	1:A:272:PHE:CZ	2.56	0.41
1:C:207:PHE:HE2	1:C:209:CYS:HB2	1.85	0.41
1:D:157:GLU:CD	1:D:159:LEU:HG	2.41	0.41
1:A:32:PHE:CG	1:A:33:GLY:N	2.87	0.41
1:C:50:HIS:CE1	1:C:298:VAL:HB	2.55	0.41
1:D:294:HIS:O	1:D:295:ARG:HG2	2.20	0.41
1:E:37:LEU:O	1:F:65:VAL:HA	2.20	0.41
1:E:168:THR:OG1	1:E:169:GLN:N	2.53	0.41
1:E:294:HIS:O	1:E:294:HIS:CG	2.73	0.41
1:G:184:ILE:HB	1:G:217:ILE:HD11	2.02	0.41
1:B:198:ASN:HD22	1:B:335:GLU:CD	2.24	0.41
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.86	0.41
1:B:232:ILE:CG2	1:B:239:ILE:HA	2.51	0.41
1:B:276:LYS:HE2	1:B:276:LYS:HB2	1.92	0.41
1:A:85:LYS:NZ	1:F:263:GLU:OE1	2.32	0.41
1:A:304:ARG:HA	1:A:304:ARG:NE	2.35	0.41
1:B:148:VAL:HG12	1:B:282:LYS:H	1.86	0.41
1:D:100:LEU:HD23	1:D:325:TYR:CE2	2.53	0.41
1:D:107:TYR:HB2	1:D:110:GLU:HB2	2.03	0.41
1:F:94:ILE:HD11	1:F:332:LEU:HD12	2.01	0.41
1:G:26:ALA:HB1	1:G:28:PHE:H	1.86	0.41
1:A:62:GLN:NE2	1:A:91:GLU:OE1	2.54	0.41
1:A:269:LYS:O	1:A:270:HIS:ND1	2.53	0.41
1:C:11:GLY:HA3	1:C:28:PHE:CE1	2.56	0.41
1:C:79:ASN:OD1	1:C:82:ASP:N	2.54	0.41
1:C:83:LYS:H	1:C:83:LYS:HZ3	1.68	0.41
1:C:176:ASP:C	1:C:178:VAL:H	2.25	0.41
1:D:59:LYS:HB3	1:D:59:LYS:HE2	1.90	0.41
1:D:99:LEU:HD11	1:D:324:LYS:HD3	2.02	0.41
1:D:125:GLN:OE1	1:E:68:ARG:HG3	2.20	0.41
1:E:199:TYR:O	1:E:200:VAL:HB	2.21	0.41
1:F:57:SER:OG	1:F:58:GLY:N	2.52	0.41
1:F:143:ALA:HB3	1:F:272:PHE:HZ	1.86	0.41
1:F:222:MET:SD	1:F:223:PRO:HD2	2.61	0.41
1:G:100:LEU:HD11	1:G:130:LEU:HG	2.03	0.41
1:A:269:LYS:HG2	1:B:73:TYR:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:HD13	1:C:139:LEU:HA	1.90	0.41
1:C:313:ARG:HB2	1:C:320:GLN:OE1	2.21	0.41
1:D:94:ILE:HD11	1:D:301:VAL:HG22	2.02	0.41
1:D:222:MET:HB3	1:D:223:PRO:HD3	2.02	0.41
1:E:116:TYR:CE1	1:E:118:VAL:HG22	2.56	0.41
1:A:161:THR:OG1	1:A:162:ALA:N	2.54	0.40
1:D:117:ASP:HA	1:D:118:VAL:CG1	2.49	0.40
1:F:25:LEU:HB3	1:F:28:PHE:HD1	1.86	0.40
1:G:237:GLY:HA3	1:G:238:SER:HA	1.68	0.40
1:A:73:TYR:OH	1:F:269:LYS:NZ	2.53	0.40
1:A:167:THR:OG1	1:A:168:THR:N	2.54	0.40
1:F:228:TYR:CG	1:F:229:ALA:N	2.89	0.40
1:A:64:PRO:O	1:F:37:LEU:HB3	2.21	0.40
1:D:231:LEU:HD13	1:D:242:VAL:HG13	2.02	0.40
1:G:214:TYR:CD1	1:G:249:GLU:HG2	2.56	0.40
1:A:224:ASN:HD22	1:B:182:LYS:HZ3	1.69	0.40
1:A:262:ARG:HG3	1:B:85:LYS:HB2	2.04	0.40
1:C:276:LYS:O	1:C:281:VAL:HG12	2.22	0.40
1:F:140:ALA:HA	1:F:272:PHE:CZ	2.57	0.40
1:A:243:MET:HE2	1:F:218:LEU:HD21	2.02	0.40
1:C:96:ILE:HG13	1:C:303:LEU:HD21	2.04	0.40
1:C:178:VAL:HG22	1:C:179:ALA:H	1.86	0.40
1:D:31:VAL:HG22	1:D:32:PHE:H	1.87	0.40
1:D:184:ILE:HD12	1:D:184:ILE:HA	1.89	0.40
1:G:16:LYS:HA	1:G:16:LYS:HD2	1.95	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	341/345 (99%)	282 (83%)	58 (17%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	341/345 (99%)	279 (82%)	53 (16%)	9 (3%)	5	35
1	C	341/345 (99%)	251 (74%)	84 (25%)	6 (2%)	8	43
1	D	341/345 (99%)	275 (81%)	63 (18%)	3 (1%)	17	57
1	E	341/345 (99%)	281 (82%)	53 (16%)	7 (2%)	7	40
1	F	341/345 (99%)	276 (81%)	57 (17%)	8 (2%)	6	38
1	G	341/345 (99%)	276 (81%)	59 (17%)	6 (2%)	8	43
All	All	2387/2415 (99%)	1920 (80%)	427 (18%)	40 (2%)	13	45

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	118	VAL
1	D	118	VAL
1	E	18	VAL
1	F	118	VAL
1	G	52	VAL
1	B	206	VAL
1	B	232	ILE
1	E	19	VAL
1	E	236	LYS
1	E	296	SER
1	F	178	VAL
1	F	206	VAL
1	F	239	ILE
1	G	232	ILE
1	B	239	ILE
1	C	118	VAL
1	C	239	ILE
1	C	281	VAL
1	D	296	SER
1	E	239	ILE
1	G	156	ILE
1	A	19	VAL
1	B	45	VAL
1	B	199	TYR
1	C	19	VAL
1	C	244	GLY
1	C	298	VAL
1	E	118	VAL
1	F	19	VAL

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Mol	Chain	Res	Type
1	F	179	ALA
1	G	204	ASP
1	G	298	VAL
1	B	200	VAL
1	E	235	GLU
1	B	296	SER
1	F	296	SER
1	B	242	VAL
1	F	247	VAL
1	D	142	ILE
1	G	234	PRO

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	259/261 (99%)	205 (79%)	54 (21%)	1 7
1	B	259/261 (99%)	206 (80%)	53 (20%)	1 7
1	C	259/261 (99%)	200 (77%)	59 (23%)	1 5
1	D	259/261 (99%)	191 (74%)	68 (26%)	0 4
1	E	259/261 (99%)	207 (80%)	52 (20%)	1 8
1	F	259/261 (99%)	205 (79%)	54 (21%)	1 7
1	G	259/261 (99%)	207 (80%)	52 (20%)	1 8
All	All	1813/1827 (99%)	1421 (78%)	392 (22%)	3 6

All (392) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	PHE
1	A	30	LYS
1	A	32	PHE
1	A	46	THR
1	A	49	ARG

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Mol	Chain	Res	Type
1	A	52	VAL
1	A	59	LYS
1	A	69	THR
1	A	80	LEU
1	A	83	LYS
1	A	84	ARG
1	A	87	ILE
1	A	89	HIS
1	A	94	ILE
1	A	103	ASP
1	A	107	TYR
1	A	114	ASN
1	A	115	HIS
1	A	128	GLU
1	A	142	ILE
1	A	152	TYR
1	A	153	ASN
1	A	159	LEU
1	A	163	THR
1	A	166	GLU
1	A	170	ASN
1	A	192	ARG
1	A	198	ASN
1	A	200	VAL
1	A	210	ASP
1	A	217	ILE
1	A	218	LEU
1	A	224	ASN
1	A	228	TYR
1	A	231	LEU
1	A	232	ILE
1	A	239	ILE
1	A	248	VAL
1	A	253	LEU
1	A	262	ARG
1	A	271	VAL
1	A	276	LYS
1	A	295	ARG
1	A	298	VAL
1	A	303	LEU
1	A	304	ARG
1	A	308	LEU

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Mol	Chain	Res	Type
1	A	322	ILE
1	A	325	TYR
1	A	332	LEU
1	A	333	ARG
1	A	341	VAL
1	A	344	VAL
1	B	28	PHE
1	B	29	LEU
1	B	32	PHE
1	B	38	THR
1	B	42	ARG
1	B	46	THR
1	B	47	THR
1	B	53	ARG
1	B	69	THR
1	B	70	GLN
1	B	73	TYR
1	B	74	LEU
1	B	78	GLU
1	B	87	ILE
1	B	88	LYS
1	B	92	LYS
1	B	94	ILE
1	B	95	THR
1	B	96	ILE
1	B	105	LEU
1	B	111	ASP
1	B	118	VAL
1	B	128	GLU
1	B	142	ILE
1	B	145	LEU
1	B	147	ASN
1	B	148	VAL
1	B	154	GLU
1	B	166	GLU
1	B	169	GLN
1	B	195	LEU
1	B	197	LYS
1	B	198	ASN
1	B	200	VAL
1	B	205	ARG
1	B	209	CYS

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Mol	Chain	Res	Type
1	B	221	LEU
1	B	241	ASN
1	B	243	MET
1	B	245	PHE
1	B	260	THR
1	B	272	PHE
1	B	280	ASN
1	B	283	VAL
1	B	291	LEU
1	B	294	HIS
1	B	298	VAL
1	B	303	LEU
1	B	320	GLN
1	B	322	ILE
1	B	325	TYR
1	B	332	LEU
1	B	333	ARG
1	C	5	THR
1	C	10	MET
1	C	13	ASN
1	C	18	VAL
1	C	24	LYS
1	C	27	LEU
1	C	30	LYS
1	C	40	PHE
1	C	46	THR
1	C	55	ILE
1	C	69	THR
1	C	73	TYR
1	C	74	LEU
1	C	80	LEU
1	C	82	ASP
1	C	83	LYS
1	C	84	ARG
1	C	89	HIS
1	C	90	THR
1	C	91	GLU
1	C	92	LYS
1	C	94	ILE
1	C	95	THR
1	C	96	ILE
1	C	100	LEU

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Mol	Chain	Res	Type
1	C	103	ASP
1	C	115	HIS
1	C	139	LEU
1	C	142	ILE
1	C	151	LYS
1	C	159	LEU
1	C	163	THR
1	C	169	GLN
1	C	171	LYS
1	C	174	LEU
1	C	183	GLU
1	C	200	VAL
1	C	205	ARG
1	C	227	ASN
1	C	232	ILE
1	C	236	LYS
1	C	243	MET
1	C	248	VAL
1	C	253	LEU
1	C	260	THR
1	C	272	PHE
1	C	276	LYS
1	C	280	ASN
1	C	281	VAL
1	C	295	ARG
1	C	298	VAL
1	C	303	LEU
1	C	304	ARG
1	C	309	GLU
1	C	312	ARG
1	C	324	LYS
1	C	325	TYR
1	C	332	LEU
1	C	333	ARG
1	D	3	SER
1	D	19	VAL
1	D	27	LEU
1	D	28	PHE
1	D	29	LEU
1	D	32	PHE
1	D	38	THR
1	D	42	ARG

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Mol	Chain	Res	Type
1	D	43	THR
1	D	50	HIS
1	D	51	MET
1	D	66	LEU
1	D	68	ARG
1	D	69	THR
1	D	73	TYR
1	D	79	ASN
1	D	81	ASP
1	D	83	LYS
1	D	84	ARG
1	D	86	ASP
1	D	91	GLU
1	D	94	ILE
1	D	105	LEU
1	D	110	GLU
1	D	114	ASN
1	D	115	HIS
1	D	117	ASP
1	D	118	VAL
1	D	126	LEU
1	D	132	MET
1	D	139	LEU
1	D	142	ILE
1	D	149	GLU
1	D	154	GLU
1	D	157	GLU
1	D	163	THR
1	D	180	LEU
1	D	184	ILE
1	D	192	ARG
1	D	200	VAL
1	D	204	ASP
1	D	218	LEU
1	D	221	LEU
1	D	231	LEU
1	D	233	ASP
1	D	235	GLU
1	D	241	ASN
1	D	245	PHE
1	D	250	VAL
1	D	262	ARG

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Mol	Chain	Res	Type
1	D	272	PHE
1	D	276	LYS
1	D	291	LEU
1	D	294	HIS
1	D	298	VAL
1	D	300	THR
1	D	306	LEU
1	D	309	GLU
1	D	310	ARG
1	D	312	ARG
1	D	315	ASN
1	D	317	GLN
1	D	324	LYS
1	D	325	TYR
1	D	332	LEU
1	D	335	GLU
1	D	341	VAL
1	D	344	VAL
1	E	18	VAL
1	E	29	LEU
1	E	38	THR
1	E	46	THR
1	E	50	HIS
1	E	70	GLN
1	E	78	GLU
1	E	82	ASP
1	E	83	LYS
1	E	86	ASP
1	E	89	HIS
1	E	90	THR
1	E	92	LYS
1	E	97	ASP
1	E	101	THR
1	E	105	LEU
1	E	107	TYR
1	E	111	ASP
1	E	119	ARG
1	E	128	GLU
1	E	142	ILE
1	E	145	LEU
1	E	147	ASN
1	E	149	GLU

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Mol	Chain	Res	Type
1	E	157	GLU
1	E	161	THR
1	E	169	GLN
1	E	174	LEU
1	E	190	LYS
1	E	192	ARG
1	E	209	CYS
1	E	210	ASP
1	E	212	ASP
1	E	231	LEU
1	E	240	ARG
1	E	263	GLU
1	E	265	THR
1	E	271	VAL
1	E	275	ASN
1	E	280	ASN
1	E	291	LEU
1	E	294	HIS
1	E	295	ARG
1	E	298	VAL
1	E	303	LEU
1	E	306	LEU
1	E	317	GLN
1	E	319	ASP
1	E	320	GLN
1	E	325	TYR
1	E	332	LEU
1	E	344	VAL
1	F	24	LYS
1	F	25	LEU
1	F	27	LEU
1	F	28	PHE
1	F	29	LEU
1	F	45	VAL
1	F	47	THR
1	F	49	ARG
1	F	50	HIS
1	F	51	MET
1	F	69	THR
1	F	81	ASP
1	F	92	LYS
1	F	95	THR

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Mol	Chain	Res	Type
1	F	96	ILE
1	F	99	LEU
1	F	105	LEU
1	F	106	ILE
1	F	108	ASP
1	F	109	ILE
1	F	116	TYR
1	F	118	VAL
1	F	128	GLU
1	F	142	ILE
1	F	153	ASN
1	F	156	ILE
1	F	159	LEU
1	F	163	THR
1	F	167	THR
1	F	170	ASN
1	F	177	GLN
1	F	192	ARG
1	F	212	ASP
1	F	222	MET
1	F	224	ASN
1	F	227	ASN
1	F	231	LEU
1	F	232	ILE
1	F	236	LYS
1	F	243	MET
1	F	252	HIS
1	F	254	THR
1	F	262	ARG
1	F	294	HIS
1	F	303	LEU
1	F	306	LEU
1	F	309	GLU
1	F	312	ARG
1	F	317	GLN
1	F	319	ASP
1	F	325	TYR
1	F	332	LEU
1	F	333	ARG
1	F	343	LYS
1	G	18	VAL
1	G	24	LYS

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Mol	Chain	Res	Type
1	G	25	LEU
1	G	31	VAL
1	G	35	GLU
1	G	38	THR
1	G	42	ARG
1	G	47	THR
1	G	50	HIS
1	G	55	ILE
1	G	62	GLN
1	G	65	VAL
1	G	66	LEU
1	G	80	LEU
1	G	83	LYS
1	G	85	LYS
1	G	89	HIS
1	G	91	GLU
1	G	97	ASP
1	G	101	THR
1	G	108	ASP
1	G	113	MET
1	G	119	ARG
1	G	142	ILE
1	G	163	THR
1	G	168	THR
1	G	169	GLN
1	G	171	LYS
1	G	190	LYS
1	G	192	ARG
1	G	195	LEU
1	G	197	LYS
1	G	199	TYR
1	G	210	ASP
1	G	228	TYR
1	G	231	LEU
1	G	235	GLU
1	G	249	GLU
1	G	271	VAL
1	G	281	VAL
1	G	288	VAL
1	G	291	LEU
1	G	295	ARG
1	G	303	LEU

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Mol	Chain	Res	Type
1	G	304	ARG
1	G	310	ARG
1	G	319	ASP
1	G	324	LYS
1	G	325	TYR
1	G	332	LEU
1	G	341	VAL
1	G	342	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	169	GLN
1	A	252	HIS
1	A	315	ASN
1	B	14	GLN
1	B	70	GLN
1	B	155	ASN
1	B	170	ASN
1	B	275	ASN
1	B	280	ASN
1	B	317	GLN
1	B	320	GLN
1	C	13	ASN
1	C	62	GLN
1	C	147	ASN
1	C	268	GLN
1	C	287	ASN
1	C	294	HIS
1	C	317	GLN
1	D	50	HIS
1	D	62	GLN
1	D	70	GLN
1	D	287	ASN
1	E	9	GLN
1	E	50	HIS
1	E	89	HIS
1	E	147	ASN
1	E	169	GLN
1	E	177	GLN
1	E	268	GLN

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Mol	Chain	Res	Type
1	E	280	ASN
1	E	287	ASN
1	F	14	GLN
1	F	114	ASN
1	F	198	ASN
1	F	252	HIS
1	G	14	GLN
1	G	62	GLN
1	G	70	GLN
1	G	89	HIS
1	G	125	GLN
1	G	155	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 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.

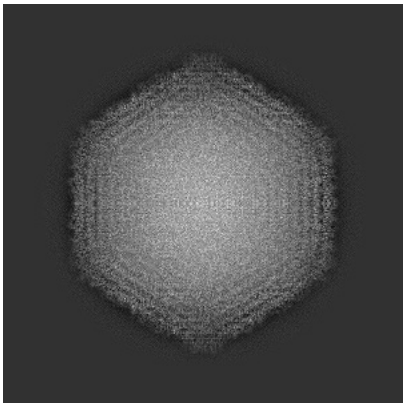
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6037. These allow visual inspection of the internal detail of the map and identification of artifacts.

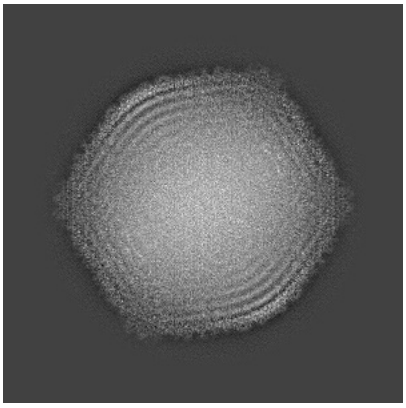
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

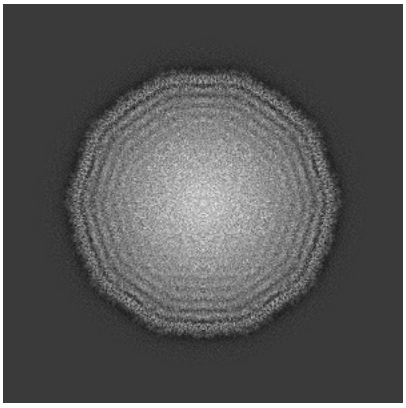
6.1.1 Primary map



X



Y

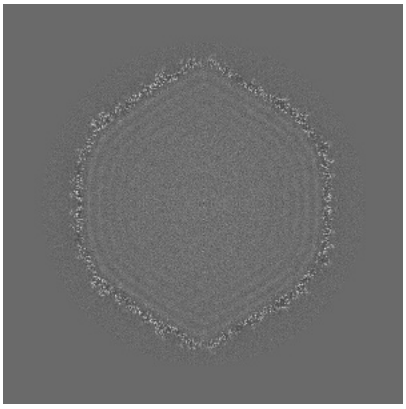


Z

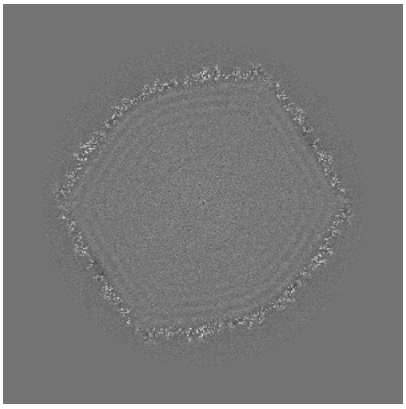
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

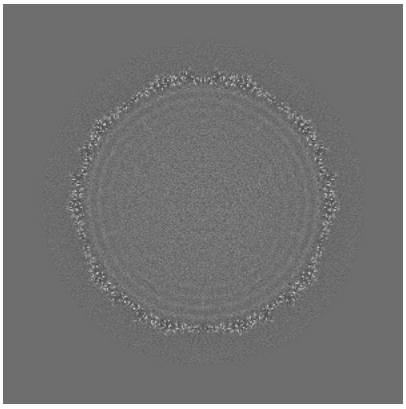
6.2.1 Primary map



X Index: 400



Y Index: 400

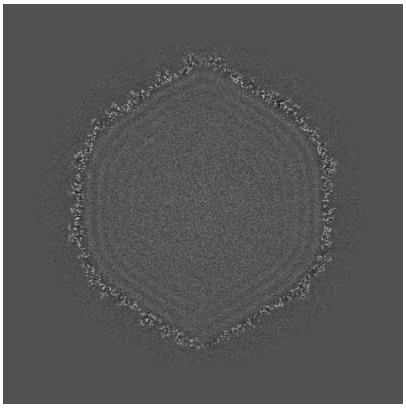


Z Index: 400

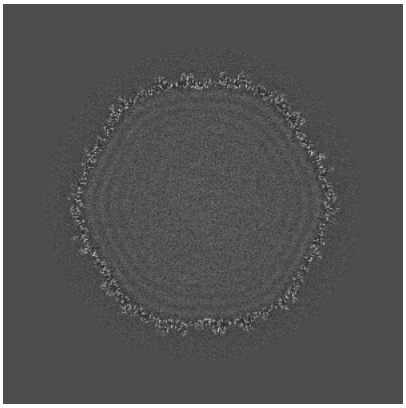
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

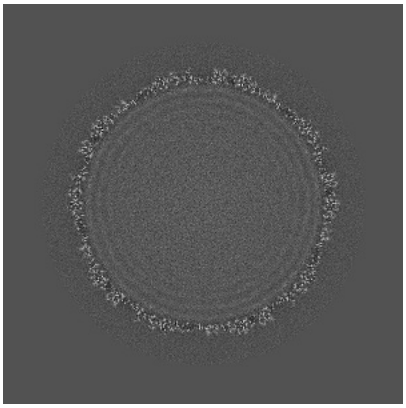
6.3.1 Primary map



X Index: 394



Y Index: 333

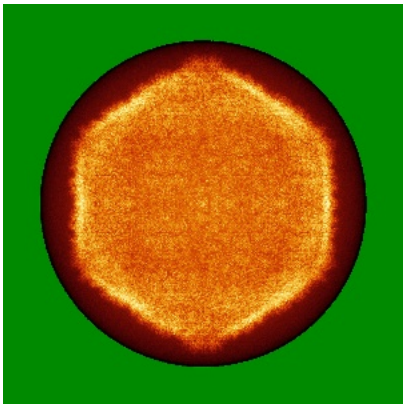


Z Index: 402

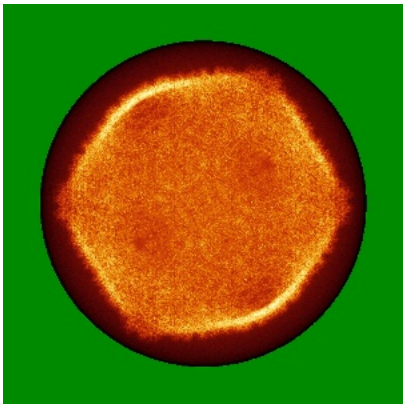
The images above show the largest variance slices of the map in three orthogonal directions.

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

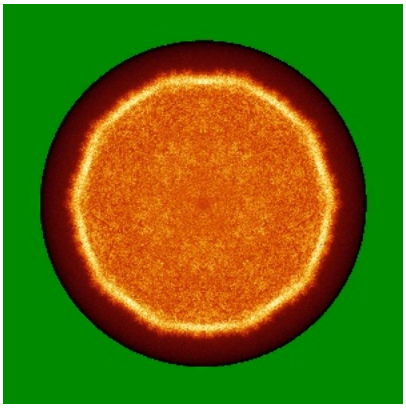
6.4.1 Primary map



X



Y

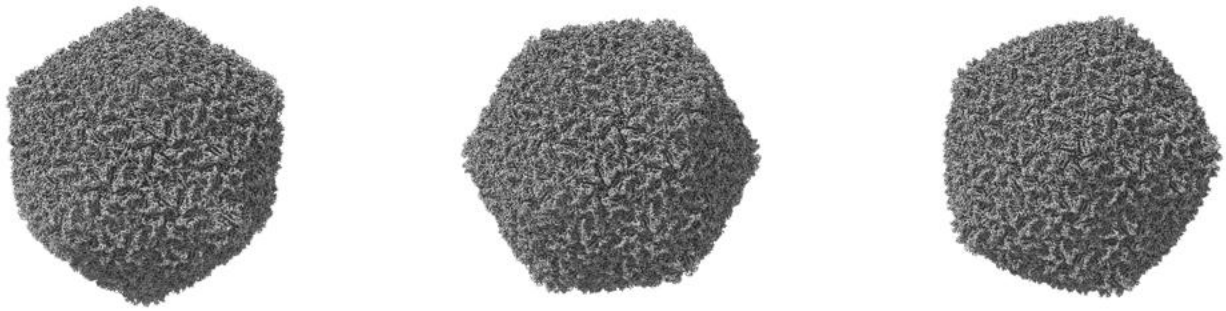


Z

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

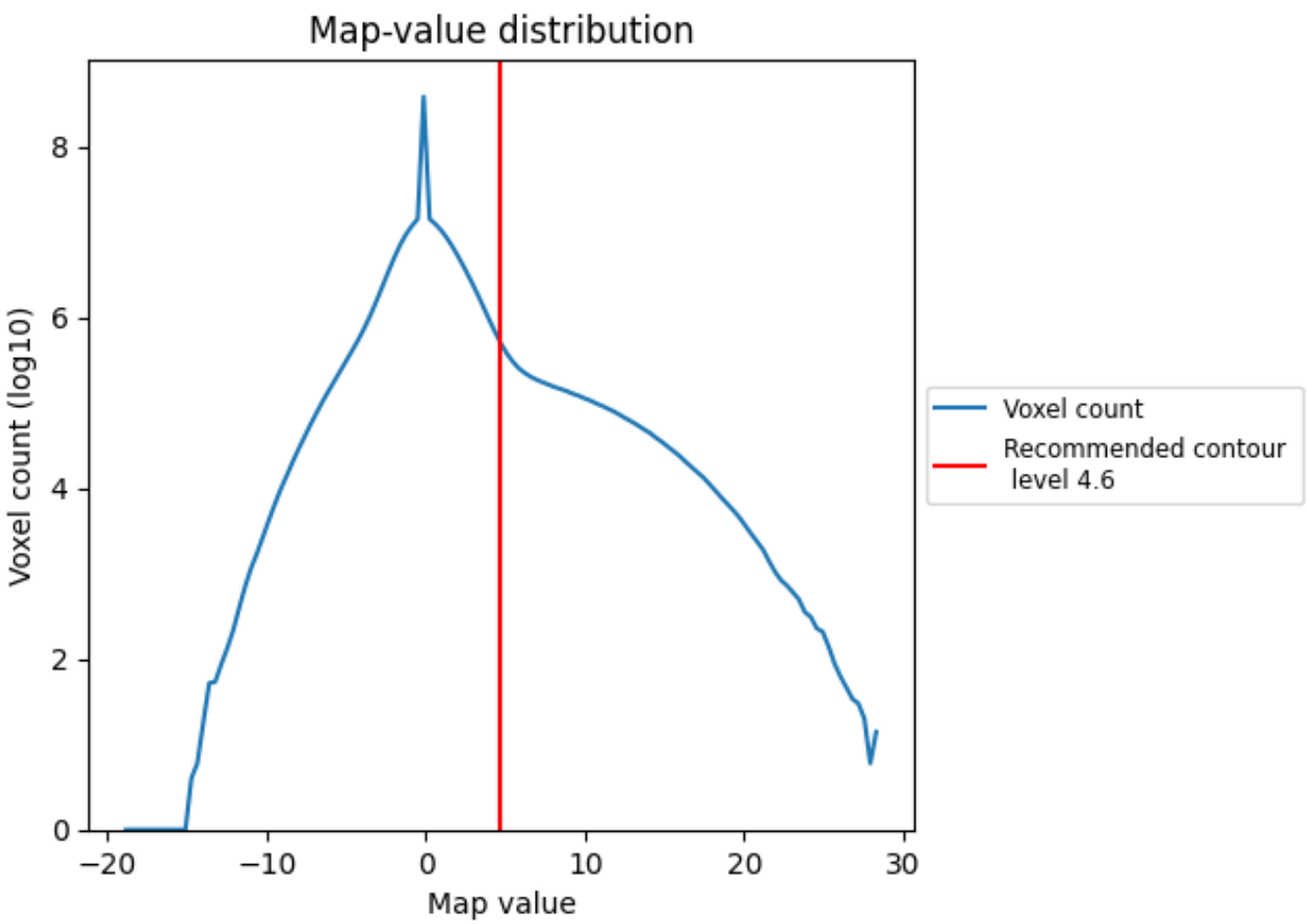
6.6 Mask visualisation (i)

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

7 Map analysis (i)

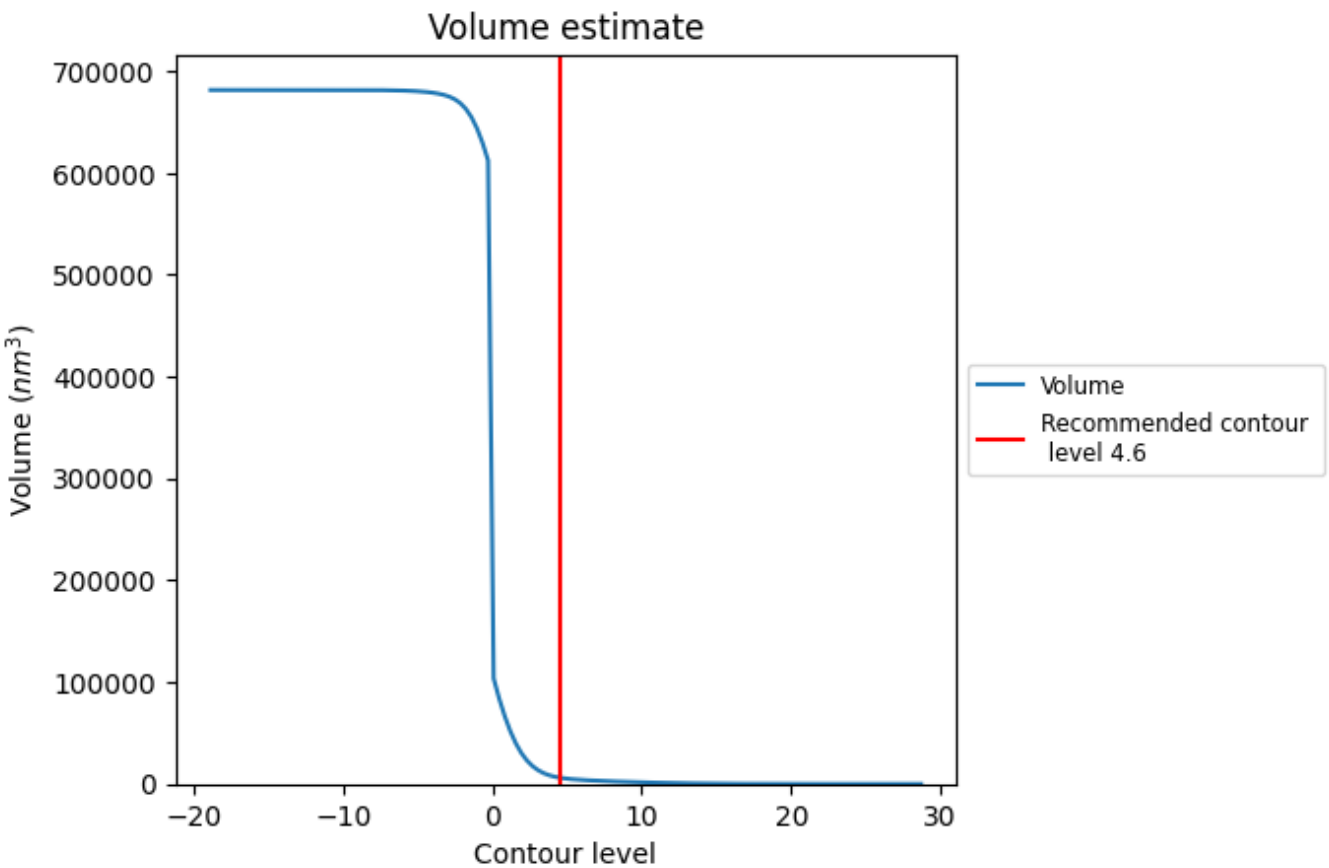
This section contains the results of statistical analysis of the map.

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.

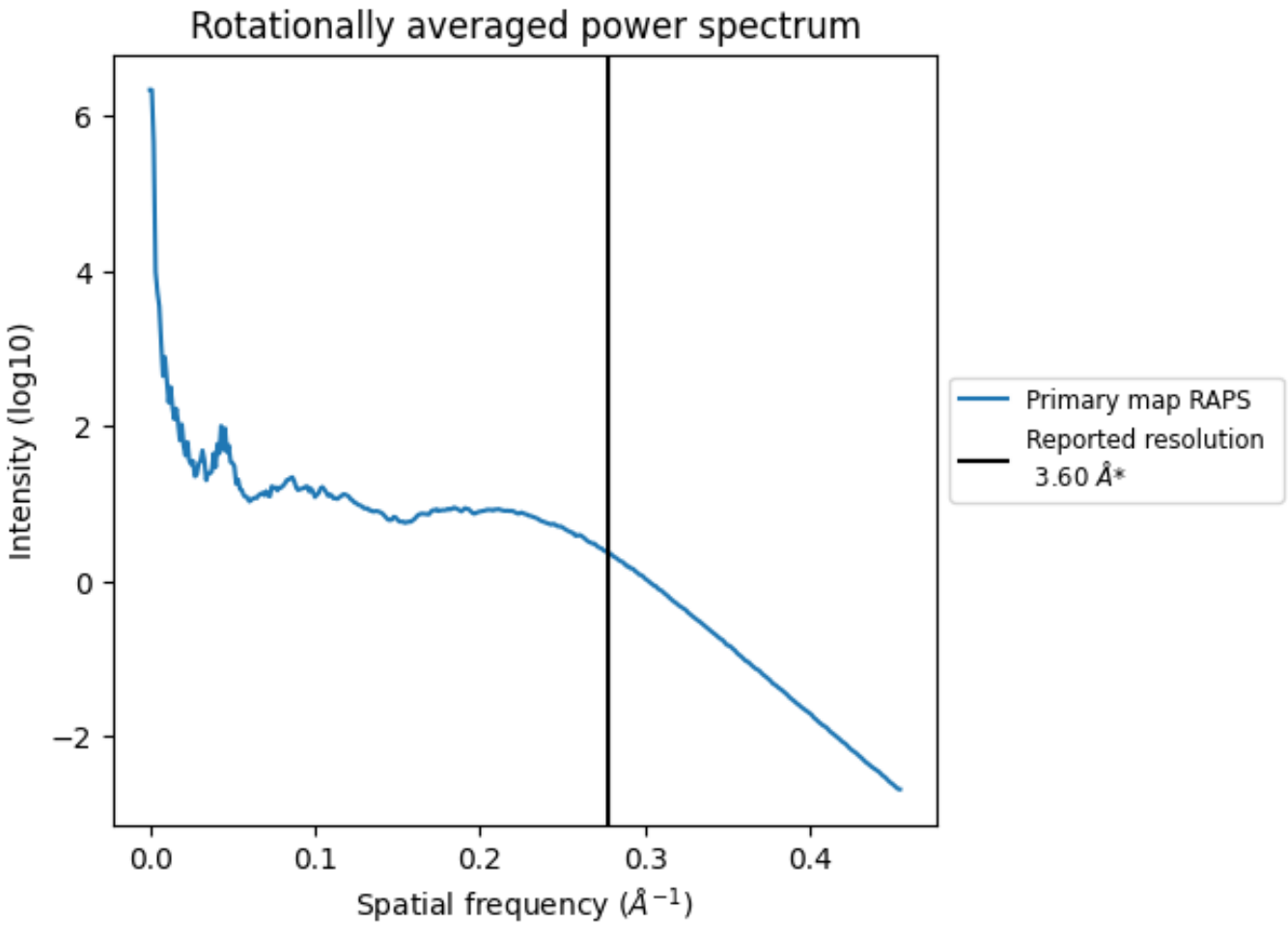
7.2 Volume estimate (i)



The volume at the recommended contour level is 5943 nm^3; this corresponds to an approximate mass of 5368 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 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

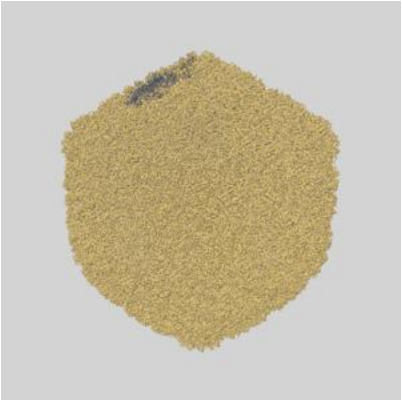
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6037 and PDB model 3J7X. Per-residue inclusion information can be found in section 3 on page 4.

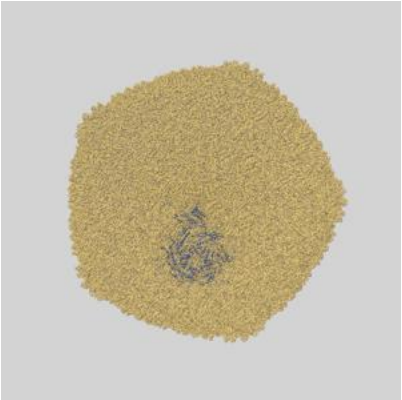
9.1 Map-model overlays

9.1.1 Map-model overlay (i)



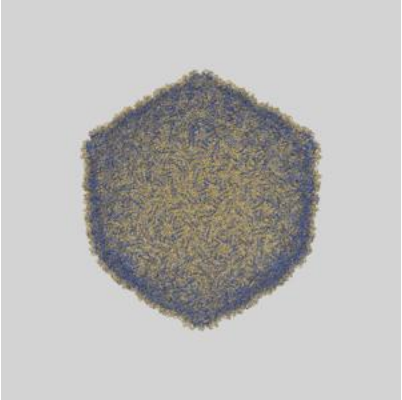
X

Y

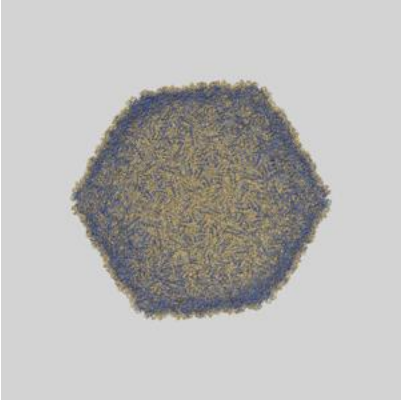


Z

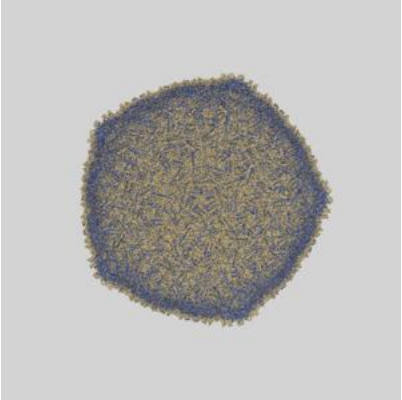
9.1.2 Map-model assembly overlay (i)



X



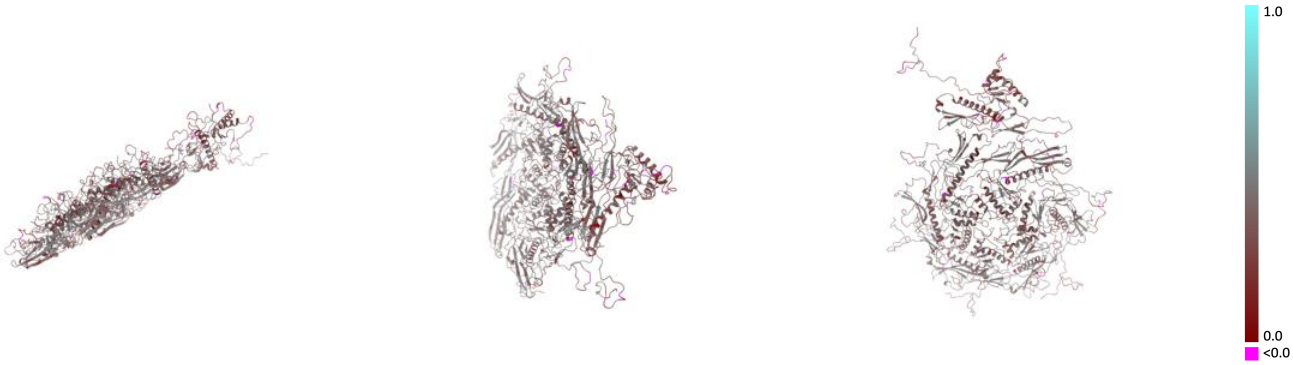
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.6 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.

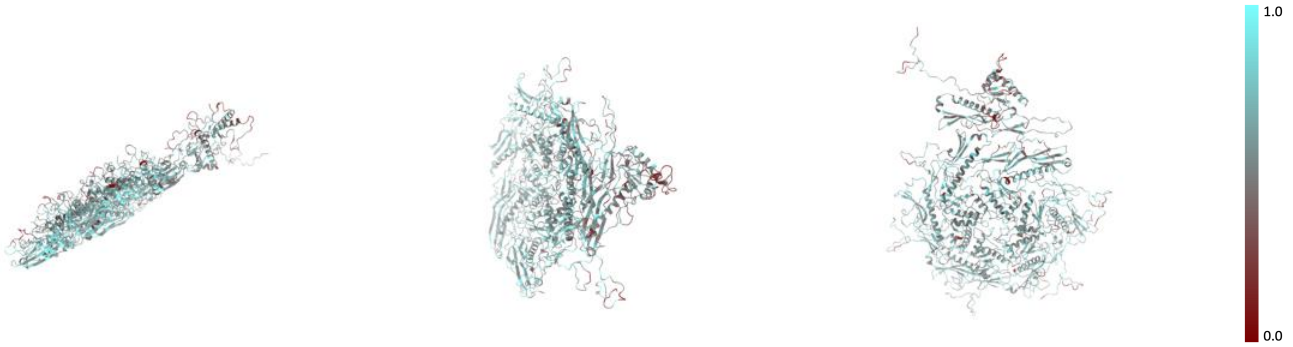
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

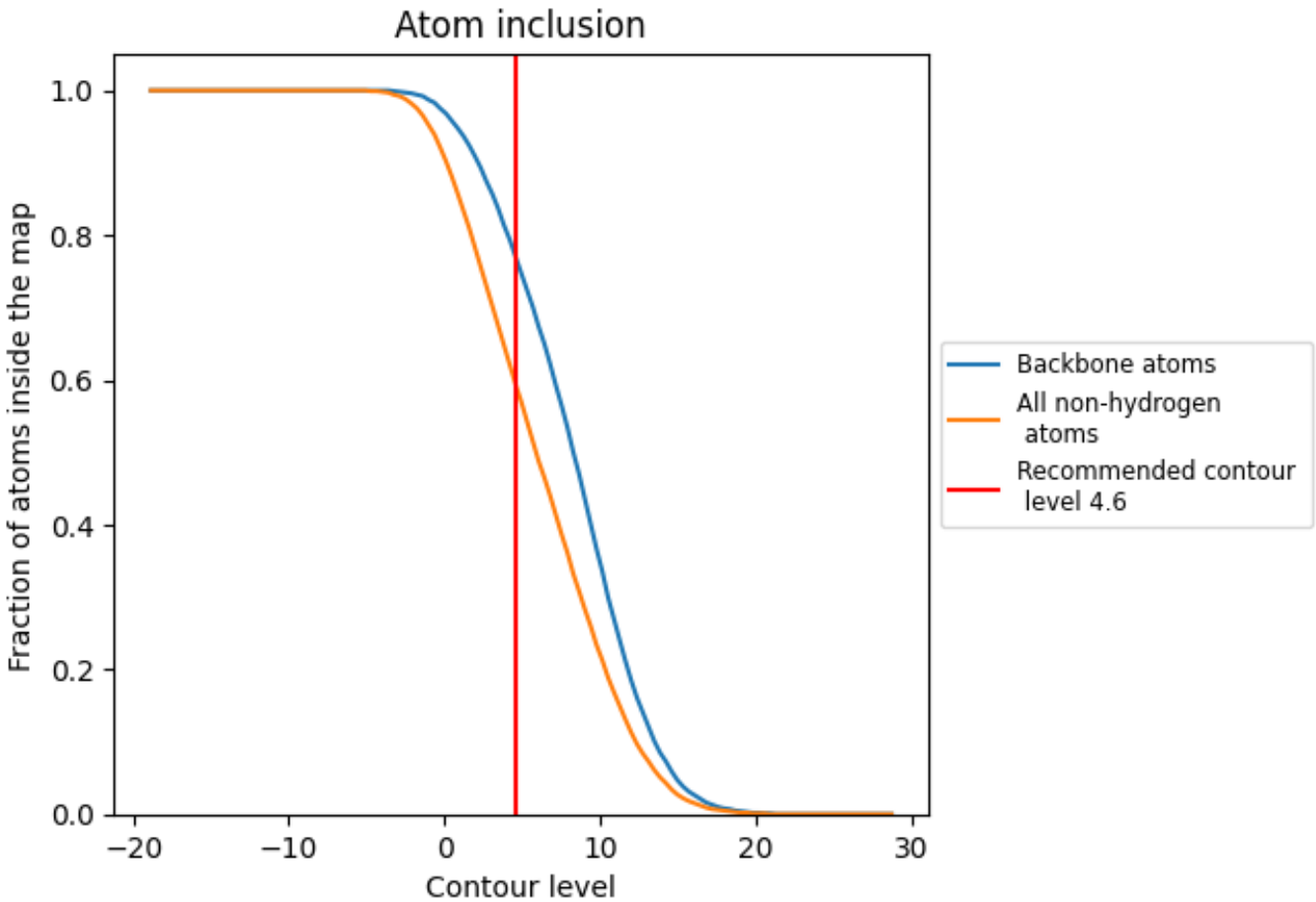
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.6).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 59% 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 (4.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5910	0.3630
A	0.5950	0.3660
B	0.6080	0.3700
C	0.6100	0.3690
D	0.6240	0.3720
E	0.6080	0.3690
F	0.6020	0.3730
G	0.4930	0.3240