Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 11:20 AM EST

PDB ID	:	3J7W
EMDB ID	:	EMD-6035
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	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

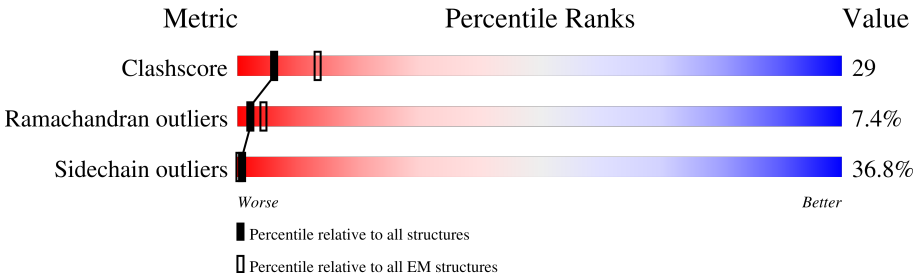
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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	9% 41% 38% 18%
1	B	345	9% 42% 37% 16%
1	C	345	8% 42% 38% 18%
1	D	345	5% 43% 40% 14%
1	E	345	10% 44% 41% 11%
1	F	345	9% 43% 36% 18%
1	G	345	17% 44% 37% 16%

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.

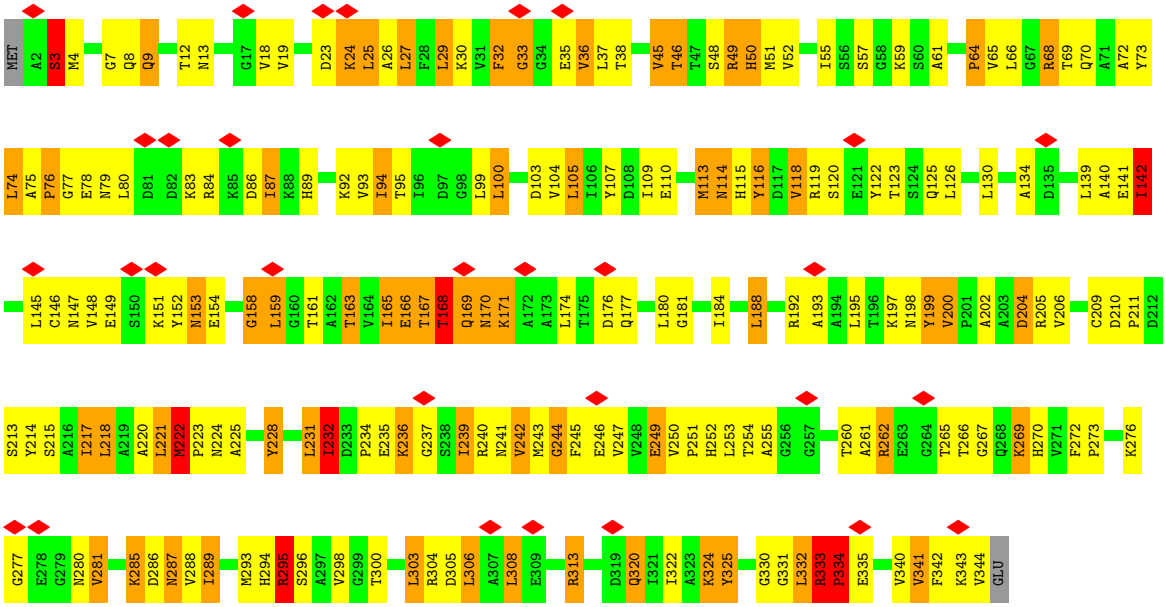
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	B	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	C	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	D	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	E	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11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

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.

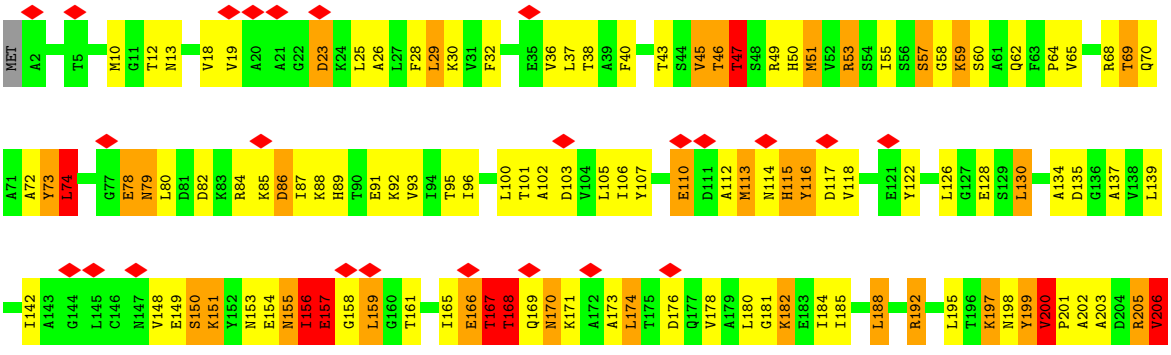
• Molecule 1: Major capsid protein 10A

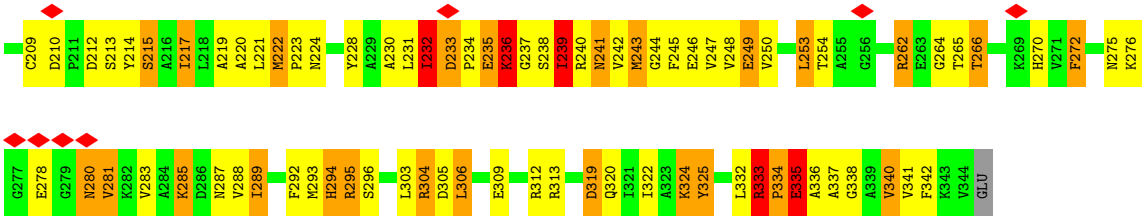
Chain A:



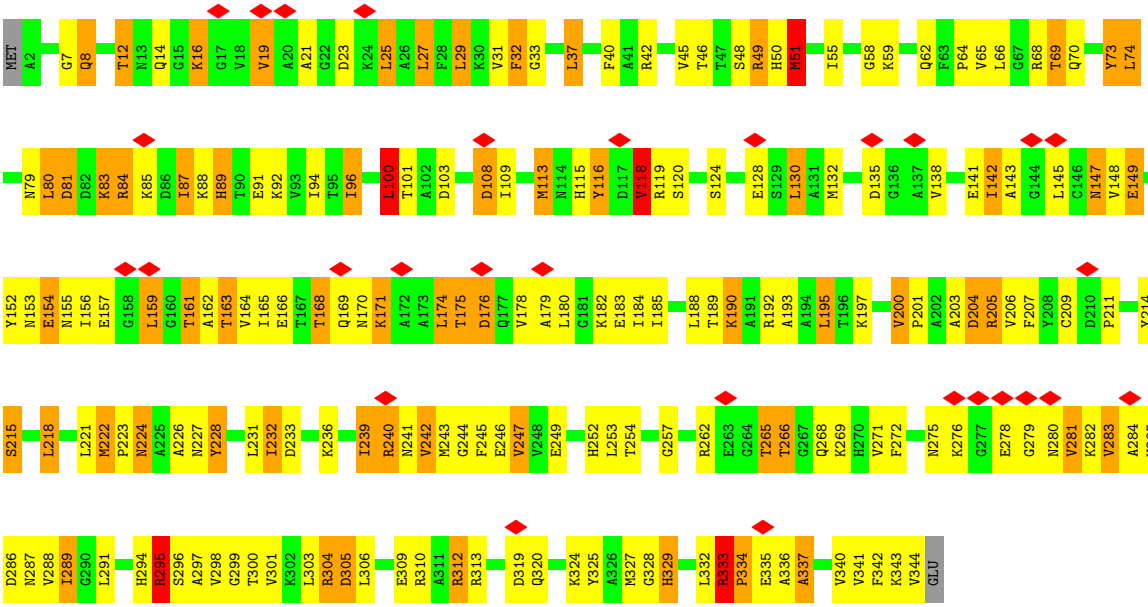
• Molecule 1: Major capsid protein 10A

Chain B:

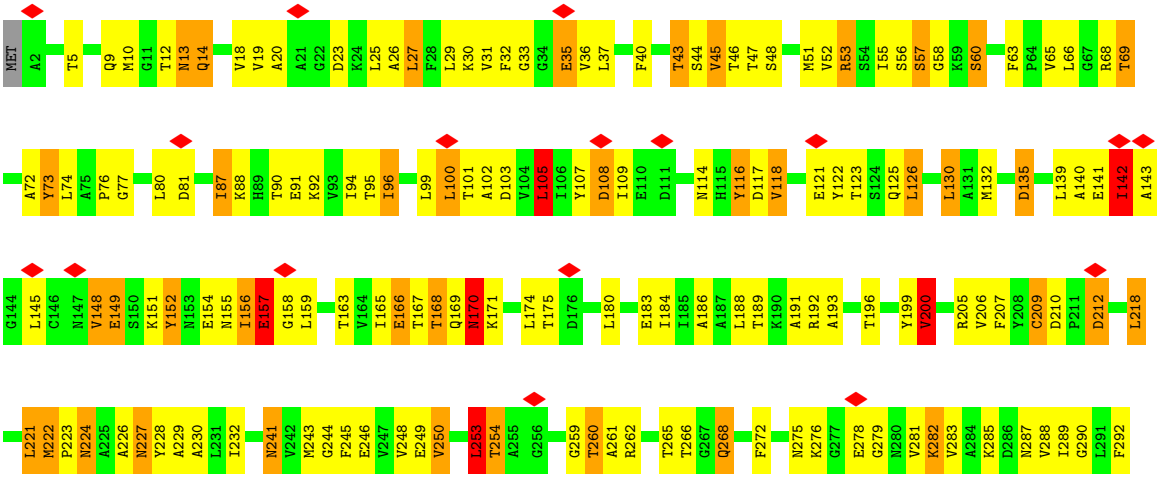


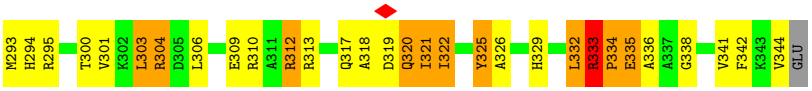


• Molecule 1: Major capsid protein 10A



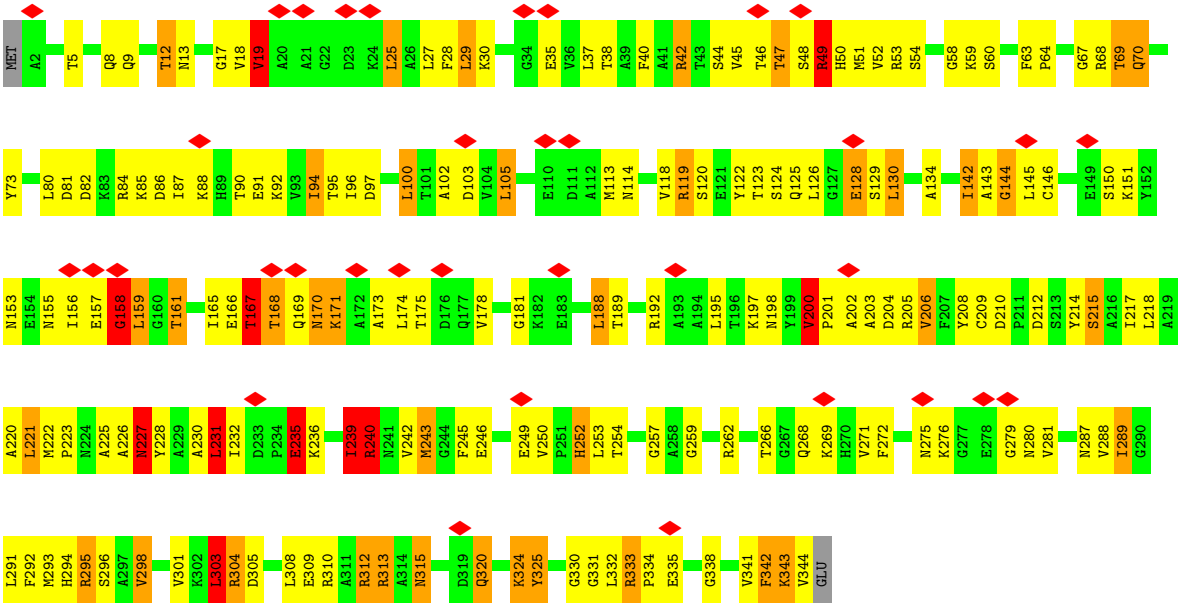
• Molecule 1: Major capsid protein 10A





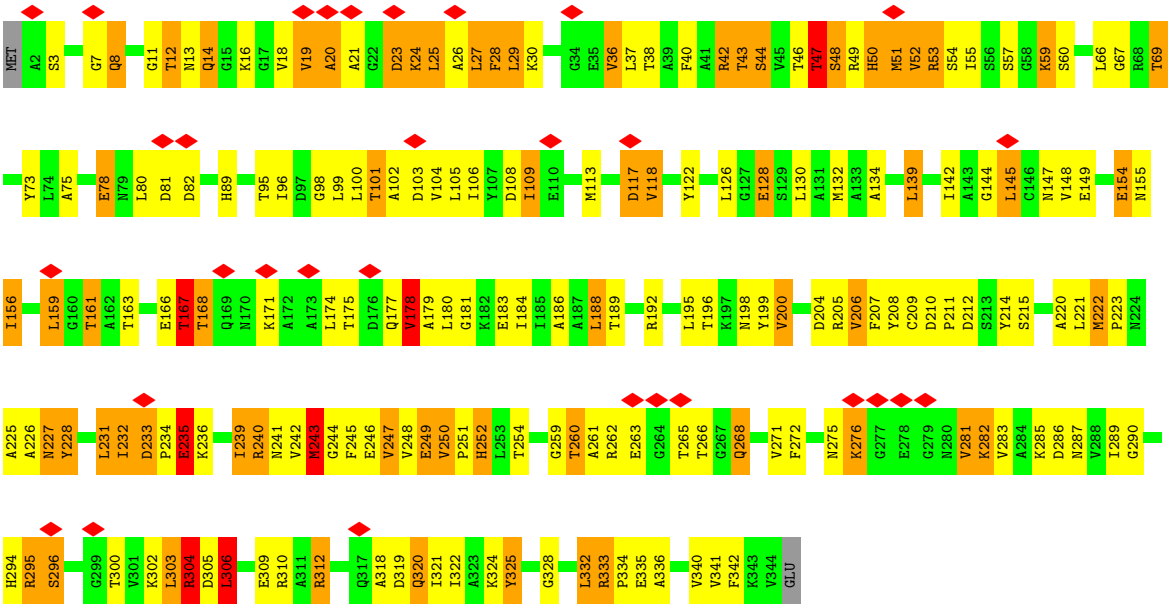
• Molecule 1: Major capsid protein 10A

Chain E:



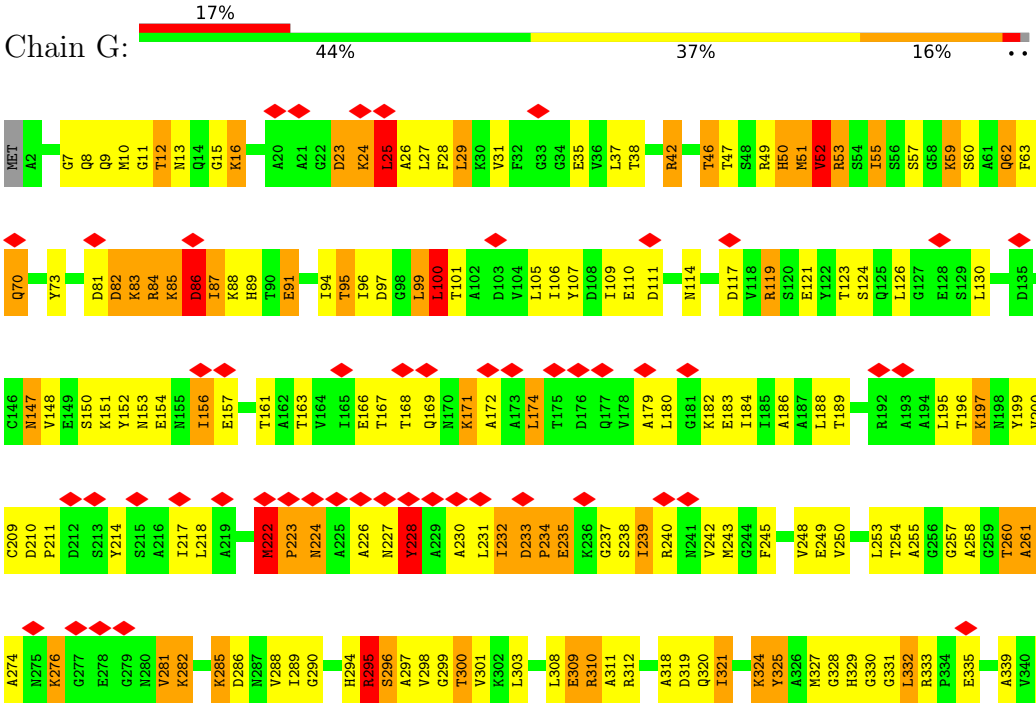
• Molecule 1: Major capsid protein 10A

Chain F:



• Molecule 1: Major capsid protein 10A

Chain G:


17%
44%
37%
16%
MET A2 G7 Q8 Q9 M10 G11 T12 N13 Q14 G15 K16 A20 A21 G22 D23 K24 L25 A26 L27 F28 L29 K30 V31 F32 G33 G34 E35 V36 L37 T38 R42 T46 T47 S48 R49 H50 M51 V52 R53 S54 I55 S56 S57 G58 K59 S60 A61 Q62 F63 P64 V65 L66 G67 R68 T69
Q70 Y73 D81 D82 K83 R84 K85 D86 I87 K88 H89 T90 E91 I94 T95 I96 D97 G98 L99 L100 T101 A102 D103 V104 L105 I106 Y107 D108 I109 E110 D111 N114 D117 V118 R119 S120 E121 Y122 T123 S124 Q125 L126 G127 E128 S129 L130 D135 L139 I142 A143 G144 L145
C146 N147 V148 E149 S150 K151 Y152 N153 E154 N155 I156 E157 T161 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 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 L218 A219 M222 P223 N224 A225 A226 N227 Y228 A229 A230 L231 I232 D233 P234 E235 K236 G237 S238 I239 R240 N241 V242 M243 G244 F245 V248 E249 V250 L253 T254 A255 G256 G257 A258 G259 T260 A261 T265 T266 G267 Q268 K269 H270 V271 F272 P273
A274 W275 K276 G277 E278 G279 N280 V281 K282 K285 D286 W287 V288 I289 G290 H294 R295 S296 A297 V298 G299 T300 V301 K302 L303 L308 E309 R310 A311 R312 A318 D319 Q320 I321 K324 Y325 A326 M327 G328 H329 G330 G331 L332 R333 P334 E335 A339 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	43417	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)	500	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	57727	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	26.777	Depositor
Minimum map value	-25.608	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	1.187	Depositor
Recommended contour level	4.3	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	0.33	1/2582 (0.0%)	0.69	5/3491 (0.1%)
1	B	0.34	1/2582 (0.0%)	0.66	2/3491 (0.1%)
1	C	0.33	1/2582 (0.0%)	0.66	3/3491 (0.1%)
1	D	0.34	0/2582	0.65	4/3491 (0.1%)
1	E	0.32	0/2582	0.62	3/3491 (0.1%)
1	F	0.31	0/2582	0.65	2/3491 (0.1%)
1	G	0.33	1/2582 (0.0%)	0.68	4/3491 (0.1%)
All	All	0.33	4/18074 (0.0%)	0.66	23/24437 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	334	PRO	N-CD	5.34	1.55	1.47
1	A	334	PRO	N-CD	5.30	1.55	1.47
1	B	334	PRO	N-CD	5.16	1.55	1.47
1	G	223	PRO	N-CD	5.00	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	74	LEU	CA-CB-CG	6.88	131.12	115.30
1	D	27	LEU	CA-CB-CG	6.70	130.71	115.30
1	G	333	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	G	100	LEU	CA-CB-CG	6.33	129.87	115.30
1	G	222	MET	C-N-CD	5.95	140.89	128.40
1	F	304	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	222	MET	C-N-CD	5.88	140.74	128.40
1	D	253	LEU	CA-CB-CG	5.86	128.77	115.30
1	D	105	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	333	ARG	C-N-CD	5.74	140.46	128.40
1	C	333	ARG	C-N-CD	5.68	140.34	128.40
1	E	303	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	333	ARG	C-N-CD	5.68	140.32	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	306	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	303	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	308	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	100	LEU	CA-CB-CG	5.30	127.50	115.30
1	G	25	LEU	CA-CB-CG	5.28	127.45	115.30
1	E	158	GLY	C-N-CA	5.27	134.87	121.70
1	A	27	LEU	CA-CB-CG	5.16	127.17	115.30
1	E	231	LEU	CA-CB-CG	5.15	127.15	115.30
1	C	27	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	158	GLY	N-CA-C	-5.04	100.49	113.10

There are no chirality outliers.

There are no planarity outliers.

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	2571	189	0
1	B	2547	0	2573	180	0
1	C	2547	0	2573	177	0
1	D	2547	0	2573	134	0
1	E	2547	0	2573	124	0
1	F	2547	0	2573	171	0
1	G	2547	0	2573	183	0
All	All	17829	0	18009	1051	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 29.

All (1051) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:CB	1:A:335:GLU:HG2	1.27	1.63
1:B:74:LEU:HD22	1:B:80:LEU:CD2	1.35	1.53
1:C:159:LEU:CD1	1:C:335:GLU:HA	1.41	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HB2	1:A:335:GLU:CD	1.33	1.47
1:A:159:LEU:CB	1:A:335:GLU:CG	1.94	1.44
1:A:159:LEU:CD2	1:A:335:GLU:HB3	1.47	1.41
1:C:159:LEU:HD13	1:C:335:GLU:CA	1.52	1.39
1:D:117:ASP:HA	1:D:118:VAL:CB	1.39	1.37
1:D:117:ASP:HA	1:D:118:VAL:CG1	1.57	1.35
1:C:296:SER:N	1:C:297:ALA:HB3	1.37	1.34
1:F:27:LEU:HD12	1:F:28:PHE:N	1.42	1.34
1:B:236:LYS:HA	1:C:243:MET:O	1.25	1.33
1:B:334:PRO:HA	1:B:335:GLU:O	1.27	1.32
1:B:74:LEU:CD2	1:B:80:LEU:HD21	1.62	1.29
1:B:236:LYS:CA	1:C:243:MET:O	1.81	1.29
1:D:117:ASP:CB	1:D:118:VAL:HG12	1.63	1.28
1:F:27:LEU:HD12	1:F:27:LEU:C	1.52	1.28
1:A:159:LEU:HD22	1:A:335:GLU:CB	1.63	1.26
1:G:85:LYS:HA	1:G:85:LYS:CE	1.50	1.25
1:A:159:LEU:HB2	1:A:335:GLU:CG	1.56	1.24
1:B:74:LEU:CD2	1:B:80:LEU:CD2	2.19	1.19
1:F:25:LEU:N	1:F:26:ALA:HB3	1.57	1.17
1:A:159:LEU:HB3	1:A:335:GLU:CG	1.63	1.17
1:C:295:ARG:C	1:C:297:ALA:HB3	1.63	1.17
1:B:40:PHE:CE1	1:C:333:ARG:NH2	2.14	1.14
1:G:85:LYS:HA	1:G:85:LYS:HE2	1.28	1.13
1:A:159:LEU:HB2	1:A:335:GLU:OE2	1.46	1.12
1:B:40:PHE:CZ	1:C:333:ARG:NH2	2.17	1.12
1:D:117:ASP:HB2	1:D:118:VAL:HG12	1.31	1.12
1:D:117:ASP:CA	1:D:118:VAL:HG12	1.79	1.12
1:G:51:MET:O	1:G:52:VAL:HG13	1.49	1.11
1:G:85:LYS:HA	1:G:85:LYS:HE3	1.22	1.11
1:G:298:VAL:HG13	1:G:331:GLY:HA2	1.25	1.10
1:B:74:LEU:HD22	1:B:80:LEU:HD23	1.23	1.10
1:G:51:MET:HG3	1:G:299:GLY:HA3	1.31	1.10
1:G:53:ARG:CG	1:G:53:ARG:HH11	1.64	1.10
1:D:117:ASP:CA	1:D:118:VAL:CB	2.30	1.10
1:G:300:THR:CG2	1:G:329:HIS:ND1	2.14	1.09
1:D:117:ASP:CA	1:D:118:VAL:HB	1.82	1.09
1:G:29:LEU:H	1:G:29:LEU:HD22	0.94	1.09
1:D:117:ASP:CA	1:D:118:VAL:CG1	2.30	1.09
1:D:222:MET:HG3	1:D:223:PRO:HD2	1.24	1.09
1:G:222:MET:HB3	1:G:223:PRO:HD2	1.33	1.08
1:B:45:VAL:HG12	1:B:46:THR:H	1.19	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:LEU:CD1	1:F:28:PHE:N	2.17	1.06
1:B:114:ASN:C	1:B:115:HIS:CD2	2.30	1.04
1:G:85:LYS:HE2	1:G:85:LYS:CA	1.86	1.04
1:G:85:LYS:CE	1:G:85:LYS:CA	2.30	1.03
1:A:332:LEU:O	1:A:332:LEU:HD22	1.60	1.02
1:B:45:VAL:HG12	1:B:46:THR:N	1.74	1.01
1:G:168:THR:O	1:G:168:THR:HG22	1.59	1.01
1:D:117:ASP:HA	1:D:118:VAL:HB	1.04	1.00
1:G:29:LEU:H	1:G:29:LEU:CD2	1.74	1.00
1:G:295:ARG:O	1:G:296:SER:OG	1.76	1.00
1:F:24:LYS:HZ3	1:F:24:LYS:HB3	1.27	0.99
1:G:300:THR:HG21	1:G:329:HIS:CE1	1.96	0.99
1:B:74:LEU:HD22	1:B:80:LEU:HD21	1.00	0.98
1:G:51:MET:C	1:G:52:VAL:HG13	1.83	0.98
1:A:168:THR:HG23	1:A:169:GLN:N	1.79	0.97
1:G:222:MET:HB3	1:G:223:PRO:CD	1.93	0.97
1:F:25:LEU:HD13	1:F:25:LEU:O	1.63	0.97
1:F:27:LEU:C	1:F:27:LEU:CD1	2.30	0.97
1:C:296:SER:HA	1:C:298:VAL:H	1.30	0.96
1:A:159:LEU:CB	1:A:335:GLU:CD	2.18	0.96
1:F:25:LEU:O	1:F:25:LEU:HD22	1.63	0.96
1:G:169:GLN:NE2	1:G:174:LEU:HD21	1.79	0.96
1:B:236:LYS:N	1:C:243:MET:O	1.98	0.95
1:G:29:LEU:HD22	1:G:29:LEU:N	1.76	0.95
1:C:296:SER:N	1:C:297:ALA:CB	2.30	0.95
1:F:25:LEU:N	1:F:26:ALA:CB	2.30	0.94
1:F:25:LEU:H	1:F:26:ALA:HB3	1.24	0.94
1:D:229:ALA:HB2	1:E:228:TYR:CZ	2.03	0.93
1:C:295:ARG:C	1:C:297:ALA:CB	2.36	0.93
1:A:146:CYS:SG	1:A:334:PRO:HB3	2.09	0.92
1:B:116:TYR:N	1:B:116:TYR:HD2	1.68	0.92
1:G:53:ARG:HH11	1:G:53:ARG:HG3	1.32	0.92
1:C:159:LEU:HD12	1:C:335:GLU:HA	1.50	0.92
1:C:159:LEU:HD13	1:C:335:GLU:HA	0.91	0.91
1:C:161:THR:HG22	1:C:334:PRO:O	1.70	0.91
1:A:332:LEU:HD13	1:A:332:LEU:H	1.35	0.90
1:B:37:LEU:HB2	1:C:65:VAL:HG12	1.54	0.90
1:A:159:LEU:HD13	1:A:335:GLU:OE1	1.73	0.89
1:A:250:VAL:HG23	1:A:253:LEU:HG	1.53	0.89
1:G:300:THR:HG21	1:G:329:HIS:ND1	1.86	0.89
1:F:249:GLU:O	1:F:249:GLU:HG2	1.69	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:LEU:HD23	1:G:29:LEU:O	1.73	0.88
1:D:116:TYR:O	1:D:118:VAL:HB	1.71	0.88
1:G:51:MET:CG	1:G:299:GLY:HA3	2.03	0.88
1:G:85:LYS:HE2	1:G:85:LYS:O	1.73	0.88
1:D:117:ASP:CB	1:D:118:VAL:CG1	2.50	0.87
1:A:254:THR:HG22	1:A:255:ALA:H	1.39	0.86
1:G:298:VAL:CG1	1:G:330:GLY:O	2.23	0.86
1:D:227:ASN:O	1:D:228:TYR:CG	2.30	0.85
1:D:222:MET:HG3	1:D:223:PRO:CD	2.08	0.84
1:D:227:ASN:O	1:D:228:TYR:CD2	2.30	0.84
1:G:297:ALA:O	1:G:332:LEU:O	1.95	0.84
1:B:114:ASN:O	1:B:115:HIS:CG	2.30	0.83
1:B:114:ASN:O	1:B:116:TYR:CE2	2.30	0.83
1:B:334:PRO:CA	1:B:335:GLU:O	2.20	0.83
1:A:159:LEU:CD2	1:A:335:GLU:CB	2.36	0.83
1:F:27:LEU:HD12	1:F:28:PHE:CA	2.06	0.83
1:C:159:LEU:HD13	1:C:335:GLU:CB	2.07	0.83
1:F:24:LYS:HB3	1:F:24:LYS:NZ	1.92	0.83
1:G:298:VAL:HG12	1:G:330:GLY:O	1.80	0.82
1:G:53:ARG:HH11	1:G:53:ARG:HG2	1.42	0.82
1:G:294:HIS:CE1	1:G:296:SER:OG	2.32	0.82
1:G:25:LEU:HB2	1:G:26:ALA:HB2	1.62	0.82
1:G:85:LYS:HE2	1:G:85:LYS:C	1.99	0.82
1:B:206:VAL:HG23	1:B:246:GLU:HB3	1.61	0.81
1:A:273:PRO:HG2	1:A:281:VAL:HG11	1.63	0.81
1:C:159:LEU:CD1	1:C:335:GLU:CA	2.29	0.81
1:B:114:ASN:O	1:B:115:HIS:CD2	2.34	0.80
1:F:249:GLU:O	1:F:249:GLU:CG	2.30	0.80
1:A:332:LEU:HD23	1:A:333:ARG:HG2	1.64	0.80
1:G:168:THR:O	1:G:168:THR:CG2	2.30	0.80
1:B:116:TYR:N	1:B:116:TYR:CD2	2.42	0.79
1:G:230:ALA:HB1	1:G:231:LEU:HD23	1.63	0.79
1:F:24:LYS:O	1:F:25:LEU:CD1	2.30	0.79
1:F:25:LEU:O	1:F:25:LEU:CD1	2.30	0.79
1:F:25:LEU:O	1:F:25:LEU:CD2	2.30	0.79
1:F:208:TYR:CD2	1:F:248:VAL:HG21	2.17	0.79
1:G:51:MET:O	1:G:52:VAL:CG1	2.30	0.79
1:F:25:LEU:CA	1:F:26:ALA:HB3	2.14	0.78
1:G:51:MET:HG3	1:G:299:GLY:CA	2.14	0.78
1:G:171:LYS:HD3	1:G:172:ALA:H	1.48	0.78
1:A:332:LEU:CD2	1:A:333:ARG:HG2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:THR:CG2	1:A:169:GLN:N	2.48	0.77
1:G:297:ALA:O	1:G:332:LEU:HD22	1.84	0.77
1:G:300:THR:CG2	1:G:329:HIS:CE1	2.63	0.77
1:A:332:LEU:O	1:A:333:ARG:HG3	1.86	0.76
1:B:114:ASN:O	1:B:116:TYR:HE2	1.65	0.76
1:G:51:MET:CG	1:G:299:GLY:CA	2.62	0.76
1:A:159:LEU:HD21	1:A:198:ASN:HB3	1.66	0.76
1:B:45:VAL:HG12	1:B:46:THR:HG22	1.66	0.76
1:A:168:THR:HG23	1:A:169:GLN:H	1.46	0.75
1:G:298:VAL:HG13	1:G:331:GLY:CA	2.13	0.75
1:C:203:ALA:HA	1:C:205:ARG:HD2	1.69	0.75
1:C:159:LEU:HB2	1:C:335:GLU:HG3	1.67	0.75
1:F:159:LEU:HB3	1:F:335:GLU:HB2	1.68	0.75
1:G:294:HIS:ND1	1:G:296:SER:OG	2.19	0.75
1:B:74:LEU:HD11	1:B:78:GLU:O	1.87	0.75
1:B:294:HIS:H	1:B:336:ALA:HB1	1.51	0.75
1:A:221:LEU:O	1:A:222:MET:HB2	1.86	0.75
1:B:159:LEU:HD11	1:B:335:GLU:H	1.51	0.74
1:D:218:LEU:HD23	1:D:232:ILE:HD11	1.67	0.74
1:D:36:VAL:HG12	1:E:64:PRO:HG2	1.68	0.74
1:A:159:LEU:HB3	1:A:335:GLU:HG2	0.74	0.74
1:A:332:LEU:HD13	1:A:332:LEU:N	2.02	0.74
1:G:295:ARG:C	1:G:296:SER:OG	2.24	0.74
1:G:294:HIS:ND1	1:G:295:ARG:O	2.20	0.73
1:G:51:MET:C	1:G:52:VAL:CG1	2.55	0.73
1:A:142:ILE:HB	1:A:298:VAL:HG21	1.70	0.73
1:A:159:LEU:HD13	1:A:335:GLU:CD	2.09	0.73
1:B:46:THR:O	1:B:47:THR:HB	1.88	0.73
1:D:287:ASN:HB3	1:D:341:VAL:HG13	1.69	0.73
1:G:51:MET:CB	1:G:299:GLY:HA2	2.19	0.73
1:C:154:GLU:HB3	1:C:334:PRO:CD	2.18	0.72
1:C:37:LEU:HD21	1:D:332:LEU:HD23	1.71	0.72
1:B:45:VAL:CG1	1:B:46:THR:H	1.93	0.72
1:B:74:LEU:CD2	1:B:80:LEU:HD23	2.07	0.72
1:F:103:ASP:OD1	1:F:262:ARG:NH2	2.23	0.71
1:C:332:LEU:O	1:C:333:ARG:HB3	1.90	0.71
1:A:159:LEU:HD22	1:A:335:GLU:HB3	0.73	0.71
1:B:114:ASN:C	1:B:115:HIS:CG	2.64	0.71
1:F:24:LYS:O	1:F:25:LEU:HD13	1.91	0.71
1:B:45:VAL:HG12	1:B:46:THR:CG2	2.21	0.70
1:C:336:ALA:O	1:C:337:ALA:CB	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:HD11	1:A:247:VAL:HB	1.73	0.70
1:G:85:LYS:O	1:G:86:ASP:CG	2.30	0.70
1:D:312:ARG:HG2	1:D:319:ASP:HB3	1.73	0.70
1:A:215:SER:OG	1:B:192:ARG:NH1	2.25	0.70
1:C:184:ILE:HD12	1:C:289:ILE:HG21	1.73	0.70
1:A:73:TYR:HD1	1:F:259:GLY:HA2	1.56	0.69
1:A:146:CYS:SG	1:A:334:PRO:CB	2.81	0.69
1:C:332:LEU:O	1:C:333:ARG:CB	2.41	0.69
1:F:248:VAL:O	1:F:249:GLU:CD	2.30	0.69
1:G:29:LEU:CD2	1:G:29:LEU:N	2.42	0.69
1:G:254:THR:HG23	1:G:272:PHE:HD2	1.55	0.69
1:D:159:LEU:HD22	1:D:335:GLU:HG2	1.75	0.69
1:D:223:PRO:HG3	1:E:230:ALA:CB	2.23	0.69
1:F:42:ARG:NH1	1:F:128:GLU:OE1	2.24	0.69
1:C:174:LEU:O	1:C:176:ASP:N	2.26	0.69
1:F:47:THR:OG1	1:F:48:SER:N	2.25	0.69
1:E:333:ARG:NH1	1:E:335:GLU:OE1	2.25	0.68
1:D:96:ILE:HD13	1:D:303:LEU:HD11	1.76	0.68
1:B:51:MET:HE1	1:B:53:ARG:HD2	1.75	0.68
1:F:27:LEU:O	1:F:28:PHE:CG	2.46	0.68
1:E:96:ILE:HD11	1:E:303:LEU:HB3	1.75	0.68
1:E:242:VAL:HG12	1:E:243:MET:HG2	1.75	0.68
1:F:24:LYS:O	1:F:25:LEU:HD12	1.93	0.68
1:F:25:LEU:O	1:F:25:LEU:CG	2.42	0.68
1:A:204:ASP:OD1	1:A:294:HIS:CD2	2.47	0.67
1:E:17:GLY:O	1:E:19:VAL:N	2.26	0.67
1:F:312:ARG:HG2	1:F:319:ASP:HB3	1.76	0.67
1:A:332:LEU:O	1:A:333:ARG:CG	2.42	0.67
1:B:45:VAL:CG1	1:B:46:THR:N	2.48	0.67
1:A:250:VAL:CG2	1:A:253:LEU:HG	2.23	0.67
1:C:154:GLU:HB3	1:C:334:PRO:HD3	1.76	0.67
1:G:26:ALA:HB1	1:G:28:PHE:H	1.59	0.67
1:E:150:SER:OG	1:E:280:ASN:ND2	2.27	0.67
1:D:226:ALA:C	1:D:227:ASN:OD1	2.33	0.67
1:B:289:ILE:HG12	1:B:340:VAL:O	1.95	0.67
1:E:202:ALA:HA	1:E:205:ARG:HH12	1.60	0.67
1:C:157:GLU:HB2	1:C:159:LEU:HB3	1.77	0.67
1:G:86:ASP:C	1:G:86:ASP:OD2	2.32	0.66
1:G:254:THR:HG22	1:G:255:ALA:H	1.61	0.66
1:D:241:ASN:OD1	1:D:241:ASN:N	2.25	0.66
1:D:51:MET:SD	1:D:53:ARG:NH1	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:LEU:HD22	1:F:59:LYS:HE3	1.77	0.66
1:E:259:GLY:HA2	1:F:73:TYR:HD1	1.59	0.66
1:C:48:SER:O	1:C:49:ARG:HD2	1.96	0.66
1:E:227:ASN:H	1:F:227:ASN:HD22	1.41	0.66
1:G:171:LYS:HD3	1:G:172:ALA:N	2.11	0.66
1:B:36:VAL:HG22	1:C:64:PRO:HG2	1.76	0.66
1:F:59:LYS:HD2	1:F:60:SER:HB2	1.78	0.66
1:B:137:ALA:HB1	1:B:270:HIS:HD2	1.61	0.66
1:A:30:LYS:HG2	1:B:60:SER:HB3	1.77	0.65
1:G:111:ASP:OD1	1:G:119:ARG:NH1	2.28	0.65
1:A:92:LYS:NZ	1:A:333:ARG:H	1.95	0.65
1:A:159:LEU:HD23	1:A:335:GLU:HB3	1.68	0.65
1:G:53:ARG:HG2	1:G:53:ARG:NH1	2.05	0.65
1:F:50:HIS:HB3	1:F:52:VAL:HG12	1.79	0.65
1:G:52:VAL:O	1:G:52:VAL:HG23	1.95	0.65
1:B:115:HIS:CD2	1:B:115:HIS:N	2.64	0.65
1:D:209:CYS:SG	1:D:210:ASP:N	2.69	0.65
1:E:97:ASP:OD2	1:E:269:LYS:NZ	2.28	0.65
1:A:35:GLU:OE2	1:B:53:ARG:NH1	2.30	0.65
1:A:87:ILE:HD11	1:F:104:VAL:HG12	1.79	0.65
1:B:222:MET:CE	1:C:243:MET:CE	2.75	0.65
1:F:43:THR:OG1	1:F:44:SER:N	2.30	0.64
1:F:276:LYS:HG3	1:F:282:LYS:HA	1.77	0.64
1:G:166:GLU:OE1	1:G:342:PHE:HB3	1.97	0.64
1:A:197:LYS:O	1:A:198:ASN:HB2	1.98	0.64
1:B:107:TYR:HB2	1:B:110:GLU:HG2	1.78	0.64
1:F:199:TYR:O	1:F:200:VAL:HB	1.97	0.64
1:D:140:ALA:HA	1:D:272:PHE:HE1	1.63	0.64
1:B:116:TYR:HD2	1:B:116:TYR:H	1.45	0.63
1:E:49:ARG:NH1	1:E:246:GLU:OE2	2.31	0.63
1:E:257:GLY:HA3	1:E:268:GLN:HG2	1.78	0.63
1:B:222:MET:CE	1:C:243:MET:HE2	2.29	0.63
1:G:42:ARG:H	1:G:42:ARG:HD3	1.62	0.63
1:D:310:ARG:HH21	1:D:321:ILE:HD11	1.64	0.63
1:G:169:GLN:HE21	1:G:174:LEU:HD21	1.60	0.63
1:E:259:GLY:HA2	1:F:73:TYR:CD1	2.34	0.63
1:F:304:ARG:HG2	1:F:304:ARG:HH11	1.64	0.63
1:C:161:THR:OG1	1:C:162:ALA:N	2.27	0.62
1:C:286:ASP:OD2	1:C:287:ASN:N	2.32	0.62
1:C:296:SER:H	1:C:297:ALA:HB3	1.51	0.62
1:F:25:LEU:HD13	1:F:25:LEU:C	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:HB3	1:C:89:HIS:HB3	1.82	0.62
1:D:262:ARG:O	1:E:70:GLN:NE2	2.31	0.62
1:F:53:ARG:HH11	1:F:53:ARG:HB3	1.63	0.62
1:C:232:ILE:HG22	1:C:233:ASP:H	1.64	0.62
1:G:70:GLN:HA	1:G:70:GLN:HE21	1.64	0.62
1:A:140:ALA:HA	1:A:272:PHE:HE1	1.65	0.62
1:C:296:SER:CA	1:C:298:VAL:H	2.09	0.62
1:F:184:ILE:HD12	1:F:289:ILE:HG21	1.82	0.62
1:A:214:TYR:HE1	1:A:239:ILE:HD12	1.65	0.62
1:B:69:THR:OG1	1:B:70:GLN:N	2.31	0.62
1:C:147:ASN:HD21	1:C:163:THR:HG21	1.65	0.62
1:F:161:THR:HG22	1:F:334:PRO:HB2	1.82	0.62
1:A:3:SER:OG	1:A:4:MET:N	2.29	0.61
1:B:59:LYS:HE3	1:B:60:SER:H	1.65	0.61
1:B:334:PRO:HA	1:B:335:GLU:C	2.10	0.61
1:F:243:MET:SD	1:F:243:MET:N	2.73	0.61
1:A:55:ILE:HD13	1:A:61:ALA:HB2	1.82	0.61
1:F:102:ALA:HB1	1:F:126:LEU:HD22	1.81	0.61
1:F:166:GLU:HG3	1:F:167:THR:O	2.01	0.61
1:C:295:ARG:CA	1:C:297:ALA:HB3	2.30	0.61
1:B:156:ILE:HG23	1:B:157:GLU:H	1.66	0.61
1:G:300:THR:HG22	1:G:329:HIS:ND1	2.12	0.61
1:E:69:THR:OG1	1:E:70:GLN:N	2.31	0.61
1:E:53:ARG:O	1:E:301:VAL:HA	2.01	0.61
1:F:105:LEU:HA	1:F:320:GLN:HB2	1.83	0.61
1:G:166:GLU:OE2	1:G:183:GLU:HB3	2.01	0.61
1:A:161:THR:HB	1:A:334:PRO:O	2.01	0.60
1:A:204:ASP:OD2	1:A:295:ARG:HG2	2.02	0.60
1:F:287:ASN:HB3	1:F:341:VAL:HG13	1.82	0.60
1:G:254:THR:HG23	1:G:272:PHE:CD2	2.35	0.60
1:A:107:TYR:HB2	1:A:110:GLU:HG2	1.82	0.60
1:B:37:LEU:HD12	1:C:333:ARG:HH12	1.66	0.60
1:D:169:GLN:O	1:D:170:ASN:ND2	2.21	0.60
1:G:207:PHE:CZ	1:G:290:GLY:HA3	2.37	0.60
1:G:312:ARG:HG2	1:G:319:ASP:HB3	1.84	0.60
1:E:231:LEU:HD23	1:E:232:ILE:HG23	1.82	0.60
1:A:221:LEU:HB3	1:A:232:ILE:HG21	1.84	0.60
1:D:142:ILE:HG23	1:D:143:ALA:H	1.66	0.60
1:G:257:GLY:HA3	1:G:268:GLN:HB3	1.84	0.60
1:B:102:ALA:HB1	1:B:126:LEU:HD22	1.83	0.60
1:B:178:VAL:HG12	1:B:182:LYS:HE2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:SER:HA	1:C:298:VAL:N	2.09	0.60
1:G:51:MET:HB2	1:G:299:GLY:HA2	1.84	0.60
1:C:50:HIS:HE1	1:C:298:VAL:C	2.05	0.60
1:E:304:ARG:HA	1:E:304:ARG:HH11	1.66	0.60
1:B:37:LEU:HD12	1:C:333:ARG:NH1	2.16	0.59
1:D:333:ARG:HG3	1:D:335:GLU:HB2	1.83	0.59
1:E:232:ILE:HG21	1:E:239:ILE:HA	1.84	0.59
1:B:232:ILE:HB	1:B:239:ILE:HA	1.84	0.59
1:C:40:PHE:HE2	1:D:335:GLU:HG3	1.67	0.59
1:D:157:GLU:OE2	1:D:158:GLY:N	2.35	0.59
1:G:169:GLN:NE2	1:G:174:LEU:CD2	2.62	0.59
1:A:294:HIS:O	1:A:295:ARG:HB3	2.01	0.59
1:C:50:HIS:HE1	1:C:298:VAL:O	1.85	0.59
1:F:305:ASP:O	1:F:325:TYR:HB2	2.03	0.59
1:G:51:MET:O	1:G:52:VAL:HG22	2.01	0.59
1:C:116:TYR:HD1	1:C:118:VAL:HG22	1.67	0.59
1:D:100:LEU:HB3	1:D:130:LEU:HD11	1.84	0.59
1:E:166:GLU:HB3	1:E:342:PHE:HA	1.84	0.59
1:B:289:ILE:HD12	1:B:342:PHE:CE1	2.38	0.59
1:A:99:LEU:HD11	1:A:324:LYS:HB2	1.84	0.59
1:B:167:THR:OG1	1:B:168:THR:N	2.35	0.59
1:F:208:TYR:CE2	1:F:248:VAL:HG21	2.38	0.59
1:G:142:ILE:HB	1:G:298:VAL:HG21	1.85	0.59
1:D:142:ILE:HD11	1:D:293:MET:HB3	1.83	0.59
1:G:184:ILE:HD12	1:G:289:ILE:HG21	1.84	0.58
1:A:167:THR:O	1:A:168:THR:HB	2.03	0.58
1:B:46:THR:HG21	1:B:139:LEU:HG	1.85	0.58
1:C:143:ALA:HB2	1:C:291:LEU:HD13	1.84	0.58
1:D:116:TYR:O	1:D:118:VAL:CB	2.49	0.58
1:A:159:LEU:CD1	1:A:335:GLU:CD	2.71	0.58
1:A:243:MET:O	1:A:245:PHE:N	2.36	0.58
1:C:166:GLU:HB3	1:C:342:PHE:HA	1.85	0.58
1:G:205:ARG:HB2	1:G:245:PHE:CD2	2.39	0.58
1:G:49:ARG:O	1:G:295:ARG:NH1	2.37	0.58
1:A:241:ASN:ND2	1:A:245:PHE:O	2.37	0.58
1:E:235:GLU:HG2	1:F:241:ASN:HB2	1.85	0.58
1:A:134:ALA:HB2	1:A:325:TYR:OH	2.04	0.58
1:F:186:ALA:O	1:F:189:THR:OG1	2.20	0.58
1:B:114:ASN:O	1:B:116:TYR:CD2	2.56	0.58
1:G:11:GLY:O	1:G:24:LYS:HB2	2.04	0.58
1:B:202:ALA:HB2	1:B:205:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:MET:HE1	1:C:243:MET:HE2	1.86	0.58
1:D:45:VAL:N	1:D:135:ASP:OD2	2.37	0.58
1:G:230:ALA:HB1	1:G:231:LEU:HA	1.85	0.58
1:B:262:ARG:HD2	1:C:84:ARG:HA	1.85	0.57
1:C:155:ASN:OD1	1:C:156:ILE:N	2.33	0.57
1:C:168:THR:OG1	1:C:169:GLN:N	2.37	0.57
1:D:260:THR:H	1:E:73:TYR:HB2	1.67	0.57
1:F:148:VAL:HG22	1:F:281:VAL:HB	1.85	0.57
1:F:289:ILE:HD11	1:F:342:PHE:HD2	1.69	0.57
1:A:104:VAL:HG23	1:A:126:LEU:HD21	1.86	0.57
1:B:23:ASP:OD2	1:B:23:ASP:N	2.37	0.57
1:A:167:THR:O	1:A:168:THR:CB	2.52	0.57
1:G:300:THR:HG23	1:G:329:HIS:ND1	2.13	0.57
1:D:332:LEU:O	1:D:333:ARG:HB2	2.03	0.57
1:E:231:LEU:H	1:E:231:LEU:HD22	1.69	0.57
1:F:232:ILE:HG12	1:F:233:ASP:N	2.19	0.57
1:F:47:THR:O	1:F:49:ARG:N	2.38	0.57
1:A:23:ASP:HA	1:A:24:LYS:HG2	1.85	0.57
1:F:207:PHE:HB2	1:F:245:PHE:HD1	1.69	0.57
1:C:51:MET:HG2	1:C:296:SER:HB2	1.87	0.57
1:C:142:ILE:HB	1:C:298:VAL:HG21	1.87	0.57
1:D:300:THR:HG22	1:D:329:HIS:ND1	2.19	0.57
1:F:231:LEU:HD23	1:F:232:ILE:HG22	1.86	0.57
1:F:294:HIS:HB3	1:F:336:ALA:HB1	1.87	0.57
1:G:53:ARG:HG3	1:G:53:ARG:NH1	2.09	0.57
1:D:243:MET:O	1:D:245:PHE:N	2.38	0.57
1:G:7:GLY:O	1:G:9:GLN:N	2.35	0.57
1:G:209:CYS:SG	1:G:210:ASP:N	2.77	0.57
1:D:212:ASP:OD1	1:D:212:ASP:N	2.36	0.56
1:B:232:ILE:HG12	1:B:233:ASP:N	2.20	0.56
1:D:223:PRO:HG3	1:E:230:ALA:HB2	1.88	0.56
1:E:49:ARG:HE	1:E:206:VAL:HG21	1.70	0.56
1:C:242:VAL:HG12	1:C:243:MET:CE	2.35	0.56
1:A:181:GLY:HA3	1:A:220:ALA:HB2	1.88	0.56
1:B:235:GLU:O	1:B:236:LYS:HB3	2.06	0.56
1:B:254:THR:HG21	1:B:285:LYS:HE3	1.86	0.56
1:D:166:GLU:HB2	1:D:342:PHE:HA	1.88	0.56
1:A:139:LEU:CD2	1:A:253:LEU:CD2	2.83	0.56
1:E:181:GLY:HA3	1:E:220:ALA:HB2	1.86	0.56
1:A:159:LEU:CG	1:A:335:GLU:CD	2.74	0.56
1:D:102:ALA:HB1	1:D:126:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:CG	1:A:204:ASP:O	2.44	0.55
1:A:231:LEU:HD23	1:A:232:ILE:H	1.70	0.55
1:A:332:LEU:N	1:A:332:LEU:CD1	2.69	0.55
1:D:148:VAL:HG13	1:D:281:VAL:HB	1.87	0.55
1:D:227:ASN:OD1	1:D:227:ASN:N	2.35	0.55
1:F:117:ASP:OD1	1:F:117:ASP:N	2.34	0.55
1:E:159:LEU:HD23	1:E:335:GLU:HG2	1.88	0.55
1:F:305:ASP:CG	1:F:306:LEU:H	2.09	0.55
1:B:134:ALA:HB2	1:B:325:TYR:OH	2.05	0.55
1:C:257:GLY:HA3	1:C:268:GLN:HB2	1.89	0.55
1:F:96:ILE:HA	1:F:328:GLY:HA3	1.89	0.55
1:A:103:ASP:H	1:A:262:ARG:HH22	1.55	0.55
1:A:214:TYR:CE1	1:A:239:ILE:HD12	2.42	0.55
1:A:254:THR:HG23	1:A:272:PHE:HB2	1.89	0.55
1:F:75:ALA:HB3	1:F:78:GLU:HG3	1.89	0.55
1:G:169:GLN:HG3	1:G:174:LEU:HD11	1.88	0.55
1:A:163:THR:O	1:A:163:THR:OG1	2.25	0.55
1:D:229:ALA:HB2	1:E:228:TYR:CE1	2.41	0.55
1:A:75:ALA:HB1	1:A:76:PRO:HD2	1.89	0.55
1:E:102:ALA:HB1	1:E:126:LEU:HD22	1.87	0.55
1:E:294:HIS:ND1	1:E:295:ARG:O	2.39	0.55
1:F:19:VAL:O	1:F:21:ALA:N	2.37	0.55
1:F:205:ARG:HB2	1:F:244:GLY:O	2.07	0.55
1:A:29:LEU:HD13	1:A:29:LEU:H	1.72	0.55
1:E:120:SER:O	1:E:123:THR:OG1	2.22	0.55
1:F:333:ARG:HH11	1:F:333:ARG:HB2	1.72	0.55
1:D:259:GLY:HA2	1:E:73:TYR:HD1	1.71	0.55
1:D:293:MET:HA	1:D:336:ALA:O	2.07	0.55
1:E:113:MET:O	1:E:114:ASN:ND2	2.40	0.55
1:F:294:HIS:O	1:F:295:ARG:HB3	2.07	0.55
1:A:166:GLU:OE1	1:A:167:THR:O	2.25	0.54
1:B:313:ARG:NH2	1:C:81:ASP:OD2	2.41	0.54
1:C:265:THR:HG22	1:C:266:THR:H	1.72	0.54
1:F:179:ALA:O	1:F:183:GLU:HG2	2.06	0.54
1:A:73:TYR:CD1	1:F:259:GLY:HA2	2.40	0.54
1:B:150:SER:O	1:B:151:LYS:HG2	2.08	0.54
1:E:289:ILE:HD11	1:E:342:PHE:CE2	2.42	0.54
1:A:262:ARG:O	1:B:70:GLN:NE2	2.41	0.54
1:B:65:VAL:HG13	1:B:91:GLU:HA	1.89	0.54
1:B:181:GLY:HA3	1:B:220:ALA:HB2	1.89	0.54
1:D:14:GLN:HE21	1:D:14:GLN:HA	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASN:HB3	1:C:182:LYS:HE2	1.90	0.54
1:C:298:VAL:HG12	1:C:299:GLY:N	2.23	0.54
1:G:50:HIS:HA	1:G:295:ARG:HH11	1.73	0.54
1:B:214:TYR:OH	1:B:237:GLY:O	2.22	0.54
1:D:159:LEU:HB3	1:D:335:GLU:HA	1.89	0.54
1:G:85:LYS:HE3	1:G:85:LYS:CA	2.15	0.54
1:G:148:VAL:HG22	1:G:282:LYS:H	1.73	0.54
1:C:242:VAL:HG12	1:C:243:MET:HE2	1.90	0.54
1:D:26:ALA:O	1:D:27:LEU:HB3	2.08	0.54
1:D:184:ILE:HD12	1:D:289:ILE:HG21	1.89	0.54
1:D:306:LEU:HD23	1:D:325:TYR:HB3	1.90	0.54
1:E:236:LYS:H	1:F:243:MET:HA	1.72	0.54
1:B:122:TYR:CD1	1:C:87:ILE:HD12	2.43	0.54
1:F:231:LEU:HD23	1:F:232:ILE:H	1.73	0.54
1:F:304:ARG:HH11	1:F:304:ARG:CG	2.21	0.54
1:G:169:GLN:HE21	1:G:174:LEU:CG	2.20	0.54
1:B:234:PRO:HB2	1:C:231:LEU:HD21	1.90	0.53
1:G:166:GLU:OE2	1:G:183:GLU:CB	2.56	0.53
1:G:169:GLN:HE21	1:G:174:LEU:CD2	2.20	0.53
1:A:197:LYS:HB3	1:F:211:PRO:HG3	1.88	0.53
1:A:254:THR:HG22	1:A:255:ALA:N	2.17	0.53
1:G:224:ASN:N	1:G:224:ASN:HD22	2.07	0.53
1:A:32:PHE:CG	1:A:33:GLY:N	2.76	0.53
1:A:252:HIS:H	1:A:252:HIS:CD2	2.26	0.53
1:C:138:VAL:O	1:C:141:GLU:HG2	2.08	0.53
1:F:214:TYR:HB2	1:F:249:GLU:HB2	1.89	0.53
1:A:72:ALA:O	1:F:100:LEU:HD23	2.09	0.53
1:E:206:VAL:HG23	1:E:246:GLU:HB3	1.90	0.53
1:G:274:ALA:HA	1:G:285:LYS:HG2	1.91	0.53
1:A:193:ALA:HB2	1:F:215:SER:HB2	1.91	0.53
1:E:228:TYR:HD1	1:E:230:ALA:H	1.57	0.53
1:G:51:MET:CB	1:G:299:GLY:CA	2.86	0.53
1:C:108:ASP:OD1	1:C:108:ASP:N	2.41	0.53
1:D:116:TYR:C	1:D:118:VAL:HB	2.29	0.53
1:F:149:GLU:CD	1:F:149:GLU:H	2.11	0.53
1:C:148:VAL:HG12	1:C:283:VAL:HG13	1.91	0.53
1:C:159:LEU:HD13	1:C:335:GLU:N	2.16	0.53
1:E:202:ALA:HA	1:E:205:ARG:NH1	2.22	0.53
1:F:19:VAL:HG22	1:F:20:ALA:H	1.73	0.53
1:F:24:LYS:O	1:F:24:LYS:HD2	2.09	0.53
1:B:222:MET:SD	1:C:243:MET:HE1	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ALA:O	1:C:337:ALA:HB2	2.08	0.53
1:A:113:MET:O	1:A:114:ASN:ND2	2.32	0.52
1:B:170:ASN:OD1	1:B:170:ASN:N	2.42	0.52
1:E:252:HIS:CD2	1:E:252:HIS:H	2.28	0.52
1:E:276:LYS:HA	1:E:281:VAL:HG13	1.91	0.52
1:F:23:ASP:OD2	1:F:26:ALA:HB2	2.09	0.52
1:F:208:TYR:CD2	1:F:248:VAL:CG2	2.90	0.52
1:A:159:LEU:HB3	1:A:335:GLU:CB	2.36	0.52
1:B:45:VAL:HB	1:B:135:ASP:OD1	2.10	0.52
1:C:33:GLY:HA3	1:D:63:PHE:CE1	2.43	0.52
1:A:158:GLY:O	1:A:159:LEU:HD12	2.08	0.52
1:A:305:ASP:CG	1:A:306:LEU:H	2.12	0.52
1:F:27:LEU:HD12	1:F:28:PHE:HA	1.91	0.52
1:A:221:LEU:HD23	1:A:232:ILE:HB	1.91	0.52
1:B:205:ARG:HA	1:B:294:HIS:HA	1.91	0.52
1:C:103:ASP:H	1:C:262:ARG:NH2	2.06	0.52
1:D:60:SER:HB3	1:D:95:THR:HG22	1.91	0.52
1:F:132:MET:HG3	1:F:252:HIS:CE1	2.44	0.52
1:A:50:HIS:CE1	1:A:300:THR:HG23	2.45	0.52
1:B:79:ASN:N	1:B:79:ASN:HD22	2.07	0.52
1:B:305:ASP:O	1:B:325:TYR:HB2	2.09	0.52
1:E:155:ASN:OD1	1:E:156:ILE:N	2.40	0.52
1:C:224:ASN:N	1:C:224:ASN:HD22	2.08	0.52
1:F:207:PHE:O	1:F:248:VAL:HG22	2.10	0.52
1:A:167:THR:CG2	1:A:168:THR:N	2.73	0.51
1:B:166:GLU:HB2	1:B:341:VAL:O	2.10	0.51
1:D:265:THR:OG1	1:D:268:GLN:OE1	2.27	0.51
1:E:42:ARG:HB3	1:F:199:TYR:CE1	2.45	0.51
1:E:105:LEU:HA	1:E:320:GLN:HB2	1.91	0.51
1:E:343:LYS:HD3	1:E:344:VAL:HG23	1.92	0.51
1:G:156:ILE:HG13	1:G:157:GLU:H	1.75	0.51
1:B:224:ASN:HA	1:C:226:ALA:HA	1.92	0.51
1:C:159:LEU:HB2	1:C:335:GLU:CG	2.36	0.51
1:C:169:GLN:HB3	1:C:343:LYS:HE2	1.92	0.51
1:D:30:LYS:HB3	1:E:60:SER:HB3	1.91	0.51
1:D:223:PRO:HB3	1:E:228:TYR:CE1	2.44	0.51
1:F:27:LEU:HD22	1:G:91:GLU:HB3	1.93	0.51
1:B:222:MET:HE3	1:C:243:MET:CE	2.39	0.51
1:E:239:ILE:HG22	1:E:240:ARG:N	2.25	0.51
1:A:222:MET:HG3	1:A:223:PRO:HD2	1.92	0.51
1:B:319:ASP:OD2	1:B:319:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLU:N	1:C:91:GLU:OE1	2.44	0.51
1:C:244:GLY:O	1:C:245:PHE:CD1	2.63	0.51
1:E:253:LEU:HD23	1:E:254:THR:N	2.26	0.51
1:F:24:LYS:NZ	1:F:24:LYS:CB	2.63	0.51
1:G:85:LYS:O	1:G:86:ASP:CB	2.59	0.51
1:A:210:ASP:HB2	1:A:211:PRO:HD2	1.92	0.51
1:A:171:LYS:HB3	1:A:342:PHE:HE2	1.74	0.51
1:B:46:THR:HG21	1:B:139:LEU:CG	2.40	0.51
1:G:151:LYS:O	1:G:153:ASN:N	2.43	0.51
1:G:180:LEU:O	1:G:184:ILE:HG12	2.10	0.51
1:A:205:ARG:HB2	1:A:244:GLY:O	2.11	0.51
1:F:174:LEU:HD11	1:F:180:LEU:HD13	1.92	0.51
1:F:207:PHE:HE2	1:F:209:CYS:HB3	1.75	0.51
1:B:46:THR:O	1:B:47:THR:CB	2.58	0.51
1:E:102:ALA:HA	1:E:262:ARG:HH22	1.76	0.51
1:A:209:CYS:SG	1:A:213:SER:HB2	2.50	0.51
1:E:214:TYR:CZ	1:E:239:ILE:HG13	2.45	0.51
1:B:29:LEU:HD13	1:B:29:LEU:H	1.76	0.51
1:C:179:ALA:O	1:C:183:GLU:HG2	2.11	0.51
1:A:35:GLU:OE2	1:B:53:ARG:HD3	2.10	0.50
1:B:171:LYS:HB3	1:B:342:PHE:CD1	2.46	0.50
1:C:306:LEU:HA	1:C:325:TYR:HB3	1.92	0.50
1:D:169:GLN:C	1:D:170:ASN:HD22	2.10	0.50
1:D:294:HIS:O	1:D:294:HIS:ND1	2.44	0.50
1:G:26:ALA:HB1	1:G:28:PHE:HB2	1.92	0.50
1:G:147:ASN:HD21	1:G:339:ALA:HB3	1.76	0.50
1:B:45:VAL:HG21	1:B:250:VAL:HG23	1.93	0.50
1:E:289:ILE:HD11	1:E:342:PHE:CD2	2.46	0.50
1:C:74:LEU:HG	1:C:80:LEU:HB2	1.93	0.50
1:D:155:ASN:CG	1:D:156:ILE:H	2.14	0.50
1:E:312:ARG:HB2	1:E:312:ARG:CZ	2.39	0.50
1:F:227:ASN:OD1	1:F:227:ASN:N	2.45	0.50
1:G:207:PHE:HE2	1:G:209:CYS:HB2	1.75	0.50
1:E:128:GLU:HG3	1:E:129:SER:N	2.26	0.50
1:F:181:GLY:HA3	1:F:220:ALA:HB2	1.92	0.50
1:C:96:ILE:HA	1:C:328:GLY:HA3	1.93	0.50
1:C:148:VAL:HB	1:C:281:VAL:HG22	1.93	0.50
1:F:248:VAL:O	1:F:249:GLU:OE2	2.30	0.50
1:G:171:LYS:HB3	1:G:342:PHE:CZ	2.46	0.50
1:G:224:ASN:HD22	1:G:224:ASN:H	1.59	0.50
1:B:49:ARG:NH2	1:B:248:VAL:HG11	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:TYR:CG	1:B:249:GLU:HG2	2.47	0.50
1:A:100:LEU:HD21	1:A:325:TYR:HE2	1.76	0.50
1:B:241:ASN:OD1	1:B:241:ASN:N	2.22	0.50
1:C:138:VAL:O	1:C:142:ILE:HG22	2.12	0.50
1:F:134:ALA:HB2	1:F:325:TYR:OH	2.11	0.50
1:G:51:MET:CG	1:G:299:GLY:HA2	2.39	0.50
1:A:94:ILE:HD13	1:A:95:THR:H	1.76	0.49
1:A:332:LEU:HD22	1:A:332:LEU:C	2.31	0.49
1:B:122:TYR:HD1	1:C:87:ILE:HD12	1.76	0.49
1:B:155:ASN:HD22	1:B:156:ILE:N	2.10	0.49
1:B:159:LEU:HD11	1:B:335:GLU:N	2.24	0.49
1:D:45:VAL:HG13	1:D:46:THR:HG23	1.92	0.49
1:D:200:VAL:HG11	1:D:335:GLU:OE2	2.11	0.49
1:F:207:PHE:CD2	1:F:247:VAL:HG12	2.47	0.49
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.78	0.49
1:C:295:ARG:CA	1:C:297:ALA:CB	2.87	0.49
1:D:180:LEU:O	1:D:184:ILE:HG12	2.12	0.49
1:G:171:LYS:CD	1:G:171:LYS:H	2.25	0.49
1:G:294:HIS:O	1:G:295:ARG:HB3	2.11	0.49
1:B:294:HIS:HB3	1:B:336:ALA:CB	2.42	0.49
1:E:170:ASN:HD21	1:E:173:ALA:HB3	1.77	0.49
1:E:171:LYS:HE2	1:E:342:PHE:CZ	2.47	0.49
1:F:159:LEU:HB3	1:F:335:GLU:CB	2.40	0.49
1:F:249:GLU:O	1:F:249:GLU:OE2	2.30	0.49
1:G:186:ALA:O	1:G:189:THR:OG1	2.23	0.49
1:C:12:THR:HG23	1:C:14:GLN:HG2	1.94	0.49
1:B:57:SER:OG	1:B:58:GLY:N	2.45	0.49
1:B:333:ARG:CG	1:B:333:ARG:HH11	2.26	0.49
1:A:45:VAL:HG22	1:A:49:ARG:HH12	1.77	0.49
1:D:87:ILE:HD13	1:D:87:ILE:H	1.77	0.49
1:D:292:PHE:CZ	1:D:338:GLY:HA3	2.46	0.49
1:G:168:THR:O	1:G:169:GLN:OE1	2.30	0.49
1:G:298:VAL:HG13	1:G:330:GLY:O	2.07	0.49
1:C:45:VAL:O	1:C:135:ASP:OD2	2.30	0.49
1:B:199:TYR:O	1:B:200:VAL:HG13	2.12	0.49
1:B:254:THR:HG22	1:B:272:PHE:CD2	2.47	0.49
1:C:276:LYS:HB2	1:C:284:ALA:HB2	1.94	0.49
1:C:343:LYS:HG2	1:C:344:VAL:H	1.77	0.49
1:D:223:PRO:HG3	1:E:230:ALA:HB1	1.93	0.49
1:E:218:LEU:O	1:E:222:MET:HG2	2.13	0.49
1:E:313:ARG:NH2	1:F:81:ASP:OD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:ARG:HG3	1:F:296:SER:N	2.26	0.49
1:G:23:ASP:OD2	1:G:23:ASP:N	2.44	0.49
1:A:214:TYR:CD2	1:A:249:GLU:HG2	2.48	0.49
1:C:189:THR:OG1	1:C:190:LYS:N	2.45	0.49
1:C:289:ILE:HG12	1:C:342:PHE:CE2	2.48	0.49
1:G:167:THR:O	1:G:169:GLN:OE1	2.30	0.49
1:A:49:ARG:O	1:A:295:ARG:HD3	2.12	0.49
1:F:46:THR:HB	1:F:47:THR:HA	1.94	0.49
1:G:25:LEU:HD13	1:G:25:LEU:H	1.76	0.49
1:G:55:ILE:HG23	1:G:301:VAL:HG13	1.95	0.49
1:C:222:MET:C	1:D:228:TYR:HH	2.16	0.48
1:D:13:ASN:HA	1:D:27:LEU:HD22	1.94	0.48
1:F:154:GLU:HG3	1:F:159:LEU:HD21	1.95	0.48
1:A:36:VAL:HG13	1:B:64:PRO:HG2	1.94	0.48
1:C:294:HIS:HD2	1:C:295:ARG:O	1.96	0.48
1:G:214:TYR:CE1	1:G:239:ILE:HD11	2.47	0.48
1:G:227:ASN:O	1:G:228:TYR:HB2	2.13	0.48
1:B:292:PHE:CZ	1:B:338:GLY:HA3	2.49	0.48
1:C:66:LEU:CB	1:C:89:HIS:HB3	2.43	0.48
1:F:154:GLU:HG3	1:F:159:LEU:HD11	1.95	0.48
1:F:207:PHE:CZ	1:F:290:GLY:HA3	2.48	0.48
1:F:304:ARG:HG2	1:F:304:ARG:NH1	2.26	0.48
1:A:72:ALA:HB2	1:F:262:ARG:CZ	2.43	0.48
1:E:144:GLY:O	1:E:146:CYS:N	2.47	0.48
1:F:8:GLN:OE1	1:G:87:ILE:HB	2.13	0.48
1:A:228:TYR:CE1	1:F:223:PRO:HA	2.49	0.48
1:G:169:GLN:HE22	1:G:174:LEU:HD21	1.71	0.48
1:A:228:TYR:HE1	1:F:223:PRO:HA	1.79	0.48
1:B:180:LEU:O	1:B:184:ILE:HG12	2.13	0.48
1:D:122:TYR:HE1	1:E:87:ILE:HG13	1.78	0.48
1:E:100:LEU:HB3	1:E:130:LEU:HD11	1.95	0.48
1:E:305:ASP:O	1:E:325:TYR:HB2	2.13	0.48
1:B:231:LEU:HD23	1:B:231:LEU:H	1.78	0.48
1:C:19:VAL:O	1:C:21:ALA:N	2.47	0.48
1:D:186:ALA:O	1:D:189:THR:OG1	2.26	0.48
1:G:143:ALA:HB3	1:G:272:PHE:CZ	2.49	0.48
1:G:148:VAL:HG13	1:G:281:VAL:HA	1.94	0.48
1:A:269:LYS:HB3	1:A:270:HIS:CD2	2.49	0.48
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.77	0.48
1:D:243:MET:HB2	1:D:245:PHE:CD1	2.48	0.48
1:E:315:ASN:HD22	1:E:315:ASN:N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:H	1:A:49:ARG:HH11	1.62	0.48
1:B:289:ILE:HD13	1:B:289:ILE:N	2.29	0.48
1:D:117:ASP:O	1:D:117:ASP:OD2	2.30	0.48
1:F:180:LEU:O	1:F:184:ILE:HG12	2.13	0.48
1:A:50:HIS:HE1	1:A:300:THR:HG23	1.78	0.47
1:A:217:ILE:HD13	1:A:217:ILE:HA	1.75	0.47
1:A:241:ASN:HB2	1:F:235:GLU:HG3	1.95	0.47
1:B:243:MET:O	1:B:245:PHE:N	2.47	0.47
1:D:207:PHE:CZ	1:D:290:GLY:HA3	2.49	0.47
1:G:300:THR:CG2	1:G:329:HIS:CG	2.95	0.47
1:A:159:LEU:CG	1:A:335:GLU:CG	2.83	0.47
1:C:103:ASP:OD1	1:C:262:ARG:NH2	2.48	0.47
1:C:164:VAL:HG12	1:C:340:VAL:HG12	1.96	0.47
1:A:165:ILE:HD13	1:A:166:GLU:H	1.78	0.47
1:A:202:ALA:HA	1:A:205:ARG:HH12	1.80	0.47
1:B:222:MET:CE	1:C:243:MET:HE1	2.43	0.47
1:C:116:TYR:CD1	1:C:118:VAL:HG22	2.48	0.47
1:A:7:GLY:C	1:A:9:GLN:H	2.17	0.47
1:A:139:LEU:HD21	1:A:253:LEU:CD2	2.44	0.47
1:A:170:ASN:OD1	1:A:170:ASN:N	2.45	0.47
1:B:197:LYS:HE3	1:B:197:LYS:HB2	1.79	0.47
1:C:180:LEU:O	1:C:184:ILE:HG12	2.13	0.47
1:F:167:THR:HG22	1:F:168:THR:H	1.80	0.47
1:G:51:MET:O	1:G:52:VAL:CB	2.62	0.47
1:A:105:LEU:HA	1:A:320:GLN:HB2	1.95	0.47
1:A:242:VAL:O	1:F:235:GLU:HA	2.13	0.47
1:B:209:CYS:SG	1:B:213:SER:HB2	2.54	0.47
1:B:253:LEU:HD13	1:B:253:LEU:HA	1.71	0.47
1:C:294:HIS:HD2	1:C:295:ARG:HG3	1.80	0.47
1:C:297:ALA:O	1:C:298:VAL:CG2	2.62	0.47
1:D:99:LEU:HD12	1:D:326:ALA:HB2	1.96	0.47
1:E:289:ILE:CD1	1:E:289:ILE:N	2.78	0.47
1:F:171:LYS:O	1:F:174:LEU:HG	2.14	0.47
1:A:159:LEU:HD11	1:A:198:ASN:HB3	1.95	0.47
1:A:218:LEU:HD21	1:A:237:GLY:O	2.14	0.47
1:A:231:LEU:HD22	1:A:231:LEU:H	1.80	0.47
1:C:195:LEU:O	1:C:200:VAL:HG13	2.14	0.47
1:G:161:THR:HA	1:G:335:GLU:HA	1.97	0.47
1:A:159:LEU:CD2	1:A:335:GLU:CG	2.88	0.47
1:A:195:LEU:HD22	1:A:205:ARG:HE	1.80	0.47
1:A:287:ASN:HD22	1:A:287:ASN:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PRO:HA	1:B:91:GLU:HB2	1.97	0.47
1:B:304:ARG:HH11	1:B:304:ARG:HA	1.80	0.47
1:C:37:LEU:HB2	1:D:65:VAL:HG12	1.95	0.47
1:D:68:ARG:O	1:D:69:THR:OG1	2.27	0.47
1:D:229:ALA:HB2	1:E:228:TYR:CE2	2.49	0.47
1:E:170:ASN:HB3	1:E:344:VAL:HB	1.96	0.47
1:E:243:MET:HA	1:E:243:MET:HE3	1.96	0.47
1:E:252:HIS:H	1:E:252:HIS:HD2	1.61	0.47
1:E:279:GLY:O	1:E:281:VAL:HG12	2.14	0.47
1:F:178:VAL:O	1:F:180:LEU:N	2.42	0.47
1:F:207:PHE:HB2	1:F:245:PHE:CD1	2.50	0.47
1:G:83:LYS:H	1:G:83:LYS:HD3	1.79	0.47
1:B:215:SER:HB2	1:C:193:ALA:HB2	1.97	0.47
1:C:118:VAL:O	1:C:120:SER:N	2.42	0.47
1:E:94:ILE:HB	1:E:330:GLY:HA3	1.97	0.47
1:G:50:HIS:O	1:G:50:HIS:ND1	2.48	0.47
1:A:139:LEU:HD22	1:A:253:LEU:CD2	2.45	0.47
1:B:59:LYS:HB3	1:B:59:LYS:HE2	1.45	0.47
1:D:43:THR:HB	1:D:44:SER:H	1.41	0.47
1:E:47:THR:HA	1:E:48:SER:HA	1.59	0.47
1:E:169:GLN:HG3	1:E:170:ASN:ND2	2.30	0.47
1:G:59:LYS:HD2	1:G:60:SER:OG	2.15	0.47
1:A:72:ALA:O	1:F:100:LEU:HA	2.15	0.47
1:B:64:PRO:HA	1:B:91:GLU:CB	2.45	0.47
1:C:244:GLY:O	1:C:245:PHE:CG	2.68	0.47
1:F:268:GLN:HE21	1:F:268:GLN:HB2	1.50	0.47
1:C:239:ILE:O	1:C:240:ARG:HB2	2.15	0.46
1:E:126:LEU:HD23	1:F:69:THR:HG21	1.96	0.46
1:F:51:MET:HG3	1:F:296:SER:HA	1.97	0.46
1:F:147:ASN:HB2	1:F:283:VAL:HG11	1.98	0.46
1:G:325:TYR:CD2	1:G:327:MET:HG3	2.50	0.46
1:A:159:LEU:CB	1:A:335:GLU:OE2	2.39	0.46
1:A:209:CYS:SG	1:A:210:ASP:N	2.87	0.46
1:B:169:GLN:HB2	1:B:173:ALA:HB3	1.97	0.46
1:C:152:TYR:O	1:C:153:ASN:ND2	2.48	0.46
1:C:200:VAL:HG23	1:C:294:HIS:ND1	2.30	0.46
1:D:40:PHE:CZ	1:E:200:VAL:HG23	2.51	0.46
1:G:289:ILE:HD11	1:G:342:PHE:CG	2.50	0.46
1:G:300:THR:HG22	1:G:329:HIS:CG	2.49	0.46
1:A:298:VAL:HG22	1:A:331:GLY:HA2	1.97	0.46
1:A:325:TYR:C	1:A:325:TYR:CD2	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:HIS:CD2	1:C:295:ARG:HG3	2.50	0.46
1:E:292:PHE:CZ	1:E:338:GLY:HA3	2.51	0.46
1:G:64:PRO:HA	1:G:91:GLU:HA	1.98	0.46
1:A:184:ILE:O	1:A:188:LEU:HB2	2.16	0.46
1:A:295:ARG:HD2	1:A:296:SER:H	1.81	0.46
1:B:205:ARG:HG2	1:B:245:PHE:CE1	2.51	0.46
1:C:336:ALA:O	1:C:337:ALA:HB3	2.13	0.46
1:D:45:VAL:HG11	1:D:250:VAL:HG11	1.97	0.46
1:D:102:ALA:O	1:D:322:ILE:HG12	2.16	0.46
1:F:27:LEU:CD1	1:F:28:PHE:CA	2.81	0.46
1:B:157:GLU:OE2	1:B:159:LEU:HB2	2.15	0.46
1:B:159:LEU:CD1	1:B:335:GLU:H	2.22	0.46
1:D:191:ALA:HB1	1:D:292:PHE:CZ	2.51	0.46
1:F:7:GLY:O	1:F:8:GLN:HB3	2.15	0.46
1:F:239:ILE:O	1:F:240:ARG:HB2	2.15	0.46
1:G:214:TYR:HE1	1:G:239:ILE:HD11	1.80	0.46
1:A:200:VAL:HG22	1:F:40:PHE:CE1	2.51	0.46
1:B:74:LEU:CD1	1:B:78:GLU:O	2.59	0.46
1:E:157:GLU:O	1:E:159:LEU:HD12	2.15	0.46
1:G:12:THR:OG1	1:G:13:ASN:N	2.49	0.46
1:F:171:LYS:HB2	1:F:342:PHE:CE1	2.51	0.46
1:A:153:ASN:N	1:A:153:ASN:OD1	2.47	0.46
1:A:171:LYS:H	1:A:171:LYS:HG2	1.55	0.46
1:B:234:PRO:O	1:C:231:LEU:HD21	2.14	0.46
1:G:53:ARG:CG	1:G:53:ARG:NH1	2.36	0.46
1:G:86:ASP:O	1:G:87:ILE:HD13	2.16	0.46
1:D:206:VAL:HG23	1:D:246:GLU:HB2	1.98	0.46
1:D:260:THR:HB	1:D:261:ALA:H	1.52	0.46
1:F:225:ALA:HA	1:F:226:ALA:HA	1.51	0.46
1:G:228:TYR:CD2	1:G:230:ALA:HB3	2.51	0.46
1:E:42:ARG:NE	1:E:128:GLU:OE1	2.38	0.45
1:E:239:ILE:HG22	1:E:240:ARG:H	1.80	0.45
1:E:304:ARG:HA	1:E:304:ARG:HD3	1.63	0.45
1:E:167:THR:O	1:E:168:THR:HG22	2.17	0.45
1:G:205:ARG:O	1:G:245:PHE:HA	2.17	0.45
1:B:265:THR:HG22	1:B:266:THR:H	1.82	0.45
1:F:109:ILE:HG12	1:G:99:LEU:HD23	1.99	0.45
1:G:166:GLU:HB3	1:G:342:PHE:HB3	1.99	0.45
1:A:166:GLU:HB2	1:A:341:VAL:O	2.17	0.45
1:A:254:THR:HG21	1:A:285:LYS:HE2	1.98	0.45
1:A:325:TYR:C	1:A:325:TYR:HD2	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:HIS:ND1	1:C:252:HIS:O	2.49	0.45
1:C:289:ILE:HD12	1:C:289:ILE:HA	1.68	0.45
1:D:45:VAL:HG22	1:D:46:THR:H	1.81	0.45
1:D:253:LEU:O	1:D:254:THR:HB	2.16	0.45
1:G:27:LEU:O	1:G:27:LEU:HG	2.16	0.45
1:B:322:ILE:HD11	1:C:80:LEU:HD11	1.98	0.45
1:D:46:THR:OG1	1:D:47:THR:N	2.49	0.45
1:D:254:THR:HG21	1:D:285:LYS:HD3	1.97	0.45
1:E:103:ASP:OD1	1:E:262:ARG:NH1	2.49	0.45
1:F:144:GLY:O	1:F:148:VAL:HB	2.16	0.45
1:C:221:LEU:HD13	1:C:221:LEU:HA	1.71	0.45
1:D:76:PRO:HA	1:D:77:GLY:HA2	1.55	0.45
1:E:29:LEU:HD22	1:E:29:LEU:H	1.82	0.45
1:E:171:LYS:HE2	1:E:342:PHE:CE1	2.52	0.45
1:E:298:VAL:HG12	1:E:331:GLY:HA2	1.98	0.45
1:F:14:GLN:HB3	1:G:88:LYS:HE2	1.99	0.45
1:F:155:ASN:CG	1:F:156:ILE:H	2.18	0.45
1:G:81:ASP:OD2	1:G:84:ARG:NH1	2.34	0.45
1:G:106:ILE:O	1:G:318:ALA:HB1	2.16	0.45
1:G:195:LEU:HD23	1:G:205:ARG:HE	1.81	0.45
1:G:276:LYS:HE2	1:G:343:LYS:HG2	1.97	0.45
1:A:105:LEU:HD13	1:A:320:GLN:HB2	1.99	0.45
1:A:141:GLU:OE2	1:A:330:GLY:HA2	2.17	0.45
1:C:69:THR:OG1	1:C:70:GLN:N	2.49	0.45
1:C:297:ALA:C	1:C:298:VAL:HG23	2.37	0.45
1:E:158:GLY:N	1:E:159:LEU:HB2	2.32	0.45
1:G:171:LYS:CD	1:G:171:LYS:N	2.78	0.45
1:A:86:ASP:OD2	1:A:86:ASP:N	2.45	0.45
1:A:332:LEU:O	1:A:332:LEU:CD2	2.48	0.45
1:D:103:ASP:N	1:D:103:ASP:OD2	2.50	0.45
1:F:98:GLY:HA2	1:F:99:LEU:HA	1.63	0.45
1:G:234:PRO:O	1:G:235:GLU:HB3	2.16	0.45
1:A:119:ARG:O	1:A:122:TYR:HB2	2.16	0.45
1:A:240:ARG:H	1:A:240:ARG:HG2	1.55	0.45
1:A:287:ASN:HD22	1:A:287:ASN:N	2.13	0.45
1:D:105:LEU:HA	1:D:320:GLN:HB2	1.97	0.45
1:E:215:SER:HB2	1:F:192:ARG:HH12	1.82	0.45
1:E:236:LYS:N	1:F:243:MET:HA	2.32	0.45
1:G:147:ASN:ND2	1:G:339:ALA:HB3	2.32	0.45
1:A:139:LEU:HD11	1:A:253:LEU:HD21	1.99	0.45
1:A:184:ILE:HD11	1:A:289:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:CG1	1:B:46:THR:HG22	2.42	0.45
1:B:157:GLU:HB2	1:B:158:GLY:H	1.56	0.45
1:B:280:ASN:N	1:B:280:ASN:HD22	2.15	0.45
1:C:215:SER:OG	1:D:193:ALA:HB2	2.16	0.45
1:D:35:GLU:CD	1:E:53:ARG:HE	2.20	0.45
1:D:289:ILE:HD11	1:D:342:PHE:CD2	2.52	0.45
1:B:46:THR:HG21	1:B:139:LEU:CD2	2.47	0.44
1:B:287:ASN:O	1:B:287:ASN:ND2	2.49	0.44
1:C:96:ILE:HG12	1:C:328:GLY:N	2.32	0.44
1:E:9:GLN:O	1:E:12:THR:HG22	2.17	0.44
1:E:49:ARG:HD3	1:E:208:TYR:OH	2.16	0.44
1:A:223:PRO:HG3	1:B:230:ALA:HB2	1.99	0.44
1:C:222:MET:C	1:D:228:TYR:OH	2.56	0.44
1:A:139:LEU:HD22	1:A:253:LEU:HD22	1.98	0.44
1:B:13:ASN:HB3	1:B:18:VAL:HG11	2.00	0.44
1:A:7:GLY:HA3	1:A:9:GLN:HE21	1.83	0.44
1:C:89:HIS:N	1:C:89:HIS:CD2	2.85	0.44
1:C:207:PHE:CE2	1:C:209:CYS:HB2	2.52	0.44
1:D:68:ARG:HA	1:D:68:ARG:HD3	1.67	0.44
1:E:143:ALA:HB2	1:E:291:LEU:HD13	2.00	0.44
1:E:325:TYR:C	1:E:325:TYR:HD2	2.21	0.44
1:F:106:ILE:O	1:F:318:ALA:HB1	2.17	0.44
1:C:159:LEU:HD13	1:C:335:GLU:HB2	1.97	0.44
1:C:185:ILE:O	1:C:189:THR:HG23	2.18	0.44
1:G:15:GLY:O	1:G:16:LYS:HD2	2.18	0.44
1:G:51:MET:O	1:G:52:VAL:CG2	2.66	0.44
1:G:82:ASP:OD1	1:G:83:LYS:HG3	2.18	0.44
1:A:92:LYS:HZ1	1:A:333:ARG:H	1.65	0.44
1:B:46:THR:HG21	1:B:139:LEU:HD21	2.00	0.44
1:B:293:MET:HA	1:B:336:ALA:O	2.17	0.44
1:E:197:LYS:HE3	1:E:197:LYS:HB2	1.71	0.44
1:E:295:ARG:O	1:E:296:SER:OG	2.35	0.44
1:G:96:ILE:HG22	1:G:328:GLY:HA3	1.98	0.44
1:G:260:THR:HG23	1:G:261:ALA:N	2.33	0.44
1:G:295:ARG:C	1:G:297:ALA:H	2.21	0.44
1:G:309:GLU:OE1	1:G:311:ALA:HB2	2.18	0.44
1:A:139:LEU:CD2	1:A:253:LEU:HD22	2.48	0.44
1:A:313:ARG:HH11	1:A:313:ARG:CG	2.30	0.44
1:D:57:SER:OG	1:D:58:GLY:N	2.49	0.44
1:D:107:TYR:HD1	1:D:318:ALA:HB2	1.83	0.44
1:F:222:MET:SD	1:F:223:PRO:HD2	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:HG22	1:B:324:LYS:HB3	1.99	0.44
1:C:188:LEU:HD13	1:C:242:VAL:HG21	1.99	0.44
1:C:239:ILE:HB	1:C:240:ARG:H	1.56	0.44
1:D:279:GLY:C	1:D:281:VAL:H	2.21	0.44
1:D:325:TYR:C	1:D:325:TYR:CD2	2.91	0.44
1:F:252:HIS:H	1:F:252:HIS:CD2	2.36	0.44
1:B:236:LYS:HA	1:C:243:MET:C	2.22	0.43
1:C:254:THR:HG23	1:C:272:PHE:CD2	2.53	0.43
1:F:145:LEU:HD22	1:F:145:LEU:HA	1.84	0.43
1:F:250:VAL:HA	1:F:251:PRO:HD3	1.77	0.43
1:G:276:LYS:HB3	1:G:276:LYS:HE3	1.62	0.43
1:C:204:ASP:OD2	1:C:295:ARG:HG2	2.18	0.43
1:E:161:THR:HB	1:E:334:PRO:O	2.18	0.43
1:F:198:ASN:HB3	1:F:335:GLU:HG2	2.01	0.43
1:G:156:ILE:HD12	1:G:156:ILE:HA	1.84	0.43
1:G:285:LYS:HB3	1:G:285:LYS:HE2	1.91	0.43
1:A:74:LEU:HG	1:F:101:THR:HG21	2.01	0.43
1:B:161:THR:HB	1:B:337:ALA:O	2.18	0.43
1:C:33:GLY:HA3	1:D:63:PHE:HE1	1.82	0.43
1:F:282:LYS:HB3	1:F:282:LYS:HE2	1.79	0.43
1:G:46:THR:CB	1:G:47:THR:HA	2.47	0.43
1:G:197:LYS:HB2	1:G:197:LYS:HE3	1.64	0.43
1:A:65:VAL:HG22	1:F:37:LEU:HB3	2.01	0.43
1:A:70:GLN:NE2	1:F:262:ARG:O	2.51	0.43
1:B:205:ARG:HB3	1:B:206:VAL:H	1.54	0.43
1:B:289:ILE:HD11	1:B:341:VAL:C	2.39	0.43
1:B:305:ASP:CG	1:B:306:LEU:H	2.20	0.43
1:C:223:PRO:HG2	1:D:221:LEU:HD11	2.00	0.43
1:E:217:ILE:O	1:E:221:LEU:HD22	2.18	0.43
1:E:325:TYR:C	1:E:325:TYR:CD2	2.92	0.43
1:F:96:ILE:HD12	1:F:303:LEU:HD11	1.99	0.43
1:F:260:THR:HB	1:F:261:ALA:H	1.55	0.43
1:G:26:ALA:HB1	1:G:28:PHE:N	2.31	0.43
1:G:86:ASP:OD2	1:G:87:ILE:N	2.51	0.43
1:B:25:LEU:HA	1:B:26:ALA:HA	1.58	0.43
1:B:159:LEU:HD13	1:B:159:LEU:HA	1.72	0.43
1:B:214:TYR:CE1	1:B:239:ILE:HD12	2.53	0.43
1:C:29:LEU:HD22	1:C:29:LEU:H	1.83	0.43
1:E:70:GLN:HE21	1:E:70:GLN:HB3	1.66	0.43
1:E:100:LEU:O	1:E:324:LYS:HA	2.19	0.43
1:A:206:VAL:HG22	1:A:246:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG13	1:B:281:VAL:HA	2.00	0.43
1:B:249:GLU:H	1:B:249:GLU:HG3	1.57	0.43
1:G:60:SER:OG	1:G:95:THR:HA	2.19	0.43
1:A:25:LEU:HA	1:A:26:ALA:HA	1.72	0.43
1:A:100:LEU:HB3	1:B:73:TYR:CD2	2.53	0.43
1:B:174:LEU:HD21	1:B:180:LEU:HD13	2.00	0.43
1:C:42:ARG:NE	1:C:128:GLU:OE1	2.31	0.43
1:C:254:THR:HG21	1:C:285:LYS:HZ3	1.83	0.43
1:D:294:HIS:O	1:D:294:HIS:CG	2.72	0.43
1:E:228:TYR:HA	1:F:228:TYR:CG	2.53	0.43
1:F:27:LEU:CD1	1:F:28:PHE:HA	2.49	0.43
1:A:23:ASP:H	1:A:24:LYS:HZ2	1.65	0.43
1:A:46:THR:O	1:A:50:HIS:HD2	2.02	0.43
1:A:199:TYR:O	1:A:200:VAL:HB	2.19	0.43
1:A:243:MET:SD	1:A:243:MET:N	2.91	0.43
1:B:232:ILE:HG21	1:B:239:ILE:HG12	2.00	0.43
1:F:178:VAL:HG13	1:F:179:ALA:N	2.34	0.43
1:B:100:LEU:HG	1:C:73:TYR:CD2	2.53	0.43
1:C:239:ILE:HG13	1:C:247:VAL:HG21	2.01	0.43
1:E:37:LEU:HD11	1:F:333:ARG:NH1	2.34	0.43
1:E:134:ALA:HB2	1:E:325:TYR:OH	2.19	0.43
1:G:232:ILE:HG22	1:G:233:ASP:H	1.84	0.43
1:G:253:LEU:HD23	1:G:254:THR:H	1.84	0.43
1:B:312:ARG:HA	1:B:319:ASP:HB3	2.01	0.43
1:E:293:MET:HG3	1:E:295:ARG:H	1.84	0.43
1:D:168:THR:HG21	1:D:174:LEU:HD23	2.00	0.42
1:D:241:ASN:HB3	1:D:245:PHE:O	2.18	0.42
1:F:139:LEU:HD13	1:F:139:LEU:HA	1.87	0.42
1:F:254:THR:HA	1:F:272:PHE:CD1	2.54	0.42
1:G:210:ASP:HB2	1:G:211:PRO:HD2	2.01	0.42
1:G:235:GLU:HG2	1:G:235:GLU:O	2.18	0.42
1:G:260:THR:HG21	1:G:266:THR:OG1	2.18	0.42
1:A:224:ASN:HA	1:A:225:ALA:HA	1.66	0.42
1:C:145:LEU:O	1:C:149:GLU:HG3	2.19	0.42
1:D:304:ARG:HH11	1:D:304:ARG:HA	1.83	0.42
1:G:59:LYS:HE2	1:G:59:LYS:HB3	1.27	0.42
1:G:179:ALA:O	1:G:183:GLU:HG2	2.19	0.42
1:B:333:ARG:CG	1:B:333:ARG:NH1	2.82	0.42
1:C:31:VAL:O	1:C:32:PHE:HB3	2.19	0.42
1:C:147:ASN:ND2	1:C:163:THR:HG21	2.33	0.42
1:C:222:MET:HB3	1:C:223:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HG22	1:A:49:ARG:NH1	2.34	0.42
1:A:262:ARG:HD3	1:B:72:ALA:HB2	2.01	0.42
1:B:222:MET:HE3	1:C:243:MET:HE2	2.00	0.42
1:C:42:ARG:HG3	1:D:199:TYR:CE1	2.55	0.42
1:D:282:LYS:H	1:D:282:LYS:HG2	1.60	0.42
1:G:99:LEU:HB3	1:G:100:LEU:H	1.41	0.42
1:B:236:LYS:HE2	1:B:238:SER:HB3	2.01	0.42
1:C:68:ARG:HD3	1:C:68:ARG:HA	1.76	0.42
1:C:84:ARG:C	1:C:85:LYS:HD3	2.40	0.42
1:F:148:VAL:HG13	1:F:281:VAL:HB	2.02	0.42
1:A:24:LYS:HD3	1:A:25:LEU:H	1.84	0.42
1:C:40:PHE:CE2	1:D:335:GLU:HG3	2.51	0.42
1:C:188:LEU:HA	1:C:188:LEU:HD23	1.84	0.42
1:D:151:LYS:HG3	1:D:152:TYR:CD2	2.54	0.42
1:E:64:PRO:HA	1:E:91:GLU:CB	2.48	0.42
1:G:46:THR:HB	1:G:47:THR:HA	2.01	0.42
1:A:49:ARG:NH2	1:A:246:GLU:OE1	2.28	0.42
1:A:64:PRO:HG2	1:F:36:VAL:HG22	2.01	0.42
1:A:75:ALA:O	1:A:77:GLY:N	2.52	0.42
1:B:171:LYS:HB2	1:B:171:LYS:HE2	1.90	0.42
1:C:50:HIS:O	1:C:51:MET:C	2.58	0.42
1:C:100:LEU:HB3	1:D:73:TYR:CD2	2.55	0.42
1:E:130:LEU:HD13	1:E:130:LEU:HA	1.78	0.42
1:F:53:ARG:HB3	1:F:53:ARG:NH1	2.30	0.42
1:F:206:VAL:HG23	1:F:246:GLU:HB2	2.00	0.42
1:G:100:LEU:HD21	1:G:258:ALA:O	2.20	0.42
1:G:205:ARG:HB2	1:G:245:PHE:HD2	1.84	0.42
1:A:139:LEU:HD21	1:A:253:LEU:HD21	2.01	0.42
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.35	0.42
1:B:46:THR:HG23	1:B:135:ASP:OD2	2.19	0.42
1:B:51:MET:HE3	1:B:51:MET:HB2	1.88	0.42
1:B:185:ILE:HD13	1:B:185:ILE:HA	1.93	0.42
1:C:7:GLY:O	1:C:8:GLN:HB2	2.19	0.42
1:A:197:LYS:O	1:A:198:ASN:CB	2.67	0.42
1:B:202:ALA:HB2	1:B:205:ARG:NH1	2.33	0.42
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.80	0.42
1:D:56:SER:OG	1:D:57:SER:N	2.53	0.42
1:D:310:ARG:NH2	1:D:321:ILE:HD11	2.31	0.42
1:D:333:ARG:C	1:D:335:GLU:H	2.23	0.42
1:E:158:GLY:CA	1:E:159:LEU:HB2	2.50	0.42
1:G:107:TYR:HA	1:G:318:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:SER:O	1:G:151:LYS:HB3	2.20	0.42
1:A:7:GLY:O	1:A:8:GLN:HB3	2.19	0.42
1:B:113:MET:O	1:B:113:MET:HG2	2.20	0.42
1:B:215:SER:CB	1:C:193:ALA:HB2	2.49	0.42
1:B:222:MET:HE2	1:B:234:PRO:HB3	2.01	0.42
1:C:227:ASN:HB3	1:C:228:TYR:H	1.57	0.42
1:C:262:ARG:NH1	1:D:72:ALA:HB2	2.35	0.42
1:E:37:LEU:HD21	1:F:332:LEU:HD23	2.02	0.42
1:A:94:ILE:HD13	1:A:95:THR:N	2.35	0.41
1:B:156:ILE:HG23	1:B:157:GLU:N	2.34	0.41
1:B:185:ILE:HG12	1:B:217:ILE:HD11	2.01	0.41
1:B:217:ILE:HD13	1:B:217:ILE:HA	1.69	0.41
1:B:294:HIS:HB3	1:B:336:ALA:HB2	2.01	0.41
1:B:304:ARG:HH11	1:B:304:ARG:CA	2.33	0.41
1:D:224:ASN:C	1:D:226:ALA:H	2.22	0.41
1:E:225:ALA:HA	1:E:226:ALA:HA	1.78	0.41
1:G:310:ARG:HB3	1:G:321:ILE:HG13	2.01	0.41
1:A:176:ASP:O	1:A:177:GLN:HB3	2.21	0.41
1:A:250:VAL:HA	1:A:251:PRO:HD2	1.88	0.41
1:B:219:ALA:HB2	1:C:189:THR:HG21	2.02	0.41
1:C:312:ARG:HG2	1:C:319:ASP:HB3	2.02	0.41
1:D:333:ARG:C	1:D:335:GLU:N	2.74	0.41
1:E:50:HIS:CG	1:E:51:MET:N	2.88	0.41
1:G:99:LEU:HA	1:G:99:LEU:HD22	1.74	0.41
1:B:285:LYS:HE2	1:B:285:LYS:O	2.20	0.41
1:C:211:PRO:O	1:C:214:TYR:HB3	2.20	0.41
1:D:14:GLN:O	1:D:14:GLN:HG3	2.19	0.41
1:D:92:LYS:HD3	1:D:332:LEU:HA	2.02	0.41
1:F:25:LEU:CA	1:F:26:ALA:CB	2.84	0.41
1:G:143:ALA:HB3	1:G:272:PHE:HZ	1.85	0.41
1:G:207:PHE:N	1:G:245:PHE:HB3	2.35	0.41
1:G:286:ASP:OD1	1:G:286:ASP:N	2.53	0.41
1:C:304:ARG:HA	1:C:304:ARG:HD3	1.60	0.41
1:D:108:ASP:HB2	1:D:317:GLN:O	2.19	0.41
1:A:13:ASN:OD1	1:A:18:VAL:HG11	2.20	0.41
1:A:100:LEU:HD22	1:B:73:TYR:CE2	2.56	0.41
1:E:67:GLY:O	1:E:68:ARG:HB3	2.20	0.41
1:E:200:VAL:HG22	1:E:201:PRO:HD2	2.02	0.41
1:F:27:LEU:HD12	1:F:27:LEU:O	2.09	0.41
1:E:37:LEU:HD12	1:E:37:LEU:HA	1.77	0.41
1:A:242:VAL:HG12	1:A:243:MET:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ASN:C	1:E:170:ASN:HD22	2.23	0.41
1:E:188:LEU:HD13	1:E:188:LEU:HA	1.72	0.41
1:G:101:THR:HG23	1:G:324:LYS:HB3	2.02	0.41
1:A:165:ILE:HD13	1:A:166:GLU:N	2.36	0.41
1:B:65:VAL:O	1:B:89:HIS:HB2	2.21	0.41
1:C:241:ASN:ND2	1:C:246:GLU:OE2	2.53	0.41
1:G:211:PRO:HA	1:G:249:GLU:OE1	2.21	0.41
1:A:75:ALA:HB3	1:A:78:GLU:OE2	2.20	0.41
1:A:87:ILE:HG13	1:F:122:TYR:CE1	2.56	0.41
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.90	0.41
1:C:141:GLU:OE2	1:C:329:HIS:HB2	2.21	0.41
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.88	0.41
1:D:207:PHE:HE2	1:D:209:CYS:HB2	1.86	0.41
1:E:142:ILE:HB	1:E:298:VAL:HG11	2.02	0.41
1:E:195:LEU:HD21	1:E:205:ARG:HD3	2.03	0.41
1:E:253:LEU:O	1:E:254:THR:HB	2.21	0.41
1:F:11:GLY:O	1:F:12:THR:HB	2.21	0.41
1:F:25:LEU:HD23	1:F:28:PHE:CE1	2.56	0.41
1:F:177:GLN:O	1:F:178:VAL:HG12	2.21	0.41
1:G:310:ARG:HE	1:G:321:ILE:HD11	1.85	0.41
1:B:201:PRO:HB2	1:B:203:ALA:HB3	2.03	0.41
1:B:295:ARG:HD2	1:B:296:SER:H	1.85	0.41
1:C:83:LYS:N	1:C:83:LYS:HD3	2.36	0.41
1:C:113:MET:N	1:C:113:MET:SD	2.90	0.41
1:C:192:ARG:HD2	1:C:243:MET:HB3	2.02	0.41
1:C:218:LEU:HD22	1:C:232:ILE:HG21	2.03	0.41
1:D:121:GLU:O	1:D:125:GLN:HG2	2.20	0.41
1:F:27:LEU:HD13	1:F:28:PHE:N	2.21	0.41
1:A:24:LYS:HG2	1:A:24:LYS:HZ2	1.81	0.40
1:A:116:TYR:HE2	1:A:118:VAL:HG23	1.85	0.40
1:B:188:LEU:HD13	1:B:188:LEU:HA	1.91	0.40
1:C:50:HIS:ND1	1:C:51:MET:N	2.69	0.40
1:D:33:GLY:HA3	1:E:63:PHE:HE1	1.85	0.40
1:B:112:ALA:O	1:B:113:MET:HG2	2.21	0.40
1:B:233:ASP:HA	1:B:234:PRO:HD3	1.77	0.40
1:C:295:ARG:C	1:C:297:ALA:HB2	2.34	0.40
1:D:333:ARG:N	1:D:334:PRO:HD2	2.36	0.40
1:E:85:LYS:HA	1:E:85:LYS:HD3	1.77	0.40
1:F:28:PHE:HB3	1:F:29:LEU:H	1.71	0.40
1:F:147:ASN:HB2	1:F:283:VAL:CG1	2.51	0.40
1:F:188:LEU:HB3	1:F:242:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:HG13	1:A:281:VAL:HA	2.04	0.40
1:C:171:LYS:H	1:C:171:LYS:HG3	1.51	0.40
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.92	0.40
1:F:234:PRO:O	1:F:235:GLU:HB3	2.21	0.40
1:G:109:ILE:HD12	1:G:109:ILE:HA	1.94	0.40
1:G:343:LYS:HD3	1:G:344:VAL:O	2.20	0.40
1:A:147:ASN:HD22	1:A:147:ASN:N	2.19	0.40
1:B:295:ARG:HD2	1:B:296:SER:N	2.37	0.40
1:C:159:LEU:HD12	1:C:161:THR:H	1.87	0.40
1:C:305:ASP:CG	1:C:306:LEU:N	2.74	0.40
1:D:228:TYR:HE1	1:D:230:ALA:HB3	1.86	0.40
1:E:227:ASN:OD1	1:E:227:ASN:N	2.55	0.40
1:F:254:THR:HG21	1:F:285:LYS:HE3	2.02	0.40
1:G:62:GLN:OE1	1:G:91:GLU:HG3	2.20	0.40
1:A:223:PRO:HG3	1:B:230:ALA:CB	2.52	0.40
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.84	0.40
1:C:16:LYS:HE3	1:C:16:LYS:HB3	1.44	0.40
1:C:332:LEU:O	1:C:332:LEU:HD12	2.21	0.40
1:D:223:PRO:O	1:D:224:ASN:CB	2.70	0.40
1:E:125:GLN:NE2	1:F:67:GLY:O	2.55	0.40
1:F:25:LEU:HA	1:F:26:ALA:HB3	2.00	0.40
1:G:25:LEU:HB2	1:G:26:ALA:CB	2.44	0.40
1:G:231:LEU:HB3	1:G:233:ASP:HB2	2.03	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%)	262 (77%)	51 (15%)	28 (8%)	1 9
1	B	341/345 (99%)	275 (81%)	40 (12%)	26 (8%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	341/345 (99%)	267 (78%)	48 (14%)	26 (8%)	1	10
1	D	341/345 (99%)	271 (80%)	46 (14%)	24 (7%)	1	12
1	E	341/345 (99%)	266 (78%)	50 (15%)	25 (7%)	1	11
1	F	341/345 (99%)	280 (82%)	38 (11%)	23 (7%)	1	13
1	G	341/345 (99%)	281 (82%)	36 (11%)	24 (7%)	1	12
All	All	2387/2415 (99%)	1902 (80%)	309 (13%)	176 (7%)	2	11

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	19	VAL
1	A	76	PRO
1	A	222	MET
1	A	236	LYS
1	A	244	GLY
1	A	277	GLY
1	A	288	VAL
1	A	295	ARG
1	B	47	THR
1	B	118	VAL
1	B	156	ILE
1	B	157	GLU
1	B	200	VAL
1	B	206	VAL
1	B	232	ILE
1	B	236	LYS
1	B	239	ILE
1	B	333	ARG
1	B	335	GLU
1	C	8	GLN
1	C	12	THR
1	C	51	MET
1	C	116	TYR
1	C	170	ASN
1	C	175	THR
1	C	240	ARG
1	C	288	VAL
1	C	295	ARG
1	C	337	ALA

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Mol	Chain	Res	Type
1	D	69	THR
1	D	118	VAL
1	D	142	ILE
1	D	148	VAL
1	D	333	ARG
1	D	334	PRO
1	E	18	VAL
1	E	19	VAL
1	E	49	ARG
1	E	159	LEU
1	E	239	ILE
1	E	288	VAL
1	F	8	GLN
1	F	12	THR
1	F	28	PHE
1	F	48	SER
1	F	118	VAL
1	F	178	VAL
1	F	240	ARG
1	F	266	THR
1	G	12	THR
1	G	52	VAL
1	G	100	LEU
1	G	117	ASP
1	G	156	ILE
1	G	222	MET
1	G	234	PRO
1	A	116	TYR
1	B	57	SER
1	B	228	TYR
1	B	235	GLU
1	B	244	GLY
1	B	288	VAL
1	C	58	GLY
1	C	118	VAL
1	C	201	PRO
1	C	266	THR
1	C	278	GLU
1	D	20	ALA
1	D	48	SER
1	D	149	GLU
1	D	244	GLY

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Mol	Chain	Res	Type
1	E	8	GLN
1	E	12	THR
1	F	19	VAL
1	F	57	SER
1	F	168	THR
1	F	243	MET
1	F	247	VAL
1	G	152	TYR
1	G	199	TYR
1	G	226	ALA
1	G	267	GLY
1	G	288	VAL
1	G	295	ARG
1	A	12	THR
1	A	33	GLY
1	A	57	SER
1	A	168	THR
1	A	261	ALA
1	B	86	ASP
1	C	19	VAL
1	C	161	THR
1	C	222	MET
1	C	228	TYR
1	C	239	ILE
1	D	12	THR
1	D	23	ASP
1	D	116	TYR
1	D	152	TYR
1	D	154	GLU
1	D	157	GLU
1	D	170	ASN
1	D	254	THR
1	D	288	VAL
1	E	13	ASN
1	E	118	VAL
1	E	119	ARG
1	E	145	LEU
1	E	227	ASN
1	F	23	ASP
1	F	175	THR
1	G	8	GLN
1	G	174	LEU

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Mol	Chain	Res	Type
1	G	228	TYR
1	G	232	ILE
1	G	238	SER
1	G	261	ALA
1	A	200	VAL
1	A	234	PRO
1	A	266	THR
1	A	267	GLY
1	A	280	ASN
1	B	12	THR
1	B	45	VAL
1	B	167	THR
1	B	266	THR
1	C	23	ASP
1	C	280	ASN
1	D	57	SER
1	D	224	ASN
1	E	167	THR
1	E	175	THR
1	E	203	ALA
1	E	235	GLU
1	E	266	THR
1	F	14	GLN
1	F	20	ALA
1	F	167	THR
1	F	200	VAL
1	F	239	ILE
1	G	233	ASP
1	G	260	THR
1	A	3	SER
1	B	74	LEU
1	B	168	THR
1	C	168	THR
1	C	242	VAL
1	D	88	LYS
1	E	58	GLY
1	E	240	ARG
1	F	235	GLU
1	G	86	ASP
1	G	239	ILE
1	A	68	ARG
1	A	142	ILE

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Mol	Chain	Res	Type
1	A	152	TYR
1	A	199	TYR
1	B	223	PRO
1	C	333	ARG
1	F	47	THR
1	B	242	VAL
1	B	264	GLY
1	A	64	PRO
1	A	232	ILE
1	E	144	GLY
1	F	206	VAL
1	G	237	GLY
1	C	279	GLY
1	D	45	VAL
1	E	158	GLY
1	E	223	PRO
1	A	242	VAL
1	E	333	ARG
1	D	200	VAL
1	E	200	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	259/261 (99%)	160 (62%)	99 (38%)	0 1
1	B	259/261 (99%)	150 (58%)	109 (42%)	0 0
1	C	259/261 (99%)	171 (66%)	88 (34%)	0 1
1	D	259/261 (99%)	167 (64%)	92 (36%)	0 1
1	E	259/261 (99%)	166 (64%)	93 (36%)	0 1
1	F	259/261 (99%)	165 (64%)	94 (36%)	0 1
1	G	259/261 (99%)	166 (64%)	93 (36%)	0 1
All	All	1813/1827 (99%)	1145 (63%)	668 (37%)	1 1

All (668) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	24	LYS
1	A	25	LEU
1	A	27	LEU
1	A	29	LEU
1	A	32	PHE
1	A	36	VAL
1	A	37	LEU
1	A	38	THR
1	A	45	VAL
1	A	46	THR
1	A	48	SER
1	A	49	ARG
1	A	50	HIS
1	A	51	MET
1	A	52	VAL
1	A	59	LYS
1	A	66	LEU
1	A	68	ARG
1	A	69	THR
1	A	74	LEU
1	A	79	ASN
1	A	80	LEU
1	A	83	LYS
1	A	84	ARG
1	A	87	ILE
1	A	89	HIS
1	A	93	VAL
1	A	94	ILE
1	A	100	LEU
1	A	105	LEU
1	A	109	ILE
1	A	113	MET
1	A	114	ASN
1	A	115	HIS
1	A	118	VAL
1	A	120	SER
1	A	123	THR
1	A	125	GLN
1	A	130	LEU
1	A	142	ILE
1	A	145	LEU

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Mol	Chain	Res	Type
1	A	149	GLU
1	A	151	LYS
1	A	153	ASN
1	A	154	GLU
1	A	159	LEU
1	A	163	THR
1	A	165	ILE
1	A	166	GLU
1	A	167	THR
1	A	168	THR
1	A	169	GLN
1	A	170	ASN
1	A	171	LYS
1	A	174	LEU
1	A	180	LEU
1	A	188	LEU
1	A	192	ARG
1	A	204	ASP
1	A	217	ILE
1	A	218	LEU
1	A	221	LEU
1	A	222	MET
1	A	228	TYR
1	A	231	LEU
1	A	232	ILE
1	A	235	GLU
1	A	236	LYS
1	A	239	ILE
1	A	249	GLU
1	A	260	THR
1	A	262	ARG
1	A	265	THR
1	A	269	LYS
1	A	276	LYS
1	A	281	VAL
1	A	285	LYS
1	A	286	ASP
1	A	287	ASN
1	A	289	ILE
1	A	293	MET
1	A	295	ARG
1	A	303	LEU

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Mol	Chain	Res	Type
1	A	304	ARG
1	A	306	LEU
1	A	308	LEU
1	A	313	ARG
1	A	320	GLN
1	A	322	ILE
1	A	324	LYS
1	A	325	TYR
1	A	332	LEU
1	A	333	ARG
1	A	334	PRO
1	A	340	VAL
1	A	341	VAL
1	A	343	LYS
1	A	344	VAL
1	B	10	MET
1	B	19	VAL
1	B	23	ASP
1	B	28	PHE
1	B	29	LEU
1	B	30	LYS
1	B	32	PHE
1	B	38	THR
1	B	43	THR
1	B	46	THR
1	B	47	THR
1	B	50	HIS
1	B	51	MET
1	B	53	ARG
1	B	55	ILE
1	B	59	LYS
1	B	62	GLN
1	B	68	ARG
1	B	69	THR
1	B	73	TYR
1	B	78	GLU
1	B	79	ASN
1	B	82	ASP
1	B	84	ARG
1	B	85	LYS
1	B	86	ASP
1	B	87	ILE

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Mol	Chain	Res	Type
1	B	88	LYS
1	B	92	LYS
1	B	93	VAL
1	B	95	THR
1	B	96	ILE
1	B	103	ASP
1	B	105	LEU
1	B	106	ILE
1	B	110	GLU
1	B	113	MET
1	B	115	HIS
1	B	116	TYR
1	B	117	ASP
1	B	128	GLU
1	B	130	LEU
1	B	142	ILE
1	B	149	GLU
1	B	150	SER
1	B	151	LYS
1	B	153	ASN
1	B	154	GLU
1	B	155	ASN
1	B	156	ILE
1	B	157	GLU
1	B	159	LEU
1	B	165	ILE
1	B	166	GLU
1	B	167	THR
1	B	168	THR
1	B	170	ASN
1	B	174	LEU
1	B	176	ASP
1	B	182	LYS
1	B	188	LEU
1	B	192	ARG
1	B	195	LEU
1	B	197	LYS
1	B	198	ASN
1	B	199	TYR
1	B	200	VAL
1	B	205	ARG
1	B	206	VAL

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Mol	Chain	Res	Type
1	B	210	ASP
1	B	212	ASP
1	B	215	SER
1	B	217	ILE
1	B	221	LEU
1	B	222	MET
1	B	232	ILE
1	B	233	ASP
1	B	236	LYS
1	B	239	ILE
1	B	240	ARG
1	B	241	ASN
1	B	243	MET
1	B	247	VAL
1	B	249	GLU
1	B	253	LEU
1	B	262	ARG
1	B	272	PHE
1	B	275	ASN
1	B	276	LYS
1	B	278	GLU
1	B	280	ASN
1	B	281	VAL
1	B	283	VAL
1	B	285	LYS
1	B	289	ILE
1	B	294	HIS
1	B	295	ARG
1	B	303	LEU
1	B	304	ARG
1	B	306	LEU
1	B	309	GLU
1	B	319	ASP
1	B	320	GLN
1	B	324	LYS
1	B	325	TYR
1	B	332	LEU
1	B	333	ARG
1	B	335	GLU
1	B	340	VAL
1	C	16	LYS
1	C	25	LEU

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Mol	Chain	Res	Type
1	C	27	LEU
1	C	29	LEU
1	C	32	PHE
1	C	37	LEU
1	C	46	THR
1	C	49	ARG
1	C	51	MET
1	C	55	ILE
1	C	59	LYS
1	C	62	GLN
1	C	69	THR
1	C	73	TYR
1	C	74	LEU
1	C	79	ASN
1	C	80	LEU
1	C	81	ASP
1	C	83	LYS
1	C	84	ARG
1	C	87	ILE
1	C	88	LYS
1	C	89	HIS
1	C	92	LYS
1	C	94	ILE
1	C	96	ILE
1	C	100	LEU
1	C	101	THR
1	C	108	ASP
1	C	109	ILE
1	C	113	MET
1	C	115	HIS
1	C	118	VAL
1	C	119	ARG
1	C	124	SER
1	C	130	LEU
1	C	132	MET
1	C	142	ILE
1	C	147	ASN
1	C	149	GLU
1	C	154	GLU
1	C	159	LEU
1	C	163	THR
1	C	165	ILE

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Mol	Chain	Res	Type
1	C	171	LYS
1	C	174	LEU
1	C	175	THR
1	C	176	ASP
1	C	178	VAL
1	C	190	LYS
1	C	195	LEU
1	C	197	LYS
1	C	200	VAL
1	C	204	ASP
1	C	205	ARG
1	C	206	VAL
1	C	215	SER
1	C	218	LEU
1	C	224	ASN
1	C	232	ILE
1	C	236	LYS
1	C	247	VAL
1	C	249	GLU
1	C	253	LEU
1	C	265	THR
1	C	269	LYS
1	C	271	VAL
1	C	275	ASN
1	C	281	VAL
1	C	282	LYS
1	C	283	VAL
1	C	289	ILE
1	C	295	ARG
1	C	300	THR
1	C	301	VAL
1	C	303	LEU
1	C	304	ARG
1	C	305	ASP
1	C	309	GLU
1	C	310	ARG
1	C	312	ARG
1	C	313	ARG
1	C	320	GLN
1	C	324	LYS
1	C	327	MET
1	C	329	HIS

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Mol	Chain	Res	Type
1	C	333	ARG
1	C	341	VAL
1	D	5	THR
1	D	9	GLN
1	D	10	MET
1	D	13	ASN
1	D	14	GLN
1	D	18	VAL
1	D	19	VAL
1	D	25	LEU
1	D	29	LEU
1	D	31	VAL
1	D	32	PHE
1	D	35	GLU
1	D	37	LEU
1	D	43	THR
1	D	52	VAL
1	D	53	ARG
1	D	55	ILE
1	D	60	SER
1	D	66	LEU
1	D	73	TYR
1	D	74	LEU
1	D	80	LEU
1	D	81	ASP
1	D	87	ILE
1	D	90	THR
1	D	91	GLU
1	D	94	ILE
1	D	96	ILE
1	D	100	LEU
1	D	101	THR
1	D	105	LEU
1	D	108	ASP
1	D	109	ILE
1	D	114	ASN
1	D	123	THR
1	D	126	LEU
1	D	130	LEU
1	D	132	MET
1	D	135	ASP
1	D	139	LEU

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Mol	Chain	Res	Type
1	D	141	GLU
1	D	142	ILE
1	D	149	GLU
1	D	156	ILE
1	D	157	GLU
1	D	163	THR
1	D	165	ILE
1	D	166	GLU
1	D	167	THR
1	D	168	THR
1	D	170	ASN
1	D	171	LYS
1	D	175	THR
1	D	183	GLU
1	D	188	LEU
1	D	192	ARG
1	D	196	THR
1	D	200	VAL
1	D	205	ARG
1	D	209	CYS
1	D	212	ASP
1	D	218	LEU
1	D	221	LEU
1	D	227	ASN
1	D	241	ASN
1	D	248	VAL
1	D	249	GLU
1	D	250	VAL
1	D	253	LEU
1	D	260	THR
1	D	266	THR
1	D	268	GLN
1	D	275	ASN
1	D	276	LYS
1	D	278	GLU
1	D	282	LYS
1	D	283	VAL
1	D	295	ARG
1	D	301	VAL
1	D	303	LEU
1	D	304	ARG
1	D	309	GLU

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Mol	Chain	Res	Type
1	D	312	ARG
1	D	313	ARG
1	D	320	GLN
1	D	321	ILE
1	D	322	ILE
1	D	325	TYR
1	D	332	LEU
1	D	333	ARG
1	D	335	GLU
1	D	344	VAL
1	E	5	THR
1	E	19	VAL
1	E	25	LEU
1	E	27	LEU
1	E	28	PHE
1	E	29	LEU
1	E	30	LYS
1	E	35	GLU
1	E	38	THR
1	E	40	PHE
1	E	42	ARG
1	E	44	SER
1	E	45	VAL
1	E	46	THR
1	E	47	THR
1	E	49	ARG
1	E	52	VAL
1	E	54	SER
1	E	59	LYS
1	E	69	THR
1	E	70	GLN
1	E	80	LEU
1	E	81	ASP
1	E	82	ASP
1	E	84	ARG
1	E	86	ASP
1	E	88	LYS
1	E	90	THR
1	E	92	LYS
1	E	94	ILE
1	E	95	THR
1	E	100	LEU

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Mol	Chain	Res	Type
1	E	105	LEU
1	E	119	ARG
1	E	122	TYR
1	E	124	SER
1	E	128	GLU
1	E	130	LEU
1	E	142	ILE
1	E	151	LYS
1	E	153	ASN
1	E	161	THR
1	E	165	ILE
1	E	167	THR
1	E	168	THR
1	E	170	ASN
1	E	171	LYS
1	E	174	LEU
1	E	178	VAL
1	E	188	LEU
1	E	189	THR
1	E	192	ARG
1	E	198	ASN
1	E	200	VAL
1	E	204	ASP
1	E	206	VAL
1	E	209	CYS
1	E	210	ASP
1	E	212	ASP
1	E	215	SER
1	E	221	LEU
1	E	227	ASN
1	E	231	LEU
1	E	235	GLU
1	E	239	ILE
1	E	240	ARG
1	E	243	MET
1	E	245	PHE
1	E	249	GLU
1	E	250	VAL
1	E	252	HIS
1	E	271	VAL
1	E	272	PHE
1	E	275	ASN

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Mol	Chain	Res	Type
1	E	287	ASN
1	E	289	ILE
1	E	295	ARG
1	E	298	VAL
1	E	303	LEU
1	E	304	ARG
1	E	308	LEU
1	E	309	GLU
1	E	310	ARG
1	E	312	ARG
1	E	313	ARG
1	E	315	ASN
1	E	320	GLN
1	E	324	LYS
1	E	325	TYR
1	E	332	LEU
1	E	341	VAL
1	E	342	PHE
1	E	343	LYS
1	F	3	SER
1	F	13	ASN
1	F	16	LYS
1	F	18	VAL
1	F	24	LYS
1	F	25	LEU
1	F	27	LEU
1	F	29	LEU
1	F	30	LYS
1	F	36	VAL
1	F	38	THR
1	F	42	ARG
1	F	43	THR
1	F	44	SER
1	F	47	THR
1	F	50	HIS
1	F	51	MET
1	F	52	VAL
1	F	53	ARG
1	F	54	SER
1	F	55	ILE
1	F	59	LYS
1	F	66	LEU

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Mol	Chain	Res	Type
1	F	69	THR
1	F	78	GLU
1	F	80	LEU
1	F	82	ASP
1	F	89	HIS
1	F	95	THR
1	F	101	THR
1	F	108	ASP
1	F	109	ILE
1	F	113	MET
1	F	117	ASP
1	F	118	VAL
1	F	128	GLU
1	F	130	LEU
1	F	139	LEU
1	F	142	ILE
1	F	145	LEU
1	F	154	GLU
1	F	156	ILE
1	F	159	LEU
1	F	161	THR
1	F	163	THR
1	F	167	THR
1	F	178	VAL
1	F	188	LEU
1	F	195	LEU
1	F	196	THR
1	F	204	ASP
1	F	210	ASP
1	F	212	ASP
1	F	221	LEU
1	F	222	MET
1	F	227	ASN
1	F	228	TYR
1	F	231	LEU
1	F	232	ILE
1	F	233	ASP
1	F	235	GLU
1	F	236	LYS
1	F	243	MET
1	F	249	GLU
1	F	250	VAL

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Mol	Chain	Res	Type
1	F	252	HIS
1	F	260	THR
1	F	263	GLU
1	F	265	THR
1	F	268	GLN
1	F	271	VAL
1	F	275	ASN
1	F	276	LYS
1	F	281	VAL
1	F	282	LYS
1	F	286	ASP
1	F	295	ARG
1	F	296	SER
1	F	300	THR
1	F	302	LYS
1	F	303	LEU
1	F	304	ARG
1	F	306	LEU
1	F	309	GLU
1	F	310	ARG
1	F	312	ARG
1	F	320	GLN
1	F	321	ILE
1	F	322	ILE
1	F	324	LYS
1	F	325	TYR
1	F	332	LEU
1	F	333	ARG
1	F	340	VAL
1	G	10	MET
1	G	16	LYS
1	G	23	ASP
1	G	24	LYS
1	G	25	LEU
1	G	29	LEU
1	G	31	VAL
1	G	35	GLU
1	G	37	LEU
1	G	38	THR
1	G	42	ARG
1	G	46	THR
1	G	50	HIS

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Mol	Chain	Res	Type
1	G	51	MET
1	G	52	VAL
1	G	53	ARG
1	G	55	ILE
1	G	57	SER
1	G	59	LYS
1	G	62	GLN
1	G	63	PHE
1	G	65	VAL
1	G	66	LEU
1	G	68	ARG
1	G	70	GLN
1	G	73	TYR
1	G	82	ASP
1	G	83	LYS
1	G	84	ARG
1	G	85	LYS
1	G	86	ASP
1	G	87	ILE
1	G	89	HIS
1	G	91	GLU
1	G	94	ILE
1	G	95	THR
1	G	97	ASP
1	G	99	LEU
1	G	105	LEU
1	G	110	GLU
1	G	114	ASN
1	G	119	ARG
1	G	121	GLU
1	G	123	THR
1	G	124	SER
1	G	126	LEU
1	G	130	LEU
1	G	139	LEU
1	G	142	ILE
1	G	145	LEU
1	G	147	ASN
1	G	154	GLU
1	G	163	THR
1	G	171	LYS
1	G	182	LYS

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Mol	Chain	Res	Type
1	G	188	LEU
1	G	196	THR
1	G	197	LYS
1	G	200	VAL
1	G	205	ARG
1	G	217	ILE
1	G	218	LEU
1	G	224	ASN
1	G	228	TYR
1	G	235	GLU
1	G	240	ARG
1	G	242	VAL
1	G	243	MET
1	G	248	VAL
1	G	250	VAL
1	G	268	GLN
1	G	269	LYS
1	G	271	VAL
1	G	272	PHE
1	G	276	LYS
1	G	281	VAL
1	G	282	LYS
1	G	285	LYS
1	G	295	ARG
1	G	296	SER
1	G	300	THR
1	G	303	LEU
1	G	308	LEU
1	G	309	GLU
1	G	310	ARG
1	G	320	GLN
1	G	321	ILE
1	G	324	LYS
1	G	325	TYR
1	G	332	LEU
1	G	341	VAL
1	G	342	PHE
1	G	343	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	50	HIS
1	A	89	HIS
1	A	125	GLN
1	A	147	ASN
1	A	252	HIS
1	A	287	ASN
1	A	294	HIS
1	A	315	ASN
1	B	79	ASN
1	B	115	HIS
1	B	155	ASN
1	B	270	HIS
1	B	275	ASN
1	B	280	ASN
1	B	287	ASN
1	B	294	HIS
1	C	50	HIS
1	C	147	ASN
1	C	153	ASN
1	C	268	GLN
1	D	14	GLN
1	D	50	HIS
1	D	89	HIS
1	D	153	ASN
1	D	252	HIS
1	D	315	ASN
1	E	50	HIS
1	E	89	HIS
1	E	114	ASN
1	E	170	ASN
1	E	280	ASN
1	E	315	ASN
1	F	147	ASN
1	F	169	GLN
1	F	227	ASN
1	F	252	HIS
1	F	268	GLN
1	F	287	ASN
1	G	70	GLN
1	G	79	ASN
1	G	114	ASN
1	G	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	147	ASN
1	G	169	GLN
1	G	224	ASN
1	G	241	ASN
1	G	315	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.

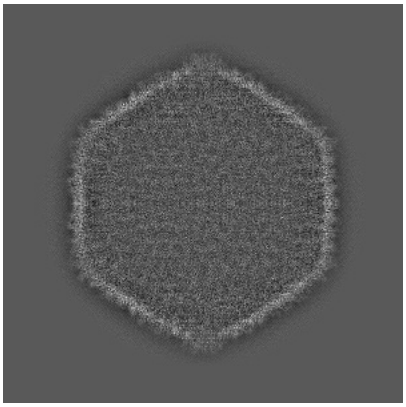
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6035. These allow visual inspection of the internal detail of the map and identification of artifacts.

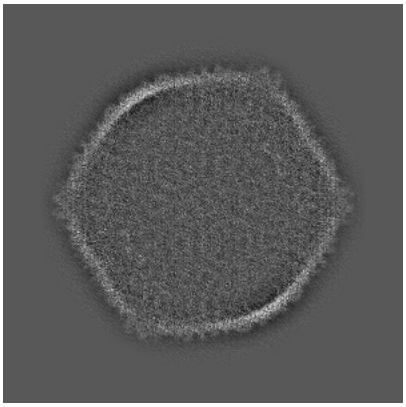
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

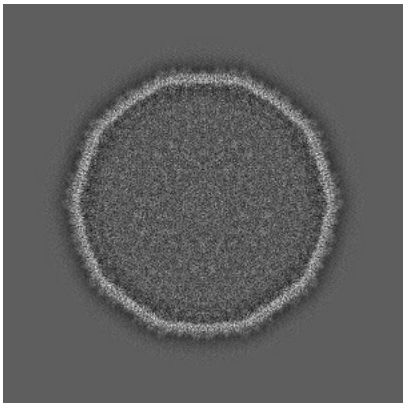
6.1.1 Primary map



X



Y

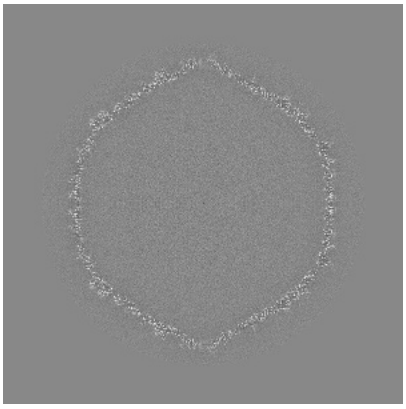


Z

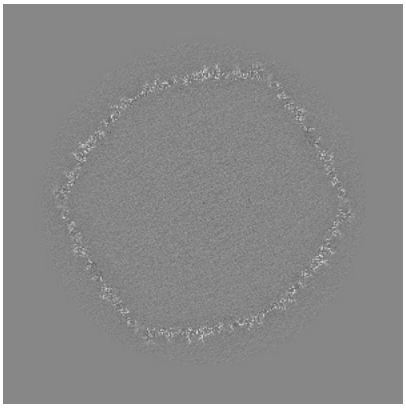
The images above show the map projected in three orthogonal directions.

6.2 Central slices

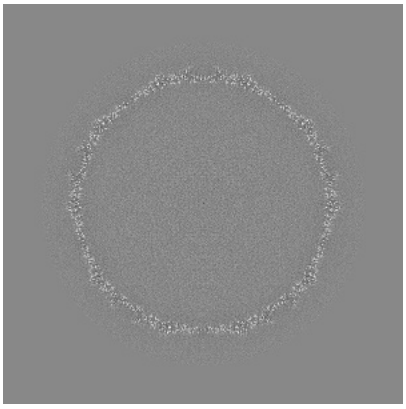
6.2.1 Primary map



X Index: 400



Y Index: 400

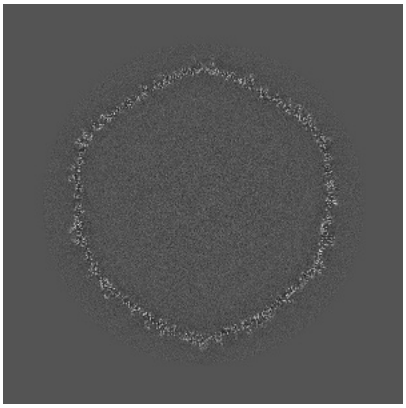


Z Index: 400

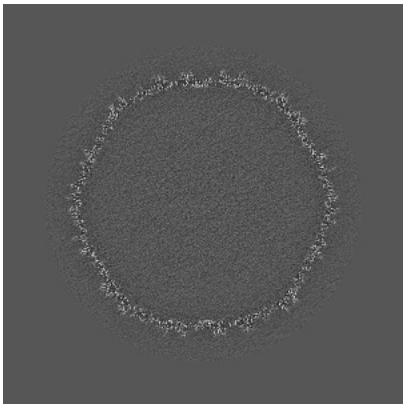
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

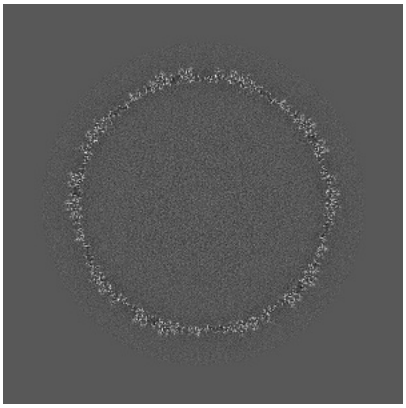
6.3.1 Primary map



X Index: 434



Y Index: 332



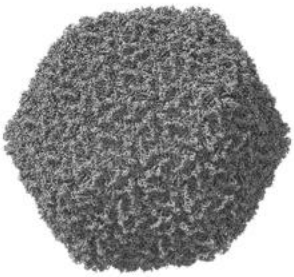
Z Index: 398

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

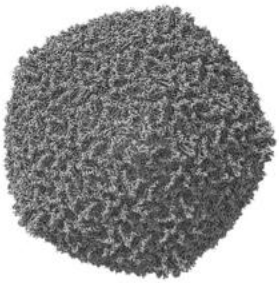
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

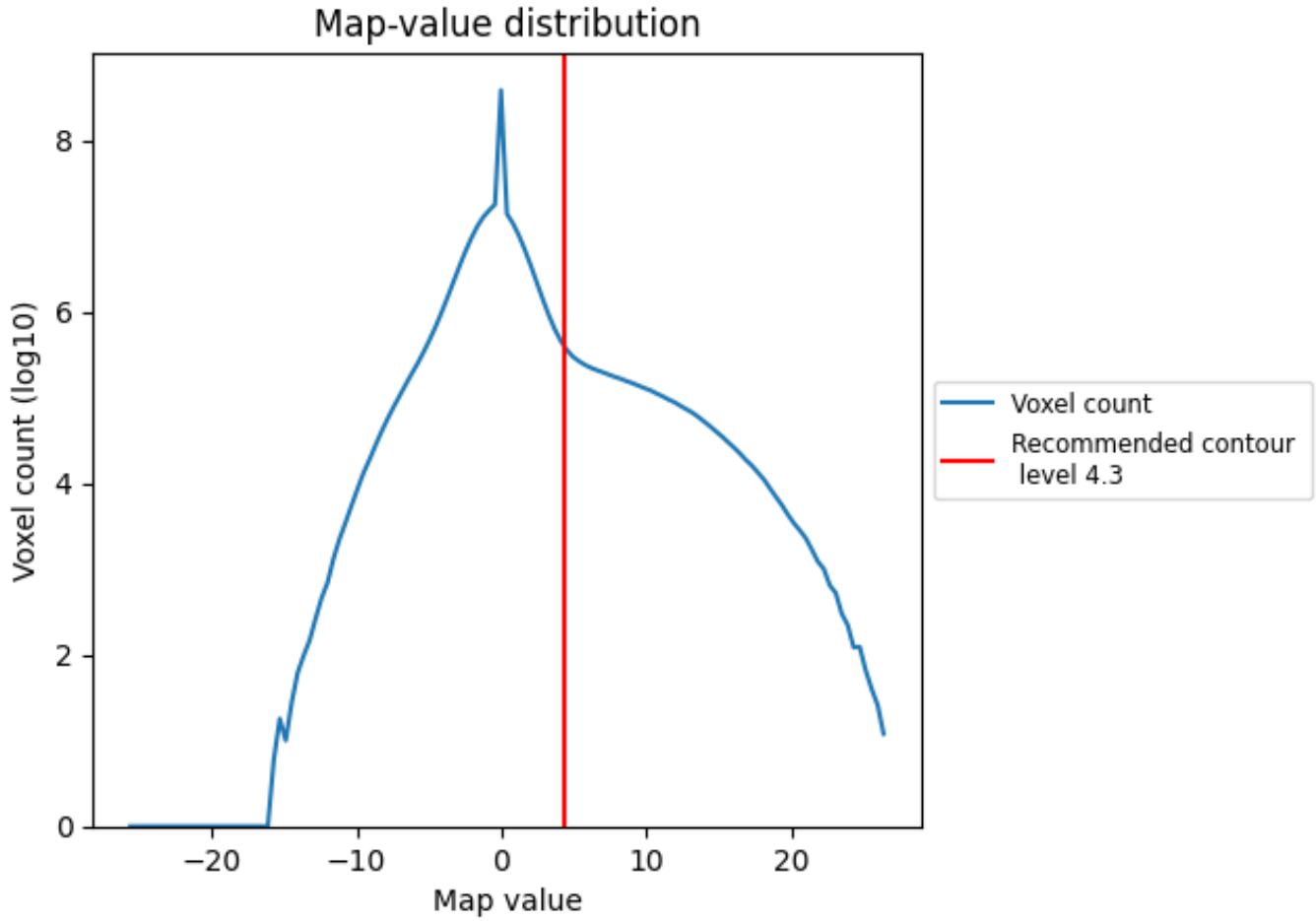
6.5 Mask visualisation (i)

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

7 Map analysis

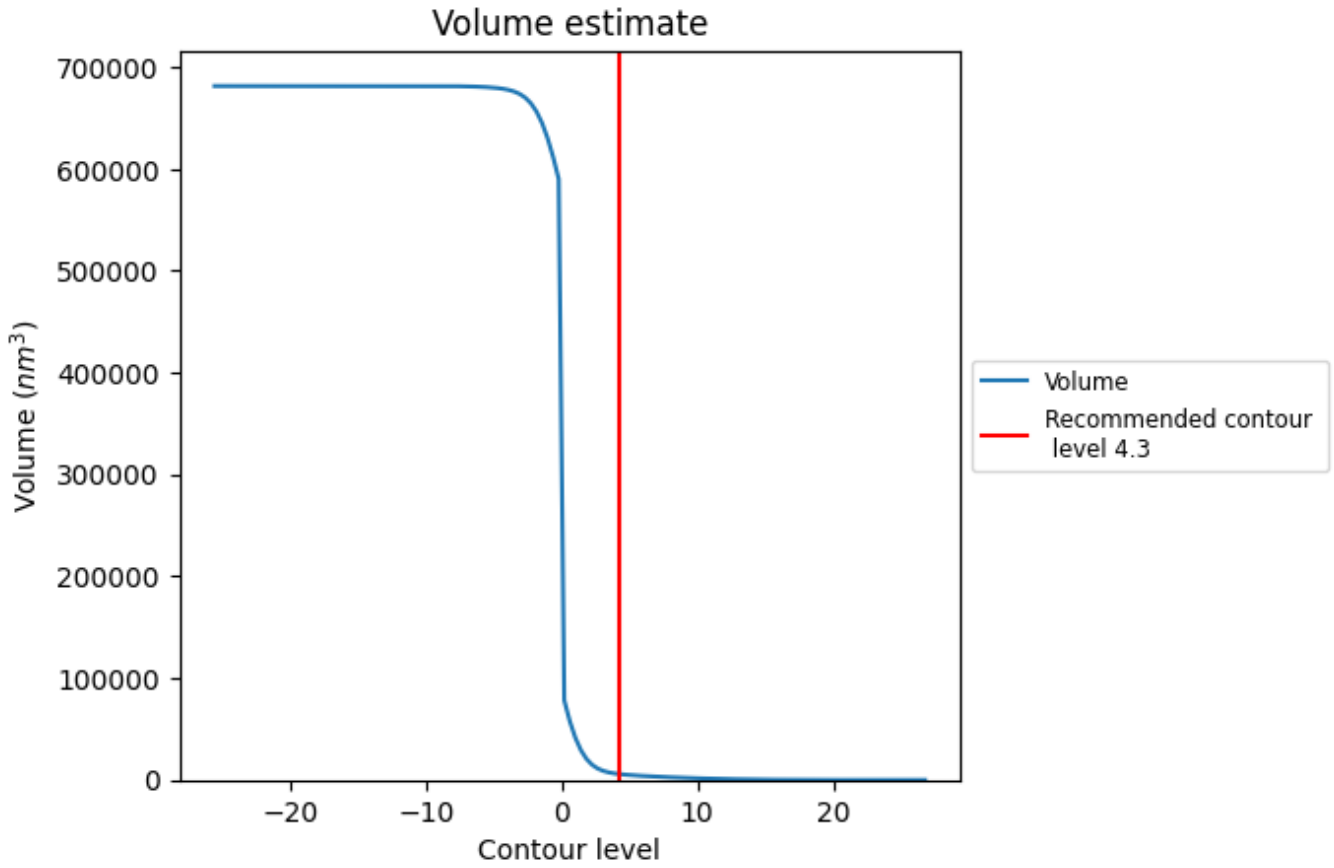
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

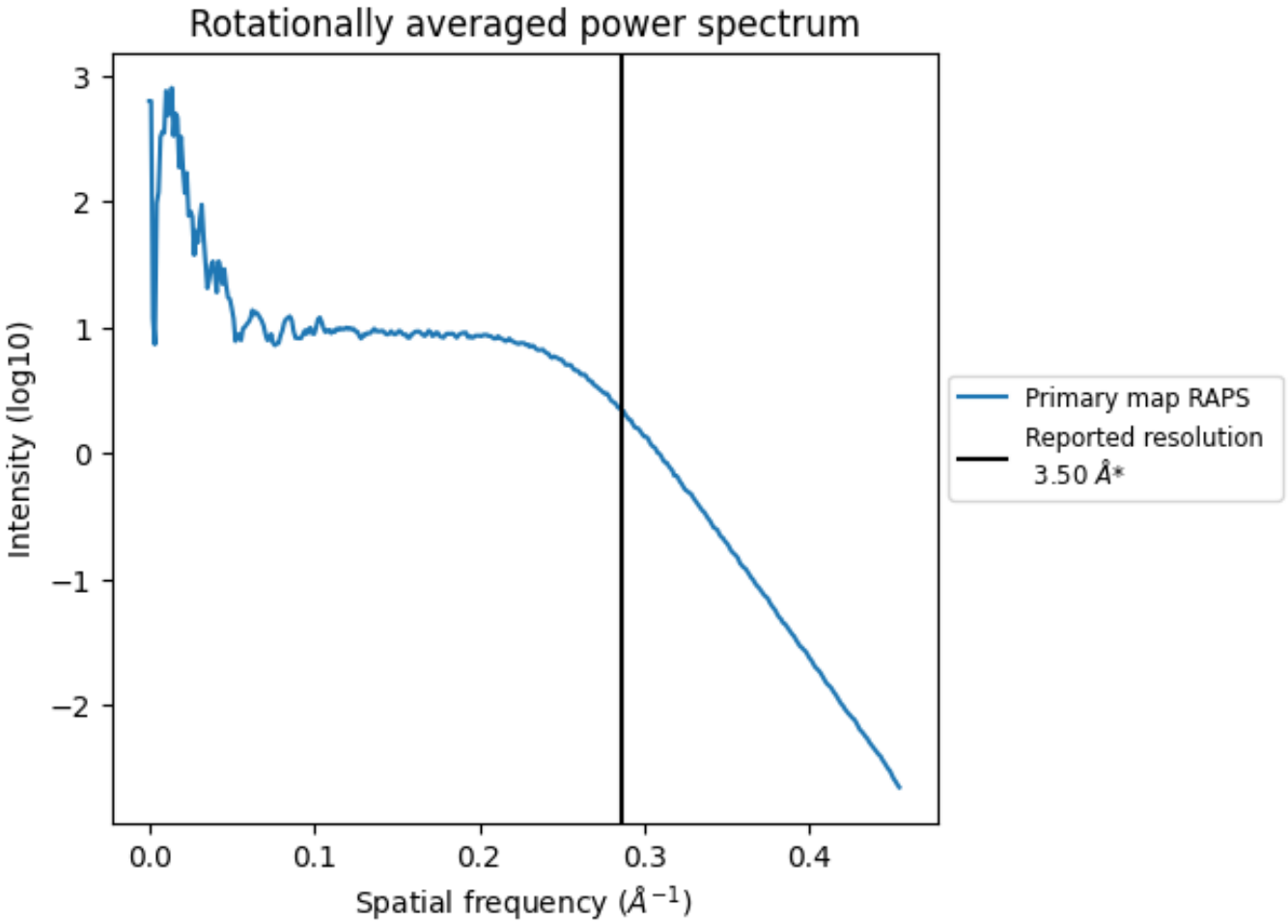
7.2 Volume estimate



The volume at the recommended contour level is 5664 nm^3; this corresponds to an approximate mass of 5116 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 0.286 $Å^{-1}$

8 Fourier-Shell correlation (i)

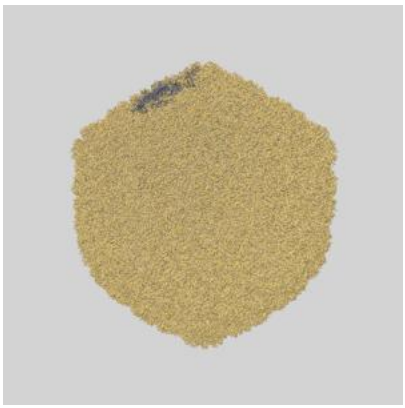
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

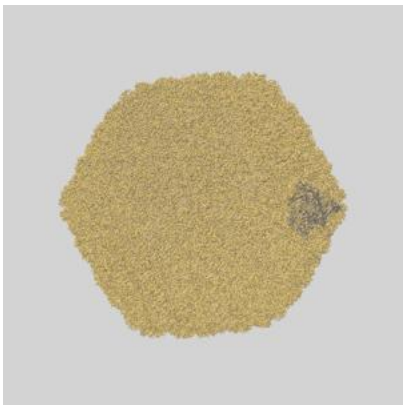
This section contains information regarding the fit between EMDB map EMD-6035 and PDB model 3J7W. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

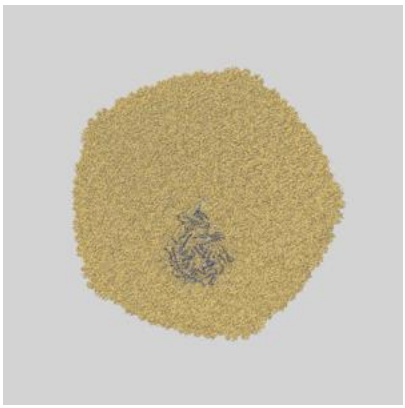
9.1.1 Map-model overlay



X

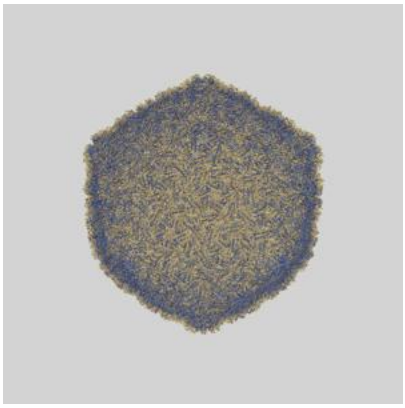


Y

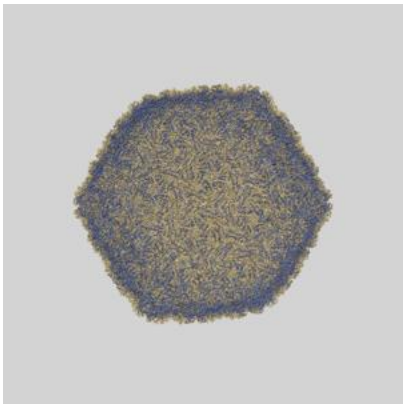


Z

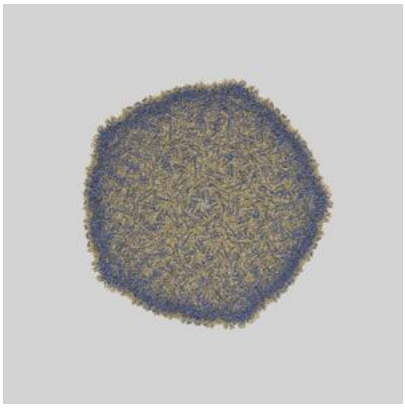
9.1.2 Map-model assembly overlay



X



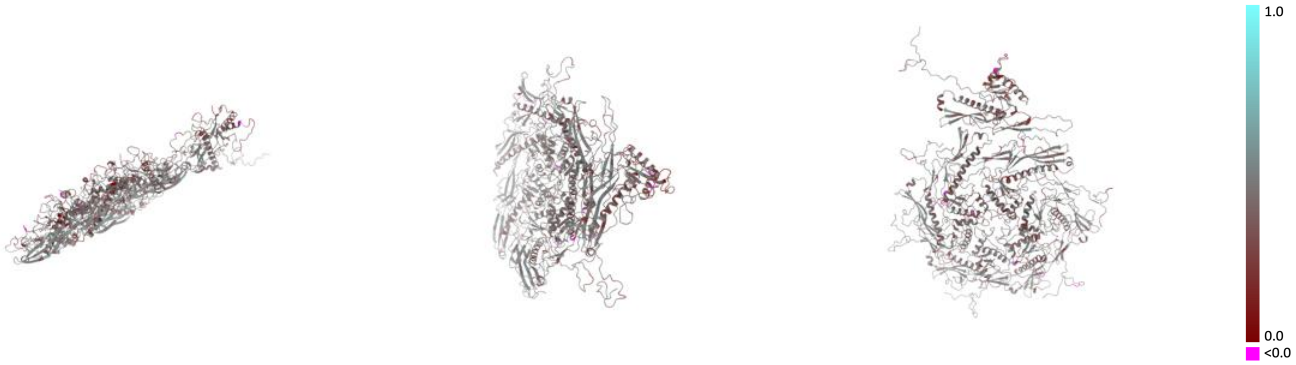
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3 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.

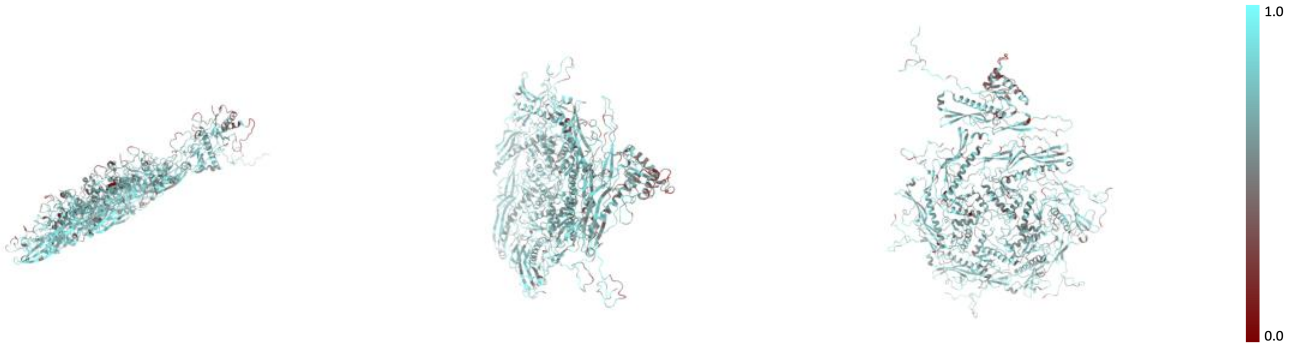
9.2 Q-score mapped to coordinate model (i)



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.

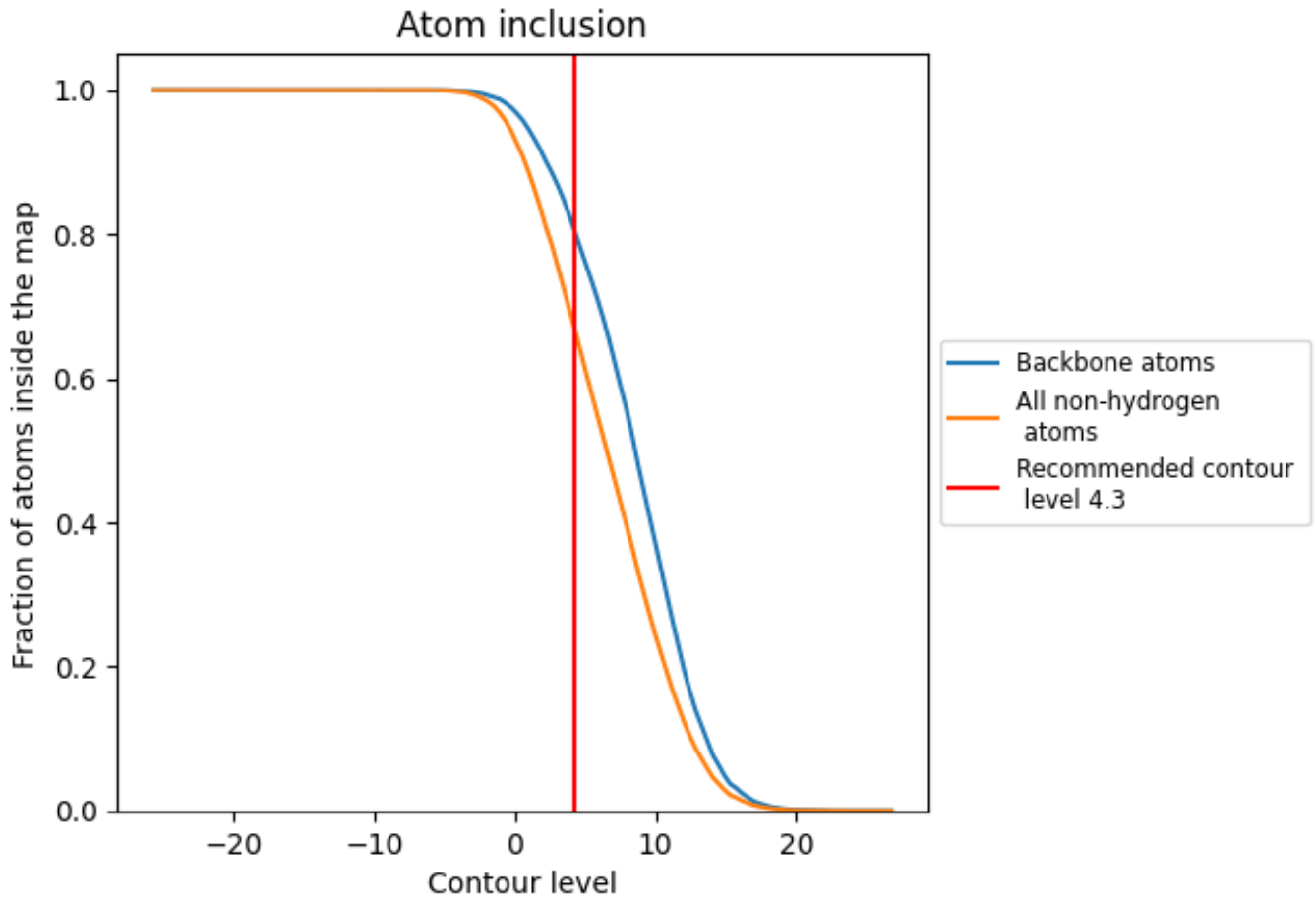
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.3).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6654	0.4180
A	0.6607	0.4210
B	0.6663	0.4170
C	0.6874	0.4180
D	0.6970	0.4320
E	0.6747	0.4300
F	0.6595	0.4100
G	0.6124	0.3990