Full wwPDB EM Validation Report (i)

Nov 12, 2022 – 09:45 AM EST

PDB ID	:	6UVN
EMDB ID	:	EMD-20908
Title	:	CryoEM structure of VcCascasde-TniQ complex
Authors	:	Chang, L.; Li, Z.; Zhang, H.
Deposited on	:	2019-11-03
Resolution	:	3.10 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:

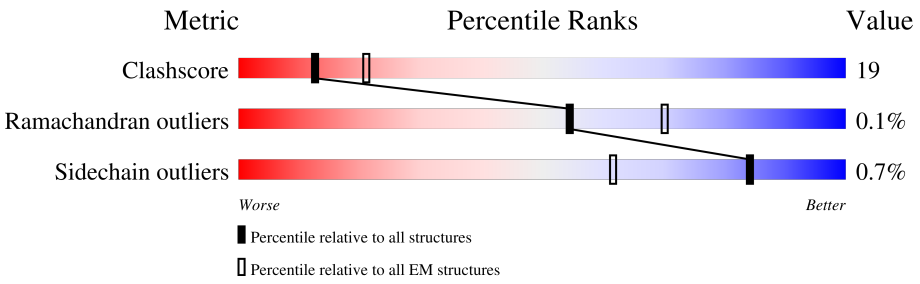
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	217	53% 37% • 9%
2	B	640	• 48% 29% 22%
3	C	355	55% 31% • 13%
3	D	355	55% 40% 5%
3	E	355	• 59% 36% 5%
3	F	355	65% 30% 5%
3	G	355	• 56% 39% • 5%
3	H	355	• 60% 35% 5%

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Mol	Chain	Length	Quality of chain
4	I	394	59% 38%
4	J	394	60% 38%
5	M	61	31% 69%
6	N	98	34% 77% 6% 17%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 29487 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 Cas6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	198	1619	1030	287	295	7	0	0

- Molecule 2 is a protein called Cas8/5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	498	3921	2481	679	743	18	0	0

- Molecule 3 is a protein called Cas7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	337	2695	1717	463	501	14	0	0
3	F	337	2695	1717	463	501	14	0	0
3	E	337	2695	1717	463	501	14	0	0
3	H	337	2695	1717	463	501	14	0	0
3	D	337	2695	1717	463	501	14	0	0
3	C	308	2495	1596	429	457	13	0	0

- Molecule 4 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	383	3124	2004	540	561	19	0	0
4	J	389	3171	2034	548	571	18	0	0

- Molecule 5 is DNA/RNA hybrid called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	M	61	1275	569	223	423	60	0	0

- Molecule 6 is a protein called Cas8_HelicalBundle.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	N	81	405	243	81	81	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

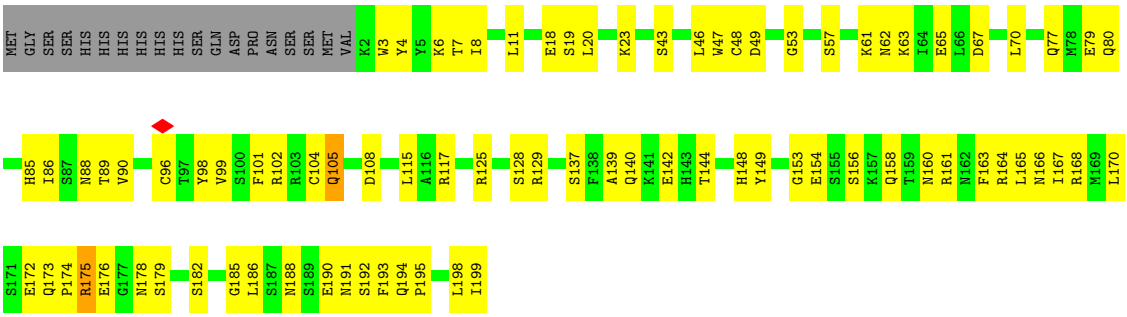
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	I	1	1	1	0
			Total	Zn	
7	J	1	1	1	0

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.

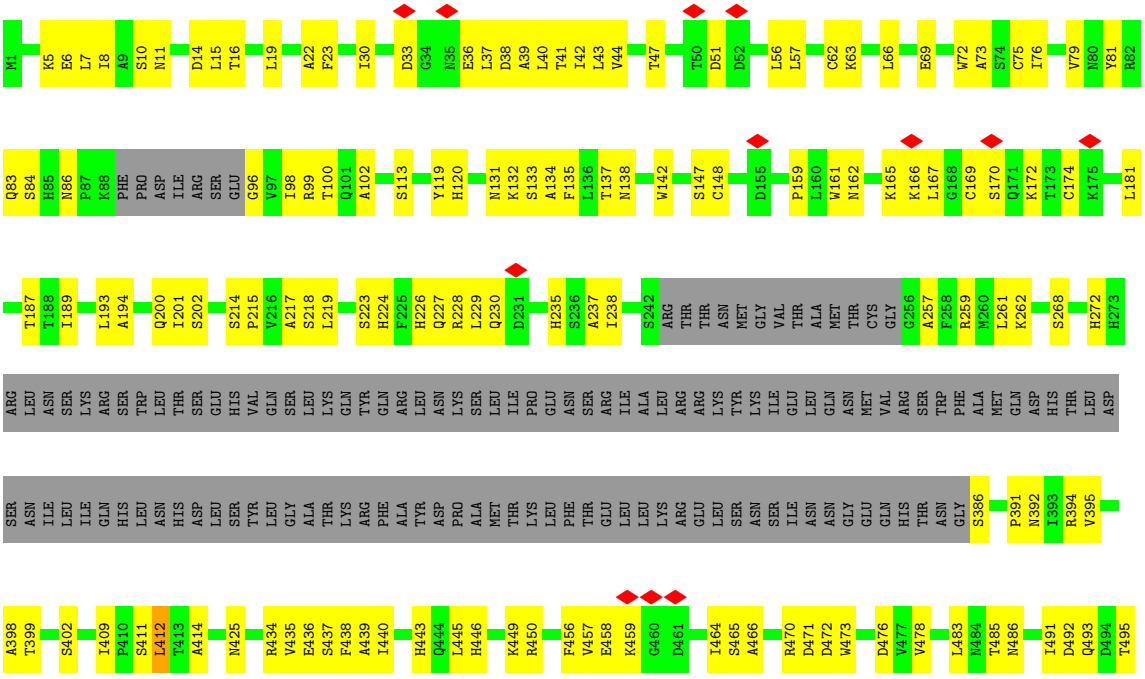
- Molecule 1: Cas6

Chain A: 53% 37% • 9%



- Molecule 2: Cas8/5

Chain B: 48% 29% 22%



L496 V497 T498 S499 R506 K510 F516 K517 H518 I519 N520 S521 T527 E530 I534 E535 W539 L540 S541 L542 L550 L553 L554 M557 T558 E559 Q562 L563 S566 C567 V568 G569 Y570 H571 L572 L573 K579 P580 N581 R584 H588 A591 L597

I598 S604 N610 T611 I612 F613 W614 S615 L616 Y619 L623 Q626 P627 R628 S629 I630 ASN ASP GLU THR THR ASP LYS SER SER LEU

• Molecule 3: Cas7

Chain G: 56% 39% • 5%

MET ALA ASP L4 P7 L10 A11 Y12 E13 R14 S15 I16 D17 D20 F24 V25 D29 D30 R31 L35 T36 Y37 N38 S39 R40 T41 L42 L43 A52 Y53 I60 K61 S62 A63 T64 A65 E66 A69 P73 C79 P82 E89 C90 S91 F92 S93 V94

S97 S98 E99 L100 R101 Q102 P103 Y104 K105 C106 N107 S108 V111 K112 Q113 T114 L115 V116 Q117 L118 Y122 E123 T124 K125 W128 T129 E130 L131 R134 Y135 L136 M137 N138 I139 C140 N141 W146 K147 W155 N156 I157 V158 L159 T160 P161 W162 P163 W164 E167 K168 V169

I174 Y178 F184 I193 M196 I197 A200 F201 S202 F210 A214 T215 L216 H217 L218 A222 M223 V224 R225 P226 S227 Q228 V229 F230 T231 GLU LYS GLU SER GLY SER LYS SER LYS SER LYS THR GLN N245 S246 R247 V248 F249 Q250 I254 P260 K266 A269

T273 I274 D275 D276 W277 Y278 P279 E280 E283 R286 V287 G288 R289 F290 G291 V292 H293 R294 E295 D296 C299 Y300 R301 H302 P303 K307 D308 F309 F310 A316 Y319 I320 L323 N326 K327 T328 P329 A330 Q331 E332 T333 I334 M335 D336 M337 L340 N343 L344 I345

G348 M349 F350 Q351 H352 K353 GLY ASP

• Molecule 3: Cas7

Chain F: 65% 30% 5%

MET ALA ASP L4 P7 T8 N9 L10 A11 Y12 E13 R14 S15 D20 F23 F24 V25 V26 D29 D30 R31 K32 T33 P34 L35 T36 Y37 R40 L43 A52 Y53 Q70 P73 H74 C79 I88 L100 R101 Q102 P103 Y104 K105 C106 N107 V116 E120

L121 Y122 I126 G127 W128 L131 L136 M137 N141 L145 W155 N156 I157 V158 L159 T160 P161 W162 P163 W164 V169 D173 I174 N177 F184 N187 W190 I193 V194 E195 M196 I197 K198 S202 I209 F210 E211 V212 R213 A214 T215 L216 P219

A222 R225 P226 V229 F230 T231 GLU LYS GLU SER GLY SER LYS SER LYS SER LYS THR GLN N245 V248 S259 P260 A269 T273 W277 Y278 P279 R286 R289 F290 G291 V292 H293 R294 E295 D296 V297 R301 H302 P303 S304 K307 D308 S311 N326 K327

T328 E332 T333 I334 M337 N343 L344 I345 G348 M349 F350 K353 GLY ASP

• Molecule 3: Cas7

Chain E: 59% 36% 5%

MET ALA ASP L4 K5 L6 P7 T8 N9 L10 E13 R14 S15 I16 D20 F23 F24 W27 P28 L35 S39 R40 T41 L42 E47 A52 Y53 D54 V55 S56 G57 Q58 T64 A65 E66 A67 L68 P73 H74 Q75 V76 H80 I88 V94 S98 E99

L100 R101 N107 V111 K112 Q113 T114 L115 V116 Q117 L118 V119 E120 L121 K125 W128 T129 T133 L136 M137 N138 I139 C140 N141 G142 K143 W144 R150 K151 W155 N156 I157 V158 L159 T160 P161 W162 P163 W164 N165 G166 V169 D173 I174 R175 T176 R181 F184

K185 W190 S191 A192 I193 V194 E195 M196 I197 K198 T199 A200 F201 S202 A208 I209 F210 E211 V212 R213 A214 T215 L216 N221 P226 V229 F230 T231 GLU LYS GLU SER GLY SER LYS SER LYS SER LYS THR GLN N245 V248 P260 I261 L262 G263 A264 F265 K266 A269

T273 I274 D275 D276 W277 Y278 P279 E280 R286 V287 G288 R289 F290 G291 R294 R301 H302 P303 K307 D308 F309 F310 Q314 H318 Y319 I320 E321 V322 L323 N326 E332 M337 N343 L344 I345 G348 K353 GLY ASP

- Molecule 3: Cas7

Chain H:

MET ALA ASP L4 P7 T8 N9 L10 S15 I16 D17 V21 W27 R31 L35 T36 R40 A49 A52 Y53 D54 V55 S56 P59 I60 A63 L68 I88 F92 S93 V94 S98 E99 L100 R101 K105 V111 K112 Q113 T114 L115 V116 Q117

L118 V119 E120 E123 T124 K125 I126 G127 W128 T133 L136 M137 N138 I139 C140 N141 L145 W146 K147 K151 W155 N156 I157 V158 L159 T160 P161 W162 P163 W164 N165 G166 E167 K168 V169 I174 F184 K188 N189 W190 I193 V194 E195 M196 I197 A200 F201 S202

L207 A208 I209 F210 E211 V212 R213 A214 T215 L216 H217 L218 P219 A222 R225 P226 F230 T231 GLU LYS GLU SER GLY SER LYS SER LYS SER LYS THR GLN N245 T253 E257 P260 T261 L262 K266 A269 A272 T273 I274 D275 D276 W277 Y278 P279 L285 R286 V287

G288 R289 F290 G291 R294 E295 C299 Y300 R301 H302 P303 K307 D308 F309 Q314 Y319 I320 E321 V322 K327 T328 P329 I334 N335 L340 I345 G348 H352 K353 GLY ASP

- Molecule 3: Cas7

Chain D:

MET ALA ASP L4 K5 L6 P7 T8 N9 L10 A11 Y12 E13 R14 S15 I16 D17 D20 F23 F24 V25 V26 W27 P28 D29 D30 R31 L35 T36 Y37 N38 S39 L42 L43 M46 A49 S50 L51 A52 Y53 D54 V55 S56 G57 Q58 P59 I60 A63 E66 P73 H74

Q75 C79 A85 S86 H87 C90 S91 F92 S98 E99 L100 R101 C106 N107 V111 T114 L118 V119 E120 L121 Y122 E123 T124 W128 T129 E130 R134 Y135 L136 N141 G142 K143 W144 L145 W146 R150 K151 A152 W155 N156 I157 V158 L159 T160 P161 W162 P163

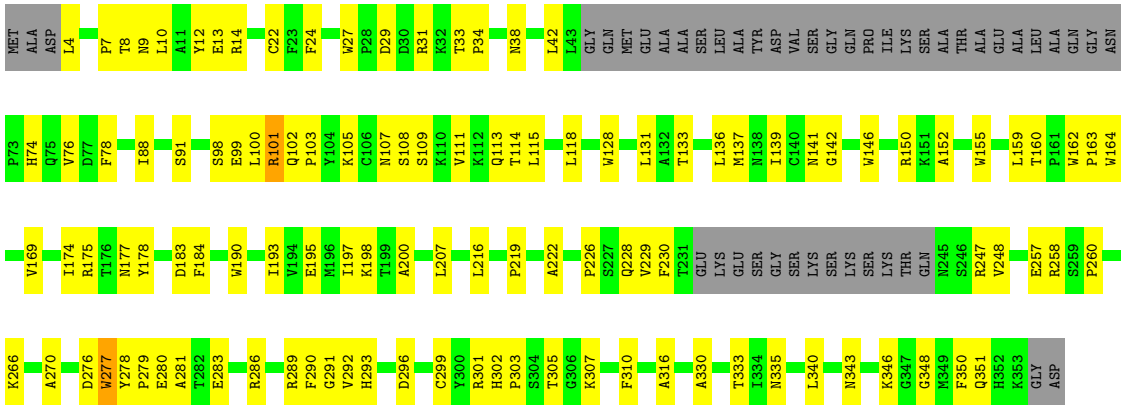
W164 V169 E172 D173 I174 R175 T176 N177 Y178 I193 M196 I197 A200 F201 S202 S203 T204 L207 A208 I209 F210 E211 V212 R213 A214 P219 A222 P226 S227 Q228 V229 F230 T231 GLU LYS GLU SER GLY SER LYS SER LYS SER LYS THR GLN N245 V248 F249 Q250

R258 S259 P260 K266 T267 G268 A269 A272 T273 I274 D275 D276 W277 Y278 P279 R286 V287 G288 R289 F290 G291 V292 H293 R294 E295 D296 V297 T298 C299 Y300 R301 H302 P303 K307 F310 Q314 Q315 A316 Y319 I320 E321 V322 L323 N326 Q331 E332 I333 I334 M337

I345 G348 M349 F350 Q351 H352 K353 GLY ASP

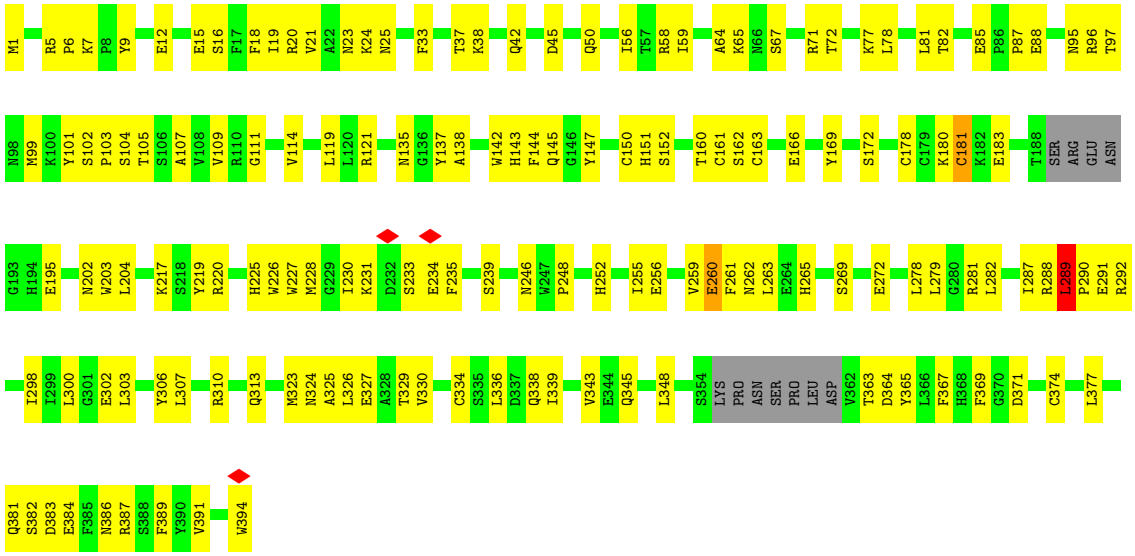
- Molecule 3: Cas7

Chain C:



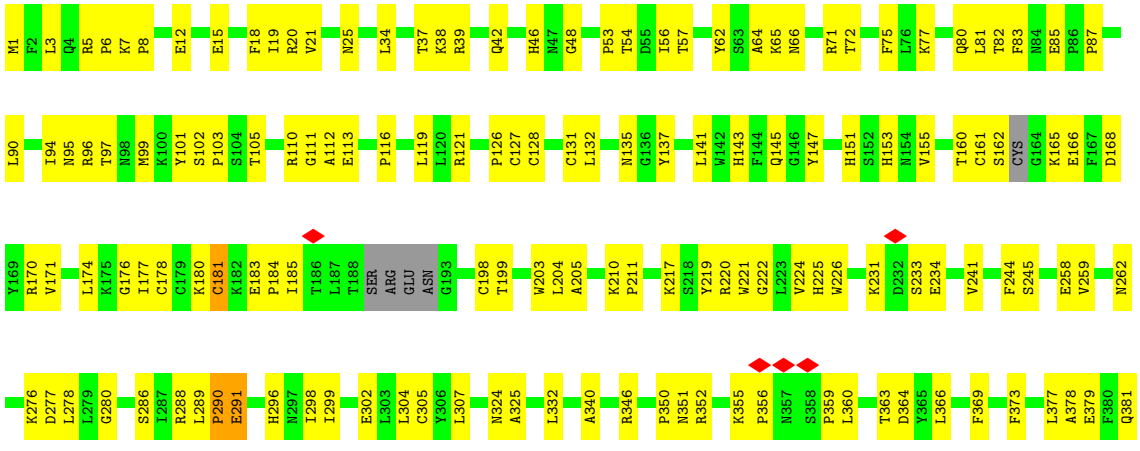
- Molecule 4: TniQ

Chain I:



- Molecule 4: TniQ

Chain J:



N386 R387 S388 F389 Y390 W394

• Molecule 5: crRNA

Chain M: 31% 69%

C1 U2 A3 A4 A8 U9 G18 U21 U22 G23 A24 U25 G26 U27 C28 C29 G30 C31 G32 U33 C34 U35 A36 U39 G40 G41 U42 U43 C44 A45 C46 U47 G48 C49 C50 G51 U52 G53 U54 A55 G56 G57 C58 A59 G60 C61

• Molecule 6: Cas8_HelicalBundle

Chain N: 34% 77% 6% 17%

X275 X284 X285 X286 X304 X305 X306 X307 X308 X309 X312 X313 X314 X321 X322 X323 X324 X325 X326 X333 X334 X343 X346 X355 X356 X357 X358 X359 X360 X361 X362 X363 X364 X365 X366 X367 X368 X369 X370 X371 X372 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

UNK UNK UNK UNK

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	582000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0215	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.48	0/1656	0.51	0/2233
2	B	0.51	0/4007	0.54	0/5438
3	C	0.58	0/2563	0.53	0/3481
3	D	0.54	0/2766	0.51	0/3759
3	E	0.49	0/2766	0.49	0/3759
3	F	0.49	0/2766	0.49	0/3759
3	G	0.48	0/2766	0.49	0/3759
3	H	0.57	0/2766	0.51	0/3759
4	I	0.42	0/3211	0.50	0/4348
4	J	0.41	0/3260	0.51	0/4416
5	M	0.97	0/1423	0.87	0/2217
All	All	0.53	0/29950	0.54	0/40928

There are no bond length outliers.

There are no bond angle outliers.

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	1619	0	1608	69	0
2	B	3921	0	3892	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2495	0	2438	99	0
3	D	2695	0	2630	112	0
3	E	2695	0	2630	97	0
3	F	2695	0	2630	86	0
3	G	2695	0	2630	114	0
3	H	2695	0	2630	97	0
4	I	3124	0	3041	165	0
4	J	3171	0	3089	136	0
5	M	1275	0	643	59	0
6	N	405	0	90	4	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
All	All	29487	0	27951	1079	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 19.

All (1079) 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)
4:I:289:LEU:HB3	4:I:290:PRO:CD	1.55	1.32
4:I:219:TYR:CD2	4:I:290:PRO:HG2	1.69	1.27
4:I:303:LEU:O	4:I:307:LEU:HD23	1.41	1.17
4:J:219:TYR:CE2	4:J:290:PRO:HG2	1.83	1.13
4:J:290:PRO:CD	4:J:291:GLU:H	1.64	1.08
4:I:255:ILE:O	4:I:259:VAL:HG12	1.55	1.04
4:J:290:PRO:HD2	4:J:291:GLU:H	0.88	1.04
4:I:289:LEU:HB3	4:I:290:PRO:HD3	1.05	1.03
4:J:290:PRO:HD2	4:J:291:GLU:N	1.70	1.02
2:B:84:SER:OG	2:B:99:ARG:HA	1.59	1.01
4:I:163:CYS:HB3	4:I:181:CYS:SG	2.02	0.99
2:B:412:LEU:HD23	2:B:614:TRP:CZ3	1.99	0.98
3:C:101:ARG:HH11	3:C:101:ARG:HB3	1.28	0.96
4:I:219:TYR:CG	4:I:290:PRO:HG2	2.01	0.96
4:I:163:CYS:CB	4:I:181:CYS:SG	2.56	0.94
4:I:289:LEU:CB	4:I:290:PRO:CD	2.46	0.94
4:I:289:LEU:CB	4:I:290:PRO:HD3	1.99	0.90
4:I:219:TYR:CE2	4:I:290:PRO:HG2	2.06	0.89
4:J:219:TYR:CD2	4:J:290:PRO:CG	2.58	0.87
1:A:160:ASN:O	1:A:161:ARG:HG2	1.75	0.86
4:I:163:CYS:O	4:I:180:LYS:HG2	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:279:PRO:HD3	3:G:307:LYS:HG3	1.58	0.86
4:I:163:CYS:SG	4:I:183:GLU:OE2	2.33	0.85
4:J:219:TYR:CD2	4:J:290:PRO:HG3	2.13	0.84
4:I:219:TYR:CD2	4:I:290:PRO:CG	2.57	0.83
4:I:143:HIS:HE2	4:I:169:TYR:HH	1.22	0.82
1:A:8:ILE:HD11	1:A:70:LEU:HD11	1.62	0.82
4:J:219:TYR:CE2	4:J:290:PRO:CG	2.64	0.81
3:D:291:GLY:H	3:D:301:ARG:HB2	1.46	0.81
3:D:289:ARG:HH12	3:D:348:GLY:HA3	1.46	0.80
4:I:261:PHE:CD1	4:I:265:HIS:CE1	2.70	0.80
3:G:352:HIS:HE1	3:H:53:TYR:O	1.64	0.80
4:I:99:MET:CE	4:I:290:PRO:O	2.29	0.79
4:I:163:CYS:HB2	4:I:178:CYS:CB	2.12	0.79
2:B:392:ASN:HD21	2:B:534:ILE:HG12	1.48	0.79
3:G:101:ARG:HH11	3:G:202:SER:HA	1.48	0.79
4:J:290:PRO:CD	4:J:291:GLU:N	2.33	0.78
3:F:70:GLN:HE21	3:F:70:GLN:HA	1.46	0.78
3:F:169:VAL:HG21	3:F:193:ILE:HD11	1.64	0.78
3:G:352:HIS:CE1	3:H:53:TYR:O	2.36	0.78
3:C:13:GLU:CD	3:C:99:GLU:OE1	2.23	0.77
1:A:6:LYS:HD2	1:A:70:LEU:HG	1.67	0.77
4:J:219:TYR:CD2	4:J:290:PRO:HG2	2.19	0.77
3:D:266:LYS:NZ	5:M:32:G:N3	2.33	0.77
2:B:412:LEU:CD2	2:B:614:TRP:CZ3	2.70	0.74
3:E:7:PRO:HG3	3:E:111:VAL:HG21	1.68	0.74
4:I:343:VAL:HG12	4:I:348:LEU:HB3	1.70	0.74
3:G:169:VAL:HG21	3:G:193:ILE:HD11	1.69	0.74
3:E:289:ARG:NH2	3:E:343:ASN:OD1	2.20	0.74
3:C:293:HIS:ND1	3:C:296:ASP:OD1	2.21	0.74
4:I:96:ARG:NH1	4:J:379:GLU:OE2	2.21	0.74
3:E:15:SER:HB2	3:E:345:ILE:HG23	1.70	0.74
3:F:159:LEU:HD11	3:F:210:PHE:HB3	1.69	0.73
4:J:340:ALA:HB2	4:J:360:LEU:HD22	1.70	0.73
3:H:291:GLY:H	3:H:301:ARG:HB2	1.50	0.73
3:F:159:LEU:HD13	3:F:212:VAL:HG22	1.70	0.73
3:E:169:VAL:HG11	3:E:193:ILE:HD11	1.70	0.73
3:D:277:TRP:O	3:D:301:ARG:NH2	2.20	0.73
3:D:159:LEU:HD11	3:D:210:PHE:HB3	1.71	0.73
4:I:279:LEU:CD1	4:I:307:LEU:HD11	2.19	0.73
4:J:258:GLU:OE2	4:J:262:ASN:ND2	2.22	0.73
4:I:163:CYS:O	4:I:180:LYS:CG	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:SER:HA	6:N:275:UNK:H2	1.54	0.72
3:G:277:TRP:O	3:G:301:ARG:NH2	2.22	0.72
4:I:99:MET:HE3	4:I:290:PRO:O	1.90	0.72
3:G:69:ALA:HB1	3:F:297:VAL:HG22	1.72	0.71
3:C:101:ARG:HH11	3:C:101:ARG:CB	2.02	0.71
4:J:62:TYR:O	4:J:96:ARG:NH2	2.23	0.71
2:B:19:LEU:HD21	2:B:43:LEU:HD22	1.71	0.71
3:E:159:LEU:HD11	3:E:210:PHE:HB3	1.73	0.71
2:B:412:LEU:CD2	2:B:614:TRP:CH2	2.73	0.71
3:E:141:ASN:HB3	3:E:184:PHE:HZ	1.55	0.71
3:E:277:TRP:O	3:E:301:ARG:NH2	2.23	0.71
3:D:169:VAL:HG21	3:D:193:ILE:HD11	1.72	0.71
3:D:101:ARG:HH11	3:D:202:SER:HA	1.56	0.71
3:G:290:PHE:HE1	3:G:308:ASP:OD2	1.72	0.70
3:G:291:GLY:H	3:G:301:ARG:HB2	1.56	0.70
3:C:118:LEU:HD21	3:C:340:LEU:HD21	1.72	0.70
3:F:307:LYS:NZ	3:F:332:GLU:OE2	2.23	0.70
3:E:291:GLY:H	3:E:301:ARG:HB2	1.55	0.70
1:A:142:GLU:OE2	3:C:258:ARG:NE	2.22	0.70
4:I:21:VAL:O	4:I:25:ASN:ND2	2.24	0.70
3:D:159:LEU:HD13	3:D:212:VAL:HG22	1.73	0.70
3:D:15:SER:HB2	3:D:345:ILE:HG23	1.74	0.70
1:A:190:GLU:OE2	1:A:191:ASN:ND2	2.24	0.70
3:E:121:LEU:HD21	3:E:320:ILE:HG12	1.73	0.70
3:D:23:PHE:HB3	3:D:35:LEU:HD12	1.73	0.70
4:J:101:TYR:HB2	4:J:105:THR:HG23	1.73	0.70
4:J:259:VAL:HG23	4:J:278:LEU:HD11	1.74	0.69
1:A:108:ASP:OD1	1:A:166:ASN:ND2	2.26	0.69
4:I:163:CYS:HB2	4:I:178:CYS:SG	2.32	0.69
3:G:289:ARG:NH2	3:G:343:ASN:OD1	2.24	0.69
4:J:21:VAL:O	4:J:25:ASN:ND2	2.26	0.69
3:F:70:GLN:HA	3:F:70:GLN:NE2	2.07	0.69
2:B:437:SER:HB3	2:B:628:ARG:HH21	1.55	0.69
4:I:217:LYS:HA	4:I:220:ARG:HG3	1.74	0.69
2:B:7:LEU:HD12	2:B:40:LEU:HD13	1.75	0.69
3:D:301:ARG:NH1	3:D:307:LYS:O	2.25	0.69
4:I:261:PHE:CE1	4:I:265:HIS:CD2	2.81	0.69
3:F:15:SER:HB2	3:F:345:ILE:HG23	1.75	0.69
3:C:301:ARG:NH1	3:C:307:LYS:O	2.26	0.69
4:I:261:PHE:CE1	4:I:265:HIS:NE2	2.61	0.69
4:I:289:LEU:HB3	4:I:290:PRO:HD2	1.67	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:125:LYS:HD3	3:E:323:LEU:HD22	1.72	0.69
2:B:391:PRO:CG	2:B:518:HIS:HB2	2.23	0.69
3:G:308:ASP:OD2	3:H:53:TYR:CE2	2.46	0.68
3:G:43:LEU:HD13	3:F:230:PHE:HE2	1.58	0.68
1:A:188:ASN:ND2	1:A:191:ASN:OD1	2.26	0.68
3:G:14:ARG:NE	3:G:17:ASP:OD1	2.21	0.68
3:C:169:VAL:HG11	3:C:193:ILE:HD11	1.73	0.68
2:B:435:VAL:HG22	2:B:485:THR:HG22	1.76	0.68
3:F:52:ALA:HB1	3:E:303:PRO:HG3	1.75	0.68
4:J:226:TRP:HB2	4:J:289:LEU:HD11	1.75	0.68
1:A:175:ARG:NH2	1:A:193:PHE:O	2.27	0.68
3:G:7:PRO:HG3	3:G:111:VAL:HG11	1.76	0.68
4:I:255:ILE:O	4:I:259:VAL:CG1	2.36	0.68
4:I:306:TYR:HD1	4:I:307:LEU:HD22	1.59	0.68
3:G:130:GLU:OE2	3:G:134:ARG:NH1	2.27	0.67
4:J:289:LEU:CB	4:J:290:PRO:HD3	2.24	0.67
3:G:164:TRP:NE1	3:G:167:GLU:O	2.28	0.67
3:E:155:TRP:HB3	3:E:216:LEU:HD13	1.75	0.67
3:G:147:LYS:NZ	3:F:13:GLU:OE1	2.27	0.67
3:F:301:ARG:NH1	3:F:307:LYS:O	2.27	0.67
3:F:225:ARG:NH1	3:E:13:GLU:OE2	2.27	0.67
3:F:289:ARG:NH2	3:F:343:ASN:OD1	2.28	0.67
2:B:425:ASN:HB3	2:B:499:SER:HB2	1.75	0.67
4:J:97:THR:HG22	4:J:99:MET:H	1.60	0.67
3:G:174:ILE:HG23	3:G:178:TYR:HB2	1.77	0.66
3:G:136:LEU:HD13	3:G:197:ILE:HD11	1.77	0.66
4:I:111:GLY:O	4:J:386:ASN:ND2	2.24	0.66
4:I:323:MET:HE1	4:I:369:PHE:HD1	1.60	0.66
4:I:102:SER:CA	4:I:288:ARG:O	2.43	0.66
2:B:39:ALA:HA	2:B:42:ILE:HD12	1.77	0.66
2:B:436:GLU:O	2:B:628:ARG:NH2	2.29	0.66
3:C:152:ALA:O	3:C:175:ARG:NH2	2.28	0.66
3:E:9:ASN:HB2	3:E:107:ASN:HB3	1.78	0.66
4:I:219:TYR:CE2	4:I:290:PRO:CG	2.77	0.66
3:D:12:TYR:CD1	3:D:350:PHE:HE2	2.13	0.66
3:E:101:ARG:HH11	3:E:202:SER:HA	1.59	0.65
5:M:43:U:H2'	5:M:44:C:C5	2.30	0.65
3:G:111:VAL:HA	3:G:114:THR:HG22	1.78	0.65
3:D:146:TRP:CD1	3:D:266:LYS:HE3	2.31	0.65
6:N:355:UNK:O	6:N:358:UNK:N	2.29	0.65
3:F:231:THR:H	5:M:21:U:H5	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:64:THR:HG23	3:E:66:GLU:H	1.61	0.65
4:I:181:CYS:SG	4:I:181:CYS:O	2.54	0.65
3:H:159:LEU:HB3	3:H:169:VAL:HG13	1.79	0.65
3:C:159:LEU:HB3	3:C:169:VAL:HG13	1.78	0.65
2:B:493:GLN:NE2	2:B:516:PHE:O	2.30	0.65
4:I:302:GLU:OE2	4:I:394:TRP:NE1	2.30	0.65
2:B:412:LEU:HD21	2:B:614:TRP:CH2	2.32	0.64
4:J:15:GLU:O	4:J:19:ILE:HG12	1.97	0.64
1:A:153:GLY:HA2	1:A:164:ARG:HG2	1.78	0.64
3:G:141:ASN:HB3	3:G:184:PHE:HZ	1.62	0.64
3:C:305:THR:HG23	3:C:307:LYS:H	1.62	0.64
4:I:163:CYS:HB2	4:I:178:CYS:HB2	1.79	0.64
1:A:101:PHE:HB3	1:A:167:ILE:HD11	1.78	0.64
3:E:94:VAL:HG11	3:E:139:ILE:HD12	1.80	0.64
4:J:34:LEU:CD2	4:J:54:THR:HA	2.28	0.64
4:I:287:ILE:HD13	4:I:330:VAL:HG12	1.80	0.64
3:G:307:LYS:NZ	3:G:332:GLU:OE2	2.31	0.64
2:B:134:ALA:O	2:B:138:ASN:ND2	2.31	0.64
3:C:162:TRP:HZ3	3:C:207:LEU:HD21	1.63	0.64
4:J:147:TYR:OH	4:J:151:HIS:ND1	2.25	0.64
3:G:279:PRO:CD	3:G:307:LYS:HG3	2.27	0.63
3:H:169:VAL:HG11	3:H:193:ILE:HD11	1.80	0.63
4:I:5:ARG:HD3	4:I:87:PRO:HB3	1.79	0.63
2:B:412:LEU:HD23	2:B:614:TRP:CE3	2.33	0.63
3:F:279:PRO:HD3	3:F:307:LYS:HG3	1.81	0.63
3:D:39:SER:HG	3:D:75:GLN:HE21	1.46	0.63
3:D:90:CYS:SG	3:D:214:ALA:HB3	2.39	0.63
3:C:22:CYS:SG	3:C:91:SER:OG	2.57	0.62
2:B:194:ALA:HA	2:B:581:ASN:HD22	1.63	0.62
4:I:147:TYR:OH	4:I:151:HIS:ND1	2.25	0.62
3:C:277:TRP:O	3:C:301:ARG:NH2	2.28	0.62
3:C:291:GLY:H	3:C:301:ARG:HB2	1.64	0.62
3:D:172:GLU:O	3:D:177:ASN:ND2	2.33	0.62
4:I:260:GLU:O	4:I:263:LEU:HG	1.99	0.62
1:A:158:GLN:HB2	5:M:61:C:O5'	1.99	0.62
3:F:161:PRO:HB3	3:F:196:MET:HE1	1.80	0.62
4:I:65:LYS:HD3	4:I:96:ARG:HH21	1.65	0.62
2:B:450:ARG:NH1	2:B:476:ASP:OD2	2.25	0.62
4:I:256:GLU:HA	4:I:259:VAL:CG1	2.30	0.62
4:J:34:LEU:HD23	4:J:34:LEU:C	2.18	0.62
4:J:34:LEU:HD22	4:J:54:THR:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:13:GLU:OE2	3:H:225:ARG:NH1	2.32	0.62
3:E:181:ARG:HG2	3:E:185:LYS:HE3	1.82	0.61
3:E:301:ARG:NH1	3:E:307:LYS:O	2.33	0.61
3:D:66:GLU:OE2	4:J:346:ARG:NH2	2.33	0.61
1:A:129:ARG:NH1	5:M:52:U:O3'	2.33	0.61
2:B:102:ALA:HA	2:B:573:LEU:HD23	1.82	0.61
2:B:579:LYS:HG3	2:B:588:HIS:HB3	1.82	0.61
3:H:277:TRP:O	3:H:301:ARG:NH2	2.33	0.61
4:J:6:PRO:O	4:J:20:ARG:NH2	2.34	0.61
3:C:229:VAL:HG12	3:C:248:VAL:HG13	1.81	0.61
3:G:308:ASP:OD2	3:H:53:TYR:HE2	1.84	0.61
3:D:12:TYR:CD1	3:D:350:PHE:CE2	2.89	0.61
3:D:319:TYR:HA	3:D:322:VAL:HG22	1.83	0.61
3:E:133:THR:HG23	3:E:190:TRP:HZ2	1.65	0.60
3:H:111:VAL:HA	3:H:114:THR:HG22	1.82	0.60
4:I:327:GLU:N	4:I:327:GLU:OE1	2.34	0.60
3:G:137:MET:O	3:G:141:ASN:ND2	2.34	0.60
4:I:261:PHE:CE1	4:I:265:HIS:CE1	2.88	0.60
1:A:11:LEU:HD21	1:A:85:HIS:HB2	1.83	0.60
1:A:77:GLN:OE1	1:A:80:GLN:NE2	2.32	0.60
2:B:470:ARG:NH1	2:B:472:ASP:OD1	2.34	0.60
3:F:293:HIS:ND1	3:F:296:ASP:OD1	2.34	0.60
3:C:10:LEU:H	3:C:351:GLN:HG2	1.66	0.60
4:J:161:CYS:SG	4:J:162:SER:N	2.74	0.60
3:F:155:TRP:HB3	3:F:216:LEU:HD13	1.82	0.60
3:D:293:HIS:ND1	3:D:296:ASP:OD1	2.35	0.60
1:A:149:TYR:OH	5:M:45:A:N1	2.30	0.60
3:C:102:GLN:OE1	3:C:102:GLN:N	2.34	0.60
4:I:102:SER:OG	4:I:103:PRO:HD3	2.00	0.60
4:J:77:LYS:O	4:J:81:LEU:HB2	2.00	0.60
3:F:229:VAL:HG22	3:F:248:VAL:HB	1.83	0.60
2:B:162:ASN:HA	2:B:165:LYS:HG2	1.83	0.60
3:F:277:TRP:O	3:F:301:ARG:NH2	2.25	0.60
2:B:142:TRP:HH2	2:B:159:PRO:HG2	1.67	0.60
3:D:142:GLY:H	3:D:155:TRP:HE1	1.49	0.60
4:I:163:CYS:SG	4:I:183:GLU:CD	2.80	0.60
4:J:34:LEU:HD23	4:J:34:LEU:O	2.02	0.60
3:H:15:SER:HB2	3:H:345:ILE:HG23	1.82	0.60
4:I:64:ALA:O	4:I:96:ARG:NH2	2.32	0.60
4:I:279:LEU:HD11	4:I:307:LEU:HD11	1.83	0.60
3:D:266:LYS:NZ	5:M:32:G:H21	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:178:CYS:HB2	4:J:181:CYS:O	2.02	0.59
2:B:84:SER:O	2:B:219:LEU:HB2	2.03	0.59
2:B:237:ALA:HB1	2:B:473:TRP:CZ2	2.37	0.59
1:A:167:ILE:HD13	1:A:186:LEU:HD13	1.84	0.59
3:F:141:ASN:HB3	3:F:184:PHE:HZ	1.65	0.59
2:B:563:LEU:HD21	2:B:597:LEU:HD13	1.85	0.59
3:F:26:VAL:HG22	3:F:32:LYS:HG2	1.83	0.59
3:H:145:LEU:HD13	3:H:216:LEU:HD22	1.84	0.59
3:F:294:ARG:HH22	5:M:22:U:H5'	1.68	0.59
3:C:155:TRP:HB3	3:C:216:LEU:HD12	1.85	0.59
4:I:163:CYS:HG	4:I:183:GLU:CD	2.05	0.59
3:E:118:LEU:HD12	3:E:121:LEU:HD11	1.84	0.59
3:H:4:LEU:HB3	3:H:314:GLN:HA	1.84	0.59
3:H:279:PRO:HD3	3:H:307:LYS:HG3	1.84	0.59
4:I:143:HIS:NE2	4:I:169:TYR:OH	2.24	0.59
2:B:394:ARG:HG3	2:B:478:VAL:HG22	1.85	0.58
4:I:325:ALA:HB2	4:I:367:PHE:HE2	1.68	0.58
4:J:233:SER:OG	4:J:234:GLU:N	2.36	0.58
2:B:395:VAL:HG11	2:B:398:ALA:HB2	1.85	0.58
3:F:137:MET:O	3:F:141:ASN:ND2	2.37	0.58
3:D:7:PRO:HG2	3:D:10:LEU:HB2	1.85	0.58
3:C:137:MET:O	3:C:141:ASN:ND2	2.35	0.58
4:I:121:ARG:NH2	4:I:144:PHE:O	2.36	0.58
4:J:5:ARG:NH1	4:J:85:GLU:O	2.36	0.58
3:E:118:LEU:HD13	3:E:320:ILE:HG13	1.85	0.58
2:B:7:LEU:HD23	2:B:10:SER:HB3	1.84	0.58
3:H:218:LEU:HB3	3:H:222:ALA:HB3	1.84	0.58
3:C:8:THR:OG1	3:C:107:ASN:ND2	2.36	0.58
4:I:227:TRP:HZ2	4:I:239:SER:HG	1.51	0.58
3:D:98:SER:OG	3:D:204:THR:O	2.21	0.58
4:I:163:CYS:O	4:I:180:LYS:CD	2.52	0.58
3:G:292:VAL:HG12	3:G:299:CYS:HB3	1.84	0.58
4:J:34:LEU:O	4:J:37:THR:HG22	2.03	0.58
4:J:289:LEU:HB3	4:J:290:PRO:HD3	1.84	0.58
3:G:107:ASN:OD1	3:G:108:SER:N	2.37	0.58
3:G:122:TYR:HB2	3:G:337:MET:HE2	1.86	0.58
3:G:301:ARG:NH1	3:G:307:LYS:O	2.36	0.58
4:I:119:LEU:HB2	4:I:145:GLN:HB2	1.85	0.58
3:C:27:TRP:HE1	3:C:33:THR:HG1	1.52	0.58
3:D:229:VAL:HG22	3:D:248:VAL:HB	1.86	0.57
4:J:116:PRO:HG2	4:J:119:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:ASP:OD2	3:C:31:ARG:NH2	2.28	0.57
1:A:48:CYS:SG	1:A:49:ASP:N	2.78	0.57
2:B:457:VAL:HG21	3:H:289:ARG:HD3	1.86	0.57
3:G:52:ALA:HB1	3:F:303:PRO:HG3	1.85	0.57
3:C:150:ARG:NH1	4:I:45:ASP:OD1	2.36	0.57
1:A:46:LEU:HB2	1:A:53:GLY:HA3	1.86	0.57
3:E:161:PRO:HB2	3:E:164:TRP:HB2	1.86	0.57
3:G:289:ARG:HD3	3:G:289:ARG:N	2.19	0.57
4:I:121:ARG:NH2	4:I:142:TRP:O	2.38	0.57
4:J:7:LYS:O	4:J:20:ARG:NH2	2.32	0.57
4:J:128:CYS:HB3	4:J:131:CYS:HB3	1.86	0.57
3:C:101:ARG:HB3	3:C:101:ARG:NH1	2.11	0.57
1:A:175:ARG:NH1	1:A:176:GLU:O	2.38	0.57
2:B:438:PHE:HE2	2:B:440:ILE:HD11	1.68	0.57
2:B:391:PRO:HG2	2:B:518:HIS:HB2	1.86	0.57
2:B:510:LYS:NZ	3:H:17:ASP:O	2.35	0.57
3:C:100:LEU:HD11	3:C:128:TRP:CH2	2.40	0.57
5:M:39:U:O2'	5:M:40:G:H5"	2.05	0.57
3:G:290:PHE:CE1	3:G:308:ASP:OD2	2.55	0.56
4:J:302:GLU:OE2	4:J:394:TRP:NE1	2.38	0.56
2:B:7:LEU:O	2:B:11:ASN:N	2.33	0.56
2:B:224:HIS:HE1	2:B:550:LEU:H	1.52	0.56
3:G:118:LEU:HD13	3:G:320:ILE:HG13	1.87	0.56
3:E:269:ALA:O	3:E:273:THR:HG23	2.06	0.56
3:H:55:VAL:O	3:H:56:SER:OG	2.11	0.56
3:H:226:PRO:HG3	3:H:260:PRO:HB2	1.87	0.56
3:D:29:ASP:OD2	3:D:31:ARG:NH2	2.38	0.56
4:I:6:PRO:O	4:I:20:ARG:NH2	2.37	0.56
4:I:102:SER:HB3	4:I:288:ARG:O	2.06	0.56
4:J:34:LEU:HD11	4:J:53:PRO:O	2.05	0.56
1:A:172:GLU:HG2	1:A:173:GLN:H	1.69	0.56
1:A:140:GLN:OE1	3:C:38:ASN:ND2	2.39	0.56
3:E:54:ASP:OD1	3:E:55:VAL:N	2.39	0.56
3:G:113:GLN:HA	3:G:116:VAL:HG12	1.87	0.56
3:G:118:LEU:HD21	3:G:340:LEU:HD21	1.87	0.56
3:E:141:ASN:HB3	3:E:184:PHE:CZ	2.39	0.56
3:D:275:ASP:HB2	3:D:287:VAL:HG12	1.88	0.56
4:J:296:HIS:O	4:J:298:ILE:N	2.39	0.56
1:A:3:TRP:CZ3	1:A:61:LYS:HG2	2.41	0.56
2:B:22:ALA:HB1	2:B:30:ILE:HG13	1.88	0.56
3:H:319:TYR:HA	3:H:322:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:TRP:O	3:C:164:TRP:N	2.39	0.56
3:E:308:ASP:OD1	3:E:308:ASP:N	2.37	0.56
5:M:22:U:O2'	5:M:23:G:O4'	2.24	0.56
2:B:100:THR:HG22	2:B:187:THR:HG23	1.88	0.55
3:G:161:PRO:HB2	3:G:164:TRP:HB2	1.87	0.55
4:I:374:CYS:HA	4:I:377:LEU:HD12	1.88	0.55
2:B:165:LYS:HA	2:B:169:CYS:SG	2.46	0.55
3:F:291:GLY:H	3:F:301:ARG:HB2	1.71	0.55
3:E:20:ASP:OD1	3:E:264:ALA:N	2.40	0.55
3:D:146:TRP:NE1	3:D:266:LYS:HE3	2.21	0.55
3:D:152:ALA:O	3:D:175:ARG:NH1	2.39	0.55
3:D:295:GLU:O	3:C:105:LYS:HA	2.06	0.55
4:I:256:GLU:O	4:I:260:GLU:HG3	2.06	0.55
4:I:287:ILE:HA	4:I:300:LEU:HD22	1.88	0.55
3:G:7:PRO:HG2	3:G:10:LEU:HB2	1.87	0.55
3:G:25:VAL:HG21	3:G:82:PRO:HD2	1.88	0.55
3:G:228:GLN:HE21	3:G:249:PHE:HE1	1.54	0.55
3:F:73:PRO:O	3:F:74:HIS:ND1	2.40	0.55
4:I:99:MET:HE2	4:I:290:PRO:O	2.06	0.55
4:I:226:TRP:CZ2	4:I:230:ILE:HD11	2.41	0.55
4:J:38:LYS:O	4:J:42:GLN:HG2	2.06	0.55
3:F:327:LYS:NZ	3:F:328:THR:O	2.39	0.55
4:J:324:ASN:HD21	4:J:363:THR:HA	1.71	0.55
3:G:53:TYR:OH	3:F:311:SER:OG	2.25	0.55
3:C:230:PHE:HA	5:M:39:U:C6	2.42	0.55
2:B:7:LEU:HG	2:B:30:ILE:HG21	1.87	0.54
3:C:296:ASP:OD1	3:C:296:ASP:N	2.38	0.54
4:J:351:ASN:ND2	4:J:366:LEU:O	2.40	0.54
3:F:226:PRO:HG3	3:F:260:PRO:HB2	1.88	0.54
4:I:248:PRO:HB3	4:I:394:TRP:CD1	2.42	0.54
4:I:279:LEU:HD13	4:I:307:LEU:HD11	1.89	0.54
3:G:308:ASP:OD2	3:H:53:TYR:OH	2.21	0.54
3:E:7:PRO:HG2	3:E:10:LEU:HB2	1.90	0.54
3:D:161:PRO:HB2	3:D:164:TRP:HB2	1.89	0.54
2:B:133:SER:OG	2:B:137:THR:OG1	2.26	0.54
3:E:159:LEU:HB3	3:E:169:VAL:HG13	1.88	0.54
3:D:26:VAL:O	3:D:86:SER:OG	2.26	0.54
3:C:178:TYR:HB3	3:C:184:PHE:CE1	2.42	0.54
3:F:173:ASP:OD1	3:F:177:ASN:ND2	2.40	0.54
3:C:195:GLU:HA	3:C:198:LYS:HD3	1.87	0.54
4:I:291:GLU:OE2	4:I:292:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:384:GLU:HA	4:I:389:PHE:HE2	1.72	0.54
4:J:12:GLU:OE2	4:J:20:ARG:HD3	2.07	0.54
3:E:159:LEU:HD13	3:E:212:VAL:HG22	1.88	0.54
3:E:275:ASP:HB2	3:E:287:VAL:HG12	1.90	0.54
3:C:276:ASP:O	3:C:281:ALA:CB	2.56	0.54
4:J:19:ILE:HG21	4:J:174:LEU:HG	1.90	0.54
3:G:15:SER:HB2	3:G:97:SER:O	2.07	0.54
3:G:162:TRP:O	3:G:164:TRP:N	2.40	0.54
4:J:307:LEU:HD23	4:J:369:PHE:CZ	2.43	0.54
2:B:36:GLU:HB2	2:B:40:LEU:HG	1.90	0.53
3:G:53:TYR:OH	3:F:308:ASP:OD2	2.20	0.53
1:A:105:GLN:HG2	5:M:58:C:C5	2.42	0.53
3:F:157:ILE:HD13	3:F:214:ALA:HB2	1.89	0.53
3:D:161:PRO:HB3	3:D:196:MET:HE1	1.89	0.53
4:J:289:LEU:CD2	4:J:299:ILE:HD11	2.38	0.53
2:B:161:TRP:O	2:B:165:LYS:HG2	2.09	0.53
3:F:158:VAL:HG11	3:F:213:ARG:HH11	1.74	0.53
3:C:226:PRO:HG3	3:C:260:PRO:HB2	1.91	0.53
4:J:231:LYS:O	4:J:233:SER:N	2.41	0.53
2:B:98:ILE:HD11	2:B:573:LEU:HD13	1.91	0.53
3:F:128:TRP:HZ3	3:F:131:LEU:HD12	1.73	0.53
3:E:302:HIS:CD2	3:E:303:PRO:HD2	2.43	0.53
3:D:146:TRP:CE2	3:D:266:LYS:HE3	2.43	0.53
4:I:102:SER:HA	4:I:288:ARG:O	2.08	0.53
4:J:64:ALA:HB2	4:J:71:ARG:CZ	2.39	0.53
2:B:402:SER:OG	2:B:409:ILE:O	2.26	0.53
2:B:438:PHE:HB3	2:B:483:LEU:HD23	1.90	0.53
3:F:269:ALA:O	3:F:273:THR:HG23	2.08	0.53
3:D:157:ILE:HD13	3:D:214:ALA:HB2	1.91	0.53
2:B:619:TYR:OH	2:B:626:GLN:NE2	2.41	0.53
3:C:14:ARG:HB3	5:M:36:A:H5"	1.90	0.53
4:I:261:PHE:HE1	4:I:265:HIS:NE2	2.07	0.53
2:B:411:SER:O	2:B:414:ALA:HB3	2.09	0.53
3:G:37:TYR:HB3	3:G:79:CYS:HB2	1.91	0.53
3:F:43:LEU:HD13	3:E:230:PHE:CE1	2.43	0.53
3:H:137:MET:O	3:H:141:ASN:ND2	2.42	0.53
3:H:155:TRP:CD1	3:H:174:ILE:HD12	2.44	0.53
3:D:266:LYS:NZ	5:M:32:G:N2	2.57	0.53
3:E:156:ASN:O	3:E:214:ALA:HA	2.08	0.53
4:I:161:CYS:SG	4:I:162:SER:N	2.77	0.53
2:B:214:SER:HB3	2:B:588:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:LYS:NZ	3:H:93:SER:O	2.42	0.53
3:H:289:ARG:HH12	3:H:348:GLY:HA3	1.73	0.53
4:I:102:SER:N	4:I:288:ARG:O	2.41	0.53
2:B:7:LEU:HD11	2:B:23:PHE:HE1	1.74	0.52
4:J:34:LEU:HD21	4:J:53:PRO:O	2.09	0.52
4:J:381:GLN:NE2	4:J:387:ARG:H	2.07	0.52
2:B:69:GLU:HA	2:B:72:TRP:HB2	1.92	0.52
3:E:307:LYS:NZ	3:E:332:GLU:OE2	2.35	0.52
3:H:162:TRP:O	3:H:164:TRP:N	2.42	0.52
3:D:307:LYS:NZ	3:D:332:GLU:OE2	2.38	0.52
3:H:101:ARG:HH11	3:H:202:SER:HA	1.73	0.52
3:H:160:THR:HG22	3:H:168:LYS:HG2	1.90	0.52
3:D:53:TYR:HE2	3:C:310:PHE:HB2	1.74	0.52
1:A:47:TRP:HH2	1:A:167:ILE:HG23	1.74	0.52
3:E:229:VAL:HG22	3:E:248:VAL:HB	1.91	0.52
3:E:318:HIS:O	3:E:322:VAL:HG23	2.10	0.52
3:D:286:ARG:NE	5:M:32:G:OP2	2.30	0.52
4:I:160:THR:HG22	4:I:166:GLU:HA	1.91	0.52
4:I:256:GLU:CA	4:I:259:VAL:HG12	2.40	0.52
2:B:86:ASN:OD1	2:B:217:ALA:HB3	2.10	0.52
3:C:98:SER:HB3	3:C:200:ALA:O	2.08	0.52
4:J:101:TYR:CG	4:J:289:LEU:O	2.62	0.52
1:A:3:TRP:CZ2	1:A:61:LYS:HE3	2.44	0.52
1:A:156:SER:HB3	5:M:60:DG:H2"	1.92	0.52
3:G:269:ALA:O	3:G:273:THR:HG23	2.10	0.52
3:E:165:ASN:OD1	3:E:166:GLY:N	2.43	0.52
3:C:34:PRO:HG2	3:C:257:GLU:OE2	2.10	0.52
2:B:409:ILE:HG22	2:B:445:LEU:HD13	1.92	0.52
3:G:25:VAL:HG23	3:G:35:LEU:HG	1.92	0.52
3:G:155:TRP:CD1	3:G:174:ILE:HD12	2.45	0.52
3:C:266:LYS:NZ	5:M:40:G:OP1	2.38	0.52
4:I:18:PHE:HA	4:I:21:VAL:HG22	1.92	0.52
3:F:195:GLU:HA	3:F:198:LYS:HG2	1.91	0.52
3:D:8:THR:OG1	3:D:107:ASN:ND2	2.43	0.52
3:C:76:VAL:HG23	3:C:78:PHE:HE1	1.75	0.52
4:I:334:CYS:SG	4:I:338:GLN:HB3	2.50	0.52
2:B:399:THR:HG21	2:B:506:ARG:HE	1.74	0.51
3:D:162:TRP:HZ3	3:D:207:LEU:HD21	1.76	0.51
3:C:277:TRP:HB3	3:C:335:ASN:HB3	1.91	0.51
4:I:16:SER:HB2	4:I:138:ALA:HB3	1.91	0.51
2:B:391:PRO:HG3	2:B:518:HIS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:ASP:O	3:C:281:ALA:HB1	2.11	0.51
4:I:33:PHE:O	4:I:37:THR:HG23	2.10	0.51
2:B:38:ASP:OD1	2:B:38:ASP:N	2.40	0.51
2:B:262:LYS:O	2:B:557:MET:HE1	2.11	0.51
3:G:40:ARG:NH1	3:F:20:ASP:OD2	2.38	0.51
4:I:386:ASN:ND2	4:J:111:GLY:O	2.34	0.51
3:D:46:MET:HB3	3:D:51:LEU:HD22	1.92	0.51
3:D:111:VAL:HA	3:D:114:THR:HG22	1.93	0.51
4:I:101:TYR:HB2	4:I:105:THR:HG23	1.93	0.51
4:I:324:ASN:OD1	4:I:325:ALA:N	2.43	0.51
2:B:142:TRP:CH2	2:B:159:PRO:HG2	2.45	0.51
2:B:230:GLN:HG2	2:B:259:ARG:HH12	1.76	0.51
2:B:614:TRP:HA	2:B:627:PRO:HA	1.92	0.51
3:F:289:ARG:NH1	3:F:348:GLY:HA3	2.25	0.51
3:E:173:ASP:OD2	3:E:176:THR:OG1	2.28	0.51
3:H:156:ASN:O	3:H:214:ALA:HA	2.10	0.51
2:B:51:ASP:N	2:B:51:ASP:OD1	2.43	0.51
2:B:76:ILE:O	2:B:79:VAL:HG12	2.11	0.51
3:G:64:THR:HG23	3:G:66:GLU:H	1.76	0.51
3:G:160:THR:O	3:G:160:THR:OG1	2.28	0.51
3:G:283:GLU:OE2	3:G:293:HIS:NE2	2.38	0.51
3:C:290:PHE:O	3:C:292:VAL:HG13	2.10	0.51
4:J:176:GLY:O	4:J:184:PRO:HA	2.11	0.51
2:B:19:LEU:HG	2:B:43:LEU:HD13	1.93	0.51
2:B:44:VAL:HG12	2:B:135:PHE:HA	1.92	0.51
3:G:250:GLN:HE21	3:H:40:ARG:HD3	1.75	0.51
3:F:126:ILE:HG21	3:F:334:ILE:HD11	1.93	0.51
3:D:226:PRO:HG2	3:D:249:PHE:CD1	2.45	0.51
3:D:289:ARG:NH1	3:D:348:GLY:HA3	2.21	0.51
4:I:67:SER:O	4:I:67:SER:OG	2.26	0.51
3:H:159:LEU:HD13	3:H:212:VAL:HG22	1.92	0.50
3:D:266:LYS:NZ	5:M:32:G:C2	2.77	0.50
3:D:266:LYS:HZ1	5:M:32:G:N2	2.08	0.50
3:C:13:GLU:CG	3:C:99:GLU:OE1	2.59	0.50
4:I:150:CYS:SG	4:I:152:SER:OG	2.59	0.50
5:M:34:C:O2'	5:M:35:U:O4'	2.22	0.50
4:J:241:VAL:O	4:J:245:SER:OG	2.27	0.50
3:C:7:PRO:HG2	3:C:10:LEU:HB2	1.93	0.50
4:J:113:GLU:OE2	4:J:221:TRP:NE1	2.42	0.50
3:F:141:ASN:HA	3:F:174:ILE:HD13	1.93	0.50
3:H:219:PRO:HG2	3:H:222:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:277:TRP:HB3	3:H:335:ASN:HB3	1.91	0.50
2:B:226:HIS:HD2	2:B:259:ARG:HB2	1.76	0.50
3:G:156:ASN:O	3:G:214:ALA:HA	2.11	0.50
4:I:6:PRO:HB3	4:I:24:LYS:HD2	1.93	0.50
3:H:275:ASP:HB2	3:H:287:VAL:HG12	1.93	0.50
4:I:18:PHE:HD2	4:I:59:ILE:HD13	1.77	0.50
3:G:290:PHE:CE1	3:G:308:ASP:CG	2.85	0.50
3:F:100:LEU:HD23	3:F:100:LEU:H	1.77	0.50
1:A:63:LYS:HD2	1:A:89:THR:HG21	1.94	0.50
2:B:14:ASP:O	2:B:16:THR:N	2.45	0.50
3:H:114:THR:HG23	3:H:115:LEU:HD12	1.92	0.50
3:D:266:LYS:HZ3	5:M:32:G:H21	1.57	0.50
3:C:137:MET:HG2	3:C:184:PHE:CD2	2.47	0.50
4:I:38:LYS:O	4:I:42:GLN:HG2	2.12	0.50
2:B:443:HIS:CE1	2:B:534:ILE:HB	2.47	0.50
3:F:156:ASN:O	3:F:214:ALA:HA	2.12	0.50
3:F:348:GLY:HA2	5:M:18:G:O4'	2.12	0.50
4:J:12:GLU:HG3	4:J:137:TYR:HB2	1.93	0.50
4:J:57:THR:HA	4:J:170:ARG:HD2	1.94	0.50
3:F:23:PHE:HB3	3:F:35:LEU:HD12	1.94	0.49
3:F:43:LEU:HD13	3:E:230:PHE:HE1	1.77	0.49
3:C:279:PRO:O	3:C:280:GLU:HG3	2.12	0.49
2:B:226:HIS:CD2	2:B:259:ARG:HE	2.30	0.49
2:B:572:LEU:HD23	2:B:591:ALA:HB2	1.93	0.49
3:E:27:TRP:HB3	3:E:28:PRO:HD2	1.93	0.49
3:H:118:LEU:HD13	3:H:320:ILE:HG13	1.93	0.49
3:D:226:PRO:HG3	3:D:260:PRO:HB2	1.93	0.49
2:B:120:HIS:CE1	2:B:227:GLN:HE22	2.30	0.49
3:F:23:PHE:HE2	3:F:226:PRO:HB3	1.77	0.49
3:D:79:CYS:SG	3:D:260:PRO:HG3	2.52	0.49
3:C:42:LEU:HB2	3:C:74:HIS:CE1	2.47	0.49
4:J:119:LEU:HB2	4:J:145:GLN:HB2	1.93	0.49
2:B:131:ASN:OD1	2:B:132:LYS:N	2.45	0.49
3:E:100:LEU:HD23	3:E:100:LEU:H	1.77	0.49
3:E:196:MET:HE2	3:E:208:ALA:HB1	1.94	0.49
3:D:348:GLY:HA2	5:M:30:G:O4'	2.12	0.49
3:C:141:ASN:HB3	3:C:184:PHE:HZ	1.77	0.49
3:C:302:HIS:O	3:C:305:THR:HG22	2.12	0.49
2:B:215:PRO:HB3	2:B:570:TYR:CE1	2.48	0.49
3:D:14:ARG:HD2	3:D:16:ILE:O	2.12	0.49
4:I:281:ARG:HG3	4:I:282:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ASN:ND2	1:A:192:SER:OG	2.45	0.49
3:G:157:ILE:HG12	3:G:174:ILE:HD11	1.95	0.49
3:E:52:ALA:HB1	3:D:303:PRO:HG3	1.93	0.49
3:E:117:GLN:HG2	3:E:121:LEU:HD23	1.94	0.49
3:H:141:ASN:HB3	3:H:184:PHE:HZ	1.78	0.49
3:D:86:SER:HG	3:D:87:HIS:CE1	2.28	0.49
4:I:307:LEU:HD22	4:I:307:LEU:N	2.26	0.49
1:A:144:THR:O	1:A:144:THR:OG1	2.30	0.49
2:B:83:GLN:NE2	2:B:96:GLY:O	2.45	0.49
2:B:491:ILE:HG23	2:B:496:LEU:HD11	1.93	0.49
2:B:584:ARG:HD3	5:M:1:C:N4	2.27	0.49
3:F:230:PHE:HA	5:M:21:U:C5	2.48	0.49
3:E:129:THR:HB	3:E:198:LYS:NZ	2.28	0.49
3:D:27:TRP:HD1	3:D:31:ARG:O	1.95	0.49
3:D:100:LEU:HD11	3:D:128:TRP:CH2	2.48	0.49
4:I:382:SER:OG	4:I:383:ASP:N	2.43	0.49
3:G:128:TRP:HZ3	3:G:131:LEU:HD12	1.77	0.49
3:H:136:LEU:HD13	3:H:197:ILE:HD11	1.94	0.49
3:H:230:PHE:HB2	5:M:9:U:C5	2.48	0.49
4:I:364:ASP:OD1	4:I:364:ASP:N	2.37	0.49
3:H:112:LYS:O	3:H:116:VAL:HG23	2.13	0.49
4:I:7:LYS:HE3	4:I:9:TYR:OH	2.13	0.49
4:I:88:GLU:OE2	4:J:387:ARG:NH1	2.46	0.49
4:J:132:LEU:HD21	4:J:174:LEU:C	2.33	0.49
4:J:356:PRO:O	4:J:359:PRO:HD3	2.12	0.49
3:E:68:LEU:HB2	3:D:299:CYS:SG	2.53	0.48
4:I:307:LEU:N	4:I:307:LEU:CD2	2.76	0.48
4:J:276:LYS:O	4:J:280:GLY:HA3	2.12	0.48
1:A:88:ASN:O	1:A:90:VAL:HG23	2.13	0.48
2:B:412:LEU:HD21	2:B:614:TRP:CZ2	2.47	0.48
3:G:98:SER:HB2	3:G:200:ALA:O	2.13	0.48
3:F:155:TRP:CD1	3:F:174:ILE:HD12	2.47	0.48
3:E:120:GLU:N	3:E:120:GLU:OE1	2.46	0.48
1:A:102:ARG:NE	1:A:170:LEU:HD12	2.28	0.48
1:A:105:GLN:HG2	5:M:58:C:H5	1.77	0.48
3:G:4:LEU:HD13	3:G:316:ALA:HB3	1.95	0.48
3:G:289:ARG:NH1	3:G:348:GLY:HA3	2.27	0.48
3:F:122:TYR:HB2	3:F:337:MET:HE2	1.95	0.48
3:C:219:PRO:HG2	3:C:222:ALA:HB2	1.95	0.48
4:I:12:GLU:OE2	4:I:20:ARG:HD3	2.13	0.48
2:B:5:LYS:NZ	2:B:10:SER:HB2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:OG	2:B:148:CYS:N	2.47	0.48
2:B:193:LEU:CD1	2:B:200:GLN:HE21	2.26	0.48
3:H:309:PHE:CE1	3:H:340:LEU:HD12	2.48	0.48
4:I:16:SER:O	4:I:20:ARG:HG2	2.14	0.48
3:F:53:TYR:OH	3:E:308:ASP:OD2	2.20	0.48
3:C:142:GLY:H	3:C:155:TRP:HE1	1.61	0.48
4:I:256:GLU:HA	4:I:259:VAL:HG12	1.94	0.48
1:A:149:TYR:HE1	3:C:42:LEU:HD11	1.78	0.48
2:B:73:ALA:HA	2:B:76:ILE:HG22	1.96	0.48
4:J:183:GLU:HG3	4:J:184:PRO:O	2.14	0.48
4:J:203:TRP:CE2	4:J:220:ARG:HD3	2.49	0.48
2:B:268:SER:CB	2:B:562:GLN:HE22	2.27	0.48
3:G:303:PRO:HG3	3:H:52:ALA:HB1	1.95	0.48
3:G:303:PRO:HB2	3:H:59:PRO:HB3	1.96	0.48
3:F:230:PHE:HA	5:M:21:U:C6	2.49	0.48
3:D:272:ALA:HB1	3:D:287:VAL:HG22	1.96	0.48
3:D:296:ASP:OD1	3:D:296:ASP:N	2.38	0.48
3:C:7:PRO:HG3	3:C:111:VAL:HG11	1.94	0.48
4:I:15:GLU:HG3	4:I:59:ILE:HD12	1.95	0.48
4:I:386:ASN:ND2	4:J:112:ALA:HA	2.28	0.48
4:J:166:GLU:O	4:J:166:GLU:HG2	2.12	0.48
1:A:102:ARG:CZ	1:A:170:LEU:HD12	2.44	0.48
1:A:163:PHE:HB3	5:M:46:C:N3	2.29	0.48
2:B:456:PHE:CD1	2:B:466:ALA:HB2	2.49	0.48
3:E:155:TRP:CD1	3:E:174:ILE:HD12	2.49	0.48
4:J:386:ASN:OD1	4:J:388:SER:N	2.43	0.48
1:A:173:GLN:O	1:A:175:ARG:N	2.47	0.48
2:B:202:SER:OG	2:B:584:ARG:NH1	2.46	0.48
3:F:37:TYR:HB3	3:F:79:CYS:HB2	1.96	0.48
3:E:42:LEU:O	3:E:73:PRO:HA	2.14	0.48
3:E:88:ILE:HG23	3:E:216:LEU:HB3	1.95	0.48
3:E:231:THR:OG1	5:M:27:U:O4	2.32	0.48
4:I:78:LEU:HD13	4:I:82:THR:HG21	1.95	0.48
4:J:121:ARG:HB2	4:J:143:HIS:O	2.13	0.48
4:J:290:PRO:HD2	4:J:291:GLU:O	2.14	0.48
3:H:169:VAL:HG11	3:H:193:ILE:CD1	2.44	0.48
3:D:100:LEU:HD23	3:D:100:LEU:H	1.78	0.48
3:G:141:ASN:HA	3:G:174:ILE:HG21	1.96	0.47
3:H:7:PRO:HG2	3:H:10:LEU:HB2	1.96	0.47
2:B:540:LEU:O	2:B:614:TRP:NE1	2.47	0.47
3:G:125:LYS:HD3	3:G:329:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:136:LEU:HD13	3:E:197:ILE:HD11	1.96	0.47
4:I:105:THR:HG21	4:I:225:HIS:CE1	2.49	0.47
4:J:96:ARG:NH1	4:J:96:ARG:HB2	2.28	0.47
3:H:120:GLU:O	3:H:124:THR:HG23	2.15	0.47
2:B:566:SER:HB2	2:B:598:ILE:HD12	1.95	0.47
3:E:133:THR:HB	3:E:181:ARG:HH21	1.79	0.47
3:E:279:PRO:O	3:E:280:GLU:HG3	2.14	0.47
3:D:49:ALA:HB2	3:C:310:PHE:CZ	2.48	0.47
3:C:281:ALA:O	4:I:58:ARG:NH2	2.48	0.47
1:A:6:LYS:HZ2	1:A:67:ASP:HA	1.79	0.47
2:B:434:ARG:O	2:B:486:ASN:ND2	2.47	0.47
3:G:89:GLU:OE2	3:G:91:SER:HB2	2.14	0.47
3:D:7:PRO:HG3	3:D:111:VAL:HG21	1.96	0.47
3:C:42:LEU:HB2	3:C:74:HIS:NE2	2.29	0.47
3:C:289:ARG:HH22	3:C:346:LYS:HD3	1.80	0.47
4:J:95:ASN:N	4:J:95:ASN:OD1	2.46	0.47
4:J:217:LYS:HA	4:J:220:ARG:HG3	1.96	0.47
3:G:29:ASP:OD1	3:G:31:ARG:NH2	2.48	0.47
4:J:178:CYS:HB2	4:J:181:CYS:SG	2.54	0.47
4:J:289:LEU:HD22	4:J:299:ILE:HD11	1.97	0.47
3:G:290:PHE:CD1	3:G:303:PRO:HD3	2.50	0.47
3:G:327:LYS:HZ3	3:G:329:PRO:HA	1.78	0.47
3:E:150:ARG:NH1	3:D:99:GLU:OE2	2.44	0.47
3:E:157:ILE:HG12	3:E:174:ILE:HD11	1.96	0.47
3:D:12:TYR:O	5:M:29:C:O2'	2.29	0.47
3:D:54:ASP:HB3	3:D:60:ILE:HD11	1.97	0.47
4:I:65:LYS:HD3	4:I:96:ARG:NH2	2.28	0.47
4:I:326:LEU:O	4:I:329:THR:OG1	2.33	0.47
3:G:17:ASP:HB2	3:H:151:LYS:HE2	1.97	0.47
3:E:53:TYR:HE2	3:D:310:PHE:HB2	1.80	0.47
3:H:302:HIS:CD2	3:H:303:PRO:HD2	2.50	0.47
3:D:331:GLN:HA	3:D:334:ILE:HG22	1.97	0.47
4:I:219:TYR:CE2	4:I:290:PRO:HD2	2.50	0.47
2:B:84:SER:OG	2:B:99:ARG:CA	2.48	0.47
2:B:170:SER:C	2:B:172:LYS:H	2.18	0.47
3:G:94:VAL:HG11	3:G:139:ILE:HD12	1.95	0.47
3:H:141:ASN:HA	3:H:174:ILE:HG21	1.97	0.47
3:C:155:TRP:CH2	3:C:175:ARG:HG3	2.50	0.47
4:I:195:GLU:OE1	4:I:195:GLU:N	2.47	0.47
4:J:277:ASP:OD1	4:J:278:LEU:N	2.44	0.47
2:B:226:HIS:CD2	2:B:259:ARG:HH21	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:223:MET:SD	3:G:223:MET:N	2.88	0.47
3:F:7:PRO:HG2	3:F:10:LEU:HB2	1.97	0.47
3:F:289:ARG:N	3:F:289:ARG:HD3	2.29	0.47
4:I:56:ILE:HG23	4:I:59:ILE:HD11	1.96	0.47
1:A:79:GLU:OE2	1:A:86:ILE:HG12	2.15	0.46
3:G:13:GLU:OE1	3:H:147:LYS:NZ	2.42	0.46
3:G:293:HIS:ND1	3:G:296:ASP:OD1	2.49	0.46
3:G:308:ASP:OD2	3:H:53:TYR:CZ	2.67	0.46
3:E:4:LEU:N	3:E:314:GLN:OE1	2.48	0.46
3:E:161:PRO:HB3	3:E:196:MET:CE	2.45	0.46
3:D:49:ALA:HB3	3:C:351:GLN:O	2.15	0.46
3:C:9:ASN:HB2	3:C:107:ASN:HB3	1.98	0.46
4:I:387:ARG:CZ	4:I:391:VAL:HG11	2.44	0.46
2:B:262:LYS:HB3	2:B:262:LYS:HE2	1.72	0.46
2:B:392:ASN:HD21	2:B:534:ILE:CG1	2.24	0.46
4:I:119:LEU:HD12	4:I:119:LEU:O	2.15	0.46
4:J:46:HIS:CD2	4:J:48:GLY:H	2.34	0.46
2:B:261:LEU:HD11	2:B:553:LEU:HD22	1.96	0.46
3:E:24:PHE:O	3:E:88:ILE:HG13	2.15	0.46
3:H:36:THR:HG22	3:H:257:GLU:OE1	2.15	0.46
3:D:90:CYS:SG	3:D:145:LEU:HD21	2.56	0.46
3:C:279:PRO:C	3:C:280:GLU:HG3	2.35	0.46
4:J:56:ILE:H	4:J:56:ILE:HD12	1.80	0.46
4:J:135:ASN:HB3	4:J:137:TYR:CE2	2.50	0.46
2:B:229:LEU:HD22	2:B:235:HIS:O	2.16	0.46
3:D:118:LEU:HD13	3:D:320:ILE:HG13	1.96	0.46
3:C:10:LEU:HD23	3:C:350:PHE:HB2	1.96	0.46
4:J:5:ARG:HE	4:J:8:PRO:HG3	1.80	0.46
4:J:141:LEU:HD12	4:J:141:LEU:H	1.81	0.46
2:B:215:PRO:HB3	2:B:570:TYR:HE1	1.80	0.46
2:B:237:ALA:HB2	2:B:262:LYS:HD2	1.97	0.46
2:B:399:THR:CG2	2:B:506:ARG:HE	2.27	0.46
3:G:20:ASP:OD2	3:H:40:ARG:NH1	2.48	0.46
3:G:101:ARG:NH1	3:G:123:GLU:OE1	2.34	0.46
3:E:348:GLY:HA2	5:M:24:A:H1'	1.98	0.46
3:H:21:VAL:HB	3:H:262:LEU:HB2	1.97	0.46
3:C:178:TYR:HA	3:C:183:ASP:HB3	1.98	0.46
4:J:1:MET:SD	4:J:1:MET:N	2.83	0.46
4:J:62:TYR:O	4:J:65:LYS:NZ	2.30	0.46
4:J:364:ASP:OD1	4:J:364:ASP:N	2.34	0.46
3:F:101:ARG:NH1	3:F:202:SER:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:191:SER:HA	3:E:194:VAL:HG12	1.97	0.46
3:E:230:PHE:HA	5:M:27:U:C6	2.50	0.46
4:I:151:HIS:HB2	4:I:202:ASN:HA	1.98	0.46
4:I:371:ASP:OD1	4:I:371:ASP:N	2.47	0.46
3:G:289:ARG:CZ	3:G:350:PHE:HE1	2.28	0.46
3:H:126:ILE:HG21	3:H:334:ILE:HD11	1.97	0.46
3:C:109:SER:HB2	3:C:113:GLN:HE22	1.81	0.46
3:C:289:ARG:NH2	3:C:343:ASN:OD1	2.49	0.46
4:I:12:GLU:OE2	4:I:20:ARG:NH1	2.45	0.46
4:I:231:LYS:O	4:I:233:SER:N	2.49	0.46
4:I:233:SER:OG	4:I:234:GLU:N	2.47	0.46
4:J:127:CYS:SG	4:J:128:CYS:N	2.89	0.46
4:J:181:CYS:SG	4:J:183:GLU:HG2	2.56	0.46
5:M:53:G:C6	5:M:55:A:C6	3.02	0.46
6:N:355:UNK:O	6:N:356:UNK:C	2.63	0.46
2:B:7:LEU:HG	2:B:30:ILE:CG2	2.46	0.46
2:B:98:ILE:HG13	2:B:189:ILE:HG12	1.96	0.46
2:B:446:HIS:HB2	3:H:253:THR:HG22	1.96	0.46
3:G:42:LEU:O	3:G:73:PRO:HA	2.16	0.46
3:F:73:PRO:HB3	3:E:230:PHE:CE2	2.51	0.46
4:I:72:THR:HG21	4:J:378:ALA:HB2	1.96	0.46
4:I:163:CYS:O	4:I:180:LYS:HD2	2.16	0.46
4:I:64:ALA:HB2	4:I:71:ARG:NH2	2.31	0.46
4:I:102:SER:CB	4:I:288:ARG:O	2.64	0.46
4:J:72:THR:HG22	4:J:90:LEU:HD11	1.97	0.46
5:M:44:C:H4'	5:M:45:A:OP2	2.15	0.46
3:G:105:LYS:HA	3:H:295:GLU:O	2.16	0.46
3:H:52:ALA:HB2	3:H:68:LEU:HD21	1.97	0.46
4:I:228:MET:HG2	4:I:235:PHE:HB2	1.97	0.46
4:J:3:LEU:HD23	4:J:82:THR:HG22	1.97	0.46
4:J:304:LEU:HD22	4:J:373:PHE:HE1	1.81	0.46
2:B:38:ASP:O	2:B:42:ILE:HG13	2.15	0.45
3:H:278:TYR:CE1	3:H:285:LEU:HD13	2.51	0.45
3:D:4:LEU:N	3:D:314:GLN:OE1	2.50	0.45
3:D:219:PRO:HG2	3:D:222:ALA:HB2	1.98	0.45
4:I:95:ASN:OD1	4:I:95:ASN:N	2.47	0.45
4:I:163:CYS:HB3	4:I:181:CYS:CB	2.46	0.45
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.83	0.45
2:B:75:CYS:SG	2:B:135:PHE:HB3	2.56	0.45
2:B:559:GLU:N	2:B:559:GLU:OE1	2.49	0.45
3:G:309:PHE:CE1	3:G:340:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:60:ILE:HG22	3:H:63:ALA:H	1.81	0.45
3:H:100:LEU:HD11	3:H:128:TRP:CH2	2.50	0.45
5:M:1:C:H3'	5:M:1:C:O2	2.16	0.45
2:B:391:PRO:HG3	2:B:518:HIS:C	2.37	0.45
3:G:319:TYR:O	3:G:323:LEU:HG	2.15	0.45
3:H:100:LEU:H	3:H:100:LEU:HD23	1.79	0.45
3:H:167:GLU:OE2	3:H:188:LYS:NZ	2.46	0.45
3:H:269:ALA:O	3:H:273:THR:HG23	2.16	0.45
3:G:159:LEU:HD11	3:G:210:PHE:HB3	1.96	0.45
3:G:309:PHE:CE1	3:G:343:ASN:HB3	2.52	0.45
3:F:161:PRO:HB2	3:F:164:TRP:HB2	1.99	0.45
3:F:162:TRP:N	3:F:209:ILE:O	2.48	0.45
3:C:160:THR:O	3:C:160:THR:OG1	2.33	0.45
4:J:324:ASN:OD1	4:J:325:ALA:N	2.49	0.45
2:B:238:ILE:HG12	2:B:259:ARG:HG3	1.98	0.45
1:A:96:CYS:O	1:A:98:TYR:N	2.46	0.45
1:A:102:ARG:CZ	1:A:193:PHE:HZ	2.30	0.45
2:B:386:SER:OG	2:B:521:SER:OG	2.34	0.45
3:G:114:THR:O	3:G:320:ILE:HD11	2.17	0.45
3:G:331:GLN:HA	3:G:334:ILE:HG22	1.98	0.45
3:E:142:GLY:H	3:E:155:TRP:HE1	1.65	0.45
4:I:121:ARG:HB2	4:I:143:HIS:O	2.16	0.45
4:J:94:ILE:HG12	4:J:110:ARG:HB2	1.97	0.45
4:J:346:ARG:HD3	4:J:346:ARG:HA	1.85	0.45
2:B:62:CYS:O	2:B:66:LEU:HG	2.17	0.45
2:B:219:LEU:HD23	2:B:219:LEU:HA	1.82	0.45
3:H:98:SER:HB2	3:H:200:ALA:O	2.16	0.45
3:D:296:ASP:O	3:D:298:THR:N	2.49	0.45
4:I:336:LEU:HA	4:I:339:ILE:HG12	1.99	0.45
2:B:458:GLU:OE1	2:B:465:SER:OG	2.25	0.45
3:F:302:HIS:CD2	3:F:303:PRO:HD2	2.52	0.45
3:E:39:SER:OG	3:E:75:GLN:NE2	2.50	0.45
3:D:162:TRP:N	3:D:209:ILE:O	2.44	0.45
2:B:201:ILE:HB	5:M:2:U:H5"	1.99	0.45
3:G:218:LEU:HB3	3:G:222:ALA:HB3	1.98	0.45
3:G:226:PRO:HG3	3:G:260:PRO:HB2	1.99	0.45
3:F:122:TYR:HD2	3:F:337:MET:HG3	1.81	0.45
3:E:114:THR:O	3:E:118:LEU:HB2	2.17	0.45
3:H:7:PRO:HG3	3:H:111:VAL:HG21	1.98	0.45
3:D:12:TYR:HD1	3:D:350:PHE:CE2	2.35	0.45
3:D:92:PHE:CE1	3:D:212:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:136:LEU:HD13	3:D:197:ILE:HD11	1.99	0.45
3:C:162:TRP:HB3	3:C:163:PRO:HD3	1.98	0.45
4:J:153:HIS:HB2	4:J:155:VAL:HG12	1.98	0.45
2:B:76:ILE:HD11	2:B:181:LEU:HG	1.98	0.45
2:B:272:HIS:ND1	2:B:535:GLU:O	2.40	0.45
3:G:229:VAL:HG22	3:G:248:VAL:HB	1.97	0.45
3:F:289:ARG:CZ	3:F:350:PHE:HE1	2.29	0.45
3:D:42:LEU:O	3:D:73:PRO:HA	2.16	0.45
3:D:230:PHE:HA	5:M:33:U:C5	2.52	0.45
4:J:132:LEU:HD11	4:J:174:LEU:HA	1.98	0.45
4:J:203:TRP:CH2	4:J:220:ARG:HB3	2.52	0.45
1:A:43:SER:OG	1:A:57:SER:HB2	2.16	0.44
3:G:92:PHE:HE2	3:G:94:VAL:HB	1.82	0.44
3:G:174:ILE:H	3:G:174:ILE:HG13	1.62	0.44
3:F:34:PRO:HB2	3:F:259:SER:OG	2.16	0.44
3:E:133:THR:HG21	3:E:181:ARG:HE	1.81	0.44
3:C:27:TRP:NE1	3:C:33:THR:OG1	2.35	0.44
4:J:168:ASP:HB3	4:J:171:VAL:HG22	1.99	0.44
3:H:272:ALA:HB1	3:H:287:VAL:HG22	1.99	0.44
4:I:261:PHE:O	4:I:265:HIS:ND1	2.49	0.44
4:J:18:PHE:HA	4:J:21:VAL:HG22	2.00	0.44
4:J:71:ARG:HG2	4:J:75:PHE:CE2	2.52	0.44
1:A:188:ASN:ND2	5:M:59:A:OP1	2.50	0.44
2:B:162:ASN:O	2:B:166:LYS:HG2	2.17	0.44
3:F:289:ARG:HA	3:F:343:ASN:HD21	1.81	0.44
3:D:5:LYS:HD3	3:D:6:LEU:H	1.83	0.44
5:M:28:C:H2'	5:M:29:C:C6	2.52	0.44
5:M:48:G:H2'	5:M:49:C:H6	1.81	0.44
3:G:106:CYS:SG	3:G:112:LYS:HB2	2.58	0.44
3:G:302:HIS:CD2	3:G:303:PRO:HD2	2.53	0.44
3:H:161:PRO:HB3	3:H:196:MET:HE1	2.00	0.44
3:H:329:PRO:HG2	3:H:334:ILE:HD13	1.98	0.44
4:I:169:TYR:HA	4:I:172:SER:HB3	1.98	0.44
4:I:324:ASN:ND2	4:I:363:THR:O	2.50	0.44
4:I:345:GLN:O	4:J:66:ASN:ND2	2.50	0.44
4:J:83:PHE:CD1	4:J:87:PRO:HG3	2.53	0.44
4:J:119:LEU:O	4:J:119:LEU:HD12	2.18	0.44
4:J:286:SER:O	4:J:286:SER:OG	2.35	0.44
2:B:527:THR:HA	2:B:530:GLU:HB3	1.98	0.44
3:E:294:ARG:NH1	5:M:26:G:N3	2.66	0.44
4:I:97:THR:HG22	4:I:107:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:220:ARG:O	4:J:224:VAL:HG23	2.17	0.44
2:B:81:TYR:O	2:B:83:GLN:N	2.50	0.44
2:B:610:ASN:O	2:B:629:SER:N	2.44	0.44
3:H:35:LEU:HG	3:H:88:ILE:HD11	2.00	0.44
3:H:160:THR:OG1	3:H:211:GLU:HB2	2.17	0.44
3:H:190:TRP:O	3:H:194:VAL:HG12	2.18	0.44
3:C:10:LEU:HA	3:C:105:LYS:O	2.18	0.44
4:I:56:ILE:HD12	4:I:56:ILE:H	1.82	0.44
4:I:109:VAL:HA	4:I:114:VAL:HA	1.99	0.44
4:I:269:SER:OG	4:I:272:GLU:OE2	2.25	0.44
4:I:324:ASN:HB3	4:I:327:GLU:OE1	2.18	0.44
3:H:159:LEU:HD11	3:H:210:PHE:HB3	2.00	0.44
3:D:302:HIS:CD2	3:D:303:PRO:HD2	2.53	0.44
4:J:204:LEU:HD23	4:J:204:LEU:HA	1.87	0.44
5:M:41:G:OP1	5:M:42:U:H1'	2.17	0.44
1:A:7:THR:HA	1:A:57:SER:HA	2.00	0.44
3:H:94:VAL:HG11	3:H:139:ILE:HD13	1.99	0.44
3:C:133:THR:HG23	3:C:190:TRP:HZ2	1.83	0.44
4:I:377:LEU:HD22	4:I:387:ARG:HD2	2.00	0.44
4:J:80:GLN:HG3	4:J:81:LEU:HD12	2.00	0.44
4:J:305:CYS:HB2	4:J:390:TYR:CD1	2.53	0.44
1:A:104:CYS:SG	1:A:168:ARG:HD2	2.57	0.43
1:A:154:GLU:HG3	1:A:165:LEU:HG	1.99	0.43
3:C:114:THR:HG23	3:C:115:LEU:HD12	2.00	0.43
4:I:324:ASN:HA	4:I:365:TYR:HA	2.00	0.43
2:B:391:PRO:CD	2:B:519:ILE:HG12	2.49	0.43
3:G:146:TRP:NE1	3:G:266:LYS:HG3	2.32	0.43
3:H:133:THR:HG23	3:H:190:TRP:HZ2	1.82	0.43
3:D:4:LEU:HD13	3:D:316:ALA:HB3	2.00	0.43
3:D:230:PHE:CE2	3:D:231:THR:HG22	2.52	0.43
1:A:115:LEU:HD23	1:A:140:GLN:HG2	2.01	0.43
1:A:149:TYR:CE1	3:C:42:LEU:HD11	2.53	0.43
2:B:37:LEU:O	2:B:41:THR:HG23	2.18	0.43
2:B:449:LYS:NZ	2:B:471:ASP:HB3	2.32	0.43
3:E:128:TRP:HB2	3:E:198:LYS:HB2	2.00	0.43
3:E:151:LYS:HE2	3:D:17:ASP:HB2	1.99	0.43
4:I:20:ARG:HA	4:I:23:ASN:OD1	2.17	0.43
4:I:310:ARG:HA	4:I:313:GLN:HG2	1.99	0.43
4:J:101:TYR:CD2	4:J:289:LEU:O	2.71	0.43
4:J:210:LYS:N	4:J:211:PRO:HD2	2.33	0.43
3:G:15:SER:OG	3:G:345:ILE:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:130:GLU:OE2	3:D:134:ARG:NH1	2.49	0.43
3:C:155:TRP:O	3:C:174:ILE:HG13	2.18	0.43
3:G:307:LYS:HZ3	3:G:336:ASP:CG	2.17	0.43
3:F:12:TYR:CE1	3:F:103:PRO:HB3	2.53	0.43
3:H:294:ARG:NH1	5:M:8:A:O2'	2.51	0.43
4:I:5:ARG:NH1	4:I:85:GLU:O	2.52	0.43
4:J:103:PRO:HD2	4:J:225:HIS:HE1	1.82	0.43
4:J:304:LEU:HD23	4:J:304:LEU:HA	1.72	0.43
6:N:343:UNK:O	6:N:346:UNK:O	2.36	0.43
1:A:117:ARG:NH1	5:M:47:U:OP2	2.39	0.43
2:B:62:CYS:SG	2:B:63:LYS:N	2.92	0.43
3:E:40:ARG:NH1	3:D:20:ASP:OD2	2.48	0.43
4:I:15:GLU:O	4:I:19:ILE:HG12	2.18	0.43
2:B:120:HIS:CG	2:B:223:SER:HG	2.36	0.43
3:E:98:SER:HB3	3:E:200:ALA:O	2.19	0.43
3:E:162:TRP:N	3:E:209:ILE:O	2.51	0.43
3:D:122:TYR:HD1	3:D:337:MET:HG3	1.84	0.43
3:C:348:GLY:HA2	5:M:36:A:O4'	2.19	0.43
1:A:4:TYR:CE2	1:A:63:LYS:HB2	2.53	0.43
1:A:99:VAL:HG22	1:A:198:LEU:HB2	2.00	0.43
2:B:438:PHE:CE2	2:B:440:ILE:HD11	2.52	0.43
2:B:495:THR:O	2:B:499:SER:OG	2.37	0.43
3:H:101:ARG:NH1	3:H:123:GLU:OE2	2.48	0.43
3:H:162:TRP:N	3:H:209:ILE:O	2.51	0.43
3:D:269:ALA:O	3:D:273:THR:HG23	2.19	0.43
4:I:262:ASN:HB2	4:I:278:LEU:HD12	2.00	0.43
4:I:381:GLN:HE21	4:I:386:ASN:CG	2.22	0.43
4:J:288:ARG:O	4:J:288:ARG:HG2	2.19	0.43
2:B:6:GLU:HB2	2:B:8:ILE:HG22	2.00	0.43
2:B:391:PRO:HD3	2:B:519:ILE:HG12	2.01	0.43
2:B:459:LYS:HD3	3:H:352:HIS:CE1	2.54	0.43
3:G:275:ASP:HB2	3:G:287:VAL:HG12	2.01	0.43
3:E:54:ASP:HB3	3:E:58:GLN:HB3	2.01	0.43
3:H:289:ARG:HA	3:H:309:PHE:HB3	1.99	0.43
3:D:322:VAL:HG23	3:D:323:LEU:HD12	2.00	0.43
4:I:104:SER:O	4:I:104:SER:OG	2.32	0.43
1:A:188:ASN:OD1	1:A:188:ASN:N	2.49	0.43
3:G:12:TYR:CE1	3:G:103:PRO:HB3	2.54	0.43
3:E:100:LEU:HD11	3:E:128:TRP:CH2	2.54	0.43
3:E:113:GLN:HA	3:E:116:VAL:HG12	2.01	0.43
3:E:137:MET:O	3:E:141:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:161:PRO:HB2	3:H:164:TRP:HB2	2.00	0.43
4:I:298:ILE:HD11	4:I:394:TRP:CH2	2.53	0.43
1:A:125:ARG:O	1:A:128:SER:OG	2.21	0.42
2:B:228:ARG:HB3	2:B:550:LEU:HD23	2.01	0.42
3:C:330:ALA:HB3	3:C:333:THR:HG22	2.00	0.42
4:I:219:TYR:CD2	4:I:290:PRO:CD	3.01	0.42
3:G:134:ARG:NH2	3:G:276:ASP:OD2	2.52	0.42
3:F:302:HIS:CE1	3:F:304:SER:HG	2.37	0.42
3:F:302:HIS:CG	3:F:303:PRO:HD2	2.54	0.42
3:E:121:LEU:HD13	3:E:323:LEU:HB2	2.00	0.42
3:C:12:TYR:CE1	3:C:103:PRO:HB3	2.54	0.42
4:J:39:ARG:O	4:J:42:GLN:HB2	2.19	0.42
5:M:48:G:H2'	5:M:49:C:C6	2.54	0.42
1:A:172:GLU:HG2	1:A:173:GLN:N	2.33	0.42
2:B:36:GLU:O	2:B:40:LEU:HG	2.19	0.42
2:B:165:LYS:NZ	2:B:174:CYS:HB2	2.34	0.42
3:F:334:ILE:HD12	3:F:334:ILE:HA	1.94	0.42
3:E:144:TRP:O	3:E:262:LEU:HD13	2.19	0.42
3:H:27:TRP:HD1	3:H:31:ARG:O	2.02	0.42
3:D:54:ASP:OD1	3:D:58:GLN:HB3	2.19	0.42
3:C:101:ARG:HH11	3:C:101:ARG:CG	2.32	0.42
3:C:280:GLU:CD	4:I:65:LYS:HB2	2.40	0.42
4:I:256:GLU:C	4:I:259:VAL:HG12	2.39	0.42
4:J:34:LEU:CD2	4:J:34:LEU:C	2.86	0.42
1:A:4:TYR:CZ	1:A:63:LYS:HB2	2.54	0.42
2:B:412:LEU:HB2	2:B:568:VAL:HG22	2.00	0.42
2:B:492:ASP:O	2:B:495:THR:HG22	2.20	0.42
3:G:228:GLN:HG2	3:G:247:ARG:HG3	2.01	0.42
3:D:27:TRP:HB3	3:D:28:PRO:HD2	2.02	0.42
3:C:10:LEU:H	3:C:351:GLN:CG	2.30	0.42
4:I:256:GLU:O	4:I:259:VAL:CG1	2.68	0.42
4:J:102:SER:HB3	4:J:103:PRO:HD3	2.01	0.42
1:A:194:GLN:NE2	1:A:195:PRO:O	2.23	0.42
2:B:412:LEU:HD22	2:B:598:ILE:HD11	2.00	0.42
3:G:73:PRO:HB3	3:F:230:PHE:CZ	2.54	0.42
3:F:187:ASN:HB3	3:F:190:TRP:HB2	2.01	0.42
3:E:42:LEU:HD13	3:E:76:VAL:HG22	2.02	0.42
3:C:4:LEU:HD13	3:C:316:ALA:HB3	2.02	0.42
3:C:289:ARG:NH2	3:C:346:LYS:HD3	2.34	0.42
4:I:135:ASN:HB3	4:I:137:TYR:CE2	2.55	0.42
2:B:539:TRP:HB3	2:B:612:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:290:PHE:O	3:G:292:VAL:HG13	2.19	0.42
3:F:40:ARG:NH1	3:E:20:ASP:OD2	2.52	0.42
3:D:161:PRO:CB	3:D:196:MET:HE1	2.48	0.42
3:D:278:TYR:HB2	3:D:279:PRO:HD2	2.00	0.42
4:J:165:LYS:HG2	4:J:180:LYS:NZ	2.35	0.42
2:B:238:ILE:CG2	2:B:257:ALA:HB1	2.50	0.42
2:B:439:ALA:HB1	2:B:612:ILE:HG22	2.02	0.42
3:D:9:ASN:O	3:D:106:CYS:HA	2.19	0.42
4:I:163:CYS:HG	4:I:183:GLU:HG2	1.85	0.42
3:F:8:THR:O	3:F:353:LYS:NZ	2.46	0.42
3:F:53:TYR:HE2	3:E:310:PHE:HB2	1.85	0.42
3:E:47:GLU:OE2	5:M:30:G:N2	2.52	0.42
3:E:245:ASN:HB2	3:E:248:VAL:HG22	2.02	0.42
3:D:143:LYS:HD2	3:D:143:LYS:HA	1.76	0.42
3:C:283:GLU:HG3	4:I:50:GLN:HB3	2.00	0.42
3:C:302:HIS:CG	3:C:303:PRO:HD2	2.54	0.42
4:I:163:CYS:HG	4:I:183:GLU:CG	2.33	0.42
4:J:131:CYS:HA	4:J:153:HIS:HE1	1.85	0.42
4:J:141:LEU:HD21	4:J:205:ALA:HB2	2.02	0.42
5:M:50:C:H2'	5:M:51:G:O4'	2.19	0.42
1:A:18:GLU:OE1	1:A:18:GLU:N	2.51	0.42
1:A:62:ASN:OD1	1:A:65:GLU:N	2.28	0.42
2:B:47:THR:HG23	2:B:56:LEU:HD21	2.02	0.42
3:F:116:VAL:HG12	3:F:120:GLU:OE2	2.20	0.42
3:H:302:HIS:CG	3:H:303:PRO:HD2	2.54	0.42
4:J:177:ILE:O	4:J:185:ILE:HD11	2.20	0.42
2:B:411:SER:CB	2:B:567:CYS:HB3	2.50	0.42
2:B:542:LEU:HD23	2:B:542:LEU:HA	1.80	0.42
3:G:302:HIS:CG	3:G:303:PRO:HD2	2.54	0.42
3:E:14:ARG:HD2	3:E:16:ILE:O	2.20	0.42
3:E:54:ASP:C	3:D:352:HIS:HE1	2.23	0.42
3:C:131:LEU:HD23	3:C:131:LEU:HA	1.84	0.42
3:C:139:ILE:HD13	3:C:139:ILE:HA	1.91	0.42
1:A:102:ARG:NH1	1:A:193:PHE:HZ	2.18	0.41
1:A:137:SER:O	1:A:139:ALA:N	2.52	0.41
2:B:62:CYS:SG	2:B:167:LEU:HD11	2.60	0.41
3:G:100:LEU:HD23	3:G:100:LEU:H	1.84	0.41
3:F:24:PHE:O	3:F:88:ILE:HG13	2.20	0.41
3:F:219:PRO:HG2	3:F:222:ALA:HB2	2.02	0.41
4:I:77:LYS:O	4:I:81:LEU:HB2	2.20	0.41
4:I:204:LEU:HD23	4:I:204:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:329:THR:HG21	4:I:336:LEU:HD12	2.02	0.41
4:J:160:THR:HG22	4:J:166:GLU:HA	2.02	0.41
1:A:49:ASP:O	1:A:148:HIS:NE2	2.48	0.41
1:A:182:SER:O	1:A:185:GLY:N	2.45	0.41
3:G:278:TYR:CE2	3:G:300:TYR:CD2	3.08	0.41
3:F:128:TRP:HB2	3:F:198:LYS:HB2	2.02	0.41
3:G:60:ILE:HG22	3:G:62:SER:H	1.85	0.41
3:G:155:TRP:HB3	3:G:216:LEU:HD13	2.02	0.41
3:F:8:THR:OG1	3:F:107:ASN:ND2	2.54	0.41
3:F:100:LEU:HD11	3:F:128:TRP:CZ2	2.55	0.41
3:D:55:VAL:O	3:D:56:SER:OG	2.29	0.41
3:C:108:SER:O	3:C:111:VAL:HG12	2.20	0.41
3:C:278:TYR:HB2	3:C:279:PRO:CD	2.51	0.41
4:J:290:PRO:O	4:J:291:GLU:HB2	2.20	0.41
4:J:332:LEU:O	4:J:332:LEU:HD12	2.20	0.41
4:J:377:LEU:HD23	4:J:377:LEU:HA	1.83	0.41
5:M:47:U:H2'	5:M:48:G:O4'	2.20	0.41
3:E:118:LEU:CD1	3:E:337:MET:HE3	2.50	0.41
3:H:159:LEU:CD1	3:H:212:VAL:HG22	2.49	0.41
1:A:98:TYR:CD2	1:A:174:PRO:HB3	2.55	0.41
1:A:102:ARG:HH11	1:A:170:LEU:HB2	1.85	0.41
3:H:230:PHE:CD1	5:M:9:U:H5	2.39	0.41
3:D:228:GLN:N	3:D:228:GLN:OE1	2.53	0.41
4:I:6:PRO:HD3	4:I:21:VAL:HG12	2.02	0.41
4:J:289:LEU:HD12	4:J:289:LEU:HA	1.86	0.41
4:J:324:ASN:ND2	4:J:363:THR:HA	2.36	0.41
4:J:355:LYS:H	4:J:355:LYS:HG2	1.54	0.41
3:G:327:LYS:NZ	3:G:329:PRO:HA	2.35	0.41
3:E:14:ARG:HB3	5:M:24:A:H5'	2.01	0.41
3:E:80:HIS:CD2	3:E:221:ASN:HD22	2.39	0.41
3:E:226:PRO:HG3	3:E:260:PRO:HB2	2.03	0.41
3:H:9:ASN:HD22	3:H:105:LYS:HE2	1.84	0.41
3:D:37:TYR:CZ	3:D:258:ARG:HD2	2.56	0.41
3:C:228:GLN:HE21	3:C:247:ARG:HG3	1.84	0.41
3:C:292:VAL:HG12	3:C:299:CYS:HB2	2.01	0.41
4:I:219:TYR:HA	4:I:290:PRO:HG3	2.03	0.41
4:J:53:PRO:HG3	4:J:71:ARG:CZ	2.51	0.41
4:J:211:PRO:O	4:J:244:PHE:HB3	2.20	0.41
5:M:55:A:H2'	5:M:56:G:O4'	2.19	0.41
1:A:160:ASN:C	1:A:161:ARG:HG2	2.37	0.41
1:A:199:ILE:H	1:A:199:ILE:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LEU:HD23	2:B:57:LEU:HA	1.86	0.41
3:H:9:ASN:ND2	3:H:105:LYS:HE2	2.36	0.41
3:H:165:ASN:OD1	3:H:166:GLY:N	2.54	0.41
3:D:150:ARG:HG2	3:C:99:GLU:OE2	2.21	0.41
4:I:302:GLU:CD	4:I:394:TRP:HE1	2.24	0.41
1:A:19:SER:O	1:A:23:LYS:HG3	2.21	0.41
3:E:231:THR:H	5:M:27:U:H5	1.67	0.41
3:H:285:LEU:HD21	3:H:300:TYR:HD2	1.86	0.41
3:H:327:LYS:HD3	3:H:328:THR:O	2.21	0.41
4:I:203:TRP:CE2	4:I:220:ARG:HD3	2.56	0.41
4:J:77:LYS:HA	4:J:77:LYS:HD2	1.78	0.41
2:B:40:LEU:O	2:B:44:VAL:HG23	2.21	0.41
2:B:119:TYR:O	2:B:120:HIS:HB2	2.20	0.41
2:B:554:LEU:HD23	2:B:554:LEU:HA	1.80	0.41
3:G:310:PHE:CZ	3:H:49:ALA:HB2	2.55	0.41
3:F:145:LEU:HD13	3:F:216:LEU:HD22	2.03	0.41
3:E:23:PHE:HB3	3:E:35:LEU:HD12	2.03	0.41
3:H:105:LYS:HD2	5:M:4:A:H2	1.86	0.41
3:D:43:LEU:HD13	3:C:230:PHE:CE2	2.56	0.41
3:D:120:GLU:O	3:D:124:THR:HG23	2.20	0.41
3:D:141:ASN:HA	3:D:174:ILE:HD13	2.03	0.41
3:C:136:LEU:HD13	3:C:197:ILE:HD11	2.03	0.41
3:C:289:ARG:NH1	3:C:348:GLY:HA3	2.36	0.41
4:I:252:HIS:ND1	4:I:306:TYR:HD2	2.18	0.41
4:J:198:CYS:SG	4:J:199:THR:N	2.94	0.41
4:J:350:PRO:O	4:J:352:ARG:N	2.54	0.41
5:M:1:C:O2	5:M:1:C:C3'	2.69	0.41
2:B:217:ALA:HB2	5:M:3:A:H61	1.86	0.41
2:B:411:SER:HB3	2:B:567:CYS:HB3	2.02	0.41
3:D:60:ILE:HG22	3:D:63:ALA:H	1.85	0.41
3:D:122:TYR:CD1	3:D:337:MET:HG3	2.56	0.41
3:D:144:TRP:HB2	3:D:267:THR:HG23	2.03	0.41
3:C:278:TYR:CZ	3:C:281:ALA:HA	2.56	0.41
4:I:219:TYR:CZ	4:I:290:PRO:HB2	2.56	0.41
4:I:339:ILE:O	4:I:343:VAL:HG13	2.22	0.41
3:G:37:TYR:O	3:G:38:ASN:ND2	2.53	0.40
3:G:125:LYS:HD2	3:G:323:LEU:HB2	2.02	0.40
3:F:136:LEU:HD13	3:F:197:ILE:HD11	2.02	0.40
3:H:146:TRP:NE1	3:H:266:LYS:HG3	2.36	0.40
4:I:246:ASN:OD1	4:I:246:ASN:N	2.50	0.40
4:J:170:ARG:HE	4:J:170:ARG:HB2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:46:C:H2'	5:M:47:U:H6	1.86	0.40
3:F:141:ASN:HB3	3:F:184:PHE:CZ	2.50	0.40
3:D:25:VAL:HG13	3:D:85:ALA:HB1	2.03	0.40
3:D:229:VAL:HG12	3:D:250:GLN:HG2	2.01	0.40
2:B:498:THR:HG23	3:H:207:LEU:HD22	2.03	0.40
2:B:616:LEU:HD21	2:B:623:LEU:HD11	2.03	0.40
3:G:161:PRO:HB3	3:G:196:MET:HE1	2.02	0.40
3:G:295:GLU:O	3:F:105:LYS:HA	2.21	0.40
3:D:290:PHE:CD1	3:D:303:PRO:HD3	2.57	0.40
3:D:292:VAL:HG22	3:D:299:CYS:HB3	2.04	0.40
3:C:24:PHE:O	3:C:88:ILE:HG13	2.21	0.40
4:I:289:LEU:HA	4:I:289:LEU:HD12	1.80	0.40
2:B:113:SER:HB3	2:B:218:SER:OG	2.21	0.40
2:B:193:LEU:HD12	2:B:200:GLN:HE21	1.85	0.40
2:B:391:PRO:CG	2:B:518:HIS:CB	2.95	0.40
2:B:464:ILE:HD11	3:H:299:CYS:SG	2.61	0.40
3:G:24:PHE:CZ	3:G:254:ILE:HD13	2.56	0.40
3:F:29:ASP:OD1	3:F:31:ARG:HG2	2.22	0.40
3:H:55:VAL:O	3:H:56:SER:CB	2.69	0.40
3:D:98:SER:HB3	3:D:200:ALA:O	2.21	0.40
3:D:174:ILE:HG23	3:D:178:TYR:HB2	2.04	0.40
3:C:146:TRP:CE2	3:C:270:ALA:HB2	2.56	0.40
3:C:177:ASN:HB2	3:C:178:TYR:CD2	2.57	0.40
4:I:163:CYS:O	4:I:180:LYS:NZ	2.45	0.40
4:I:227:TRP:CE3	4:I:227:TRP:HA	2.56	0.40
4:J:121:ARG:HD3	4:J:126:PRO:HD3	2.04	0.40
1:A:61:LYS:HG3	1:A:179:SER:OG	2.21	0.40
1:A:98:TYR:CE2	1:A:174:PRO:HB3	2.56	0.40
2:B:563:LEU:HG	2:B:597:LEU:HD22	2.04	0.40
3:E:266:LYS:NZ	5:M:26:G:N3	2.46	0.40
3:H:157:ILE:HD13	3:H:214:ALA:HB2	2.04	0.40
4:J:101:TYR:CE2	4:J:222:GLY:HA2	2.56	0.40
4:J:102:SER:CB	4:J:103:PRO:HD3	2.51	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	196/217 (90%)	178 (91%)	18 (9%)	0	100	100
2	B	490/640 (77%)	436 (89%)	52 (11%)	2 (0%)	34	69
3	C	302/355 (85%)	285 (94%)	17 (6%)	0	100	100
3	D	333/355 (94%)	309 (93%)	24 (7%)	0	100	100
3	E	333/355 (94%)	311 (93%)	22 (7%)	0	100	100
3	F	333/355 (94%)	311 (93%)	22 (7%)	0	100	100
3	G	333/355 (94%)	316 (95%)	17 (5%)	0	100	100
3	H	333/355 (94%)	310 (93%)	23 (7%)	0	100	100
4	I	377/394 (96%)	336 (89%)	40 (11%)	1 (0%)	41	73
4	J	383/394 (97%)	340 (89%)	41 (11%)	2 (0%)	29	64
All	All	3413/3775 (90%)	3132 (92%)	276 (8%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	289	LEU
4	J	290	PRO
2	B	15	LEU
4	J	291	GLU
2	B	33	ASP

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	180/198 (91%)	178 (99%)	2 (1%)	73	89
2	B	442/573 (77%)	441 (100%)	1 (0%)	93	97
3	C	276/310 (89%)	273 (99%)	3 (1%)	73	89
3	D	295/310 (95%)	294 (100%)	1 (0%)	92	96
3	E	295/310 (95%)	292 (99%)	3 (1%)	76	90
3	F	295/310 (95%)	294 (100%)	1 (0%)	92	96
3	G	295/310 (95%)	291 (99%)	4 (1%)	67	86
3	H	295/310 (95%)	293 (99%)	2 (1%)	84	93
4	I	345/356 (97%)	341 (99%)	4 (1%)	71	88
4	J	351/356 (99%)	350 (100%)	1 (0%)	92	96
All	All	3069/3343 (92%)	3047 (99%)	22 (1%)	84	93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	175	ARG
2	B	412	LEU
3	G	225	ARG
3	G	277	TRP
3	G	286	ARG
3	G	327	LYS
3	F	286	ARG
3	E	5	LYS
3	E	286	ARG
3	E	290	PHE
3	H	92	PHE
3	H	286	ARG
3	D	286	ARG
3	C	101	ARG
3	C	277	TRP
3	C	286	ARG
4	I	1	MET
4	I	181	CYS
4	I	260	GLU
4	I	289	LEU
4	J	181	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	A	160	ASN
1	A	178	ASN
2	B	224	HIS
2	B	227	GLN
2	B	392	ASN
2	B	420	HIS
2	B	446	HIS
2	B	486	ASN
2	B	493	GLN
2	B	562	GLN
2	B	621	ASN
2	B	626	GLN
3	G	38	ASN
3	G	221	ASN
3	G	250	GLN
3	G	318	HIS
3	G	331	GLN
3	G	335	ASN
3	G	338	HIS
3	G	352	HIS
3	F	70	GLN
3	F	141	ASN
3	F	182	GLN
3	F	245	ASN
3	F	335	ASN
3	F	338	HIS
3	E	75	GLN
3	E	182	GLN
3	E	221	ASN
3	E	335	ASN
3	E	352	HIS
3	H	74	HIS
3	H	80	HIS
3	H	331	GLN
3	H	335	ASN
3	H	338	HIS
3	H	343	ASN
3	D	80	HIS
3	D	107	ASN
3	D	182	GLN
3	D	217	HIS
3	D	221	ASN

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Mol	Chain	Res	Type
3	D	335	ASN
3	D	338	HIS
3	D	352	HIS
3	C	38	ASN
3	C	113	GLN
3	C	314	GLN
3	C	318	HIS
3	C	331	GLN
3	C	335	ASN
3	C	338	HIS
3	C	352	HIS
4	I	46	HIS
4	I	66	ASN
4	I	135	ASN
4	I	225	HIS
4	I	262	ASN
4	I	381	GLN
4	J	46	HIS
4	J	47	ASN
4	J	80	GLN
4	J	207	HIS
4	J	381	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	N	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	300:UNK	C	304:UNK	N	13.31
1	N	346:UNK	C	355:UNK	N	11.87
1	N	326:UNK	C	333:UNK	N	7.08

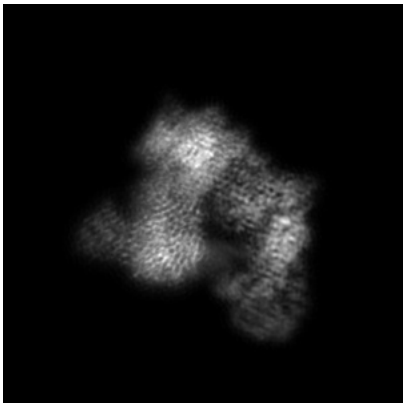
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20908. These allow visual inspection of the internal detail of the map and identification of artifacts.

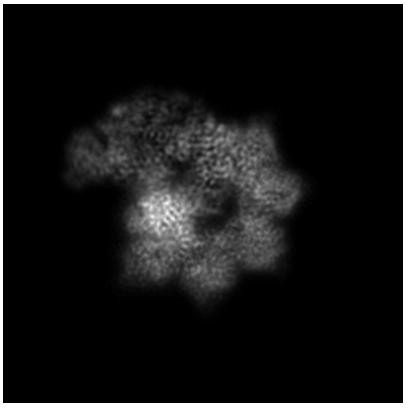
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

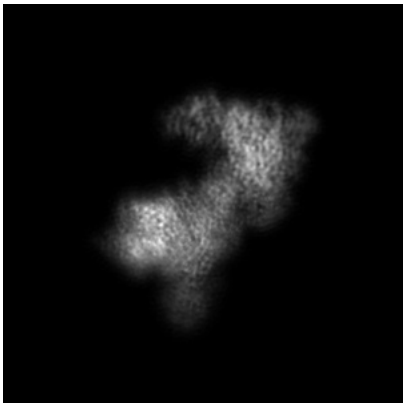
6.1.1 Primary map



X



Y

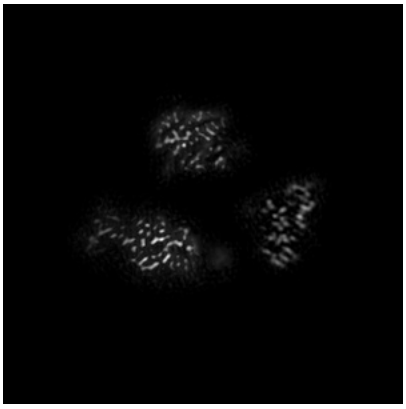


Z

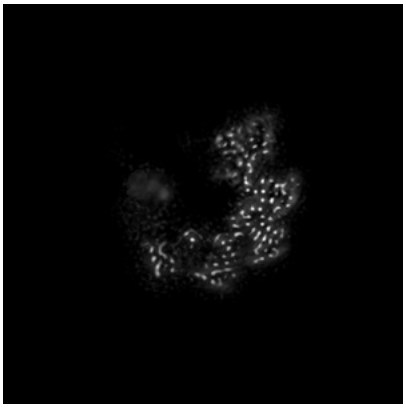
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

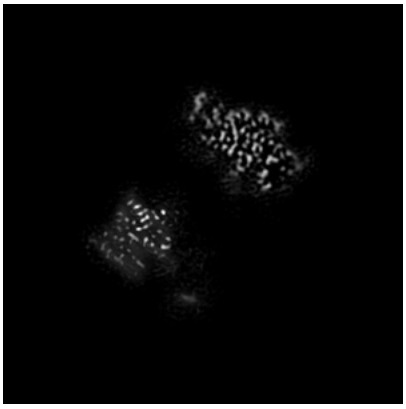
6.2.1 Primary map



X Index: 128



Y Index: 128

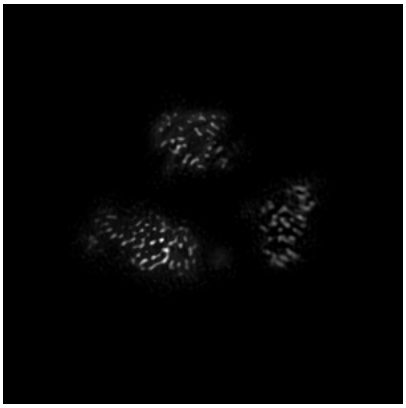


Z Index: 128

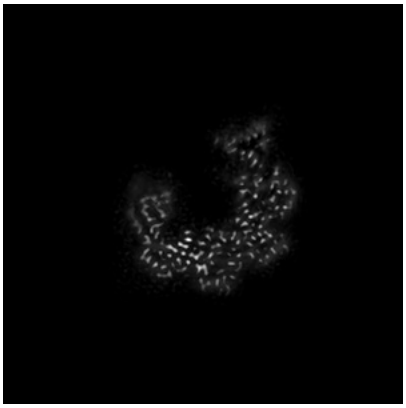
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

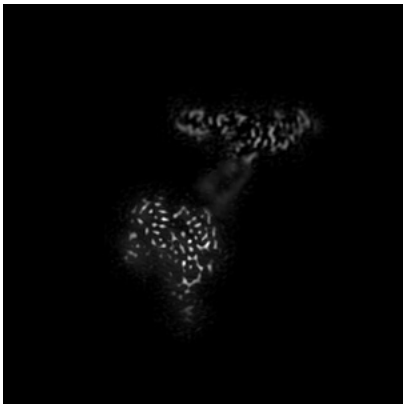
6.3.1 Primary map



X Index: 127



Y Index: 121

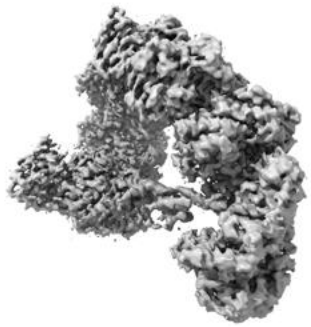


Z Index: 95

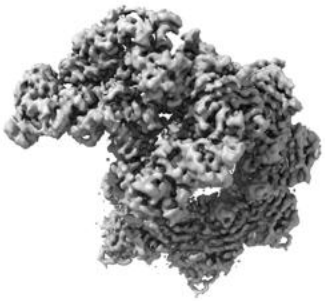
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

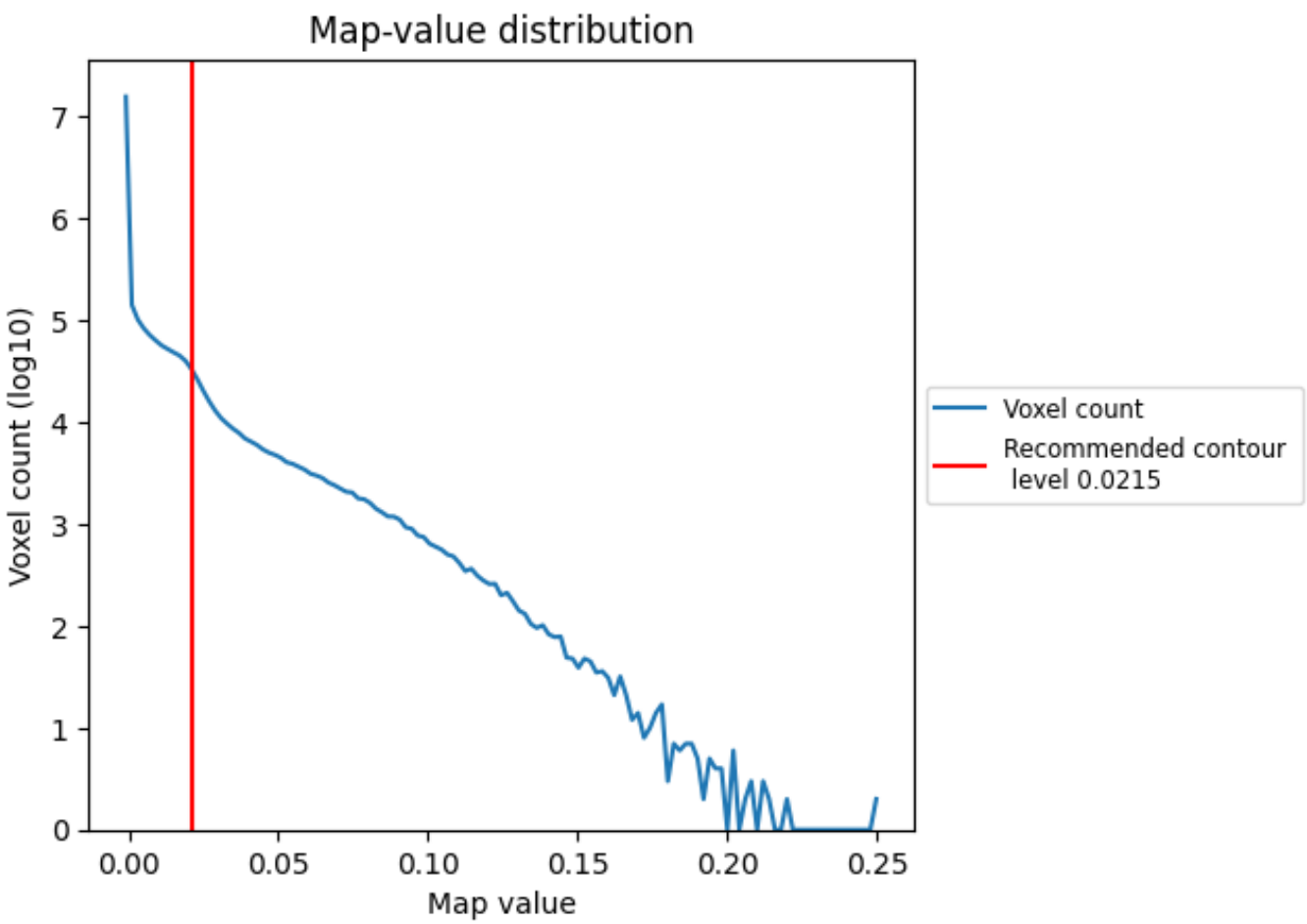
6.5 Mask visualisation (i)

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

7 Map analysis (i)

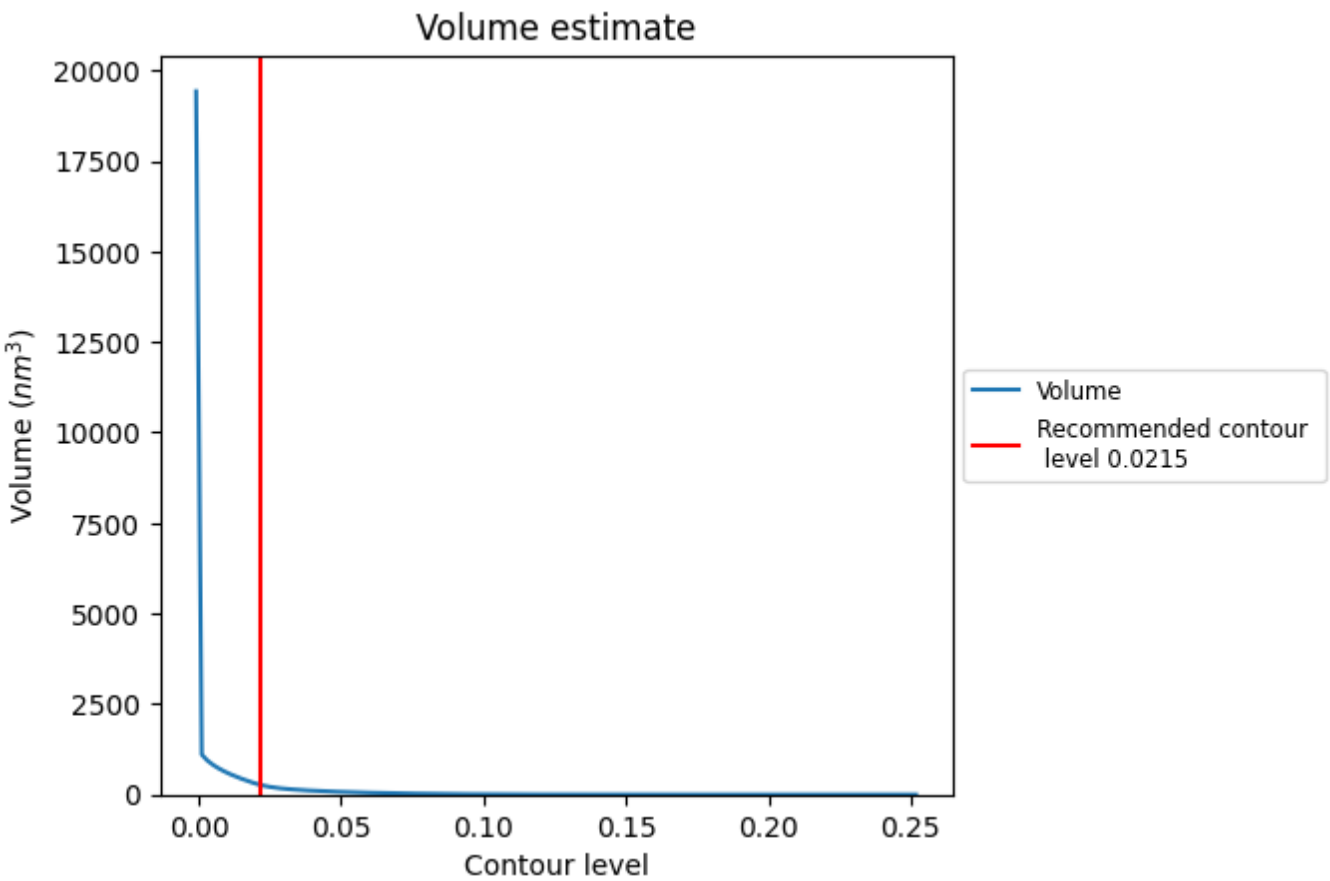
This section contains the results of statistical analysis of the map.

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.

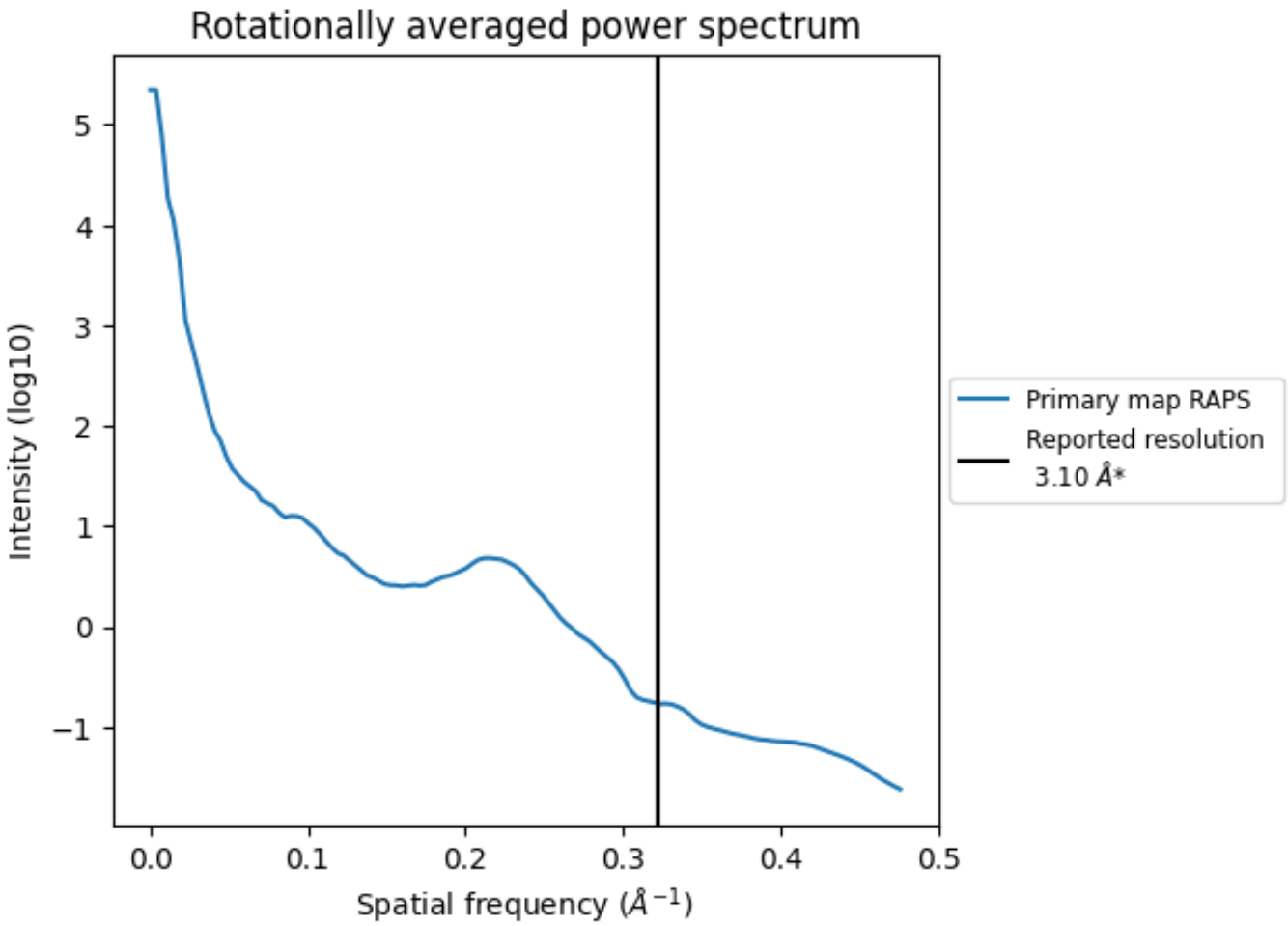
7.2 Volume estimate (i)



The volume at the recommended contour level is 271 nm^3; this corresponds to an approximate mass of 245 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 0.323 Å^{-1}

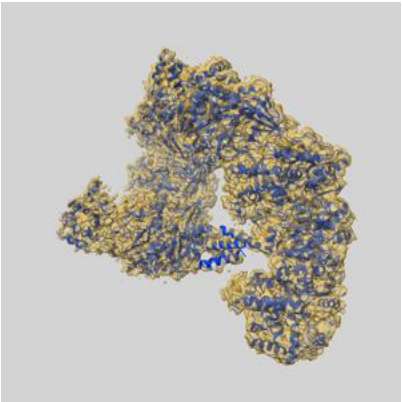
8 Fourier-Shell correlation (i)

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

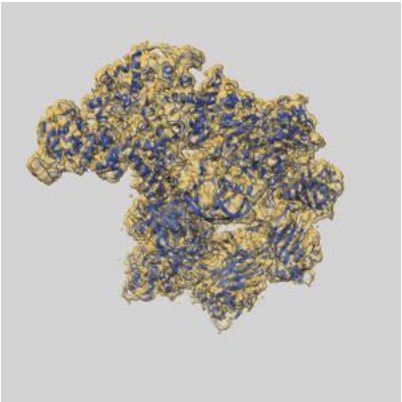
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20908 and PDB model 6UVN. Per-residue inclusion information can be found in section 3 on page 6.

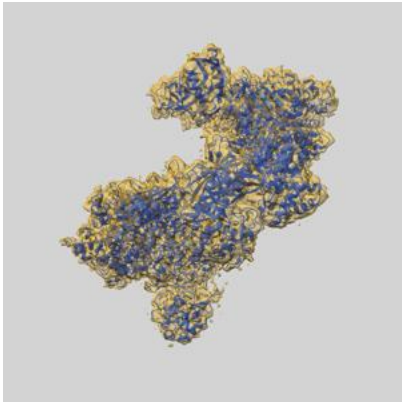
9.1 Map-model overlay (i)



X



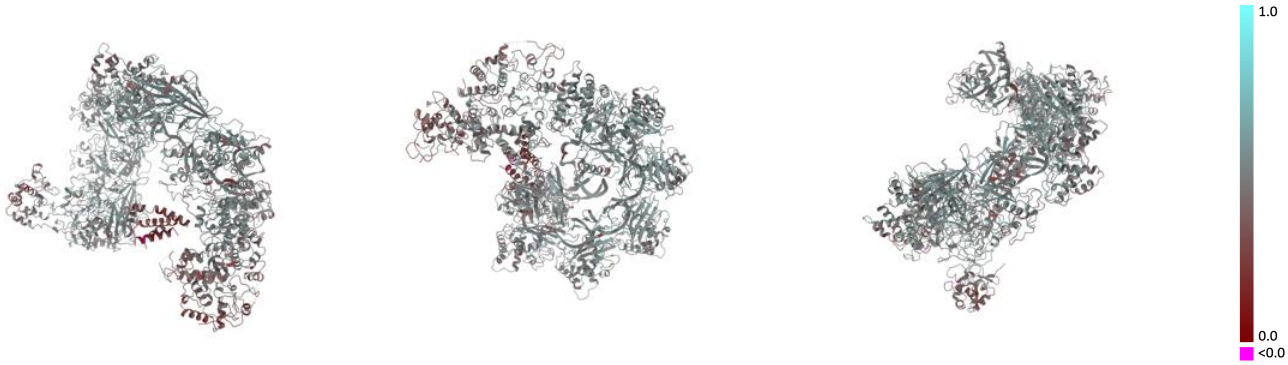
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0215 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.

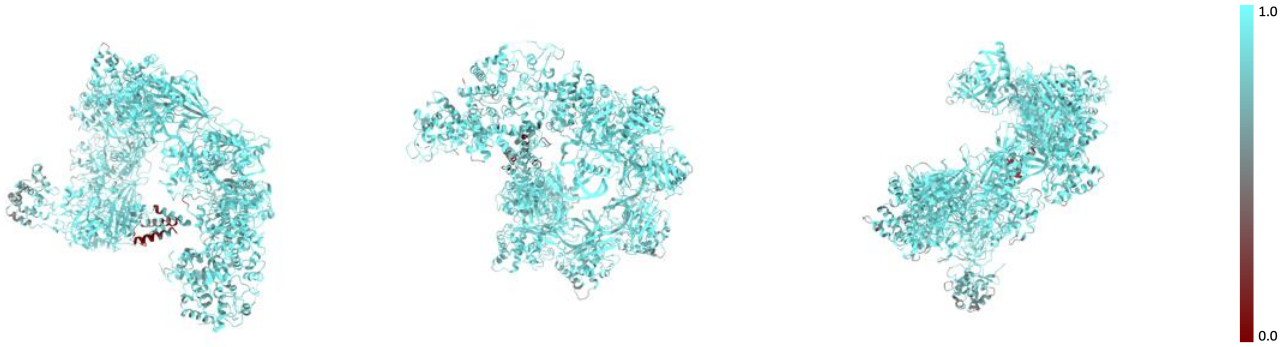
9.2 Q-score mapped to coordinate model (i)



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.

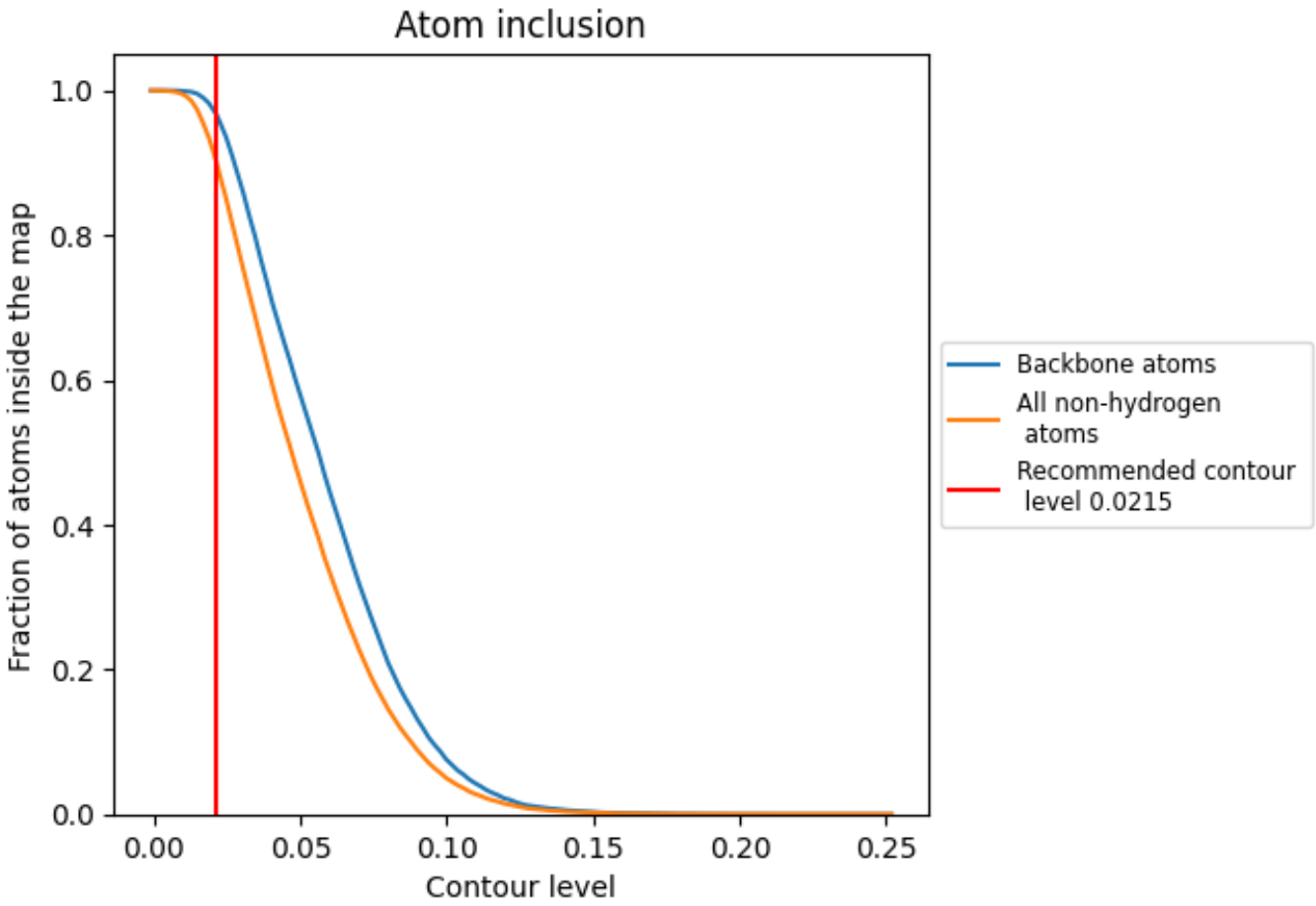
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0215).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9001	0.4860
A	0.8976	0.4790
B	0.8712	0.4710
C	0.9419	0.5170
D	0.9319	0.5150
E	0.9266	0.5150
F	0.9107	0.5100
G	0.9016	0.5010
H	0.9228	0.4970
I	0.8757	0.4600
J	0.8682	0.4440
M	0.9663	0.5060
N	0.5481	0.2250