WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Oct 12, 2021 – 09:58 am BST

PDB ID	:	7OCK
EMDB ID	:	EMD-12809
Title	:	MAT in complex with SAMH
Authors	:	Simon, H.; Kleiner, D.; Shmulevich, F.; Zarivach, R.; Zalk, R.; Tang, H.; Ding, F.; Bershtein, S.
Deposited on	:	2021-04-27
Resolution	:	3.60 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:
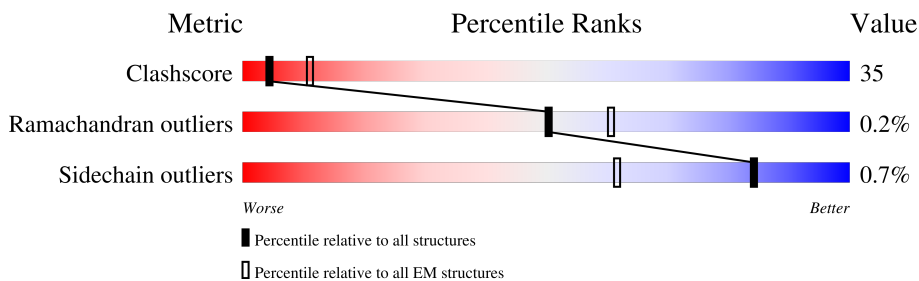
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
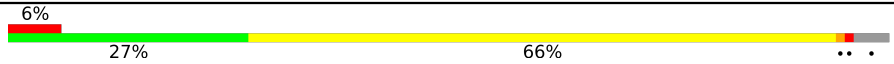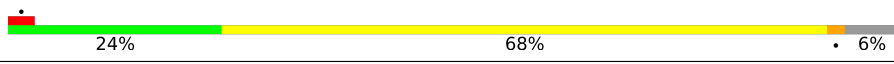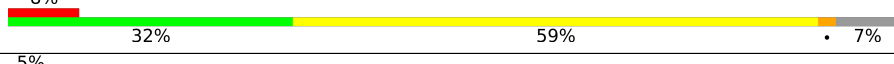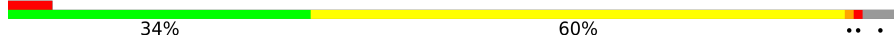
Metric	Percentile Ranks	Value
Clashscore		35
Ramachandran outliers		0.2%
Sidechain outliers		0.7%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	B	390	49% 48%
1	C	390	47% 51%
1	D	390	40% 58%
1	E	390	5% 44% 53%
1	F	390	42% 55%
1	G	390	42% 56%
1	H	390	7% 36% 61%
1	I	390	36% 62%

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Mol	Chain	Length	Quality of chain
2	A	158	6% / 27% / 66% / •• •
2	J	158	• / 24% / 68% / • 6%
2	K	158	8% / 32% / 59% / • 7%
2	L	158	5% / 34% / 60% / •• •

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 28276 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 S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	384	Total	C	N	O	S	0	0
			2951	1862	506	570	13		
1	C	384	Total	C	N	O	S	0	0
			2951	1862	506	570	13		
1	D	383	Total	C	N	O	S	0	0
			2941	1856	503	569	13		
1	E	383	Total	C	N	O	S	0	0
			2941	1856	503	569	13		
1	F	384	Total	C	N	O	S	0	0
			2951	1862	506	570	13		
1	G	383	Total	C	N	O	S	0	0
			2941	1856	503	569	13		
1	H	383	Total	C	N	O	S	0	0
			2941	1856	503	569	13		
1	I	383	Total	C	N	O	S	0	0
			2941	1856	503	569	13		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	384	HIS	-	expression tag	UNP A0A4S5B2W6
B	385	HIS	-	expression tag	UNP A0A4S5B2W6
B	386	HIS	-	expression tag	UNP A0A4S5B2W6
B	387	HIS	-	expression tag	UNP A0A4S5B2W6
B	388	HIS	-	expression tag	UNP A0A4S5B2W6
B	389	HIS	-	expression tag	UNP A0A4S5B2W6
C	384	HIS	-	expression tag	UNP A0A4S5B2W6
C	385	HIS	-	expression tag	UNP A0A4S5B2W6
C	386	HIS	-	expression tag	UNP A0A4S5B2W6
C	387	HIS	-	expression tag	UNP A0A4S5B2W6
C	388	HIS	-	expression tag	UNP A0A4S5B2W6
C	389	HIS	-	expression tag	UNP A0A4S5B2W6
D	384	HIS	-	expression tag	UNP A0A4S5B2W6
D	385	HIS	-	expression tag	UNP A0A4S5B2W6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	386	HIS	-	expression tag	UNP A0A4S5B2W6
D	387	HIS	-	expression tag	UNP A0A4S5B2W6
D	388	HIS	-	expression tag	UNP A0A4S5B2W6
D	389	HIS	-	expression tag	UNP A0A4S5B2W6
E	384	HIS	-	expression tag	UNP A0A4S5B2W6
E	385	HIS	-	expression tag	UNP A0A4S5B2W6
E	386	HIS	-	expression tag	UNP A0A4S5B2W6
E	387	HIS	-	expression tag	UNP A0A4S5B2W6
E	388	HIS	-	expression tag	UNP A0A4S5B2W6
E	389	HIS	-	expression tag	UNP A0A4S5B2W6
F	384	HIS	-	expression tag	UNP A0A4S5B2W6
F	385	HIS	-	expression tag	UNP A0A4S5B2W6
F	386	HIS	-	expression tag	UNP A0A4S5B2W6
F	387	HIS	-	expression tag	UNP A0A4S5B2W6
F	388	HIS	-	expression tag	UNP A0A4S5B2W6
F	389	HIS	-	expression tag	UNP A0A4S5B2W6
G	384	HIS	-	expression tag	UNP A0A4S5B2W6
G	385	HIS	-	expression tag	UNP A0A4S5B2W6
G	386	HIS	-	expression tag	UNP A0A4S5B2W6
G	387	HIS	-	expression tag	UNP A0A4S5B2W6
G	388	HIS	-	expression tag	UNP A0A4S5B2W6
G	389	HIS	-	expression tag	UNP A0A4S5B2W6
H	384	HIS	-	expression tag	UNP A0A4S5B2W6
H	385	HIS	-	expression tag	UNP A0A4S5B2W6
H	386	HIS	-	expression tag	UNP A0A4S5B2W6
H	387	HIS	-	expression tag	UNP A0A4S5B2W6
H	388	HIS	-	expression tag	UNP A0A4S5B2W6
H	389	HIS	-	expression tag	UNP A0A4S5B2W6
I	384	HIS	-	expression tag	UNP A0A4S5B2W6
I	385	HIS	-	expression tag	UNP A0A4S5B2W6
I	386	HIS	-	expression tag	UNP A0A4S5B2W6
I	387	HIS	-	expression tag	UNP A0A4S5B2W6
I	388	HIS	-	expression tag	UNP A0A4S5B2W6
I	389	HIS	-	expression tag	UNP A0A4S5B2W6

- Molecule 2 is a protein called SAM hydrolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	152	Total 1194	C 748	N 215	O 223	S 8	0	0
2	A	151	Total 1186	C 742	N 214	O 222	S 8	0	0

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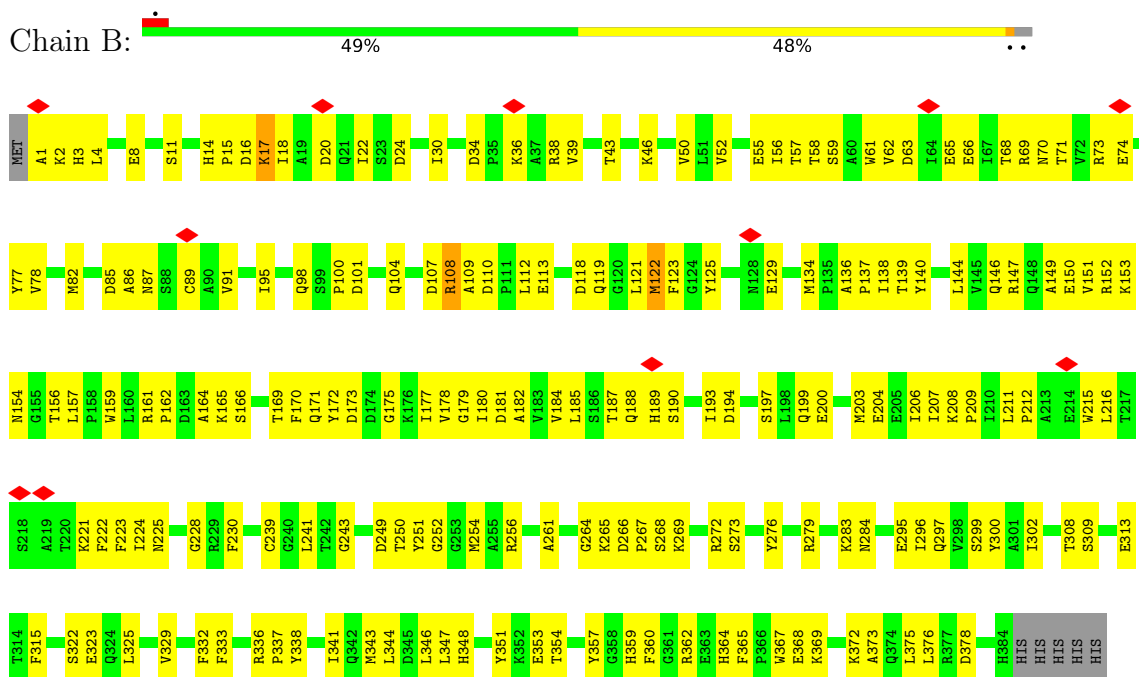| Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	147	Total 1164	C 730	N 210	O 216	S 8	0	0
2	J	149	Total 1174	C 736	N 212	O 218	S 8	0	0

There are 28 discrepancies between the modelled and reference sequences:

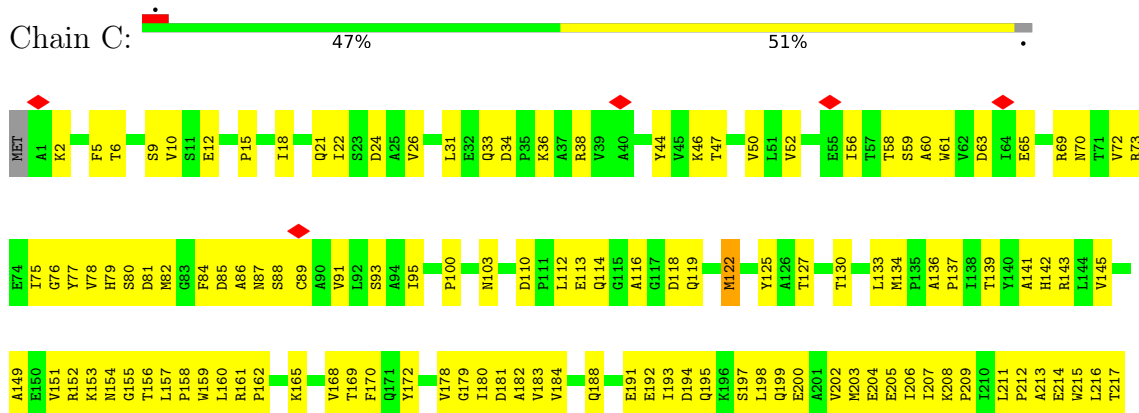| Chain	Residue	Modelled	Actual	Comment	Reference
L	9	ASN	HIS	conflict	UNP P07693
L	153	HIS	-	expression tag	UNP P07693
L	154	HIS	-	expression tag	UNP P07693
L	155	HIS	-	expression tag	UNP P07693
L	156	HIS	-	expression tag	UNP P07693
L	157	HIS	-	expression tag	UNP P07693
L	158	HIS	-	expression tag	UNP P07693
A	9	ASN	HIS	conflict	UNP P07693
A	153	HIS	-	expression tag	UNP P07693
A	154	HIS	-	expression tag	UNP P07693
A	155	HIS	-	expression tag	UNP P07693
A	156	HIS	-	expression tag	UNP P07693
A	157	HIS	-	expression tag	UNP P07693
A	158	HIS	-	expression tag	UNP P07693
K	9	ASN	HIS	conflict	UNP P07693
K	153	HIS	-	expression tag	UNP P07693
K	154	HIS	-	expression tag	UNP P07693
K	155	HIS	-	expression tag	UNP P07693
K	156	HIS	-	expression tag	UNP P07693
K	157	HIS	-	expression tag	UNP P07693
K	158	HIS	-	expression tag	UNP P07693
J	9	ASN	HIS	conflict	UNP P07693
J	153	HIS	-	expression tag	UNP P07693
J	154	HIS	-	expression tag	UNP P07693
J	155	HIS	-	expression tag	UNP P07693
J	156	HIS	-	expression tag	UNP P07693
J	157	HIS	-	expression tag	UNP P07693
J	158	HIS	-	expression tag	UNP P07693

3　Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

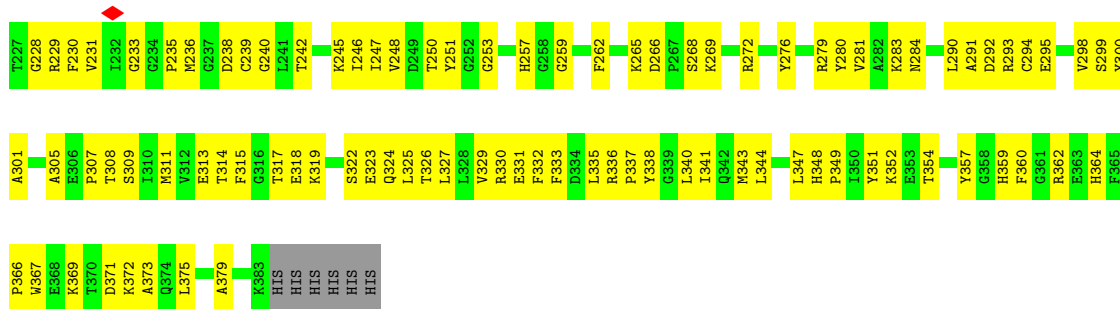- Molecule 1: S-adenosylmethionine synthase
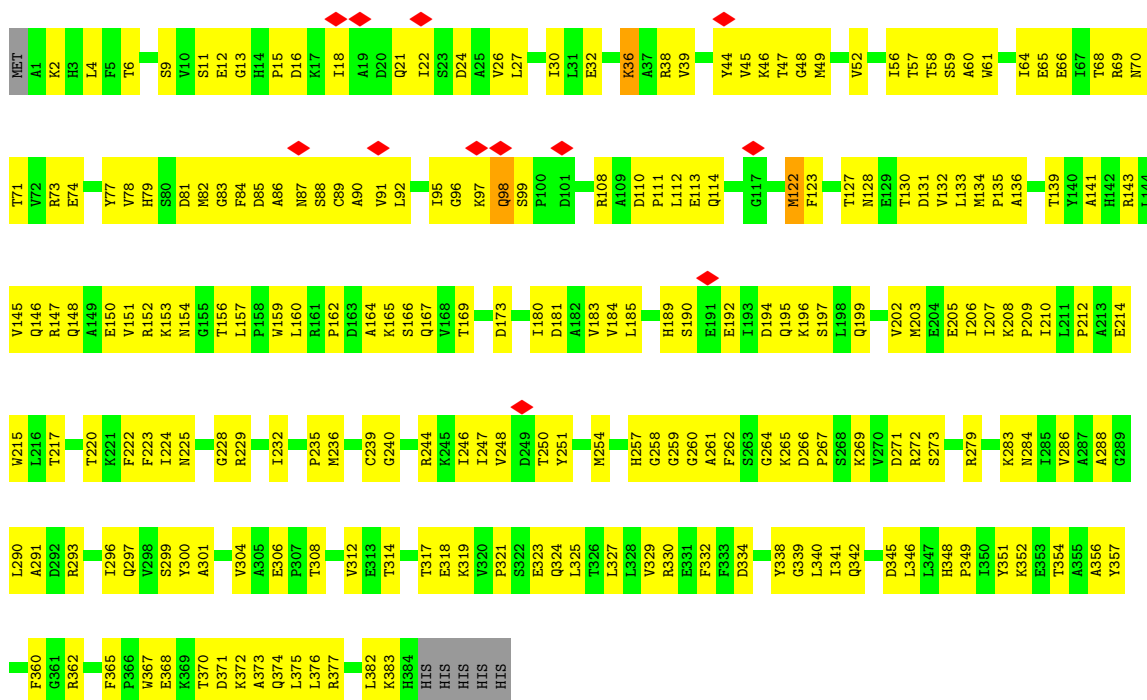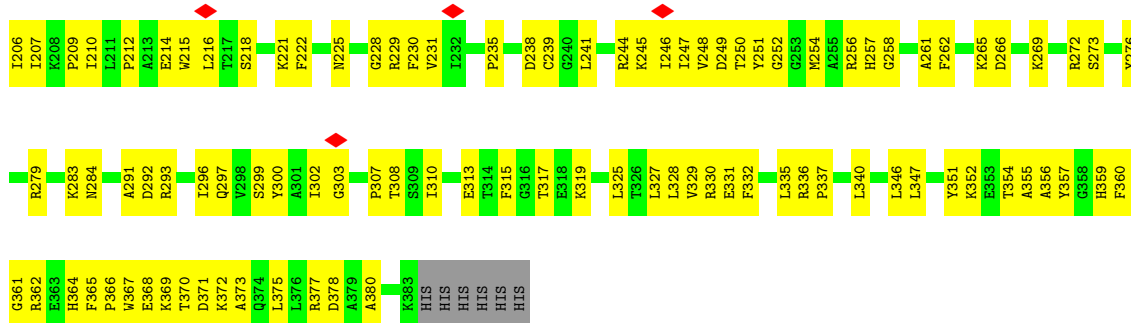
Chain B:

- Molecule 1: S-adenosylmethionine synthase

Chain C:

• Molecule 1: S-adenosylmethionine synthase

Chain D:

• Molecule 1: S-adenosylmethionine synthase

Chain E:

T227 G228 R229 F230 V231 I232 G233 G234 P235 M236 G237 D238 C239 G240 L241 T242 K245 I246 I247 V248 D249 T250 Y251 G252 G253 H257 G258 G259 F262 K265 D266 P267 S268 K269 R272 Y276 R279 Y280 V281 A282 K283 N284 L290 A291 D292 R293 C294 E295 V298 S299 Y300

A301 A305 E306 P307 T308 S309 I310 M311 V312 E313 T314 F315 G316 T317 E318 K319 S322 E323 Q324 L325 T326 L327 L328 V329 R330 E331 F332 F333 D334 L335 R336 P337 Y338 G339 L340 I341 Q342 M343 L344 L347 H348 P349 I350 Y351 K352 E353 T354 Y357 G358 H359 F360 G361 R362 E363 H364 F365

P366 W367 E368 K369 T370 D371 K372 A373 Q374 L375 A379 K383 HIS HIS HIS HIS HIS HIS

• Molecule 1: S-adenosylmethionine synthase

Chain F: 42% 55%

MET A1 K2 H3 L4 F5 T6 S9 V10 S11 E12 G13 H14 P15 D16 K17 I18 A19 D20 Q21 I22 S23 D24 A25 V26 L27 I30 L31 E32 K36 A37 R38 V39 Y44 V45 K46 T47 G48 M49 V52 I56 T57 T58 S59 A60 W61 I64 E65 E66 I67 T68 R69 N70

T71 V72 R73 E74 Y77 V78 H79 S80 D81 M82 G83 F84 D85 A86 N87 S88 C89 A90 V91 L92 I95 G96 K97 Q98 S99 P100 D101 R108 A109 D110 P111 L112 E113 Q114 G117 M122 F123 T127 N128 E129 T130 D131 V132 L133 M134 P135 A136 T139 Y140 A141 H142 R143 L144

V145 Q146 R147 Q148 A149 E150 V151 R152 K153 N154 G155 T156 L157 P158 W159 L160 R161 P162 D163 A164 K165 S166 Q167 V168 T169 D173 I180 D181 A182 V183 V184 L185 H189 S190 E191 E192 I193 D194 Q195 K196 S197 L198 Q199 V202 M203 E204 E205 I206 I207 K208 P209 I210 L211 P212 A213 E214

W215 L216 T217 T220 K221 F222 F223 I224 N225 G228 R229 I232 P235 M236 C239 G240 R244 K245 I246 I247 V248 D249 T250 Y251 M254 H257 G258 G259 G260 A261 F262 S263 G264 K265 D266 P267 S268 K269 V270 D271 R272 S273 R279 K283 N284 I285 V286 A287 A288 G289

L290 A291 D292 R293 I296 Q297 V298 S299 Y300 A301 V304 A305 E306 P307 T308 V312 E313 T314 T317 E318 K319 V320 P321 S322 E323 Q324 L325 T326 L327 L328 V329 R330 E331 F332 F333 D334 Y338 G339 L340 I341 Q342 D345 L346 L347 H348 P349 I350 Y351 K352 E353 T354 A355 A356 Y357

F360 G361 R362 F365 P366 W367 E368 K369 T370 D371 K372 A373 Q374 L375 L376 R377 L382 K383 H384 HIS HIS HIS HIS HIS

• Molecule 1: S-adenosylmethionine synthase

Chain G: 42% 56%

MET A1 F5 T6 S7 S11 E12 G13 H14 P15 D16 K17 I18 A19 D20 Q21 I22 S23 D24 A25 V26 L27 D28 L31 E32 Q33 D34 P35 K36 A37 R38 V39 A40 C41 E42 T43 Y44 V45 K46 T47 G48 M49 V52 G53 G54 E55 I56 T57 T58 S59 A60 D63 I64 E65 E66

I67 T68 R69 N70 T71 V72 R73 E74 I75 G76 Y77 M82 G83 F84 D85 A86 N87 S88 C89 A90 V91 L92 S93 A94 I95 G96 K97 Q98 S99 P100 D101 I102 N103 Q104 G105 V106 D107 R108 A109 D110 P111 L112 E113 Q114 G115 A116 G117 D118 Q119 G120 L121 M122 F123 E129 T130 D131 V132 L133

M134 P135 A136 P137 I138 T139 R143 Q146 A149 E150 V151 R152 K153 N154 G155 T156 L157 P158 W159 L160 R161 P162 D163 A164 Q167 V168 T169 F170 Q171 I177 I180 D181 A182 V183 V184 T187 Q188 H189 S190 E191 E192 I193 D194 Q195 K196 S197 L198 Q199 V202 M203 E204 E205
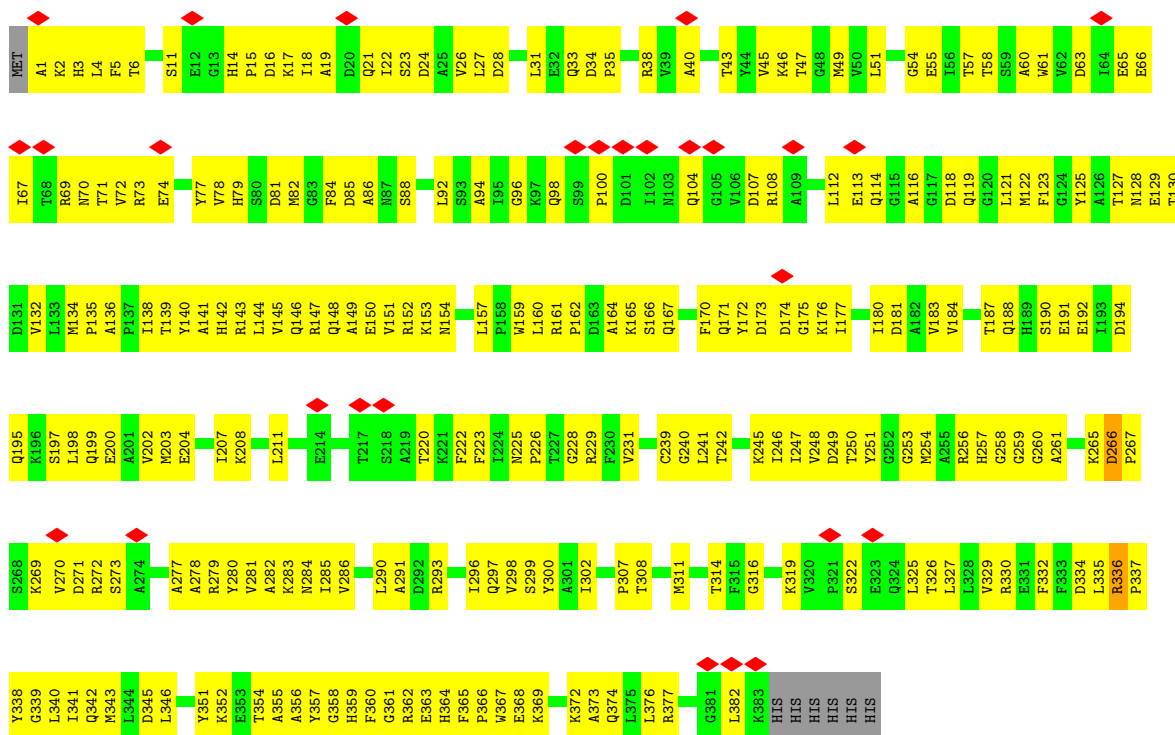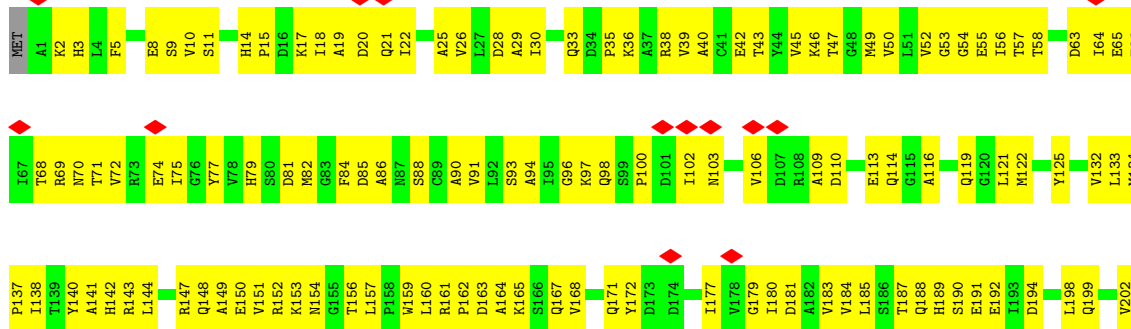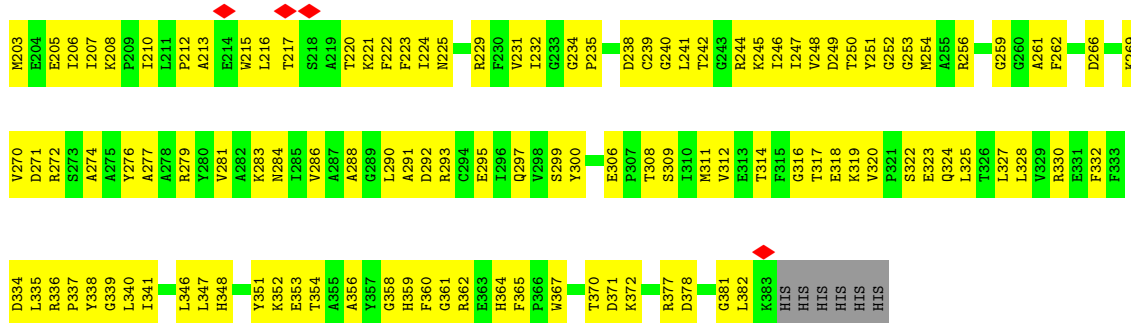
• Molecule 1: S-adenosylmethionine synthase

Chain H:

• Molecule 1: S-adenosylmethionine synthase

Chain I:

M203 E204 E205 I206 I207 K208 P209 I210 L211 P212 A213 E214 W215 L216 T217 S218 A219 T220 K221 F222 F223 I224 N225 R229 F230 V231 I232 G233 G234 P235 D238 C239 G240 L241 T242 G243 R244 K245 I246 I247 V248 D249 T250 Y251 G252 G253 M254 A255 R256 G259 G260 A261 F262 D266 K269

V270 D271 R272 S273 A274 A275 Y276 A277 A278 R279 Y280 V281 A282 K283 N284 I285 V286 A287 A288 G289 L290 A291 D292 R293 C294 E295 I296 Q297 V298 S299 Y300 E306 P307 T308 S309 I310 M311 V312 E313 T314 F315 G316 T317 E318 K319 V320 P321 S322 E323 Q324 L325 T326 L327 L328 V329 R330 E331 F332 F333

D334 L335 R336 P337 Y338 G339 L340 I341 L346 L347 H348 Y351 K352 E353 T354 A355 A356 Y357 G358 H359 F360 G361 R362 E363 H364 F365 P366 W367 T370 D371 K372 R377 D378 G381 L382 K383 HIS HIS HIS HIS HIS HIS

• Molecule 2: SAM hydrolase

Chain L:

MET I2 F3 T4 K5 E6 P7 A8 N9 V10 F11 Y12 V13 L14 A17 F18 R19 S20 N21 L22 C23 D24 E25 V26 N27 M28 S29 R30 H31 R32 H33 M34 V35 S36 T37 P42 G46 S47 V48 T51 D52 L53 T54 G55 C56 Y57 R58 E59 A60 I61 S62 S63 A64 P65 T66 E67

E68 K69 T70 V73 R74 C75 K76 D77 K78 A79 Q80 A81 L82 N83 R86 C89 N90 E91 W92 E93 Q94 D95 C96 V97 L98 V99 Y100 K101 S102 Q103 A107 G108 L109 V110 Y111 A112 K113 G114 I115 D116 G117 V118 K119 R122 L123 P124 G125 S126 F127 Q128 E129 V130 P131 K132 G133

A134 P135 L136 Q137 G138 C139 F140 G146 R147 R148 W149 Q150 V151 Q152 H153 HIS HIS HIS HIS HIS

• Molecule 2: SAM hydrolase

Chain A:

MET ILE F3 T4 K5 E6 P7 A8 N9 V10 F11 Y12 V13 L14 A17 F18 R19 S20 N21 L22 C23 D24 E25 V26 N27 M28 S29 R30 H31 R32 H33 M34 V35 S36 T37 L38 R39 P42 Y45 G46 S47 V48 E49 S50 T51 D52 L53 T54 G55 C56 Y57 R58 E59 A60 I61 S62

P65 T66 E67 E68 K69 T70 V71 R72 V73 R74 C75 K76 D77 K78 A79 Q80 A81 L82 N83 V84 A85 R86 L87 A88 C89 N90 E91 W92 E93 Q94 D95 C96 V97 L98 V99 Y100 Q103 T104 H105 T106 A107 G108 L109 V110 Y111 A112 K113 G114 Y118 K119 A120 E121 R122 L123 P124 G125 S126 F127

Q128 E129 V130 P135 L136 Q137 G138 C139 F140 T141 I142 D143 E144 F145 G146 R147 R148 W149 Q150 V151 Q152 H153 HIS HIS HIS HIS HIS

• Molecule 2: SAM hydrolase

Chain K:

MET I2 F3 T4 K5 E6 P7 A8 N9 V10 F11 Y12 V13 L14 V15 S16 A17 F18 R19 S20 C23 D24 E25 V26 N27 M28 S29 R30 H31 R32 H33 M34 V35 S36 T37 L38 R39 A40 A41 P42 G43 L44 Y45 G46 S47 V48 E49 D52 L53 T54 G55 C56 E59 ALA ILE SER SER

ALA P65 K69 T70 V71 R72 V73 R74 C75 K76 D77 K78 A79 Q80 A81 L82 N83 R86 L87 N90 E91 W92 E93 Q94 D95 C96 V97 L98 V99 Y100 Q103 T104 H105 T106 A107 G108 L109 V110 Y111 A112 K113 G114 I115 D116 G117 V118 K119 A120 E121 R122 L123 P124 G125 S126 F127 Q128

E129 V130 P131 K132 Q137 G138 C139 I142 F145 G146 R147 R148 W149 Q150 V151 Q152 H153 HIS HIS HIS HIS

- Molecule 2: SAM hydrolase

Chain J:

24%　　　　　　　　　　　68%　　　　　　6%

MET I2 F3 T4 K5 E6 N9 V10 F11 Y12 V13 L14 A17 F18 R19 S20 C23 D24 E25 V26 N27 M28 S29 R30 H31 R32 H33 M34 V35 S36 T37 L38 R39 A40 A41 P42 G43 L44 Y45 G46 S47 V48 E49 S50 T51 D52 L53 T54 G55 C56 Y57 R58 E59 A60 ILE SER SER

A64 P65 T66 E67 E68 K69 T70 V71 R72 V73 R74 C75 K76 D77 K78 A81 L82 N83 V84 A85 R86 L87 A88 C89 N90 E91 W92 E93 Q94 D95 C96 V97 L98 V99 Y100 K101 S102 Q103 T104 H105 T106 A107 G108 L109 V110 Y111 A112 K113 G114 G117 Y118 K119 A120 E121 R122 L123 S126

F127 Q128 E129 V130 P131 Q137 G138 C139 F140 T141 F145 G146 R147 R148 W149 Q150 V151 Q152 H153 HIS HIS HIS HIS HIS

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65950	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	80	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	0.893	Depositor
Minimum map value	-0.375	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	B	0.51	0/3011	0.54	0/4083
1	C	0.52	0/3011	0.52	0/4083
1	D	0.45	0/3000	0.50	0/4068
1	E	0.46	0/3000	0.51	0/4068
1	F	0.43	0/3011	0.50	0/4083
1	G	0.44	0/3000	0.50	0/4068
1	H	0.32	0/3000	0.47	0/4068
1	I	0.33	0/3000	0.46	0/4068
2	A	0.44	0/1211	0.60	0/1638
2	J	0.43	0/1198	0.57	0/1619
2	K	0.41	0/1188	0.58	1/1604 (0.1%)
2	L	0.43	0/1219	0.65	2/1649 (0.1%)
All	All	0.43	0/28849	0.52	3/39099 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
2	L	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	139	CYS	CA-CB-SG	7.47	127.45	114.00
2	K	56	CYS	CA-CB-SG	5.86	124.54	114.00
2	L	56	CYS	CA-CB-SG	5.76	124.36	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	9	ASN	Peptide
2	L	23	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2951	0	2915	166	0
1	C	2951	0	2915	179	0
1	D	2941	0	2908	205	0
1	E	2941	0	2908	184	0
1	F	2951	0	2915	209	0
1	G	2941	0	2908	205	0
1	H	2941	0	2908	219	0
1	I	2941	0	2908	232	0
2	A	1186	0	1159	116	0
2	J	1174	0	1148	140	0
2	K	1164	0	1139	110	0
2	L	1194	0	1170	104	0
All	All	28276	0	27901	1970	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 35.

All (1970) 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:H:2:LYS:HA	1:H:172:TYR:O	1.49	1.10
2:L:56:CYS:O	2:L:139:CYS:HB3	1.64	0.98
1:F:184:VAL:HG12	1:F:223:PHE:HB2	1.42	0.98
1:H:3:HIS:HB2	1:I:311:MET:HG3	1.50	0.93
2:A:128:GLN:O	2:A:147:ARG:NH1	2.02	0.91
1:F:357:TYR:HB2	1:F:362:ARG:HH21	1.36	0.91
1:G:187:THR:H	1:G:225:ASN:HD21	1.22	0.88
1:G:134:MET:SD	1:G:279:ARG:NH1	2.47	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:77:ASP:HB2	2:A:81:ALA:H	1.40	0.86
2:A:58:ARG:HA	2:A:65:PRO:HA	1.58	0.84
1:H:273:SER:HB2	1:H:341:ILE:HD11	1.59	0.84
2:L:89:CYS:HB2	2:L:94:GLN:HB3	1.60	0.84
1:I:57:THR:HA	1:I:98:GLN:HA	1.59	0.83
1:D:356:ALA:O	1:D:362:ARG:NH2	2.12	0.83
1:E:322:SER:HA	1:E:325:LEU:HD12	1.59	0.82
1:H:247:ILE:HD13	1:I:259:GLY:HA3	1.60	0.82
1:I:121:LEU:HD11	1:I:297:GLN:HG3	1.61	0.82
1:I:74:GLU:O	1:I:153:LYS:NZ	2.13	0.82
1:C:134:MET:SD	1:C:279:ARG:NH1	2.53	0.82
1:B:279:ARG:HE	1:B:283:LYS:HG3	1.44	0.81
1:E:69:ARG:NH1	1:E:86:ALA:O	2.13	0.81
1:G:327:LEU:HA	1:G:330:ARG:HE	1.45	0.81
2:L:96:CYS:SG	2:J:122:ARG:NH1	2.53	0.81
1:F:321:PRO:O	1:F:324:GLN:NE2	2.14	0.80
2:K:79:ALA:O	2:K:83:ASN:N	2.14	0.80
1:D:297:GLN:NE2	1:D:311:MET:SD	2.54	0.80
1:I:125:TYR:O	1:I:251:TYR:OH	1.99	0.80
1:F:133:LEU:HD13	1:F:283:LYS:HE3	1.64	0.80
1:D:317:THR:O	1:D:319:LYS:NZ	2.15	0.80
1:C:36:LYS:O	1:C:38:ARG:NH1	2.15	0.79
2:K:127:PHE:HA	2:K:149:TRP:HA	1.63	0.79
1:F:356:ALA:O	1:F:362:ARG:NH2	2.16	0.78
2:A:127:PHE:HA	2:A:149:TRP:HA	1.64	0.78
2:A:128:GLN:HG3	2:A:147:ARG:HD3	1.64	0.78
1:B:194:ASP:OD1	1:B:197:SER:OG	2.00	0.78
1:D:152:ARG:HH21	1:D:153:LYS:HZ3	1.31	0.78
1:B:181:ASP:OD1	1:B:221:LYS:NZ	2.17	0.78
1:G:273:SER:HB2	1:G:340:LEU:HD11	1.65	0.78
2:A:110:VAL:HG23	2:A:119:LYS:HB2	1.65	0.78
2:A:28:MET:HB2	2:A:32:ARG:HH21	1.49	0.78
1:G:229:ARG:HH12	1:G:231:VAL:H	1.28	0.78
2:J:42:PRO:O	2:J:46:GLY:N	2.16	0.78
1:E:144:LEU:HG	1:E:210:ILE:HG21	1.66	0.78
1:E:134:MET:SD	1:E:279:ARG:NH1	2.57	0.77
1:G:195:GLN:NE2	1:G:228:GLY:O	2.16	0.77
1:I:52:VAL:HG11	1:I:64:ILE:HG21	1.66	0.77
1:I:28:ASP:OD2	1:I:352:LYS:N	2.12	0.77
1:G:203:MET:HG2	1:G:207:ILE:HD12	1.67	0.77
1:E:79:HIS:HD2	1:E:81:ASP:H	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:GLN:HG2	1:I:224:ILE:HB	1.67	0.76
1:C:21:GLN:HG2	1:C:355:ALA:HB1	1.67	0.76
1:I:15:PRO:HD3	1:I:234:GLY:HA2	1.67	0.76
1:D:313:GLU:OE2	1:D:315:PHE:N	2.18	0.76
2:A:21:ASN:ND2	2:A:23:CYS:SG	2.58	0.76
2:L:127:PHE:HA	2:L:149:TRP:HA	1.67	0.76
2:A:30:ARG:HB3	2:A:34:MET:HE3	1.66	0.76
1:I:249:ASP:HA	1:I:358:GLY:HA2	1.68	0.75
1:G:130:THR:HG1	1:G:134:MET:H	1.33	0.75
1:I:180:ILE:HD11	1:I:212:PRO:HD2	1.68	0.75
2:L:100:TYR:HA	2:L:107:ALA:HB3	1.69	0.75
2:K:94:GLN:NE2	2:K:96:CYS:SG	2.59	0.75
2:J:77:ASP:HB2	2:J:81:ALA:H	1.51	0.75
2:L:51:THR:OG1	2:L:69:LYS:NZ	2.20	0.75
2:L:124:PRO:HG2	2:L:151:VAL:HG13	1.69	0.75
1:F:195:GLN:HB3	1:F:199:GLN:HE22	1.50	0.74
1:F:95:ILE:HG13	1:F:96:GLY:H	1.51	0.74
1:E:65:GLU:OE2	1:E:69:ARG:NE	2.19	0.74
1:E:63:ASP:OD1	1:E:66:GLU:N	2.18	0.74
2:A:89:CYS:HB2	2:A:94:GLN:HB3	1.69	0.74
2:J:83:ASN:HA	2:J:86:ARG:HD3	1.70	0.74
1:F:6:THR:H	1:G:297:GLN:HE22	1.36	0.73
1:F:214:GLU:OE2	2:L:101:LYS:NZ	2.21	0.73
1:F:69:ARG:HB3	1:F:73:ARG:HH22	1.54	0.73
1:F:194:ASP:OD1	1:F:197:SER:OG	2.03	0.73
1:G:229:ARG:HH22	1:G:231:VAL:HB	1.53	0.73
1:I:189:HIS:HE1	1:I:229:ARG:HH21	1.37	0.73
1:H:207:ILE:HG23	1:H:211:LEU:HD12	1.71	0.73
1:C:184:VAL:HG22	1:C:223:PHE:HB2	1.69	0.73
1:D:283:LYS:NZ	1:D:368:GLU:OE2	2.21	0.73
1:G:52:VAL:HG23	1:G:95:ILE:HD11	1.71	0.73
1:I:221:LYS:NZ	1:I:222:PHE:O	2.21	0.73
2:J:130:VAL:HG12	2:J:147:ARG:HH12	1.53	0.73
1:D:94:ALA:O	1:E:46:LYS:NZ	2.19	0.73
1:D:322:SER:HA	1:D:325:LEU:HD12	1.70	0.73
1:H:46:LYS:HB3	1:H:49:MET:HG3	1.70	0.73
1:C:266:ASP:OD2	1:C:268:SER:N	2.18	0.72
1:G:28:ASP:OD2	1:G:352:LYS:N	2.19	0.72
1:E:10:VAL:HG11	1:E:245:LYS:HE3	1.69	0.72
1:E:257:HIS:HD2	1:E:259:GLY:H	1.34	0.72
1:D:266:ASP:OD2	1:D:268:SER:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:150:GLN:NE2	2:A:151:VAL:O	2.23	0.72
1:B:256:ARG:NH1	1:C:254:MET:O	2.23	0.72
2:A:8:ALA:O	2:A:103:GLN:NE2	2.23	0.72
2:A:55:GLY:O	2:A:67:GLU:HA	1.89	0.72
1:B:151:VAL:HG13	1:B:156:THR:HB	1.71	0.72
2:L:9:ASN:O	2:L:11:PHE:N	2.23	0.72
1:B:147:ARG:NH1	1:B:150:GLU:OE1	2.22	0.72
1:B:272:ARG:HH22	1:B:351:TYR:HB3	1.55	0.72
1:C:317:THR:O	1:C:319:LYS:NZ	2.23	0.72
1:D:280:TYR:O	1:D:284:ASN:ND2	2.23	0.72
1:B:39:VAL:HG22	1:B:56:ILE:HG12	1.71	0.72
2:K:97:VAL:HG23	2:K:110:VAL:HG13	1.71	0.72
1:D:144:LEU:HG	1:D:210:ILE:HG21	1.72	0.71
1:D:293:ARG:HG2	1:D:317:THR:HG21	1.72	0.71
1:F:52:VAL:HG11	1:F:64:ILE:HG21	1.72	0.71
1:F:69:ARG:NH1	1:F:86:ALA:O	2.21	0.71
2:A:18:PHE:N	2:A:94:GLN:OE1	2.21	0.71
1:B:180:ILE:H	1:B:215:TRP:HB3	1.54	0.71
1:G:214:GLU:OE1	1:G:214:GLU:N	2.23	0.71
2:K:128:GLN:O	2:K:147:ARG:NH1	2.23	0.71
1:C:112:LEU:HB3	1:C:336:ARG:HH11	1.56	0.71
1:F:134:MET:SD	1:F:279:ARG:NH1	2.63	0.71
1:B:254:MET:HA	1:C:256:ARG:HH21	1.54	0.71
1:I:351:TYR:HA	1:I:354:THR:HG22	1.72	0.71
2:J:9:ASN:O	2:J:11:PHE:N	2.23	0.71
1:C:211:LEU:HB3	1:C:216:LEU:HD21	1.73	0.71
1:F:374:GLN:O	1:F:377:ARG:HB2	1.91	0.71
2:L:13:VAL:HG12	2:L:74:ARG:HG2	1.73	0.71
2:J:58:ARG:HG3	2:J:65:PRO:HG3	1.71	0.71
1:B:299:SER:HG	1:B:308:THR:HG1	1.34	0.71
1:D:362:ARG:HB3	1:D:364:HIS:CE1	2.26	0.71
1:I:72:VAL:HA	1:I:75:ILE:HD12	1.72	0.71
2:J:146:GLY:HA3	2:J:148:ARG:HH11	1.55	0.71
1:B:11:SER:HB3	1:B:164:ALA:HB3	1.71	0.70
1:G:299:SER:OG	1:G:308:THR:OG1	2.09	0.70
1:F:92:LEU:HD12	1:H:92:LEU:HD12	1.73	0.70
1:F:279:ARG:HH21	1:F:283:LYS:HD2	1.55	0.70
1:H:28:ASP:OD2	1:H:352:LYS:N	2.18	0.70
1:B:138:ILE:HB	1:B:252:GLY:HA3	1.73	0.70
1:D:3:HIS:HB2	1:E:311:MET:HG3	1.72	0.70
2:J:127:PHE:HA	2:J:149:TRP:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:ARG:NH1	1:G:276:TYR:OH	2.23	0.70
1:I:266:ASP:H	1:I:269:LYS:HD3	1.56	0.70
1:H:161:ARG:HB2	1:H:188:GLN:HB3	1.72	0.70
1:H:280:TYR:HB2	1:H:367:TRP:HA	1.73	0.70
1:H:38:ARG:HH21	1:H:57:THR:HG23	1.57	0.70
1:H:327:LEU:HG	1:H:330:ARG:HH21	1.56	0.70
1:D:377:ARG:NH1	1:D:381:GLY:O	2.25	0.70
1:H:332:PHE:O	1:H:372:LYS:NZ	2.24	0.70
1:F:39:VAL:HG22	1:F:56:ILE:HG23	1.74	0.69
1:H:249:ASP:HA	1:H:358:GLY:HA2	1.74	0.69
1:H:280:TYR:O	1:H:284:ASN:ND2	2.22	0.69
2:L:56:CYS:O	2:L:139:CYS:CB	2.40	0.69
1:I:246:ILE:HD13	1:I:261:ALA:HA	1.75	0.69
2:L:86:ARG:NH2	2:L:115:ILE:O	2.24	0.69
1:D:327:LEU:HA	1:D:330:ARG:HE	1.58	0.69
1:I:110:ASP:HB3	1:I:113:GLU:HB3	1.73	0.69
2:L:20:SER:HB2	2:J:119:LYS:HD2	1.74	0.69
1:F:261:ALA:O	1:F:265:LYS:NZ	2.24	0.69
1:G:299:SER:HG	1:G:308:THR:HG1	1.40	0.69
1:I:288:ALA:O	1:I:377:ARG:NH1	2.24	0.69
1:C:332:PHE:HD2	1:C:372:LYS:HD2	1.58	0.69
1:D:152:ARG:CZ	1:D:162:PRO:HA	2.23	0.69
1:E:202:VAL:HG23	1:E:206:ILE:HD13	1.75	0.69
1:G:313:GLU:OE2	1:G:315:PHE:N	2.16	0.69
1:H:11:SER:HB3	1:H:164:ALA:HB3	1.74	0.69
2:A:129:GLU:OE1	2:A:129:GLU:N	2.25	0.69
2:K:125:GLY:HA3	2:K:151:VAL:HA	1.74	0.69
2:K:128:GLN:HA	2:K:147:ARG:HB3	1.75	0.69
1:B:122:MET:SD	1:B:122:MET:N	2.66	0.69
1:C:192:GLU:OE1	1:C:192:GLU:N	2.20	0.69
1:E:265:LYS:O	1:E:272:ARG:NH1	2.26	0.69
1:F:357:TYR:HB2	1:F:362:ARG:NH2	2.07	0.68
1:G:66:GLU:OE1	1:G:70:ASN:ND2	2.25	0.68
1:I:161:ARG:HE	1:I:190:SER:HA	1.56	0.68
2:A:9:ASN:O	2:A:11:PHE:N	2.27	0.68
1:H:164:ALA:HB2	1:H:187:THR:HG23	1.76	0.68
1:D:150:GLU:O	1:D:153:LYS:N	2.27	0.68
1:B:3:HIS:O	1:B:172:TYR:HB2	1.93	0.68
1:G:118:ASP:OD1	1:G:119:GLN:N	2.27	0.68
1:H:299:SER:O	1:H:308:THR:N	2.27	0.68
2:A:77:ASP:HB3	2:A:80:GLN:HB2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:ILE:HG13	2:K:3:PHE:H	1.56	0.68
1:I:314:THR:HG23	1:I:316:GLY:H	1.59	0.68
2:J:110:VAL:HA	2:J:120:ALA:HA	1.76	0.68
1:E:46:LYS:HG3	1:E:47:THR:H	1.57	0.68
1:H:297:GLN:HE22	1:I:5:PHE:HA	1.59	0.68
1:D:94:ALA:HB1	1:E:46:LYS:HZ2	1.59	0.68
2:A:45:TYR:O	2:A:47:SER:OG	2.09	0.67
2:K:82:LEU:HG	2:K:86:ARG:HH11	1.59	0.67
1:G:202:VAL:HG23	1:G:206:ILE:HD13	1.76	0.67
1:G:99:SER:OG	1:G:101:ASP:OD1	2.11	0.67
1:G:150:GLU:OE1	1:G:154:ASN:ND2	2.27	0.67
1:E:317:THR:O	1:E:319:LYS:NZ	2.22	0.67
1:H:300:TYR:OH	1:H:335:LEU:O	2.10	0.67
2:L:126:SER:OG	2:L:129:GLU:OE1	2.13	0.67
2:A:3:PHE:HE2	2:A:104:THR:HA	1.59	0.67
2:K:128:GLN:HG3	2:K:147:ARG:HD3	1.76	0.67
1:C:288:ALA:O	1:C:377:ARG:NH1	2.28	0.67
1:H:184:VAL:HG13	1:H:223:PHE:HB2	1.75	0.67
1:I:2:LYS:NZ	1:I:3:HIS:O	2.28	0.67
1:C:33:GLN:NE2	1:C:61:TRP:O	2.25	0.67
1:D:378:ASP:HA	1:D:382:LEU:HD13	1.76	0.67
2:J:24:ASP:OD1	2:J:24:ASP:N	2.24	0.67
2:J:34:MET:O	2:J:37:THR:OG1	2.10	0.67
1:E:276:TYR:OH	1:E:359:HIS:ND1	2.25	0.66
1:C:373:ALA:HA	1:C:376:LEU:HD12	1.75	0.66
1:F:202:VAL:HG11	1:F:224:ILE:HG21	1.77	0.66
1:G:134:MET:HE3	1:G:135:PRO:HD2	1.77	0.66
1:H:121:LEU:HD11	1:H:297:GLN:HG3	1.77	0.66
1:H:341:ILE:O	1:H:345:ASP:N	2.24	0.66
1:E:150:GLU:OE2	1:E:154:ASN:ND2	2.28	0.66
2:L:137:GLN:NE2	2:L:149:TRP:O	2.25	0.66
2:J:103:GLN:OE1	2:J:103:GLN:N	2.26	0.66
1:D:231:VAL:HG23	1:D:232:ILE:HD12	1.77	0.66
1:E:323:GLU:OE1	1:E:323:GLU:N	2.25	0.66
1:G:136:ALA:O	1:G:139:THR:OG1	2.14	0.66
1:D:44:TYR:HE1	1:D:46:LYS:HB2	1.60	0.66
1:H:374:GLN:HA	1:H:377:ARG:HD3	1.75	0.66
1:I:332:PHE:O	1:I:372:LYS:NZ	2.27	0.66
1:C:246:ILE:HG12	1:C:257:HIS:HE1	1.60	0.66
1:D:7:SER:HB3	1:D:137:PRO:HB2	1.78	0.66
1:D:276:TYR:HB3	1:D:367:TRP:CG	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:GLU:OE1	1:E:229:ARG:NH2	2.29	0.66
1:E:338:TYR:HA	1:E:341:ILE:HD12	1.77	0.66
1:F:133:LEU:HD22	1:F:283:LYS:HG2	1.78	0.66
1:H:69:ARG:NH1	1:H:86:ALA:O	2.28	0.66
1:D:108:ARG:NH1	1:D:114:GLN:OE1	2.29	0.66
1:H:19:ALA:HA	1:H:22:ILE:HD12	1.77	0.66
2:J:112:ALA:HA	2:J:117:GLY:HA3	1.78	0.66
1:E:188:GLN:NE2	1:E:231:VAL:O	2.26	0.66
1:G:300:TYR:OH	1:G:335:LEU:O	2.10	0.66
2:L:124:PRO:O	2:L:152:GLN:NE2	2.29	0.66
2:A:14:LEU:HB3	2:A:99:VAL:HG23	1.77	0.66
1:E:25:ALA:HB2	1:E:352:LYS:HD3	1.78	0.66
2:L:54:THR:HG22	2:L:69:LYS:HA	1.77	0.66
1:B:129:GLU:O	2:A:3:PHE:HB2	1.97	0.65
1:E:257:HIS:CD2	1:E:259:GLY:H	2.13	0.65
1:E:266:ASP:OD2	1:E:268:SER:N	2.20	0.65
1:I:164:ALA:HB2	1:I:187:THR:HG23	1.79	0.65
1:D:299:SER:O	1:D:308:THR:N	2.28	0.65
2:A:82:LEU:HD21	2:A:99:VAL:HG21	1.77	0.65
1:D:168:VAL:HG12	1:D:183:VAL:HG22	1.77	0.65
1:F:6:THR:HG21	1:F:167:GLN:HE21	1.61	0.65
1:H:132:VAL:HG13	1:H:134:MET:HG3	1.78	0.65
1:G:54:GLY:O	1:G:96:GLY:N	2.28	0.65
2:A:150:GLN:O	2:A:152:GLN:NE2	2.29	0.65
2:L:28:MET:HB3	2:L:32:ARG:HH21	1.61	0.65
1:E:362:ARG:HB3	1:E:364:HIS:CE1	2.32	0.65
1:C:85:ASP:OD2	1:C:88:SER:N	2.28	0.65
1:E:293:ARG:HG2	1:E:317:THR:HG21	1.79	0.65
2:L:150:GLN:NE2	2:L:151:VAL:O	2.29	0.65
1:B:203:MET:HA	1:B:207:ILE:HD12	1.79	0.65
1:G:212:PRO:HG3	2:K:103:GLN:HG3	1.77	0.65
1:B:254:MET:SD	1:C:256:ARG:NH2	2.70	0.65
1:C:65:GLU:HA	1:C:91:VAL:HG11	1.79	0.65
1:E:313:GLU:OE2	1:E:315:PHE:N	2.30	0.65
2:A:24:ASP:N	2:A:24:ASP:OD1	2.26	0.65
2:K:79:ALA:HA	2:K:82:LEU:HD23	1.79	0.65
1:H:173:ASP:N	1:H:176:LYS:O	2.30	0.65
2:K:14:LEU:HB3	2:K:99:VAL:HG13	1.79	0.65
1:B:254:MET:O	1:C:256:ARG:NE	2.29	0.64
1:I:19:ALA:HA	1:I:22:ILE:HD12	1.78	0.64
1:G:40:ALA:HB2	1:G:269:LYS:HE2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:HIS:ND1	1:G:190:SER:O	2.29	0.64
2:L:57:TYR:O	2:L:65:PRO:HA	1.96	0.64
1:B:313:GLU:OE2	1:B:315:PHE:N	2.26	0.64
1:I:150:GLU:OE1	1:I:154:ASN:ND2	2.28	0.64
1:H:15:PRO:HA	1:H:18:ILE:HD12	1.79	0.64
1:H:46:LYS:HD3	1:H:47:THR:H	1.63	0.64
2:J:34:MET:HG2	2:J:92:TRP:CE2	2.33	0.64
1:E:299:SER:OG	1:E:309:SER:OG	2.10	0.64
1:C:203:MET:HA	1:C:207:ILE:HD12	1.77	0.64
1:F:246:ILE:HD11	1:F:257:HIS:NE2	2.13	0.64
1:I:356:ALA:O	1:I:362:ARG:NH2	2.31	0.64
2:L:24:ASP:N	2:L:24:ASP:OD1	2.29	0.64
2:J:10:VAL:HA	2:J:103:GLN:NE2	2.12	0.64
1:G:63:ASP:OD2	1:G:66:GLU:N	2.23	0.64
1:H:54:GLY:O	1:H:96:GLY:N	2.23	0.64
1:G:58:THR:HG23	1:G:97:LYS:HE3	1.78	0.64
1:G:130:THR:OG1	1:G:134:MET:N	2.18	0.64
1:I:152:ARG:CZ	1:I:162:PRO:HA	2.28	0.64
2:A:121:GLU:OE2	2:A:121:GLU:N	2.23	0.64
1:C:6:THR:HG23	1:C:169:THR:HG22	1.78	0.64
1:D:116:ALA:O	1:D:303:GLY:N	2.26	0.64
1:D:213:ALA:HA	1:D:216:LEU:HD12	1.80	0.64
2:K:20:SER:OG	2:K:30:ARG:NH2	2.31	0.64
1:B:43:THR:HG22	1:B:52:VAL:HG22	1.80	0.63
1:I:46:LYS:HB3	1:I:49:MET:HB3	1.80	0.63
2:J:111:TYR:N	2:J:119:LYS:O	2.25	0.63
1:B:299:SER:OG	1:B:308:THR:OG1	2.04	0.63
1:G:69:ARG:NH1	1:G:89:CYS:SG	2.71	0.63
1:H:4:LEU:O	1:I:309:SER:OG	2.16	0.63
1:I:134:MET:SD	1:I:279:ARG:NH1	2.68	0.63
2:A:128:GLN:HG3	2:A:147:ARG:HH11	1.63	0.63
1:B:150:GLU:O	1:B:154:ASN:ND2	2.30	0.63
1:F:279:ARG:NH2	1:F:368:GLU:OE2	2.32	0.63
1:G:299:SER:O	1:G:308:THR:N	2.30	0.63
1:H:373:ALA:O	1:H:376:LEU:HB3	1.98	0.63
1:F:85:ASP:OD2	1:F:88:SER:N	2.20	0.63
1:G:210:ILE:O	2:K:9:ASN:ND2	2.31	0.63
1:I:299:SER:O	1:I:308:THR:N	2.31	0.63
2:L:79:ALA:O	2:L:83:ASN:N	2.23	0.63
1:G:366:PRO:HA	1:G:369:LYS:HE2	1.80	0.63
1:I:19:ALA:HB1	1:I:43:THR:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:290:LEU:O	1:I:319:LYS:NZ	2.30	0.63
1:B:112:LEU:HB3	1:B:336:ARG:HH11	1.64	0.63
1:D:171:GLN:NE2	1:D:178:VAL:O	2.32	0.63
1:B:309:SER:OG	1:C:6:THR:OG1	2.15	0.63
1:I:247:ILE:HG22	1:I:252:GLY:HA2	1.79	0.63
2:J:34:MET:HE2	2:J:92:TRP:HB3	1.81	0.63
2:L:75:CYS:HB2	2:L:81:ALA:HB3	1.81	0.62
1:C:202:VAL:HG11	1:C:224:ILE:HG21	1.80	0.62
1:C:323:GLU:N	1:C:323:GLU:OE2	2.32	0.62
1:I:353:GLU:HB3	1:I:365:PHE:HZ	1.64	0.62
2:A:56:CYS:HA	2:A:66:THR:O	1.99	0.62
2:J:101:LYS:O	2:J:105:HIS:N	2.27	0.62
1:D:110:ASP:O	1:D:113:GLU:HG2	1.99	0.62
1:F:203:MET:HB3	1:F:208:LYS:HZ1	1.64	0.62
1:F:373:ALA:HA	1:F:376:LEU:HD12	1.81	0.62
1:H:281:VAL:O	1:H:285:ILE:HG12	1.98	0.62
1:I:69:ARG:NH1	1:I:86:ALA:O	2.31	0.62
2:L:30:ARG:HE	2:L:34:MET:HE3	1.63	0.62
1:D:28:ASP:OD2	1:D:352:LYS:N	2.24	0.62
1:H:283:LYS:NZ	1:H:363:GLU:OE2	2.28	0.62
2:A:79:ALA:O	2:A:83:ASN:N	2.25	0.62
1:F:4:LEU:HD12	1:G:310:ILE:H	1.64	0.62
1:F:44:TYR:HE1	1:F:46:LYS:HB2	1.65	0.62
1:I:54:GLY:O	1:I:96:GLY:N	2.32	0.62
2:J:101:LYS:HB3	2:J:103:GLN:NE2	2.14	0.62
2:A:33:HIS:O	2:A:36:SER:OG	2.17	0.62
1:B:125:TYR:N	1:B:251:TYR:OH	2.30	0.62
1:B:200:GLU:O	1:B:204:GLU:HG2	2.00	0.62
1:D:134:MET:SD	1:D:279:ARG:NH1	2.73	0.62
2:K:77:ASP:HB3	2:K:80:GLN:HB2	1.80	0.62
1:C:10:VAL:HG12	1:C:165:LYS:HG2	1.82	0.62
1:G:332:PHE:O	1:G:372:LYS:NZ	2.32	0.62
1:G:354:THR:OG1	1:G:359:HIS:ND1	2.33	0.62
1:H:259:GLY:HA3	1:I:247:ILE:HG12	1.81	0.62
1:F:254:MET:O	1:G:256:ARG:NH1	2.33	0.61
1:F:314:THR:HG21	1:F:318:GLU:HB3	1.81	0.61
2:J:83:ASN:O	2:J:87:LEU:HG	1.99	0.61
2:K:77:ASP:HB2	2:K:81:ALA:H	1.63	0.61
1:D:24:ASP:OD2	1:D:272:ARG:NH2	2.30	0.61
1:G:362:ARG:HB3	1:G:364:HIS:CE1	2.35	0.61
1:H:173:ASP:O	1:H:176:LYS:NZ	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:17:ALA:N	2:J:94:GLN:OE1	2.32	0.61
1:D:2:LYS:HA	1:D:172:TYR:O	2.00	0.61
1:I:300:TYR:OH	1:I:335:LEU:O	2.09	0.61
1:H:122:MET:HA	1:H:258:GLY:HA3	1.82	0.61
1:H:337:PRO:O	1:H:341:ILE:HG12	2.00	0.61
2:K:44:LEU:HG	2:K:45:TYR:H	1.65	0.61
1:D:9:SER:HA	1:D:248:VAL:HG21	1.82	0.61
1:E:299:SER:O	1:E:308:THR:N	2.34	0.61
1:E:300:TYR:OH	1:E:335:LEU:O	2.17	0.61
1:F:167:GLN:HB3	1:F:184:VAL:HG23	1.82	0.61
1:F:167:GLN:NE2	1:G:299:SER:HB2	2.16	0.61
1:G:19:ALA:HA	1:G:22:ILE:HD12	1.82	0.61
1:G:72:VAL:HA	1:G:75:ILE:HD12	1.82	0.61
2:A:84:VAL:HA	2:A:87:LEU:HD12	1.83	0.61
2:K:126:SER:HB3	2:K:150:GLN:HB2	1.82	0.61
2:J:118:TYR:H	2:J:119:LYS:HZ3	1.49	0.61
1:D:55:GLU:N	1:D:55:GLU:OE1	2.33	0.61
1:D:85:ASP:OD2	1:D:88:SER:N	2.33	0.61
1:D:290:LEU:O	1:D:319:LYS:N	2.34	0.61
1:E:6:THR:HG23	1:E:169:THR:HB	1.83	0.61
1:E:327:LEU:HA	1:E:330:ARG:HE	1.64	0.61
2:A:17:ALA:HA	2:A:70:THR:HG22	1.83	0.61
1:B:15:PRO:HA	1:B:18:ILE:HD12	1.83	0.61
1:C:46:LYS:HG3	1:C:47:THR:H	1.65	0.61
1:E:110:ASP:OD2	1:E:113:GLU:N	2.33	0.61
1:E:212:PRO:HB2	1:E:215:TRP:HB2	1.83	0.61
1:B:56:ILE:HD12	1:B:95:ILE:HG21	1.83	0.61
1:F:341:ILE:O	1:F:345:ASP:N	2.27	0.61
1:G:53:GLY:HA2	1:G:95:ILE:HG13	1.82	0.61
1:I:125:TYR:HB2	1:I:295:GLU:HG3	1.83	0.61
2:L:23:CYS:HB2	2:L:27:ASN:HB2	1.83	0.61
2:J:102:SER:HA	2:J:105:HIS:CD2	2.36	0.61
2:J:109:LEU:HD23	2:J:109:LEU:H	1.66	0.61
1:E:344:LEU:HD13	1:E:367:TRP:HB3	1.83	0.60
1:F:225:ASN:HB3	1:F:228:GLY:HA2	1.82	0.60
1:D:192:GLU:N	1:D:192:GLU:OE1	2.34	0.60
1:F:323:GLU:OE2	1:F:323:GLU:N	2.24	0.60
1:I:45:VAL:HG22	1:I:50:VAL:HG12	1.82	0.60
2:A:21:ASN:HD21	2:K:116:ASP:HB3	1.67	0.60
1:B:261:ALA:O	1:B:265:LYS:NZ	2.24	0.60
1:C:136:ALA:O	1:C:139:THR:OG1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:GLN:OE1	1:G:108:ARG:NH1	2.33	0.60
1:H:45:VAL:HB	1:H:240:GLY:HA3	1.83	0.60
2:J:51:THR:OG1	2:J:69:LYS:NZ	2.33	0.60
1:G:218:SER:O	1:G:221:LYS:NZ	2.34	0.60
1:H:134:MET:HG2	1:H:279:ARG:HH22	1.65	0.60
2:J:30:ARG:HG2	2:J:34:MET:HE1	1.82	0.60
1:E:299:SER:HG	1:E:309:SER:HG	1.43	0.60
1:F:262:PHE:O	1:F:272:ARG:HD2	2.01	0.60
2:J:117:GLY:HA2	2:J:119:LYS:NZ	2.16	0.60
1:H:256:ARG:NE	1:I:253:GLY:O	2.24	0.60
1:H:300:TYR:CZ	1:H:307:PRO:HG3	2.36	0.60
1:I:187:THR:N	1:I:225:ASN:OD1	2.31	0.60
1:C:63:ASP:OD1	1:C:65:GLU:N	2.34	0.60
1:C:85:ASP:OD1	1:C:86:ALA:N	2.34	0.60
1:C:152:ARG:HH21	1:C:153:LYS:HZ3	1.50	0.60
1:F:297:GLN:HE22	1:G:6:THR:H	1.49	0.60
1:G:159:TRP:O	1:G:190:SER:N	2.34	0.60
1:I:25:ALA:HB2	1:I:352:LYS:HD3	1.84	0.60
1:E:157:LEU:HB3	1:E:159:TRP:CZ2	2.36	0.60
1:G:225:ASN:O	1:G:228:GLY:N	2.33	0.60
1:E:246:ILE:HG12	1:E:257:HIS:CE1	2.37	0.60
1:F:136:ALA:O	1:F:139:THR:OG1	2.18	0.60
1:G:238:ASP:OD1	1:G:239:CYS:N	2.35	0.60
1:H:18:ILE:HA	1:H:21:GLN:NE2	2.17	0.60
1:B:297:GLN:HE22	1:B:299:SER:HB3	1.67	0.60
1:C:79:HIS:ND1	1:C:81:ASP:OD1	2.34	0.60
1:D:265:LYS:NZ	1:D:271:ASP:OD1	2.27	0.60
1:F:122:MET:N	1:F:122:MET:SD	2.75	0.60
1:G:249:ASP:HB3	1:G:359:HIS:HD2	1.67	0.60
1:H:63:ASP:OD1	1:H:66:GLU:N	2.24	0.60
1:H:157:LEU:HB2	1:H:160:LEU:HD23	1.84	0.60
1:H:191:GLU:OE1	1:H:229:ARG:NH2	2.35	0.60
1:I:121:LEU:HD13	1:I:299:SER:HB3	1.84	0.60
2:L:22:LEU:HD23	2:L:22:LEU:H	1.65	0.60
1:B:8:GLU:OE2	1:C:119:GLN:NE2	2.35	0.59
1:F:47:THR:HG22	1:F:236:MET:HA	1.82	0.59
2:A:58:ARG:HE	2:A:60:ALA:H	1.50	0.59
1:C:194:ASP:OD1	1:C:197:SER:N	2.35	0.59
1:C:357:TYR:O	1:C:362:ARG:NH2	2.35	0.59
1:E:194:ASP:OD1	1:E:197:SER:N	2.27	0.59
1:G:131:ASP:HB2	2:K:4:THR:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:ASP:OD2	1:I:351:TYR:N	2.35	0.59
2:J:18:PHE:O	2:J:30:ARG:NH2	2.35	0.59
1:F:78:VAL:N	1:F:82:MET:SD	2.75	0.59
1:I:11:SER:HB3	1:I:164:ALA:HB3	1.83	0.59
1:H:130:THR:OG1	1:H:134:MET:N	2.31	0.59
1:I:238:ASP:OD2	1:I:239:CYS:N	2.35	0.59
1:H:16:ASP:OD1	1:H:241:LEU:N	2.33	0.59
1:H:148:GLN:HE21	1:H:160:LEU:HD12	1.65	0.59
2:L:95:ASP:HA	2:L:113:LYS:HD2	1.83	0.59
1:F:84:PHE:CD1	1:F:235:PRO:HG2	2.38	0.59
1:F:157:LEU:HD22	1:F:159:TRP:HE1	1.67	0.59
2:A:123:LEU:HB3	2:A:124:PRO:HD2	1.83	0.59
1:D:194:ASP:OD2	1:D:197:SER:OG	2.17	0.59
1:G:39:VAL:HG22	1:G:56:ILE:HG23	1.84	0.59
2:A:20:SER:OG	2:K:119:LYS:HA	2.03	0.59
2:A:20:SER:OG	2:K:118:TYR:O	2.14	0.59
2:A:53:LEU:HA	2:A:141:THR:O	2.02	0.59
2:K:4:THR:O	2:K:6:GLU:N	2.35	0.59
1:H:251:TYR:OH	1:H:279:ARG:HD3	2.03	0.59
2:A:126:SER:OG	2:A:129:GLU:OE2	2.17	0.59
1:F:325:LEU:O	1:F:329:VAL:HG23	2.02	0.59
1:I:8:GLU:OE1	1:I:167:GLN:HB2	2.03	0.59
2:L:9:ASN:O	2:L:102:SER:OG	2.21	0.59
2:L:55:GLY:O	2:L:67:GLU:HA	2.03	0.59
1:C:114:GLN:HB2	1:C:338:TYR:CE1	2.38	0.58
1:F:79:HIS:N	1:F:82:MET:SD	2.76	0.58
1:F:147:ARG:NH2	1:F:205:GLU:OE2	2.36	0.58
1:I:109:ALA:O	1:I:114:GLN:NE2	2.35	0.58
2:L:77:ASP:HB2	2:L:81:ALA:H	1.68	0.58
2:J:31:HIS:O	2:J:35:VAL:HG23	2.03	0.58
2:J:33:HIS:O	2:J:37:THR:HG23	2.03	0.58
1:I:312:VAL:HG21	1:I:325:LEU:HD11	1.84	0.58
2:J:130:VAL:HG23	2:J:148:ARG:HH12	1.68	0.58
1:E:9:SER:HA	1:E:248:VAL:HG21	1.86	0.58
1:E:327:LEU:HA	1:E:330:ARG:HH21	1.68	0.58
1:F:70:ASN:O	1:F:74:GLU:HG3	2.03	0.58
2:L:101:LYS:HG3	2:L:107:ALA:HB2	1.85	0.58
1:F:365:PHE:HB3	1:F:367:TRP:CE2	2.38	0.58
1:H:6:THR:H	1:I:297:GLN:NE2	2.00	0.58
1:B:134:MET:HG2	1:B:279:ARG:HH12	1.69	0.58
1:D:188:GLN:NE2	1:D:231:VAL:O	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ARG:NH2	1:E:205:GLU:O	2.36	0.58
2:J:4:THR:HG21	2:J:105:HIS:CE1	2.39	0.58
2:J:19:ARG:NH1	2:J:28:MET:SD	2.77	0.58
1:D:2:LYS:HZ1	1:D:171:GLN:HB2	1.67	0.58
2:L:130:VAL:HG12	2:L:132:LYS:H	1.67	0.58
1:D:301:ALA:HB3	1:D:308:THR:HG21	1.86	0.58
1:F:65:GLU:O	1:F:68:THR:OG1	2.21	0.58
1:I:207:ILE:HD11	1:I:224:ILE:HD11	1.85	0.58
1:I:359:HIS:O	1:I:367:TRP:NE1	2.37	0.58
1:B:338:TYR:HA	1:B:341:ILE:HD12	1.84	0.58
1:G:102:ILE:O	1:G:106:VAL:HG23	2.03	0.58
1:I:151:VAL:HG23	1:I:156:THR:HB	1.85	0.58
2:A:42:PRO:O	2:A:46:GLY:N	2.37	0.58
2:K:48:VAL:O	2:K:73:VAL:HA	2.04	0.58
1:B:136:ALA:O	1:B:139:THR:OG1	2.18	0.58
1:B:362:ARG:HB2	1:B:365:PHE:CE2	2.39	0.58
1:C:214:GLU:H	1:C:214:GLU:CD	2.06	0.58
1:D:46:LYS:NZ	1:D:239:CYS:HB2	2.19	0.58
1:C:69:ARG:NH1	1:C:86:ALA:O	2.35	0.57
1:G:27:LEU:HD13	1:G:39:VAL:HG11	1.85	0.57
1:G:97:LYS:N	1:I:65:GLU:OE1	2.37	0.57
2:L:48:VAL:O	2:L:73:VAL:HA	2.04	0.57
2:L:108:GLY:HA3	2:L:122:ARG:HA	1.86	0.57
1:D:314:THR:OG1	1:D:318:GLU:OE2	2.19	0.57
1:H:43:THR:O	1:H:242:THR:OG1	2.18	0.57
2:A:109:LEU:H	2:A:109:LEU:HD23	1.69	0.57
1:G:246:ILE:HD11	1:G:257:HIS:CE1	2.39	0.57
1:H:67:ILE:O	1:H:71:THR:OG1	2.16	0.57
1:D:84:PHE:CG	1:D:235:PRO:HG2	2.39	0.57
1:E:214:GLU:N	1:E:214:GLU:OE2	2.34	0.57
1:G:284:ASN:OD1	1:G:373:ALA:N	2.36	0.57
1:C:279:ARG:NH1	1:C:360:PHE:HB3	2.19	0.57
1:D:23:SER:OG	1:D:263:SER:OG	2.23	0.57
1:E:151:VAL:HG23	1:E:156:THR:HB	1.85	0.57
1:G:77:TYR:O	1:G:86:ALA:N	2.36	0.57
1:I:179:GLY:HA2	1:I:215:TRP:CD1	2.39	0.57
1:C:125:TYR:N	1:C:251:TYR:OH	2.26	0.57
1:E:207:ILE:HG23	1:E:211:LEU:HD23	1.85	0.57
1:F:371:ASP:OD1	1:F:372:LYS:N	2.37	0.57
1:G:307:PRO:HG2	1:G:335:LEU:HB3	1.87	0.57
2:K:94:GLN:HE21	2:K:96:CYS:H	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:NH1	1:B:86:ALA:O	2.37	0.57
1:D:39:VAL:HG22	1:D:56:ILE:HG12	1.86	0.57
1:D:43:THR:HG22	1:D:52:VAL:HG12	1.85	0.57
1:D:132:VAL:O	1:D:283:LYS:NZ	2.33	0.57
1:F:61:TRP:HB3	1:H:61:TRP:CD2	2.40	0.57
1:B:63:ASP:OD1	1:B:65:GLU:N	2.38	0.57
1:C:161:ARG:HB2	1:C:188:GLN:HB3	1.87	0.57
1:E:262:PHE:O	1:E:272:ARG:NH2	2.36	0.57
1:H:363:GLU:HA	1:H:368:GLU:HB3	1.87	0.57
2:J:47:SER:HA	2:J:74:ARG:O	2.05	0.57
1:D:38:ARG:HB2	1:D:57:THR:OG1	2.05	0.57
1:D:118:ASP:OD1	1:D:119:GLN:N	2.38	0.57
1:H:17:LYS:NZ	1:H:355:ALA:O	2.36	0.57
1:C:203:MET:O	1:C:208:LYS:HG2	2.04	0.56
1:F:167:GLN:HB3	1:F:184:VAL:CG2	2.35	0.56
1:G:180:ILE:H	1:G:215:TRP:HB3	1.69	0.56
2:L:12:TYR:HB2	2:L:75:CYS:SG	2.45	0.56
2:L:135:PRO:O	2:L:148:ARG:NH1	2.37	0.56
1:C:110:ASP:HB3	1:C:113:GLU:HB2	1.87	0.56
1:C:371:ASP:OD1	1:C:372:LYS:N	2.37	0.56
1:D:138:ILE:HB	1:D:252:GLY:HA3	1.86	0.56
1:H:130:THR:HG1	1:H:134:MET:H	1.53	0.56
1:I:10:VAL:HG12	1:I:165:LYS:HG2	1.87	0.56
2:A:11:PHE:CE1	2:A:76:LYS:HB3	2.39	0.56
2:K:17:ALA:HB2	2:K:70:THR:HG22	1.88	0.56
2:J:60:ALA:O	2:J:64:ALA:N	2.39	0.56
1:D:11:SER:HB3	1:D:164:ALA:HB3	1.87	0.56
1:H:351:TYR:HA	1:H:354:THR:HG22	1.86	0.56
1:I:247:ILE:H	1:I:247:ILE:HD12	1.70	0.56
2:L:19:ARG:O	2:L:27:ASN:ND2	2.37	0.56
2:A:21:ASN:ND2	2:K:116:ASP:HB3	2.20	0.56
1:F:16:ASP:OD1	1:F:240:GLY:HA2	2.06	0.56
1:F:46:LYS:HD3	1:F:47:THR:H	1.71	0.56
1:H:81:ASP:OD1	1:H:82:MET:N	2.38	0.56
1:I:77:TYR:CZ	1:I:162:PRO:HB2	2.40	0.56
1:B:3:HIS:HB2	1:C:311:MET:HG3	1.88	0.56
1:B:188:GLN:HA	1:B:230:PHE:HD2	1.70	0.56
1:C:281:VAL:HG23	1:C:333:PHE:CZ	2.39	0.56
1:F:6:THR:O	1:G:297:GLN:NE2	2.38	0.56
1:I:64:ILE:O	1:I:68:THR:OG1	2.18	0.56
1:B:187:THR:H	1:B:225:ASN:HD21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:TYR:CE2	1:E:162:PRO:HB2	2.40	0.56
1:I:53:GLY:HA2	1:I:94:ALA:O	2.05	0.56
2:L:9:ASN:HA	2:L:103:GLN:OE1	2.05	0.56
2:L:18:PHE:HA	2:L:94:GLN:HE21	1.70	0.56
2:K:44:LEU:HD23	2:K:44:LEU:H	1.70	0.56
2:J:127:PHE:CD2	2:J:128:GLN:HG2	2.41	0.56
2:J:131:PRO:HD2	2:J:148:ARG:HH21	1.70	0.56
1:D:366:PRO:HD2	1:D:367:TRP:CZ3	2.41	0.56
1:E:77:TYR:HE2	1:E:162:PRO:HB2	1.71	0.56
1:F:147:ARG:O	1:F:151:VAL:HG23	2.06	0.56
2:L:31:HIS:O	2:L:35:VAL:HG23	2.05	0.56
1:B:367:TRP:CD1	1:B:368:GLU:HG2	2.40	0.56
1:E:69:ARG:NH2	1:E:89:CYS:O	2.38	0.56
1:E:85:ASP:OD1	1:E:86:ALA:N	2.39	0.56
1:H:125:TYR:OH	1:H:293:ARG:NE	2.29	0.56
1:H:144:LEU:HD21	1:H:211:LEU:HD21	1.87	0.56
2:A:3:PHE:HB3	2:A:5:LYS:NZ	2.21	0.56
1:C:279:ARG:HH11	1:C:360:PHE:HB3	1.70	0.56
1:D:101:ASP:OD1	1:D:101:ASP:N	2.37	0.56
1:G:15:PRO:HA	1:G:18:ILE:HD12	1.87	0.56
1:G:22:ILE:O	1:G:26:VAL:HG23	2.07	0.56
1:I:202:VAL:HG11	1:I:224:ILE:HG21	1.87	0.56
1:B:86:ALA:HA	1:B:89:CYS:SG	2.46	0.55
1:H:203:MET:HB3	1:H:208:LYS:NZ	2.21	0.55
1:D:119:GLN:HA	1:D:300:TYR:O	2.06	0.55
1:E:11:SER:HB3	1:E:164:ALA:HB3	1.87	0.55
1:G:266:ASP:N	1:G:266:ASP:OD1	2.38	0.55
1:H:100:PRO:HB2	1:H:104:GLN:HE22	1.72	0.55
2:L:21:ASN:O	2:L:27:ASN:ND2	2.39	0.55
1:C:122:MET:N	1:C:122:MET:SD	2.78	0.55
1:E:72:VAL:HA	1:E:75:ILE:HD12	1.89	0.55
1:H:121:LEU:HD13	1:H:299:SER:HB2	1.87	0.55
1:I:18:ILE:O	1:I:22:ILE:HG13	2.06	0.55
2:L:59:GLU:HG2	2:J:120:ALA:HB3	1.87	0.55
1:B:184:VAL:HG22	1:B:223:PHE:HB2	1.87	0.55
1:C:239:CYS:SG	1:C:240:GLY:N	2.79	0.55
1:E:46:LYS:HG3	1:E:47:THR:N	2.21	0.55
2:K:34:MET:O	2:K:37:THR:OG1	2.22	0.55
1:D:297:GLN:HB3	1:D:311:MET:HB3	1.89	0.55
2:L:138:GLY:HA3	2:L:149:TRP:CH2	2.41	0.55
1:C:204:GLU:O	1:C:209:PRO:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:THR:OG1	1:E:251:TYR:N	2.37	0.55
1:H:338:TYR:O	1:H:342:GLN:HG2	2.06	0.55
1:I:68:THR:O	1:I:71:THR:OG1	2.21	0.55
2:A:34:MET:HG2	2:A:92:TRP:CE2	2.42	0.55
1:C:151:VAL:HA	1:C:154:ASN:HD21	1.72	0.55
1:D:203:MET:O	1:D:207:ILE:HB	2.07	0.55
1:D:279:ARG:NH1	1:D:360:PHE:HB3	2.21	0.55
1:D:332:PHE:CG	1:D:376:LEU:HG	2.42	0.55
1:D:338:TYR:HA	1:D:341:ILE:HD12	1.88	0.55
1:B:325:LEU:O	1:B:329:VAL:HG23	2.07	0.55
1:E:225:ASN:O	1:E:228:GLY:N	2.33	0.55
1:E:337:PRO:O	1:E:340:LEU:HG	2.06	0.55
1:F:372:LYS:HA	1:F:375:LEU:HD13	1.88	0.55
1:G:279:ARG:NH1	1:G:360:PHE:HB3	2.22	0.55
1:G:300:TYR:HE2	1:G:337:PRO:HD3	1.72	0.55
1:G:337:PRO:O	1:G:340:LEU:HG	2.06	0.55
1:I:150:GLU:O	1:I:154:ASN:ND2	2.40	0.55
2:L:19:ARG:HH21	2:L:68:GLU:HA	1.71	0.55
2:L:20:SER:HB2	2:J:119:LYS:CD	2.37	0.55
2:L:67:GLU:OE1	2:L:67:GLU:N	2.40	0.55
1:D:203:MET:HG3	1:D:207:ILE:HD12	1.89	0.55
1:G:135:PRO:HB3	1:G:254:MET:HG2	1.88	0.55
1:H:346:LEU:HB3	1:H:351:TYR:OH	2.07	0.55
1:I:148:GLN:HG2	1:I:160:LEU:HD21	1.89	0.55
2:L:139:CYS:HA	2:L:148:ARG:CZ	2.37	0.55
2:A:80:GLN:H	2:A:80:GLN:CD	2.11	0.55
2:J:23:CYS:O	2:J:27:ASN:N	2.29	0.55
1:B:65:GLU:HA	1:B:91:VAL:HG11	1.89	0.55
1:I:337:PRO:O	1:I:340:LEU:HG	2.07	0.55
2:J:141:THR:HB	2:J:146:GLY:HA2	1.89	0.55
1:B:272:ARG:HH21	1:B:359:HIS:HE1	1.53	0.54
1:B:346:LEU:O	1:B:351:TYR:OH	2.25	0.54
1:C:9:SER:HA	1:C:248:VAL:HG21	1.89	0.54
1:C:61:TRP:HB3	1:E:61:TRP:CD2	2.43	0.54
1:C:149:ALA:O	1:C:153:LYS:HG2	2.06	0.54
1:D:81:ASP:OD1	1:D:82:MET:N	2.40	0.54
1:F:39:VAL:HG13	1:F:56:ILE:HG12	1.88	0.54
1:I:56:ILE:HG22	1:I:58:THR:HG23	1.89	0.54
2:L:95:ASP:OD1	2:L:96:CYS:N	2.40	0.54
1:F:13:GLY:O	1:F:77:TYR:OH	2.20	0.54
1:F:60:ALA:O	1:F:98:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:LEU:O	1:G:351:TYR:OH	2.25	0.54
1:D:121:LEU:HD13	1:E:6:THR:HB	1.90	0.54
1:G:261:ALA:O	1:G:265:LYS:NZ	2.38	0.54
2:L:127:PHE:O	2:L:129:GLU:HG3	2.07	0.54
2:K:3:PHE:HD2	2:K:5:LYS:HZ3	1.52	0.54
1:B:266:ASP:OD2	1:B:268:SER:N	2.33	0.54
1:D:199:GLN:HG2	1:D:224:ILE:HB	1.89	0.54
1:E:332:PHE:CE2	1:E:375:LEU:HG	2.42	0.54
1:G:31:LEU:HD12	1:G:35:PRO:HA	1.90	0.54
1:I:100:PRO:HA	1:I:103:ASN:HB2	1.88	0.54
2:A:39:ARG:HD3	2:A:49:GLU:OE2	2.07	0.54
1:C:383:LYS:O	1:C:384:HIS:ND1	2.41	0.54
1:F:24:ASP:OD1	1:F:264:GLY:N	2.35	0.54
1:H:27:LEU:HD11	1:H:266:ASP:HA	1.90	0.54
1:H:266:ASP:OD1	1:H:269:LYS:N	2.39	0.54
1:I:35:PRO:HB2	1:I:36:LYS:HD3	1.89	0.54
2:A:21:ASN:OD1	2:A:22:LEU:N	2.40	0.54
1:F:327:LEU:HG	1:F:330:ARG:HH21	1.73	0.54
1:G:129:GLU:O	2:K:2:ILE:N	2.41	0.54
1:H:362:ARG:HB3	1:H:364:HIS:CE1	2.43	0.54
2:K:72:ARG:HH21	2:K:142:ILE:HD13	1.72	0.54
1:B:140:TYR:CE2	2:A:5:LYS:HE3	2.43	0.54
1:B:151:VAL:HA	1:B:154:ASN:HD21	1.73	0.54
1:D:167:GLN:HG2	1:D:184:VAL:HB	1.90	0.54
1:E:81:ASP:OD1	1:E:82:MET:N	2.39	0.54
1:F:334:ASP:OD2	1:F:339:GLY:HA3	2.08	0.54
1:F:338:TYR:HA	1:F:341:ILE:HD12	1.89	0.54
2:L:21:ASN:HA	2:J:118:TYR:HD1	1.72	0.54
2:A:48:VAL:O	2:A:73:VAL:HA	2.07	0.54
2:A:100:TYR:HA	2:A:107:ALA:HB3	1.89	0.54
1:B:332:PHE:O	1:B:372:LYS:NZ	2.37	0.54
1:G:22:ILE:HG23	1:G:68:THR:HG22	1.89	0.54
1:G:157:LEU:O	1:G:160:LEU:HB2	2.08	0.54
1:G:357:TYR:O	1:G:362:ARG:NH1	2.41	0.54
2:J:118:TYR:C	2:J:119:LYS:HD3	2.29	0.54
1:C:56:ILE:HD13	1:C:95:ILE:HG23	1.89	0.54
1:E:281:VAL:HG21	1:E:329:VAL:HG13	1.90	0.54
1:G:116:ALA:O	1:G:303:GLY:N	2.39	0.54
1:G:196:LYS:HA	1:G:199:GLN:OE1	2.07	0.54
1:I:5:PHE:HD1	1:I:137:PRO:HG2	1.72	0.54
2:L:137:GLN:NE2	2:L:148:ARG:HB2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ARG:HD3	1:D:351:TYR:HE1	1.73	0.54
1:F:97:LYS:O	1:F:99:SER:OG	2.19	0.54
1:F:143:ARG:HE	2:L:5:LYS:NZ	2.06	0.54
1:H:135:PRO:HB2	1:H:138:ILE:HG22	1.90	0.54
1:C:152:ARG:CZ	1:C:162:PRO:HA	2.38	0.53
1:D:110:ASP:OD2	1:D:113:GLU:N	2.41	0.53
1:D:229:ARG:HE	1:D:231:VAL:HG22	1.73	0.53
1:H:134:MET:HE3	1:H:279:ARG:HH12	1.71	0.53
1:H:253:GLY:O	1:I:256:ARG:NE	2.36	0.53
1:I:180:ILE:HG13	1:I:215:TRP:HB3	1.90	0.53
1:I:251:TYR:OH	1:I:279:ARG:NH1	2.40	0.53
1:E:213:ALA:HA	1:E:216:LEU:HD12	1.89	0.53
1:G:246:ILE:O	1:G:250:THR:HG23	2.08	0.53
1:H:85:ASP:OD1	1:H:86:ALA:N	2.42	0.53
1:I:272:ARG:NH2	1:I:351:TYR:HB3	2.23	0.53
1:D:163:ASP:HB3	1:D:188:GLN:HB2	1.90	0.53
1:F:38:ARG:HB2	1:F:57:THR:HB	1.90	0.53
1:F:45:VAL:HB	1:F:240:GLY:HA3	1.89	0.53
1:F:202:VAL:HG23	1:F:206:ILE:HD13	1.90	0.53
1:G:168:VAL:HG23	1:G:183:VAL:HG22	1.89	0.53
1:G:229:ARG:NH1	1:G:231:VAL:H	2.03	0.53
1:H:161:ARG:HH21	1:H:190:SER:HA	1.74	0.53
1:H:167:GLN:HE21	1:H:184:VAL:HG21	1.73	0.53
1:H:203:MET:HB3	1:H:208:LYS:HZ3	1.74	0.53
1:I:20:ASP:OD1	1:I:242:THR:HA	2.08	0.53
1:I:323:GLU:O	1:I:327:LEU:HG	2.08	0.53
2:J:117:GLY:HA2	2:J:119:LYS:HZ3	1.71	0.53
1:D:1:ALA:N	1:D:174:ASP:H	2.07	0.53
1:D:58:THR:OG1	1:D:59:SER:N	2.41	0.53
1:D:181:ASP:OD1	1:D:221:LYS:NZ	2.36	0.53
1:E:366:PRO:HD2	1:E:367:TRP:CZ3	2.43	0.53
1:F:30:ILE:HG21	1:F:39:VAL:HG21	1.90	0.53
2:L:21:ASN:HA	2:J:118:TYR:HB3	1.90	0.53
2:A:108:GLY:HA2	2:A:123:LEU:HG	1.90	0.53
2:A:149:TRP:HE1	2:K:123:LEU:HD22	1.73	0.53
1:F:151:VAL:HG13	1:F:156:THR:HB	1.90	0.53
1:H:40:ALA:HB2	1:H:269:LYS:HE2	1.89	0.53
1:H:239:CYS:SG	1:I:42:GLU:HG3	2.48	0.53
1:H:314:THR:HG23	1:H:316:GLY:H	1.73	0.53
1:I:292:ASP:HB2	1:I:317:THR:HB	1.90	0.53
2:K:49:GLU:N	2:K:49:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ILE:O	1:C:26:VAL:HG23	2.09	0.53
1:D:257:HIS:CE1	1:D:259:GLY:H	2.27	0.53
1:E:219:ALA:O	1:E:221:LYS:NZ	2.29	0.53
2:A:75:CYS:HB3	2:A:81:ALA:HB3	1.90	0.53
1:D:27:LEU:HD13	1:D:39:VAL:HG11	1.89	0.53
1:F:81:ASP:OD1	1:F:81:ASP:N	2.42	0.53
1:H:296:ILE:HG22	1:H:298:VAL:HG13	1.90	0.53
2:J:103:GLN:HG2	2:J:104:THR:HG23	1.89	0.53
1:G:49:MET:HA	1:G:90:ALA:HB3	1.90	0.53
1:I:122:MET:HE3	1:I:271:ASP:HA	1.91	0.53
1:I:138:ILE:HD11	1:I:252:GLY:HA3	1.91	0.53
1:I:163:ASP:HB3	1:I:188:GLN:HB2	1.90	0.53
2:J:84:VAL:HA	2:J:87:LEU:HD12	1.91	0.53
1:B:38:ARG:HG2	1:B:269:LYS:NZ	2.24	0.53
1:B:57:THR:HB	1:B:98:GLN:NE2	2.23	0.53
1:E:214:GLU:HG2	1:E:215:TRP:HD1	1.74	0.53
1:G:46:LYS:HB3	1:G:49:MET:HB3	1.91	0.53
1:H:366:PRO:HA	1:H:369:LYS:HE2	1.90	0.53
2:L:4:THR:O	2:L:7:PRO:HD2	2.09	0.53
1:B:344:LEU:HB2	1:B:346:LEU:HG	1.91	0.53
1:C:213:ALA:HA	1:C:216:LEU:HB2	1.91	0.53
2:J:17:ALA:H	2:J:94:GLN:CD	2.12	0.53
2:J:19:ARG:HB2	2:J:68:GLU:HB3	1.89	0.53
1:B:112:LEU:HD12	1:B:336:ARG:HD2	1.90	0.52
1:D:113:GLU:HA	1:D:336:ARG:CZ	2.39	0.52
1:F:58:THR:OG1	1:F:59:SER:N	2.43	0.52
1:F:92:LEU:HD13	1:H:94:ALA:HB2	1.90	0.52
1:F:212:PRO:HG2	1:F:215:TRP:CE3	2.44	0.52
1:H:119:GLN:OE1	1:I:167:GLN:HB3	2.09	0.52
1:H:194:ASP:OD1	1:H:197:SER:OG	2.17	0.52
1:H:241:LEU:HD21	1:I:42:GLU:HB3	1.91	0.52
1:I:22:ILE:O	1:I:26:VAL:HG23	2.09	0.52
2:J:39:ARG:NE	2:J:49:GLU:OE2	2.41	0.52
1:D:336:ARG:O	1:D:340:LEU:HG	2.09	0.52
1:E:71:THR:O	1:E:75:ILE:HG13	2.09	0.52
1:E:167:GLN:HB3	1:E:184:VAL:HB	1.91	0.52
1:H:70:ASN:O	1:H:74:GLU:HG3	2.09	0.52
1:I:212:PRO:HG2	1:I:215:TRP:CE3	2.45	0.52
2:J:102:SER:HA	2:J:105:HIS:HD2	1.73	0.52
1:B:85:ASP:CG	1:B:87:ASN:HD22	2.13	0.52
1:H:365:PHE:HB3	1:H:367:TRP:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:ALA:HA	2:L:70:THR:HG22	1.92	0.52
2:A:60:ALA:CB	2:K:108:GLY:H	2.23	0.52
2:K:126:SER:OG	2:K:127:PHE:N	2.42	0.52
1:B:180:ILE:N	1:B:215:TRP:HB3	2.21	0.52
1:C:122:MET:HA	1:C:258:GLY:HA3	1.90	0.52
1:D:229:ARG:HE	1:D:231:VAL:CG2	2.22	0.52
1:E:77:TYR:HB3	1:E:84:PHE:O	2.09	0.52
1:E:280:TYR:O	1:E:284:ASN:ND2	2.41	0.52
1:G:149:ALA:O	1:G:153:LYS:HG2	2.09	0.52
1:H:1:ALA:HB3	1:H:174:ASP:HA	1.91	0.52
1:H:72:VAL:HG21	1:H:84:PHE:HE2	1.74	0.52
1:I:65:GLU:HA	1:I:91:VAL:HG11	1.92	0.52
1:I:142:HIS:CE1	1:I:248:VAL:HG22	2.45	0.52
2:L:98:LEU:HD13	2:L:109:LEU:HB3	1.92	0.52
2:A:6:GLU:OE1	2:A:6:GLU:N	2.27	0.52
1:C:24:ASP:OD1	1:C:352:LYS:HA	2.09	0.52
1:D:157:LEU:HB3	1:D:159:TRP:CE2	2.45	0.52
1:F:180:ILE:HG21	1:F:183:VAL:HG23	1.90	0.52
1:G:229:ARG:NH2	1:G:231:VAL:HB	2.22	0.52
1:H:23:SER:OG	1:H:24:ASP:N	2.43	0.52
1:H:251:TYR:HB3	1:H:254:MET:HB3	1.92	0.52
1:I:266:ASP:OD2	1:I:269:LYS:N	2.42	0.52
1:I:330:ARG:HG2	1:I:335:LEU:HD21	1.92	0.52
1:B:169:THR:OG1	1:B:182:ALA:N	2.43	0.52
1:E:63:ASP:CG	1:E:66:GLU:HG2	2.30	0.52
1:E:326:THR:HG22	1:E:330:ARG:HD3	1.92	0.52
1:E:332:PHE:HE2	1:E:375:LEU:HG	1.75	0.52
1:F:189:HIS:ND1	1:F:190:SER:O	2.42	0.52
1:G:66:GLU:HB3	1:I:97:LYS:HD2	1.91	0.52
1:H:6:THR:H	1:I:297:GLN:HE22	1.56	0.52
1:H:22:ILE:O	1:H:26:VAL:HG23	2.10	0.52
1:H:46:LYS:HD3	1:H:47:THR:HG23	1.90	0.52
1:H:140:TYR:O	1:H:144:LEU:HG	2.09	0.52
1:I:184:VAL:HG22	1:I:223:PHE:HD2	1.74	0.52
1:I:192:GLU:OE1	1:I:192:GLU:N	2.34	0.52
2:L:53:LEU:HG	2:L:70:THR:OG1	2.10	0.52
1:B:14:HIS:CE1	1:B:16:ASP:H	2.27	0.52
1:B:65:GLU:OE1	1:B:69:ARG:NE	2.41	0.52
1:B:166:SER:OG	1:B:185:LEU:HD13	2.10	0.52
1:I:72:VAL:HB	1:I:86:ALA:HB2	1.90	0.52
1:I:362:ARG:HB3	1:I:364:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PRO:HG2	1:B:215:TRP:CZ3	2.45	0.52
1:G:65:GLU:O	1:G:68:THR:OG1	2.27	0.52
1:D:174:ASP:HB2	1:D:176:LYS:HG2	1.92	0.52
1:D:333:PHE:HD1	1:D:343:MET:SD	2.33	0.52
1:I:50:VAL:HG23	1:I:91:VAL:HA	1.90	0.52
1:I:202:VAL:HG23	1:I:206:ILE:HD12	1.92	0.52
2:J:33:HIS:O	2:J:36:SER:OG	2.19	0.52
1:B:364:HIS:O	1:B:369:LYS:NZ	2.43	0.52
1:F:151:VAL:HA	1:F:154:ASN:HD21	1.75	0.52
1:G:40:ALA:O	1:G:54:GLY:HA3	2.11	0.52
1:G:110:ASP:N	1:G:113:GLU:OE1	2.36	0.52
1:G:138:ILE:HB	1:G:252:GLY:HA3	1.92	0.52
1:I:68:THR:O	1:I:72:VAL:HG23	2.10	0.52
1:E:325:LEU:O	1:E:329:VAL:HG23	2.10	0.51
1:G:356:ALA:O	1:G:362:ARG:NH1	2.36	0.51
2:K:44:LEU:HG	2:K:45:TYR:N	2.25	0.51
1:B:284:ASN:OD1	1:B:373:ALA:N	2.44	0.51
1:C:44:TYR:HE1	1:C:46:LYS:HB2	1.75	0.51
1:E:188:GLN:HA	1:E:230:PHE:HD2	1.74	0.51
1:F:338:TYR:O	1:F:342:GLN:HG2	2.11	0.51
1:I:29:ALA:O	1:I:33:GLN:HG2	2.10	0.51
1:I:317:THR:O	1:I:319:LYS:NZ	2.37	0.51
1:I:324:GLN:HE22	1:I:328:LEU:HD11	1.74	0.51
2:L:86:ARG:HH22	2:L:115:ILE:C	2.13	0.51
1:B:46:LYS:NZ	1:B:239:CYS:HB2	2.25	0.51
1:C:217:THR:OG1	1:C:220:THR:N	2.43	0.51
1:C:266:ASP:O	1:C:269:LYS:HB2	2.10	0.51
1:E:57:THR:HA	1:E:98:GLN:O	2.11	0.51
1:E:323:GLU:O	1:E:327:LEU:HG	2.11	0.51
1:F:297:GLN:NE2	1:G:6:THR:H	2.09	0.51
1:H:283:LYS:NZ	1:H:368:GLU:OE2	2.43	0.51
2:J:50:SER:HB2	2:J:72:ARG:HG3	1.91	0.51
1:B:24:ASP:OD1	1:B:264:GLY:N	2.41	0.51
1:B:58:THR:OG1	1:B:59:SER:N	2.43	0.51
1:D:1:ALA:O	1:D:3:HIS:ND1	2.43	0.51
2:J:146:GLY:HA3	2:J:148:ARG:NH1	2.25	0.51
1:B:170:PHE:CD1	1:B:180:ILE:HG12	2.46	0.51
1:D:66:GLU:OE2	1:D:70:ASN:ND2	2.38	0.51
1:H:152:ARG:CZ	1:H:162:PRO:HA	2.41	0.51
1:I:39:VAL:HG22	1:I:56:ILE:HG23	1.92	0.51
1:B:15:PRO:O	1:B:18:ILE:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:GLN:HA	1:E:224:ILE:HG21	1.93	0.51
1:H:3:HIS:CE1	1:H:175:GLY:HA2	2.46	0.51
2:A:135:PRO:HA	2:A:148:ARG:HH12	1.76	0.51
1:B:1:ALA:O	1:B:173:ASP:HA	2.11	0.51
1:D:52:VAL:HG21	1:D:64:ILE:HG21	1.93	0.51
1:D:161:ARG:HB2	1:D:188:GLN:HB3	1.93	0.51
1:D:300:TYR:OH	1:D:307:PRO:HG3	2.11	0.51
1:G:38:ARG:HB2	1:G:57:THR:OG1	2.11	0.51
2:A:23:CYS:O	2:A:27:ASN:N	2.34	0.51
2:K:109:LEU:O	2:K:121:GLU:HB2	2.10	0.51
1:B:308:THR:OG1	1:B:309:SER:N	2.44	0.51
1:D:125:TYR:HB2	1:D:295:GLU:HG3	1.93	0.51
1:D:327:LEU:HA	1:D:330:ARG:HH21	1.76	0.51
1:F:32:GLU:HB2	1:F:349:PRO:HG3	1.91	0.51
1:H:152:ARG:HH21	1:H:153:LYS:NZ	2.09	0.51
1:I:194:ASP:O	1:I:198:LEU:HB2	2.11	0.51
2:L:18:PHE:HE1	2:L:89:CYS:HA	1.76	0.51
2:A:96:CYS:HB3	2:A:111:TYR:HB3	1.93	0.51
2:A:130:VAL:HG11	2:A:148:ARG:HG2	1.92	0.51
1:C:225:ASN:O	1:C:228:GLY:N	2.44	0.51
1:E:172:TYR:HA	1:E:177:ILE:HA	1.93	0.51
1:F:373:ALA:O	1:F:377:ARG:N	2.34	0.51
1:G:327:LEU:HG	1:G:330:ARG:HH21	1.75	0.51
1:I:229:ARG:HA	1:I:229:ARG:HE	1.76	0.51
1:F:143:ARG:HA	1:F:146:GLN:NE2	2.25	0.51
1:G:325:LEU:O	1:G:329:VAL:HG23	2.11	0.51
2:K:130:VAL:HG22	2:K:132:LYS:H	1.76	0.51
1:B:250:THR:OG1	1:B:251:TYR:N	2.44	0.50
1:D:159:TRP:CE3	1:D:193:ILE:HG21	2.47	0.50
1:D:272:ARG:HD3	1:D:351:TYR:CE1	2.46	0.50
1:E:151:VAL:HA	1:E:154:ASN:ND2	2.26	0.50
1:G:122:MET:N	1:G:122:MET:SD	2.84	0.50
1:G:198:LEU:O	1:G:202:VAL:HG12	2.10	0.50
1:I:144:LEU:HG	1:I:210:ILE:HG21	1.92	0.50
2:J:83:ASN:HA	2:J:86:ARG:CD	2.41	0.50
1:D:171:GLN:HE21	1:D:179:GLY:HA3	1.76	0.50
1:E:366:PRO:HA	1:E:369:LYS:HD3	1.92	0.50
1:I:272:ARG:NH2	1:I:359:HIS:HE1	2.10	0.50
1:B:185:LEU:O	1:B:224:ILE:HA	2.11	0.50
1:D:282:ALA:O	1:D:286:VAL:HG23	2.12	0.50
1:D:371:ASP:OD1	1:D:372:LYS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:SER:HB3	1:F:164:ALA:HB3	1.93	0.50
2:L:130:VAL:HB	2:L:146:GLY:O	2.10	0.50
1:B:104:GLN:HA	1:B:107:ASP:OD1	2.12	0.50
1:E:124:GLY:O	1:E:295:GLU:HA	2.11	0.50
1:G:284:ASN:HD21	1:G:370:THR:HA	1.77	0.50
1:H:322:SER:HA	1:H:325:LEU:HD12	1.92	0.50
1:I:46:LYS:HG3	1:I:47:THR:H	1.76	0.50
1:I:262:PHE:O	1:I:272:ARG:NH1	2.43	0.50
2:L:47:SER:HB3	2:L:73:VAL:HB	1.94	0.50
2:A:12:TYR:HB2	2:A:82:LEU:HD11	1.92	0.50
2:A:96:CYS:HB2	2:A:109:LEU:HD12	1.92	0.50
2:J:23:CYS:HB3	2:J:26:VAL:HG13	1.94	0.50
1:B:165:LYS:HB3	1:C:119:GLN:HE22	1.76	0.50
1:C:2:LYS:HA	1:C:172:TYR:O	2.12	0.50
1:C:75:ILE:O	1:C:153:LYS:NZ	2.43	0.50
1:C:246:ILE:HG12	1:C:257:HIS:CE1	2.44	0.50
1:E:238:ASP:OD1	1:E:239:CYS:N	2.45	0.50
1:F:203:MET:HG2	1:F:207:ILE:HD12	1.93	0.50
1:H:229:ARG:HH11	1:H:229:ARG:HA	1.76	0.50
1:H:229:ARG:HA	1:H:229:ARG:NH1	2.25	0.50
2:J:56:CYS:SG	2:J:65:PRO:HB3	2.52	0.50
1:B:20:ASP:OD1	1:B:243:GLY:N	2.36	0.50
1:B:308:THR:HG1	1:B:309:SER:N	2.10	0.50
1:E:135:PRO:O	1:E:139:THR:HG23	2.11	0.50
1:E:294:CYS:SG	1:E:295:GLU:N	2.84	0.50
1:E:347:LEU:O	1:E:348:HIS:ND1	2.45	0.50
1:F:143:ARG:HB3	1:F:143:ARG:HH11	1.76	0.50
1:F:169:THR:O	1:F:181:ASP:N	2.45	0.50
1:H:266:ASP:OD1	1:H:269:LYS:HG2	2.12	0.50
1:H:267:PRO:HG3	1:H:351:TYR:OH	2.12	0.50
1:I:191:GLU:OE1	1:I:231:VAL:HG21	2.12	0.50
2:K:128:GLN:N	2:K:148:ARG:O	2.44	0.50
2:J:53:LEU:HD23	2:J:54:THR:N	2.26	0.50
1:B:199:GLN:OE1	1:B:224:ILE:HB	2.12	0.50
1:D:136:ALA:O	1:D:139:THR:OG1	2.20	0.50
1:D:214:GLU:HG2	1:D:215:TRP:N	2.26	0.50
1:E:33:GLN:CD	1:E:61:TRP:H	2.14	0.50
1:F:244:ARG:NH2	1:G:42:GLU:OE2	2.43	0.50
1:G:130:THR:HB	2:K:5:LYS:HG3	1.94	0.50
1:H:171:GLN:O	1:H:177:ILE:HA	2.12	0.50
2:K:45:TYR:O	2:K:81:ALA:HB1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:VAL:HG12	1:C:306:GLU:H	1.77	0.50
1:C:354:THR:OG1	1:C:359:HIS:ND1	2.36	0.50
1:D:194:ASP:OD1	1:D:196:LYS:N	2.44	0.50
1:E:23:SER:OG	1:E:41:CYS:O	2.30	0.50
1:E:157:LEU:O	1:E:159:TRP:N	2.44	0.50
1:I:5:PHE:CD1	1:I:137:PRO:HG2	2.47	0.50
1:I:140:TYR:N	1:I:143:ARG:HH21	2.09	0.50
1:I:272:ARG:HG2	1:I:276:TYR:CE2	2.47	0.50
2:L:33:HIS:O	2:L:36:SER:OG	2.23	0.50
2:K:87:LEU:HD13	2:K:115:ILE:HD12	1.93	0.50
1:E:8:GLU:HB2	1:E:166:SER:O	2.12	0.50
1:H:141:ALA:O	1:H:145:VAL:HG22	2.12	0.50
2:L:59:GLU:CG	2:J:120:ALA:HB3	2.42	0.50
1:F:6:THR:H	1:G:297:GLN:NE2	2.08	0.49
1:F:38:ARG:HE	1:F:57:THR:HG21	1.77	0.49
1:F:362:ARG:HD2	1:F:365:PHE:CZ	2.47	0.49
1:G:7:SER:OG	1:G:137:PRO:HB2	2.12	0.49
1:I:165:LYS:O	1:I:185:LEU:HD12	2.12	0.49
2:L:112:ALA:HB2	2:L:119:LYS:H	1.76	0.49
2:K:119:LYS:NZ	2:K:120:ALA:H	2.09	0.49
1:E:113:GLU:HA	1:E:336:ARG:CZ	2.41	0.49
1:E:371:ASP:N	1:E:371:ASP:OD1	2.44	0.49
1:G:123:PHE:HA	1:G:296:ILE:O	2.12	0.49
1:H:139:THR:OG1	1:H:143:ARG:NH2	2.45	0.49
1:H:141:ALA:HA	1:H:144:LEU:HD12	1.94	0.49
1:H:147:ARG:HH21	1:H:150:GLU:HB2	1.76	0.49
1:I:377:ARG:HG2	1:I:382:LEU:HD12	1.94	0.49
2:A:126:SER:OG	2:A:127:PHE:N	2.45	0.49
1:D:14:HIS:CG	1:D:15:PRO:HD2	2.47	0.49
1:E:161:ARG:HB2	1:E:188:GLN:HB3	1.94	0.49
1:F:247:ILE:O	1:F:250:THR:OG1	2.22	0.49
1:G:157:LEU:HB2	1:G:160:LEU:HD12	1.94	0.49
1:G:354:THR:HG1	1:G:359:HIS:CE1	2.30	0.49
1:I:168:VAL:HG23	1:I:183:VAL:HG22	1.93	0.49
2:A:96:CYS:HA	2:A:111:TYR:HA	1.94	0.49
2:K:126:SER:OG	2:K:129:GLU:OE2	2.22	0.49
2:J:137:GLN:OE1	2:J:137:GLN:N	2.45	0.49
1:B:112:LEU:HB3	1:B:336:ARG:NH1	2.26	0.49
1:B:308:THR:HG1	1:B:309:SER:H	1.59	0.49
1:B:375:LEU:O	1:B:378:ASP:HB2	2.12	0.49
1:H:57:THR:HA	1:H:98:GLN:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:23:CYS:HB3	2:A:26:VAL:HG23	1.93	0.49
2:A:127:PHE:CE2	2:A:128:GLN:HB2	2.47	0.49
1:C:72:VAL:HG11	1:C:84:PHE:HE2	1.78	0.49
1:C:143:ARG:NE	2:J:5:LYS:HE2	2.26	0.49
1:D:250:THR:HG22	1:D:251:TYR:CG	2.47	0.49
1:E:43:THR:N	1:E:242:THR:OG1	2.43	0.49
1:E:188:GLN:OE1	1:E:233:GLY:HA3	2.13	0.49
1:F:147:ARG:HH11	1:F:210:ILE:HD11	1.78	0.49
1:G:247:ILE:O	1:G:250:THR:N	2.44	0.49
2:A:4:THR:HG21	2:A:105:HIS:CE1	2.47	0.49
1:C:69:ARG:NH2	1:C:89:CYS:O	2.37	0.49
1:C:85:ASP:OD1	1:C:87:ASN:N	2.29	0.49
1:E:351:TYR:O	1:E:354:THR:HG22	2.13	0.49
1:F:12:GLU:HB3	1:F:357:TYR:CE2	2.47	0.49
1:H:157:LEU:HB3	1:H:159:TRP:CE2	2.47	0.49
1:I:55:GLU:HA	1:I:96:GLY:HA3	1.94	0.49
1:I:134:MET:HG2	1:I:279:ARG:HH22	1.76	0.49
2:L:33:HIS:O	2:L:37:THR:HG23	2.12	0.49
1:G:152:ARG:CZ	1:G:162:PRO:HA	2.43	0.49
1:I:147:ARG:HG2	1:I:206:ILE:HA	1.94	0.49
2:K:4:THR:HG21	2:K:105:HIS:CE1	2.47	0.49
2:J:151:VAL:HG22	2:J:152:GLN:H	1.78	0.49
1:C:143:ARG:NH1	2:J:5:LYS:HG2	2.27	0.49
1:C:288:ALA:HB1	1:C:377:ARG:HB2	1.94	0.49
1:E:198:LEU:O	1:E:202:VAL:HG12	2.12	0.49
2:J:56:CYS:HB3	2:J:139:CYS:O	2.12	0.49
2:J:78:LYS:O	2:J:82:LEU:HD21	2.13	0.49
1:C:193:ILE:HG21	1:C:198:LEU:HD12	1.93	0.49
1:C:300:TYR:CZ	1:C:307:PRO:HG3	2.47	0.49
1:E:14:HIS:CG	1:E:15:PRO:HD2	2.48	0.49
1:F:83:GLY:HA2	1:F:236:MET:HE3	1.95	0.49
1:F:266:ASP:OD1	1:F:269:LYS:NZ	2.46	0.49
1:F:346:LEU:O	1:F:351:TYR:OH	2.25	0.49
1:H:134:MET:HE1	1:H:360:PHE:HB2	1.95	0.49
1:H:257:HIS:CE1	1:H:259:GLY:H	2.30	0.49
1:H:279:ARG:HG2	1:H:360:PHE:CD1	2.47	0.49
1:I:161:ARG:NE	1:I:190:SER:HA	2.26	0.49
2:J:105:HIS:CG	2:J:128:GLN:HG3	2.47	0.49
1:D:212:PRO:HG2	1:D:215:TRP:CE3	2.48	0.49
1:F:22:ILE:O	1:F:26:VAL:HG23	2.13	0.49
1:G:317:THR:O	1:G:319:LYS:HE3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:LYS:HG3	1:I:21:GLN:NE2	2.28	0.49
1:I:42:GLU:HB2	1:I:53:GLY:O	2.12	0.49
1:I:85:ASP:OD2	1:I:88:SER:N	2.45	0.49
2:L:60:ALA:HB1	2:J:107:ALA:HB1	1.95	0.49
2:K:90:ASN:ND2	2:K:114:GLY:H	2.11	0.49
2:J:10:VAL:C	2:J:78:LYS:HZ2	2.16	0.49
1:B:161:ARG:CZ	1:B:190:SER:HA	2.42	0.48
1:D:19:ALA:HB1	1:D:43:THR:OG1	2.13	0.48
1:H:122:MET:N	1:H:122:MET:SD	2.86	0.48
1:H:181:ASP:O	1:H:220:THR:HA	2.13	0.48
2:L:137:GLN:HE21	2:L:148:ARG:HB2	1.77	0.48
2:J:12:TYR:CE1	2:J:78:LYS:HD2	2.49	0.48
2:J:56:CYS:N	2:J:139:CYS:O	2.39	0.48
1:C:5:PHE:O	1:C:169:THR:HA	2.13	0.48
1:C:85:ASP:CG	1:C:87:ASN:H	2.14	0.48
1:E:265:LYS:HD3	1:E:269:LYS:HZ3	1.78	0.48
1:F:24:ASP:OD2	1:F:272:ARG:NH2	2.41	0.48
1:G:241:LEU:HB3	1:G:244:ARG:HG3	1.95	0.48
1:H:11:SER:HA	1:H:357:TYR:HE1	1.76	0.48
1:H:161:ARG:NH2	1:H:190:SER:HA	2.28	0.48
1:H:167:GLN:NE2	1:I:308:THR:HG21	2.28	0.48
1:H:200:GLU:O	1:H:204:GLU:HG2	2.13	0.48
2:J:30:ARG:HG2	2:J:34:MET:CE	2.43	0.48
2:J:52:ASP:N	2:J:52:ASP:OD1	2.46	0.48
1:E:206:ILE:O	1:E:209:PRO:HD2	2.14	0.48
1:E:280:TYR:OH	1:E:372:LYS:HD3	2.13	0.48
1:H:43:THR:HA	1:H:51:LEU:O	2.13	0.48
1:H:281:VAL:HG23	1:H:296:ILE:HG13	1.94	0.48
1:I:185:LEU:O	1:I:225:ASN:N	2.40	0.48
1:F:66:GLU:O	1:F:70:ASN:ND2	2.46	0.48
1:H:150:GLU:OE1	1:H:154:ASN:ND2	2.37	0.48
2:L:30:ARG:CG	2:L:34:MET:HE3	2.43	0.48
2:A:33:HIS:HE1	2:A:92:TRP:CZ2	2.31	0.48
2:K:80:GLN:O	2:K:83:ASN:HB3	2.13	0.48
1:B:70:ASN:HA	1:B:73:ARG:NH1	2.28	0.48
1:C:149:ALA:HA	1:C:152:ARG:NH1	2.28	0.48
1:C:351:TYR:CD2	1:C:351:TYR:N	2.82	0.48
1:D:17:LYS:HD2	1:D:356:ALA:HA	1.96	0.48
1:E:204:GLU:OE2	1:E:208:LYS:HG3	2.14	0.48
1:F:257:HIS:CG	1:F:258:GLY:N	2.82	0.48
1:G:327:LEU:HA	1:G:330:ARG:NE	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:PHE:HB3	1:H:172:TYR:CE2	2.48	0.48
1:H:192:GLU:OE2	1:H:192:GLU:N	2.33	0.48
1:I:291:ALA:HB2	1:I:318:GLU:OE2	2.12	0.48
2:K:33:HIS:O	2:K:37:THR:HG23	2.14	0.48
2:K:110:VAL:HG23	2:K:119:LYS:O	2.14	0.48
2:J:56:CYS:O	2:J:139:CYS:N	2.47	0.48
1:E:204:GLU:O	1:E:208:LYS:HB2	2.13	0.48
1:E:212:PRO:O	1:E:216:LEU:N	2.47	0.48
1:G:38:ARG:HA	1:G:266:ASP:OD2	2.13	0.48
1:H:28:ASP:OD2	1:H:351:TYR:N	2.46	0.48
1:H:149:ALA:HA	1:H:152:ARG:NH1	2.28	0.48
1:I:22:ILE:HD12	1:I:43:THR:HG21	1.96	0.48
1:I:102:ILE:H	1:I:102:ILE:HD12	1.78	0.48
1:I:262:PHE:HB3	1:I:272:ARG:NE	2.28	0.48
2:A:136:LEU:HG	2:A:137:GLN:H	1.78	0.48
2:K:53:LEU:HD12	2:K:54:THR:N	2.28	0.48
1:B:208:LYS:HB2	1:B:209:PRO:HD3	1.96	0.48
1:C:21:GLN:HA	1:C:24:ASP:OD2	2.13	0.48
1:C:58:THR:OG1	1:C:59:SER:N	2.45	0.48
1:C:79:HIS:HB3	1:C:82:MET:HG2	1.94	0.48
1:E:79:HIS:CD2	1:E:81:ASP:H	2.22	0.48
1:F:192:GLU:OE1	1:F:192:GLU:N	2.42	0.48
1:H:107:ASP:OD2	1:H:108:ARG:N	2.46	0.48
1:H:203:MET:HA	1:H:207:ILE:HD12	1.94	0.48
2:A:19:ARG:O	2:A:27:ASN:ND2	2.37	0.48
2:K:146:GLY:O	2:K:147:ARG:HG3	2.13	0.48
1:B:365:PHE:HB3	1:B:367:TRP:CE2	2.48	0.48
1:D:152:ARG:NH2	1:D:153:LYS:HZ3	2.06	0.48
1:G:5:PHE:O	1:G:169:THR:HA	2.14	0.48
1:G:206:ILE:C	1:G:209:PRO:HD2	2.33	0.48
1:H:195:GLN:O	1:H:199:GLN:HG3	2.14	0.48
1:I:18:ILE:HD11	1:I:77:TYR:CE2	2.49	0.48
2:K:3:PHE:C	2:K:5:LYS:H	2.16	0.48
1:B:323:GLU:OE2	1:B:323:GLU:N	2.36	0.48
1:C:116:ALA:N	1:C:304:VAL:O	2.37	0.48
1:E:204:GLU:O	1:E:209:PRO:HD3	2.13	0.48
1:E:279:ARG:HG2	1:E:360:PHE:CD1	2.49	0.48
1:F:123:PHE:HA	1:F:296:ILE:O	2.14	0.48
1:G:39:VAL:O	1:G:269:LYS:NZ	2.25	0.48
1:I:39:VAL:HB	1:I:266:ASP:HB3	1.96	0.48
1:I:46:LYS:HZ3	1:I:239:CYS:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:13:VAL:HG12	2:K:74:ARG:HB3	1.95	0.48
1:B:225:ASN:O	1:B:228:GLY:N	2.39	0.48
1:B:256:ARG:HG2	1:B:295:GLU:OE2	2.13	0.48
1:B:299:SER:OG	1:B:309:SER:OG	2.19	0.48
1:E:157:LEU:HB3	1:E:159:TRP:CE2	2.49	0.48
1:F:127:THR:OG1	1:F:128:ASN:N	2.47	0.48
1:H:123:PHE:HB2	1:H:257:HIS:HA	1.96	0.48
1:H:307:PRO:HG2	1:H:335:LEU:HD12	1.95	0.48
1:I:79:HIS:NE2	1:I:81:ASP:OD1	2.47	0.48
1:I:338:TYR:HA	1:I:341:ILE:HD12	1.96	0.48
2:L:19:ARG:HB2	2:L:68:GLU:CD	2.35	0.48
2:L:124:PRO:HB2	2:L:152:GLN:HE21	1.78	0.48
2:K:100:TYR:OH	2:K:128:GLN:NE2	2.41	0.48
1:D:204:GLU:O	1:D:209:PRO:HD3	2.14	0.47
1:G:187:THR:H	1:G:225:ASN:ND2	2.01	0.47
1:H:265:LYS:HD3	1:H:269:LYS:HB3	1.96	0.47
1:I:98:GLN:HE21	1:I:103:ASN:CG	2.18	0.47
1:I:299:SER:OG	1:I:309:SER:HB3	2.13	0.47
1:C:151:VAL:HA	1:C:154:ASN:ND2	2.29	0.47
1:D:174:ASP:O	1:D:176:LYS:NZ	2.28	0.47
1:D:203:MET:O	1:D:208:LYS:HG2	2.14	0.47
1:F:122:MET:HA	1:F:258:GLY:HA3	1.96	0.47
1:H:229:ARG:HH12	1:H:231:VAL:HG13	1.78	0.47
1:I:266:ASP:N	1:I:269:LYS:HD3	2.28	0.47
1:I:306:GLU:OE2	1:I:336:ARG:NE	2.47	0.47
2:J:19:ARG:HA	2:J:27:ASN:OD1	2.14	0.47
1:B:71:THR:HA	1:B:74:GLU:OE1	2.14	0.47
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.70	0.47
1:C:122:MET:SD	1:C:298:VAL:HG23	2.54	0.47
1:D:214:GLU:HG2	1:D:215:TRP:H	1.79	0.47
1:D:266:ASP:OD2	1:D:268:SER:OG	2.23	0.47
1:D:298:VAL:HA	1:D:309:SER:O	2.14	0.47
1:E:69:ARG:NH1	1:E:89:CYS:SG	2.87	0.47
1:E:331:GLU:HB2	1:E:332:PHE:HD1	1.78	0.47
1:G:85:ASP:HB3	1:G:88:SER:OG	2.14	0.47
2:L:130:VAL:HG23	2:L:148:ARG:H	1.80	0.47
2:A:92:TRP:O	2:A:93:GLU:HG2	2.13	0.47
2:A:127:PHE:CG	2:A:128:GLN:N	2.82	0.47
1:C:112:LEU:HB3	1:C:336:ARG:NH1	2.26	0.47
1:C:216:LEU:HD12	1:C:222:PHE:HZ	1.80	0.47
1:D:335:LEU:HA	1:D:340:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:HIS:O	1:D:369:LYS:NZ	2.47	0.47
1:F:267:PRO:HB3	1:F:346:LEU:HD12	1.95	0.47
1:F:314:THR:O	1:F:317:THR:OG1	2.17	0.47
1:H:16:ASP:HB2	1:H:245:LYS:HE2	1.96	0.47
1:H:85:ASP:O	1:H:88:SER:OG	2.27	0.47
2:J:38:LEU:HD12	2:J:39:ARG:N	2.29	0.47
1:C:257:HIS:HD2	1:C:258:GLY:H	1.62	0.47
1:F:351:TYR:HA	1:F:354:THR:HG22	1.95	0.47
1:G:15:PRO:O	1:G:18:ILE:HB	2.15	0.47
1:G:19:ALA:HB1	1:G:43:THR:HB	1.95	0.47
1:G:364:HIS:O	1:G:369:LYS:NZ	2.47	0.47
1:H:173:ASP:OD2	1:H:176:LYS:NZ	2.45	0.47
1:I:15:PRO:HA	1:I:18:ILE:HD12	1.97	0.47
2:A:34:MET:O	2:A:37:THR:OG1	2.28	0.47
2:J:56:CYS:HB3	2:J:139:CYS:HB2	1.31	0.47
1:C:34:ASP:OD1	1:C:36:LYS:N	2.47	0.47
1:E:291:ALA:HA	1:E:317:THR:O	2.14	0.47
1:F:2:LYS:HB2	1:F:173:ASP:OD1	2.14	0.47
1:F:290:LEU:O	1:F:319:LYS:N	2.41	0.47
1:G:11:SER:HB3	1:G:164:ALA:HB3	1.97	0.47
1:G:293:ARG:HG2	1:G:317:THR:HG21	1.96	0.47
1:G:347:LEU:HD12	1:G:347:LEU:HA	1.71	0.47
2:L:42:PRO:O	2:L:46:GLY:N	2.47	0.47
2:J:128:GLN:CD	2:J:147:ARG:HD3	2.35	0.47
1:B:110:ASP:OD1	1:B:112:LEU:N	2.48	0.47
1:B:134:MET:HG2	1:B:279:ARG:NH1	2.30	0.47
1:B:169:THR:OG1	1:B:169:THR:O	2.33	0.47
1:B:267:PRO:O	1:B:273:SER:OG	2.21	0.47
1:C:70:ASN:HA	1:C:73:ARG:NH1	2.30	0.47
1:C:262:PHE:O	1:C:272:ARG:NH1	2.48	0.47
1:C:292:ASP:OD1	1:C:319:LYS:NZ	2.44	0.47
1:D:323:GLU:O	1:D:327:LEU:HD13	2.14	0.47
1:E:115:GLY:HA2	1:E:305:ALA:HA	1.95	0.47
1:E:121:LEU:HD13	1:E:299:SER:HB3	1.96	0.47
1:E:307:PRO:HG2	1:E:335:LEU:HD13	1.95	0.47
1:F:133:LEU:HD23	1:F:286:VAL:HB	1.97	0.47
1:F:273:SER:HB3	1:F:340:LEU:HD11	1.96	0.47
1:G:151:VAL:HA	1:G:154:ASN:HD21	1.80	0.47
1:H:151:VAL:HA	1:H:154:ASN:HD21	1.80	0.47
1:H:277:ALA:O	1:H:281:VAL:HG13	2.14	0.47
2:L:96:CYS:HG	2:J:122:ARG:HH12	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:86:ARG:NH1	2:A:114:GLY:O	2.34	0.47
2:J:29:SER:HA	2:J:32:ARG:HD2	1.97	0.47
2:J:103:GLN:HG2	2:J:104:THR:N	2.29	0.47
2:J:140:PHE:HB2	2:J:147:ARG:O	2.15	0.47
1:B:30:ILE:HG12	1:B:62:VAL:HG21	1.97	0.47
1:B:189:HIS:HE2	1:B:230:PHE:H	1.62	0.47
1:C:52:VAL:O	1:C:93:SER:HA	2.15	0.47
1:C:100:PRO:HA	1:C:103:ASN:OD1	2.14	0.47
1:D:75:ILE:O	1:D:153:LYS:NZ	2.33	0.47
1:D:172:TYR:CZ	1:D:177:ILE:HG13	2.50	0.47
1:D:295:GLU:HB3	1:D:313:GLU:HB3	1.97	0.47
1:D:351:TYR:HA	1:D:354:THR:HG22	1.97	0.47
1:E:213:ALA:O	1:E:216:LEU:HB2	2.14	0.47
1:G:97:LYS:HB3	1:I:63:ASP:OD2	2.15	0.47
1:G:101:ASP:O	1:G:104:GLN:HG3	2.15	0.47
1:H:54:GLY:N	1:I:46:LYS:HZ2	2.13	0.47
2:K:25:GLU:OE1	2:K:25:GLU:N	2.39	0.47
2:K:32:ARG:HA	2:K:35:VAL:HG12	1.97	0.47
2:J:121:GLU:OE1	2:J:122:ARG:N	2.45	0.47
1:B:14:HIS:CD2	1:B:15:PRO:HD2	2.50	0.47
1:C:362:ARG:HB3	1:C:365:PHE:CD2	2.50	0.47
1:D:181:ASP:O	1:D:220:THR:HA	2.15	0.47
1:F:143:ARG:HE	2:L:5:LYS:HZ3	1.62	0.47
1:G:130:THR:HG22	2:K:5:LYS:HE2	1.95	0.47
1:G:293:ARG:HG3	1:G:315:PHE:CD1	2.50	0.47
1:H:38:ARG:HB3	1:H:57:THR:OG1	2.15	0.47
1:H:272:ARG:HH21	1:H:359:HIS:CE1	2.32	0.47
1:I:11:SER:OG	1:I:164:ALA:N	2.48	0.47
2:L:75:CYS:HB2	2:L:81:ALA:CB	2.45	0.47
2:J:3:PHE:CD1	2:J:104:THR:HA	2.50	0.47
1:B:159:TRP:O	1:B:190:SER:N	2.45	0.47
1:D:20:ASP:O	1:D:23:SER:OG	2.33	0.47
1:D:165:LYS:NZ	1:E:119:GLN:HG2	2.29	0.47
1:E:12:GLU:HB2	1:E:21:GLN:OE1	2.15	0.47
1:F:217:THR:OG1	1:F:220:THR:OG1	2.24	0.47
1:G:365:PHE:HB3	1:G:367:TRP:CE2	2.49	0.47
1:H:132:VAL:HG21	1:H:361:GLY:HA2	1.96	0.47
1:I:159:TRP:CZ3	1:I:198:LEU:HG	2.50	0.47
1:I:250:THR:OG1	1:I:251:TYR:N	2.45	0.47
2:A:127:PHE:CD2	2:A:128:GLN:HB2	2.50	0.47
2:K:5:LYS:HD2	2:K:5:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:127:PHE:CD2	2:K:128:GLN:HB2	2.49	0.47
1:B:134:MET:SD	1:B:360:PHE:HB2	2.56	0.46
1:C:151:VAL:HG23	1:C:156:THR:HB	1.97	0.46
1:E:279:ARG:HE	1:E:283:LYS:HB2	1.79	0.46
1:F:15:PRO:HA	1:F:18:ILE:HD12	1.96	0.46
1:F:95:ILE:HG13	1:F:96:GLY:N	2.26	0.46
1:G:101:ASP:OD1	1:G:102:ILE:N	2.48	0.46
1:H:147:ARG:O	1:H:151:VAL:HG23	2.14	0.46
2:A:24:ASP:O	2:A:28:MET:HG3	2.15	0.46
1:B:149:ALA:O	1:B:153:LYS:HG2	2.15	0.46
1:B:322:SER:O	1:B:325:LEU:HB3	2.14	0.46
1:C:180:ILE:HG13	1:C:215:TRP:HB3	1.98	0.46
1:C:269:LYS:HD3	1:C:269:LYS:HA	1.61	0.46
1:D:19:ALA:HA	1:D:22:ILE:HD12	1.97	0.46
1:E:45:VAL:HG12	1:E:235:PRO:HB3	1.97	0.46
1:G:189:HIS:CE1	1:G:231:VAL:HG23	2.50	0.46
1:G:246:ILE:HD11	1:G:257:HIS:HE1	1.78	0.46
2:K:14:LEU:HB2	2:K:98:LEU:O	2.16	0.46
2:J:89:CYS:HB2	2:J:94:GLN:HB3	1.97	0.46
1:D:64:ILE:O	1:D:68:THR:HG23	2.16	0.46
1:E:188:GLN:HG3	1:E:230:PHE:O	2.15	0.46
1:F:152:ARG:CZ	1:F:162:PRO:HA	2.44	0.46
1:G:71:THR:O	1:G:75:ILE:HG13	2.15	0.46
1:G:163:ASP:O	1:G:188:GLN:N	2.47	0.46
1:G:375:LEU:HA	1:G:378:ASP:OD1	2.14	0.46
2:A:19:ARG:HB2	2:A:68:GLU:OE1	2.16	0.46
2:J:100:TYR:HA	2:J:107:ALA:HB3	1.97	0.46
2:J:129:GLU:HA	2:J:147:ARG:HH11	1.80	0.46
1:B:22:ILE:HD13	1:B:68:THR:HG23	1.97	0.46
1:D:375:LEU:HA	1:D:378:ASP:OD1	2.15	0.46
1:F:38:ARG:HA	1:F:266:ASP:OD2	2.16	0.46
1:F:143:ARG:HB3	1:F:143:ARG:NH1	2.30	0.46
1:I:79:HIS:HB3	1:I:82:MET:HG3	1.96	0.46
1:I:98:GLN:HE21	1:I:103:ASN:ND2	2.13	0.46
2:A:3:PHE:CE2	2:A:104:THR:HA	2.46	0.46
2:A:86:ARG:HD3	2:A:113:LYS:HA	1.98	0.46
2:J:49:GLU:HA	2:J:73:VAL:HG12	1.98	0.46
1:B:39:VAL:H	1:B:266:ASP:HB2	1.81	0.46
1:C:80:SER:OG	1:C:81:ASP:N	2.48	0.46
1:C:282:ALA:HB2	1:C:296:ILE:HG12	1.97	0.46
1:D:344:LEU:HD13	1:D:367:TRP:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:THR:HA	1:F:74:GLU:OE2	2.16	0.46
1:H:38:ARG:NH2	1:H:55:GLU:HG3	2.30	0.46
1:H:113:GLU:H	1:H:336:ARG:HG2	1.79	0.46
1:B:134:MET:CG	1:B:279:ARG:HH12	2.28	0.46
1:C:31:LEU:HA	1:C:34:ASP:O	2.15	0.46
1:D:56:ILE:HD12	1:D:95:ILE:HG21	1.96	0.46
1:D:64:ILE:H	1:D:64:ILE:HD12	1.79	0.46
1:D:94:ALA:HB1	1:E:46:LYS:NZ	2.27	0.46
1:D:341:ILE:HG12	1:D:346:LEU:HD12	1.97	0.46
1:F:299:SER:O	1:F:308:THR:N	2.49	0.46
1:G:188:GLN:HA	1:G:230:PHE:HD2	1.80	0.46
1:G:375:LEU:H	1:G:375:LEU:HD12	1.80	0.46
1:H:118:ASP:OD2	1:H:119:GLN:N	2.49	0.46
1:I:249:ASP:HB3	1:I:359:HIS:CD2	2.50	0.46
1:I:250:THR:HA	1:I:360:PHE:CE2	2.51	0.46
2:K:99:VAL:O	2:K:107:ALA:HB3	2.16	0.46
2:K:121:GLU:HG3	2:K:122:ARG:N	2.31	0.46
2:K:127:PHE:CE2	2:K:128:GLN:HB2	2.51	0.46
2:J:28:MET:HB3	2:J:32:ARG:HH21	1.80	0.46
2:J:58:ARG:HA	2:J:65:PRO:HA	1.98	0.46
1:C:12:GLU:HB2	1:C:21:GLN:NE2	2.30	0.46
1:C:199:GLN:OE1	1:C:224:ILE:HB	2.16	0.46
1:C:335:LEU:HD13	1:C:335:LEU:HA	1.78	0.46
1:D:292:ASP:HB2	1:D:317:THR:HB	1.96	0.46
1:E:284:ASN:HA	1:E:373:ALA:HB2	1.98	0.46
1:E:351:TYR:HA	1:E:354:THR:HG22	1.97	0.46
1:H:130:THR:HG1	1:H:134:MET:N	2.10	0.46
1:I:232:ILE:HD12	1:I:232:ILE:HA	1.81	0.46
1:B:50:VAL:HG13	1:B:91:VAL:HA	1.98	0.46
1:B:343:MET:HE2	1:B:344:LEU:HG	1.97	0.46
1:C:240:GLY:C	1:C:241:LEU:HD12	2.36	0.46
1:E:47:THR:HG23	1:E:236:MET:HA	1.97	0.46
1:E:290:LEU:O	1:E:319:LYS:HG2	2.16	0.46
1:F:46:LYS:HB3	1:F:49:MET:HG3	1.96	0.46
1:F:61:TRP:HB3	1:H:61:TRP:CE2	2.51	0.46
1:F:89:CYS:SG	1:F:90:ALA:N	2.88	0.46
1:H:33:GLN:OE1	1:H:60:ALA:HB1	2.15	0.46
1:I:40:ALA:H	1:I:56:ILE:CD1	2.28	0.46
1:I:45:VAL:HB	1:I:240:GLY:HA3	1.97	0.46
1:I:122:MET:HG3	1:I:274:ALA:HB3	1.98	0.46
2:L:90:ASN:HA	2:L:113:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLN:NE2	1:C:165:LYS:HE2	2.31	0.46
1:D:15:PRO:O	1:D:18:ILE:HB	2.15	0.46
1:D:169:THR:HG1	1:D:182:ALA:H	1.63	0.46
1:F:145:VAL:HG13	1:F:166:SER:OG	2.16	0.46
1:I:189:HIS:O	1:I:231:VAL:HA	2.16	0.46
2:J:127:PHE:CG	2:J:128:GLN:N	2.83	0.46
1:B:34:ASP:OD1	1:B:36:LYS:N	2.49	0.46
1:B:159:TRP:CG	1:B:193:ILE:HD13	2.51	0.46
1:C:257:HIS:CD2	1:C:258:GLY:H	2.34	0.46
1:D:332:PHE:HE2	1:D:375:LEU:HG	1.80	0.46
1:E:79:HIS:HB3	1:E:81:ASP:OD1	2.15	0.46
1:F:362:ARG:HD2	1:F:365:PHE:CE2	2.51	0.46
1:I:121:LEU:HD12	1:I:122:MET:N	2.30	0.46
1:I:346:LEU:O	1:I:348:HIS:N	2.49	0.46
1:I:371:ASP:OD1	1:I:371:ASP:N	2.46	0.46
2:L:61:ILE:O	2:L:63:SER:N	2.49	0.46
2:K:121:GLU:HG3	2:K:122:ARG:H	1.80	0.46
1:E:195:GLN:O	1:E:199:GLN:HG3	2.16	0.45
1:F:203:MET:O	1:F:208:LYS:HG2	2.16	0.45
1:F:291:ALA:HB1	1:F:317:THR:OG1	2.15	0.45
1:F:323:GLU:HG2	1:F:324:GLN:H	1.80	0.45
1:H:33:GLN:NE2	1:H:61:TRP:H	2.15	0.45
2:A:118:TYR:O	2:A:119:LYS:HD3	2.16	0.45
2:K:83:ASN:HA	2:K:86:ARG:CZ	2.46	0.45
1:B:61:TRP:HB3	1:D:61:TRP:CE3	2.51	0.45
1:B:313:GLU:HG3	1:B:315:PHE:CE1	2.51	0.45
1:D:14:HIS:CD2	1:D:15:PRO:HD2	2.51	0.45
1:E:2:LYS:HA	1:E:172:TYR:O	2.17	0.45
1:F:130:THR:OG1	1:F:131:ASP:N	2.48	0.45
1:G:110:ASP:O	1:G:113:GLU:HG2	2.16	0.45
1:I:2:LYS:HA	1:I:172:TYR:O	2.16	0.45
2:J:90:ASN:HD21	2:J:114:GLY:N	2.15	0.45
1:B:119:GLN:HA	1:B:300:TYR:O	2.16	0.45
1:D:133:LEU:HB2	1:D:283:LYS:HE3	1.99	0.45
1:D:148:GLN:NE2	1:D:187:THR:OG1	2.50	0.45
1:F:69:ARG:HB3	1:F:73:ARG:NH2	2.28	0.45
1:F:247:ILE:O	1:F:250:THR:N	2.50	0.45
1:H:147:ARG:HA	1:H:147:ARG:NE	2.31	0.45
2:L:14:LEU:HB2	2:L:99:VAL:HG22	1.99	0.45
2:L:127:PHE:CD2	2:L:128:GLN:HG2	2.51	0.45
2:J:17:ALA:HA	2:J:70:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:76:LYS:HG3	2:J:77:ASP:N	2.32	0.45
1:C:157:LEU:HD11	1:C:205:GLU:HG3	1.98	0.45
1:F:134:MET:SD	1:F:360:PHE:HB2	2.56	0.45
1:G:13:GLY:HA3	1:G:163:ASP:HA	1.99	0.45
1:G:351:TYR:O	1:G:354:THR:HG22	2.16	0.45
1:G:372:LYS:HA	1:G:375:LEU:HD13	1.98	0.45
1:E:118:ASP:OD2	1:E:119:GLN:N	2.48	0.45
1:F:44:TYR:CE1	1:F:46:LYS:HB2	2.48	0.45
1:G:71:THR:HG22	1:G:352:LYS:HZ1	1.81	0.45
1:H:251:TYR:OH	1:H:279:ARG:NH1	2.50	0.45
1:H:339:GLY:O	1:H:343:MET:HG3	2.17	0.45
1:I:46:LYS:NZ	1:I:239:CYS:HB2	2.31	0.45
1:I:324:GLN:NE2	1:I:328:LEU:HD11	2.31	0.45
2:K:15:VAL:HG13	2:K:98:LEU:HD13	1.97	0.45
2:K:33:HIS:O	2:K:36:SER:OG	2.25	0.45
2:K:47:SER:OG	2:K:73:VAL:HB	2.16	0.45
2:J:18:PHE:HB3	2:J:34:MET:SD	2.56	0.45
1:C:178:VAL:HG23	1:C:179:GLY:H	1.82	0.45
1:C:191:GLU:OE1	1:C:229:ARG:NH1	2.46	0.45
1:C:211:LEU:HD13	1:C:211:LEU:HA	1.83	0.45
1:F:58:THR:HG23	1:F:60:ALA:H	1.81	0.45
1:H:165:LYS:HE2	1:I:119:GLN:NE2	2.31	0.45
1:H:225:ASN:O	1:H:228:GLY:N	2.48	0.45
1:I:217:THR:HG23	1:I:220:THR:H	1.82	0.45
1:I:324:GLN:O	1:I:328:LEU:HG	2.15	0.45
2:J:55:GLY:N	2:J:67:GLU:OE1	2.50	0.45
1:B:152:ARG:CZ	1:B:162:PRO:HA	2.46	0.45
1:C:366:PRO:HA	1:C:369:LYS:HD3	1.99	0.45
1:D:227:THR:HG23	1:D:229:ARG:H	1.82	0.45
1:E:121:LEU:HD12	1:E:298:VAL:O	2.17	0.45
1:F:65:GLU:HG3	1:F:91:VAL:HG11	1.98	0.45
1:F:84:PHE:CG	1:F:235:PRO:HG2	2.52	0.45
1:F:196:LYS:HA	1:F:199:GLN:OE1	2.16	0.45
1:G:84:PHE:CD1	1:G:235:PRO:HG2	2.51	0.45
1:G:327:LEU:HG	1:G:330:ARG:NH2	2.31	0.45
1:H:165:LYS:HE2	1:I:119:GLN:HE21	1.81	0.45
1:H:357:TYR:HB2	1:H:362:ARG:NH2	2.31	0.45
1:I:125:TYR:OH	1:I:293:ARG:NE	2.32	0.45
2:L:19:ARG:HE	2:L:68:GLU:HA	1.81	0.45
2:A:34:MET:HG2	2:A:92:TRP:NE1	2.32	0.45
2:K:23:CYS:O	2:K:27:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:147:ARG:HG2	2:K:147:ARG:HH11	1.82	0.45
2:J:129:GLU:CA	2:J:147:ARG:HH11	2.29	0.45
1:B:85:ASP:OD1	1:B:86:ALA:N	2.50	0.45
1:B:110:ASP:HB3	1:B:113:GLU:CG	2.47	0.45
1:B:161:ARG:O	1:B:188:GLN:HB3	2.17	0.45
1:F:74:GLU:O	1:F:153:LYS:NZ	2.34	0.45
1:F:110:ASP:HB3	1:F:113:GLU:OE1	2.16	0.45
1:F:148:GLN:HE21	1:F:160:LEU:HD22	1.82	0.45
1:G:36:LYS:HD2	1:G:347:LEU:HD21	1.98	0.45
1:H:136:ALA:O	1:H:140:TYR:HB2	2.17	0.45
1:H:340:LEU:HA	1:H:343:MET:SD	2.57	0.45
2:K:4:THR:C	2:K:6:GLU:H	2.20	0.45
1:B:125:TYR:HB3	1:B:251:TYR:CZ	2.52	0.45
1:B:333:PHE:HZ	1:B:376:LEU:HD11	1.82	0.45
1:B:337:PRO:O	1:B:341:ILE:HG13	2.17	0.45
1:B:351:TYR:O	1:B:354:THR:N	2.50	0.45
1:D:244:ARG:NH1	1:E:42:GLU:OE1	2.39	0.45
1:E:332:PHE:CZ	1:E:379:ALA:HB2	2.52	0.45
1:H:354:THR:OG1	1:H:359:HIS:HA	2.17	0.45
2:L:56:CYS:C	2:L:139:CYS:HB3	2.34	0.45
2:K:47:SER:OG	2:K:48:VAL:N	2.49	0.45
1:B:61:TRP:CE3	1:D:61:TRP:HB3	2.52	0.45
1:C:142:HIS:ND1	1:C:357:TYR:HA	2.32	0.45
1:C:152:ARG:NH2	1:C:153:LYS:HZ3	2.15	0.45
1:C:194:ASP:CG	1:C:197:SER:H	2.20	0.45
1:C:212:PRO:HA	2:J:10:VAL:HG12	1.98	0.45
1:C:325:LEU:O	1:C:329:VAL:HG23	2.17	0.45
1:D:307:PRO:HB2	1:D:310:ILE:HG13	1.98	0.45
1:H:77:TYR:CE1	1:H:162:PRO:HD2	2.52	0.45
1:I:151:VAL:HA	1:I:154:ASN:HD21	1.82	0.45
1:I:191:GLU:HB2	1:I:231:VAL:HG11	1.97	0.45
1:I:286:VAL:HA	1:I:291:ALA:O	2.16	0.45
2:K:28:MET:HG3	2:K:32:ARG:HH21	1.81	0.45
2:J:19:ARG:HH22	2:J:24:ASP:HA	1.82	0.45
2:J:48:VAL:O	2:J:73:VAL:HA	2.16	0.45
1:C:284:ASN:ND2	1:C:372:LYS:HB3	2.32	0.44
1:D:77:TYR:CZ	1:D:162:PRO:HB2	2.52	0.44
1:E:122:MET:SD	1:E:122:MET:N	2.90	0.44
1:E:314:THR:O	1:E:317:THR:OG1	2.30	0.44
1:F:48:GLY:HA3	1:I:90:ALA:N	2.32	0.44
1:G:214:GLU:HG2	1:G:215:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:ASP:HA	1:H:302:ILE:HB	1.99	0.44
1:H:151:VAL:HA	1:H:154:ASN:ND2	2.32	0.44
1:I:187:THR:H	1:I:225:ASN:CG	2.20	0.44
2:L:34:MET:HE1	2:L:92:TRP:HB3	1.98	0.44
2:A:39:ARG:HB2	2:A:49:GLU:OE1	2.18	0.44
2:A:92:TRP:O	2:A:94:GLN:N	2.49	0.44
2:K:3:PHE:HB2	2:K:5:LYS:CD	2.47	0.44
2:K:19:ARG:NH1	2:K:69:LYS:H	2.15	0.44
1:C:357:TYR:HB2	1:C:362:ARG:NH2	2.33	0.44
1:D:291:ALA:HA	1:D:317:THR:O	2.17	0.44
1:D:330:ARG:HB2	1:D:330:ARG:CZ	2.46	0.44
1:F:288:ALA:HB1	1:F:377:ARG:HH21	1.82	0.44
1:H:28:ASP:OD1	1:H:351:TYR:HD2	1.99	0.44
1:I:63:ASP:OD2	1:I:66:GLU:HG2	2.17	0.44
1:I:181:ASP:O	1:I:220:THR:HA	2.17	0.44
1:I:347:LEU:HD12	1:I:347:LEU:O	2.17	0.44
2:A:57:TYR:CE2	2:A:59:GLU:HG2	2.51	0.44
2:K:23:CYS:SG	2:K:24:ASP:N	2.89	0.44
2:K:29:SER:HA	2:K:32:ARG:NH1	2.32	0.44
1:B:353:GLU:OE1	1:B:364:HIS:NE2	2.49	0.44
1:C:168:VAL:HG12	1:C:183:VAL:HG22	1.99	0.44
1:D:43:THR:O	1:D:242:THR:OG1	2.33	0.44
1:D:225:ASN:O	1:D:228:GLY:N	2.48	0.44
1:F:108:ARG:HE	1:F:108:ARG:HB2	1.63	0.44
1:H:326:THR:O	1:H:329:VAL:HG12	2.16	0.44
1:I:102:ILE:O	1:I:106:VAL:HG13	2.17	0.44
1:I:277:ALA:O	1:I:281:VAL:HG13	2.17	0.44
2:A:3:PHE:HB3	2:A:5:LYS:HZ3	1.81	0.44
2:J:118:TYR:O	2:J:119:LYS:HD3	2.17	0.44
1:B:2:LYS:NZ	1:B:173:ASP:OD1	2.40	0.44
1:B:17:LYS:HD3	1:B:17:LYS:HA	1.66	0.44
1:C:139:THR:HB	2:J:5:LYS:HE3	1.99	0.44
1:C:232:ILE:H	1:C:232:ILE:HD12	1.82	0.44
1:D:160:LEU:HA	1:D:160:LEU:HD23	1.70	0.44
1:D:195:GLN:NE2	1:D:228:GLY:O	2.51	0.44
1:D:292:ASP:H	1:D:317:THR:HB	1.81	0.44
1:E:85:ASP:HB3	1:E:88:SER:OG	2.17	0.44
1:F:165:LYS:O	1:F:185:LEU:HD12	2.18	0.44
2:J:82:LEU:O	2:J:86:ARG:HD3	2.18	0.44
2:J:99:VAL:O	2:J:107:ALA:HB3	2.16	0.44
2:J:146:GLY:CA	2:J:148:ARG:HH11	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:GLN:HG3	1:C:311:MET:HB3	1.99	0.44
1:E:229:ARG:HA	1:E:229:ARG:HD2	1.84	0.44
1:F:57:THR:HG23	1:F:99:SER:O	2.17	0.44
1:F:304:VAL:HG12	1:F:306:GLU:H	1.82	0.44
1:F:352:LYS:HD2	1:F:352:LYS:HA	1.62	0.44
1:G:134:MET:HG2	1:G:279:ARG:HH22	1.82	0.44
1:H:58:THR:H	1:H:98:GLN:HB2	1.82	0.44
1:H:112:LEU:HD13	1:H:336:ARG:HH12	1.83	0.44
1:I:177:ILE:H	1:I:177:ILE:HD12	1.82	0.44
1:I:262:PHE:HB2	1:I:359:HIS:CE1	2.52	0.44
1:C:118:ASP:OD1	1:C:119:GLN:N	2.50	0.44
1:C:141:ALA:O	1:C:145:VAL:HG22	2.18	0.44
1:D:8:GLU:HA	1:D:167:GLN:HA	2.00	0.44
1:F:97:LYS:O	1:F:99:SER:N	2.50	0.44
1:F:141:ALA:O	1:F:145:VAL:HG22	2.17	0.44
1:F:284:ASN:HD21	1:F:370:THR:HA	1.83	0.44
1:G:54:GLY:H	1:G:95:ILE:HA	1.82	0.44
1:H:14:HIS:CG	1:H:15:PRO:HD2	2.52	0.44
1:H:327:LEU:HA	1:H:330:ARG:HE	1.81	0.44
2:L:80:GLN:OE1	2:L:80:GLN:N	2.43	0.44
2:J:41:ALA:O	2:J:45:TYR:HD2	2.00	0.44
2:J:148:ARG:O	2:J:150:GLN:NE2	2.51	0.44
1:B:169:THR:O	1:B:181:ASP:N	2.46	0.44
1:D:68:THR:OG1	1:D:69:ARG:N	2.51	0.44
1:D:196:LYS:HA	1:D:199:GLN:OE1	2.18	0.44
1:D:199:GLN:HA	1:D:224:ILE:HG21	2.00	0.44
1:F:6:THR:N	1:G:297:GLN:HE22	2.10	0.44
1:F:130:THR:HG23	1:F:132:VAL:N	2.32	0.44
1:G:66:GLU:O	1:G:70:ASN:ND2	2.51	0.44
1:H:81:ASP:OD1	1:H:82:MET:HG3	2.18	0.44
1:H:363:GLU:HA	1:H:368:GLU:CB	2.47	0.44
1:I:14:HIS:CG	1:I:15:PRO:HD2	2.53	0.44
1:I:279:ARG:HE	1:I:283:LYS:HD2	1.83	0.44
2:L:9:ASN:OD1	2:L:103:GLN:NE2	2.51	0.44
2:A:33:HIS:HE1	2:A:92:TRP:HZ2	1.65	0.44
1:B:55:GLU:OE1	1:B:55:GLU:N	2.50	0.44
1:C:79:HIS:O	1:C:82:MET:HB2	2.17	0.44
1:C:191:GLU:OE1	1:C:231:VAL:HG21	2.17	0.44
1:D:193:ILE:HG13	1:D:194:ASP:O	2.18	0.44
1:D:307:PRO:HG3	1:D:335:LEU:HB3	2.00	0.44
1:F:284:ASN:ND2	1:F:370:THR:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:ILE:HG13	1:G:95:ILE:HD13	1.99	0.44
1:H:31:LEU:HD23	1:H:35:PRO:HA	2.00	0.44
1:H:183:VAL:O	1:H:222:PHE:HA	2.18	0.44
2:J:23:CYS:C	2:J:27:ASN:HB2	2.38	0.44
1:C:152:ARG:NH1	1:C:162:PRO:HA	2.33	0.44
1:C:365:PHE:HB3	1:C:367:TRP:CZ2	2.52	0.44
1:D:381:GLY:HA2	1:D:383:LYS:NZ	2.32	0.44
1:F:111:PRO:HA	1:F:114:GLN:HG3	1.98	0.44
1:F:338:TYR:O	1:F:341:ILE:HB	2.17	0.44
1:H:116:ALA:HB1	1:H:270:VAL:HG11	2.00	0.44
2:K:79:ALA:HA	2:K:82:LEU:HB3	1.98	0.44
2:K:82:LEU:HG	2:K:86:ARG:NH1	2.29	0.44
2:J:19:ARG:HD3	2:J:69:LYS:N	2.33	0.44
1:C:221:LYS:HG3	1:C:223:PHE:HE2	1.82	0.43
1:D:64:ILE:HA	1:D:67:ILE:HD12	2.00	0.43
1:D:332:PHE:CE2	1:D:375:LEU:HG	2.53	0.43
1:G:84:PHE:CG	1:G:235:PRO:HG2	2.53	0.43
1:I:132:VAL:HG11	1:I:361:GLY:HA2	2.00	0.43
1:I:290:LEU:O	1:I:318:GLU:HA	2.18	0.43
2:L:110:VAL:HA	2:L:119:LYS:O	2.17	0.43
2:A:90:ASN:ND2	2:A:114:GLY:O	2.51	0.43
2:K:119:LYS:HA	2:K:119:LYS:HD2	1.86	0.43
2:J:12:TYR:HB2	2:J:75:CYS:O	2.18	0.43
1:B:66:GLU:OE2	1:B:70:ASN:ND2	2.50	0.43
1:D:28:ASP:OD2	1:D:351:TYR:N	2.51	0.43
1:D:180:ILE:O	1:D:220:THR:OG1	2.22	0.43
1:D:319:LYS:HA	1:D:319:LYS:HD3	1.69	0.43
1:G:241:LEU:HD12	1:G:241:LEU:HA	1.74	0.43
1:H:33:GLN:HB3	1:H:60:ALA:HB1	1.99	0.43
1:H:38:ARG:HH11	1:H:269:LYS:NZ	2.16	0.43
1:H:127:THR:OG1	1:H:129:GLU:HG3	2.18	0.43
1:I:245:LYS:O	1:I:248:VAL:HG12	2.18	0.43
2:A:19:ARG:HB3	2:A:27:ASN:HD21	1.83	0.43
2:A:20:SER:OG	2:K:119:LYS:HD2	2.18	0.43
2:K:19:ARG:HG3	2:K:31:HIS:HB2	2.00	0.43
1:B:187:THR:H	1:B:225:ASN:ND2	2.16	0.43
1:D:46:LYS:CG	1:D:47:THR:H	2.32	0.43
1:E:362:ARG:HB3	1:E:364:HIS:HE1	1.82	0.43
1:F:127:THR:HA	1:F:293:ARG:HA	2.00	0.43
1:F:203:MET:HB3	1:F:208:LYS:NZ	2.31	0.43
2:L:23:CYS:HB3	2:L:26:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:86:ARG:HA	2:L:89:CYS:SG	2.58	0.43
2:A:51:THR:O	2:A:51:THR:OG1	2.36	0.43
2:J:44:LEU:HG	2:J:84:VAL:HG11	1.99	0.43
1:B:107:ASP:O	1:B:109:ALA:N	2.51	0.43
1:B:119:GLN:N	1:B:302:ILE:HB	2.32	0.43
1:C:180:ILE:HD11	1:C:215:TRP:HE3	1.83	0.43
1:D:338:TYR:O	1:D:342:GLN:HG2	2.19	0.43
1:F:169:THR:OG1	1:F:181:ASP:HB3	2.19	0.43
1:G:110:ASP:O	1:G:114:GLN:HG3	2.18	0.43
1:H:198:LEU:O	1:H:202:VAL:HG12	2.19	0.43
1:I:290:LEU:HD13	1:I:320:VAL:HG21	2.00	0.43
2:L:21:ASN:HA	2:J:118:TYR:CD1	2.52	0.43
2:K:83:ASN:O	2:K:87:LEU:HG	2.18	0.43
1:B:78:VAL:N	1:B:82:MET:SD	2.84	0.43
1:C:257:HIS:CD2	1:C:258:GLY:N	2.87	0.43
1:C:351:TYR:O	1:C:354:THR:HG22	2.18	0.43
1:D:46:LYS:HZ3	1:D:239:CYS:HB2	1.83	0.43
1:E:33:GLN:NE2	1:E:61:TRP:H	2.16	0.43
1:F:79:HIS:HB3	1:F:81:ASP:OD1	2.17	0.43
1:F:147:ARG:HH12	1:F:209:PRO:HB2	1.83	0.43
1:G:44:TYR:HE1	1:G:46:LYS:HE2	1.84	0.43
1:G:191:GLU:OE1	1:G:191:GLU:N	2.36	0.43
1:H:286:VAL:HA	1:H:291:ALA:O	2.17	0.43
1:I:70:ASN:O	1:I:74:GLU:HG2	2.19	0.43
1:I:147:ARG:NE	1:I:205:GLU:O	2.51	0.43
1:I:229:ARG:HA	1:I:229:ARG:NE	2.33	0.43
1:I:311:MET:HG2	1:I:312:VAL:N	2.33	0.43
2:K:87:LEU:O	2:K:90:ASN:HB3	2.18	0.43
2:K:128:GLN:HG2	2:K:147:ARG:NH1	2.34	0.43
2:J:67:GLU:OE1	2:J:68:GLU:N	2.52	0.43
1:B:85:ASP:OD1	1:B:87:ASN:ND2	2.42	0.43
1:B:152:ARG:C	1:B:153:LYS:HE2	2.39	0.43
1:C:76:GLY:O	1:C:78:VAL:N	2.52	0.43
1:E:116:ALA:HB3	1:E:301:ALA:O	2.18	0.43
1:E:142:HIS:ND1	1:E:357:TYR:HA	2.33	0.43
1:E:364:HIS:O	1:E:369:LYS:NZ	2.51	0.43
1:F:130:THR:HG23	1:F:132:VAL:H	1.83	0.43
1:F:132:VAL:O	1:F:132:VAL:HG12	2.19	0.43
1:G:216:LEU:HD13	1:G:222:PHE:HZ	1.84	0.43
1:H:246:ILE:O	1:H:250:THR:HG22	2.17	0.43
1:I:58:THR:O	1:I:98:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:151:VAL:HG22	1:I:157:LEU:H	1.83	0.43
1:I:354:THR:OG1	1:I:359:HIS:HA	2.19	0.43
1:B:63:ASP:CG	1:B:66:GLU:H	2.22	0.43
1:C:169:THR:O	1:C:181:ASP:N	2.50	0.43
1:F:382:LEU:HD12	1:F:383:LYS:H	1.83	0.43
1:H:148:GLN:HE22	1:H:152:ARG:HH11	1.66	0.43
1:H:152:ARG:NH1	1:H:162:PRO:HA	2.34	0.43
1:I:149:ALA:O	1:I:153:LYS:HG2	2.18	0.43
2:L:58:ARG:HA	2:L:65:PRO:HG3	2.01	0.43
2:A:26:VAL:O	2:A:30:ARG:HG3	2.18	0.43
2:A:31:HIS:CE1	2:A:69:LYS:HG2	2.54	0.43
2:K:145:PHE:HD2	2:K:147:ARG:NE	2.16	0.43
1:C:300:TYR:OH	1:C:335:LEU:O	2.20	0.43
1:D:71:THR:HA	1:D:74:GLU:OE1	2.19	0.43
1:D:130:THR:O	1:D:133:LEU:HD12	2.19	0.43
1:D:337:PRO:O	1:D:341:ILE:HG13	2.19	0.43
1:E:127:THR:O	1:E:133:LEU:HA	2.19	0.43
1:F:91:VAL:C	1:F:92:LEU:HD22	2.39	0.43
1:F:157:LEU:HD22	1:F:159:TRP:NE1	2.32	0.43
2:A:53:LEU:HB2	2:A:142:ILE:HB	2.01	0.43
2:K:96:CYS:HA	2:K:111:TYR:CE1	2.54	0.43
1:B:101:ASP:N	1:B:101:ASP:OD1	2.52	0.43
1:B:118:ASP:HA	1:B:302:ILE:HD12	2.01	0.43
1:B:165:LYS:HD3	1:C:119:GLN:NE2	2.34	0.43
1:C:284:ASN:HB3	1:C:376:LEU:CD1	2.48	0.43
1:D:110:ASP:HB3	1:D:113:GLU:CD	2.39	0.43
1:E:14:HIS:O	1:E:18:ILE:HG13	2.18	0.43
1:E:76:GLY:O	1:E:78:VAL:HG13	2.19	0.43
1:F:15:PRO:O	1:F:18:ILE:HB	2.19	0.43
1:G:21:GLN:HG2	1:G:355:ALA:HB1	1.99	0.43
1:G:161:ARG:HG3	1:G:189:HIS:C	2.38	0.43
1:H:73:ARG:NH1	1:H:73:ARG:HB2	2.34	0.43
1:I:133:LEU:HD23	1:I:283:LYS:HE3	1.99	0.43
1:I:290:LEU:HD21	1:I:381:GLY:HA3	2.00	0.43
1:I:334:ASP:OD2	1:I:339:GLY:HA3	2.19	0.43
2:A:19:ARG:HA	2:A:27:ASN:OD1	2.19	0.43
2:K:127:PHE:CG	2:K:128:GLN:N	2.87	0.43
1:C:65:GLU:HG2	1:C:91:VAL:HG21	2.00	0.43
1:C:82:MET:SD	1:C:161:ARG:NH1	2.92	0.43
1:D:280:TYR:OH	1:D:372:LYS:HD3	2.19	0.43
1:D:295:GLU:O	1:D:296:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:HIS:CD2	1:E:15:PRO:HD2	2.54	0.43
1:E:110:ASP:O	1:E:113:GLU:HG3	2.19	0.43
1:F:151:VAL:HA	1:F:154:ASN:ND2	2.33	0.43
1:F:246:ILE:HD11	1:F:257:HIS:CD2	2.53	0.43
1:F:296:ILE:HD13	1:F:296:ILE:HA	1.81	0.43
1:G:25:ALA:HB2	1:G:352:LYS:HZ2	1.83	0.43
1:I:132:VAL:O	1:I:132:VAL:HG12	2.19	0.43
2:L:18:PHE:CE1	2:L:92:TRP:HD1	2.37	0.43
2:L:46:GLY:O	2:L:75:CYS:HA	2.19	0.43
2:A:148:ARG:HG3	2:A:149:TRP:O	2.18	0.43
2:J:126:SER:N	2:J:150:GLN:O	2.52	0.43
2:J:145:PHE:HB3	2:J:147:ARG:NH2	2.34	0.43
1:B:121:LEU:HB2	1:B:297:GLN:HE21	1.84	0.42
1:B:203:MET:HA	1:B:207:ILE:CD1	2.49	0.42
1:E:266:ASP:OD2	1:E:268:SER:OG	2.36	0.42
1:G:133:LEU:HB2	1:G:283:LYS:HE3	2.00	0.42
1:G:212:PRO:HG2	1:G:215:TRP:CZ3	2.54	0.42
1:H:3:HIS:O	1:H:172:TYR:HB2	2.19	0.42
1:H:121:LEU:HD12	1:H:298:VAL:O	2.18	0.42
1:H:146:GLN:NE2	1:H:362:ARG:HH21	2.17	0.42
1:I:378:ASP:HA	1:I:382:LEU:HD22	2.01	0.42
2:K:11:PHE:CE2	2:K:74:ARG:HB2	2.54	0.42
2:K:18:PHE:CE1	2:K:92:TRP:HD1	2.37	0.42
2:K:29:SER:HA	2:K:32:ARG:CZ	2.49	0.42
2:K:75:CYS:HB2	2:K:81:ALA:HB3	1.99	0.42
2:J:29:SER:HB2	2:J:33:HIS:NE2	2.34	0.42
1:B:125:TYR:HB3	1:B:251:TYR:CE1	2.55	0.42
1:B:172:TYR:HD1	1:B:175:GLY:HA2	1.84	0.42
1:B:216:LEU:HD22	1:B:222:PHE:HZ	1.84	0.42
1:B:249:ASP:HB3	1:B:359:HIS:HD2	1.84	0.42
1:C:58:THR:OG1	1:C:60:ALA:N	2.53	0.42
1:C:169:THR:OG1	1:C:182:ALA:N	2.52	0.42
1:C:214:GLU:OE1	1:C:214:GLU:N	2.42	0.42
1:D:22:ILE:HD13	1:D:50:VAL:HG21	2.01	0.42
1:D:213:ALA:O	1:D:216:LEU:HB2	2.19	0.42
1:F:65:GLU:HB2	1:F:91:VAL:HG21	2.00	0.42
1:F:267:PRO:O	1:F:273:SER:OG	2.28	0.42
1:G:6:THR:HA	1:G:168:VAL:O	2.19	0.42
1:G:112:LEU:HD13	1:G:336:ARG:NH1	2.33	0.42
1:G:257:HIS:CD2	1:G:258:GLY:H	2.37	0.42
1:G:291:ALA:HA	1:G:317:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:ASN:N	1:H:226:PRO:HD3	2.35	0.42
1:I:109:ALA:C	1:I:114:GLN:HE21	2.22	0.42
2:A:13:VAL:HG13	2:A:100:TYR:CZ	2.53	0.42
1:C:15:PRO:O	1:C:18:ILE:HB	2.19	0.42
1:C:332:PHE:HB3	1:C:372:LYS:NZ	2.35	0.42
1:D:125:TYR:CD2	1:D:255:ALA:HB2	2.55	0.42
1:D:351:TYR:O	1:D:354:THR:HG22	2.19	0.42
1:E:103:ASN:HB2	1:E:106:VAL:HG23	2.00	0.42
1:F:135:PRO:HG2	1:F:251:TYR:HB3	2.01	0.42
1:F:247:ILE:HD13	1:F:247:ILE:HA	1.82	0.42
1:F:299:SER:O	1:F:308:THR:OG1	2.25	0.42
1:G:159:TRP:CZ3	1:G:193:ILE:HD13	2.54	0.42
1:G:171:GLN:HE21	1:G:181:ASP:HA	1.84	0.42
1:G:249:ASP:HB3	1:G:359:HIS:CD2	2.50	0.42
2:A:26:VAL:HA	2:A:29:SER:OG	2.19	0.42
2:A:60:ALA:HB1	2:K:107:ALA:HB1	2.01	0.42
2:A:98:LEU:HA	2:A:109:LEU:HA	2.01	0.42
2:K:137:GLN:OE1	2:K:150:GLN:NE2	2.53	0.42
2:J:128:GLN:OE1	2:J:147:ARG:HD3	2.19	0.42
1:C:313:GLU:OE2	1:C:315:PHE:N	2.51	0.42
1:C:351:TYR:HA	1:C:354:THR:HG22	2.02	0.42
1:D:300:TYR:OH	1:D:335:LEU:HB3	2.19	0.42
1:E:157:LEU:HB2	1:E:160:LEU:HD12	2.01	0.42
1:E:191:GLU:CD	1:E:229:ARG:HH22	2.20	0.42
1:F:38:ARG:HH21	1:F:57:THR:HG21	1.83	0.42
1:H:260:GLY:HA3	1:H:271:ASP:OD2	2.19	0.42
1:I:40:ALA:H	1:I:56:ILE:HD13	1.84	0.42
1:I:203:MET:SD	1:I:208:LYS:HE3	2.59	0.42
2:A:108:GLY:HA2	2:A:123:LEU:CG	2.49	0.42
2:K:19:ARG:HH11	2:K:69:LYS:H	1.67	0.42
2:K:147:ARG:C	2:K:148:ARG:HD2	2.40	0.42
1:C:200:GLU:O	1:C:204:GLU:HG2	2.20	0.42
1:C:319:LYS:HA	1:C:319:LYS:HD3	1.83	0.42
1:D:125:TYR:HE1	1:D:293:ARG:HB2	1.85	0.42
1:E:18:ILE:O	1:E:22:ILE:HG13	2.18	0.42
1:E:185:LEU:O	1:E:224:ILE:HA	2.20	0.42
1:E:324:GLN:HA	1:E:327:LEU:HG	2.01	0.42
1:E:337:PRO:O	1:E:341:ILE:HG13	2.19	0.42
1:G:143:ARG:HA	1:G:146:GLN:HE21	1.84	0.42
1:G:377:ARG:O	1:G:380:ALA:HB3	2.20	0.42
1:H:128:ASN:OD1	1:H:128:ASN:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:282:ALA:O	1:H:286:VAL:HG23	2.19	0.42
1:I:9:SER:OG	1:I:141:ALA:HB1	2.18	0.42
2:A:53:LEU:HD23	2:A:54:THR:N	2.35	0.42
2:K:3:PHE:HB2	2:K:5:LYS:HD2	2.00	0.42
2:J:11:PHE:HE2	2:J:74:ARG:C	2.22	0.42
1:D:127:THR:OG1	1:D:128:ASN:N	2.51	0.42
1:D:279:ARG:HG2	1:D:360:PHE:CD1	2.55	0.42
1:F:131:ASP:HB2	2:L:4:THR:HA	2.01	0.42
1:F:345:ASP:CG	1:F:348:HIS:HE1	2.23	0.42
1:G:82:MET:HG2	1:G:161:ARG:HH11	1.82	0.42
2:L:152:GLN:O	2:J:153:HIS:HB2	2.19	0.42
2:A:30:ARG:O	2:A:34:MET:HG3	2.19	0.42
2:A:58:ARG:HH21	2:A:60:ALA:HA	1.84	0.42
1:C:12:GLU:O	1:C:18:ILE:HG13	2.20	0.42
1:C:82:MET:SD	1:C:161:ARG:HD3	2.59	0.42
1:C:250:THR:HG21	1:C:257:HIS:CE1	2.54	0.42
1:C:277:ALA:O	1:C:281:VAL:HG12	2.18	0.42
1:F:288:ALA:O	1:F:377:ARG:NH2	2.53	0.42
1:G:17:LYS:C	1:G:21:GLN:HE21	2.23	0.42
1:I:65:GLU:O	1:I:69:ARG:HG3	2.19	0.42
2:K:127:PHE:CD1	2:K:128:GLN:N	2.88	0.42
1:B:241:LEU:HG	1:C:241:LEU:HD23	2.02	0.42
1:C:61:TRP:HB3	1:E:61:TRP:CE3	2.55	0.42
1:C:155:GLY:O	1:C:158:PRO:HD3	2.20	0.42
1:D:2:LYS:HD2	1:D:172:TYR:O	2.19	0.42
1:D:153:LYS:HD2	1:D:153:LYS:HA	1.82	0.42
1:E:247:ILE:HD11	1:E:253:GLY:HA3	2.02	0.42
1:F:323:GLU:HG2	1:F:324:GLN:N	2.34	0.42
1:F:375:LEU:H	1:F:375:LEU:HD12	1.84	0.42
1:H:356:ALA:HB1	1:H:357:TYR:CD2	2.55	0.42
1:I:164:ALA:HA	1:I:187:THR:HA	2.02	0.42
2:L:23:CYS:O	2:L:27:ASN:N	2.38	0.42
2:J:44:LEU:O	2:J:84:VAL:HG21	2.19	0.42
1:B:2:LYS:HD3	1:B:2:LYS:HA	1.92	0.42
1:C:137:PRO:HB3	1:C:170:PHE:CE1	2.54	0.42
1:D:163:ASP:OD1	1:D:164:ALA:N	2.52	0.42
1:E:281:VAL:HG23	1:E:333:PHE:CE2	2.54	0.42
1:G:92:LEU:HD13	1:G:92:LEU:HA	1.86	0.42
1:G:250:THR:OG1	1:G:251:TYR:N	2.52	0.42
1:H:78:VAL:N	1:H:82:MET:SD	2.86	0.42
1:H:290:LEU:O	1:H:319:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:PHE:HB3	1:I:172:TYR:CE2	2.54	0.42
1:I:116:ALA:HB1	1:I:270:VAL:HG11	2.02	0.42
1:I:322:SER:O	1:I:325:LEU:HG	2.19	0.42
2:K:53:LEU:HG	2:K:70:THR:OG1	2.20	0.42
2:J:34:MET:HG2	2:J:92:TRP:CD2	2.54	0.42
2:J:68:GLU:O	2:J:70:THR:HG23	2.20	0.42
1:B:161:ARG:NH1	1:B:190:SER:HA	2.35	0.42
1:D:122:MET:HG3	1:D:274:ALA:HB3	2.02	0.42
1:D:197:SER:HA	1:D:200:GLU:HB3	2.01	0.42
1:D:333:PHE:HB3	1:D:343:MET:HE3	2.01	0.42
1:E:225:ASN:N	1:E:226:PRO:HD3	2.35	0.42
1:G:143:ARG:HA	1:G:146:GLN:HG2	2.02	0.42
1:G:170:PHE:HA	1:G:180:ILE:HA	2.02	0.42
1:G:330:ARG:CZ	1:G:330:ARG:HB2	2.50	0.42
1:H:119:GLN:HB3	1:H:302:ILE:H	1.85	0.42
2:A:19:ARG:NH1	2:A:28:MET:HA	2.35	0.42
2:K:95:ASP:OD2	2:K:111:TYR:HB3	2.19	0.42
2:J:146:GLY:O	2:J:148:ARG:NH1	2.53	0.42
1:C:195:GLN:NE2	1:C:228:GLY:O	2.53	0.41
1:E:198:LEU:HD22	1:E:225:ASN:ND2	2.35	0.41
1:F:229:ARG:HH12	1:F:232:ILE:HD12	1.85	0.41
1:G:161:ARG:HB2	1:G:188:GLN:HB3	2.01	0.41
1:H:140:TYR:N	1:H:143:ARG:HH21	2.18	0.41
1:H:204:GLU:HA	1:H:208:LYS:HD3	2.00	0.41
2:L:19:ARG:HE	2:L:68:GLU:CA	2.32	0.41
2:L:77:ASP:CG	2:L:80:GLN:HB2	2.40	0.41
2:A:145:PHE:O	2:A:147:ARG:HG3	2.20	0.41
2:J:10:VAL:HG23	2:J:78:LYS:HZ1	1.85	0.41
2:J:20:SER:OG	2:J:94:GLN:HA	2.20	0.41
1:B:123:PHE:HA	1:B:296:ILE:O	2.21	0.41
1:D:171:GLN:CD	1:D:178:VAL:HG23	2.41	0.41
1:E:293:ARG:HG3	1:E:315:PHE:CD1	2.55	0.41
1:E:340:LEU:HA	1:E:343:MET:HB3	2.01	0.41
1:F:225:ASN:O	1:F:228:GLY:N	2.53	0.41
1:F:332:PHE:HE2	1:F:375:LEU:HB3	1.84	0.41
1:G:112:LEU:HD13	1:G:336:ARG:HH11	1.85	0.41
1:H:17:LYS:O	1:H:21:GLN:HG3	2.20	0.41
1:H:167:GLN:HE22	1:I:308:THR:HG21	1.84	0.41
1:I:39:VAL:N	1:I:266:ASP:OD1	2.31	0.41
2:L:59:GLU:HG2	2:L:59:GLU:O	2.19	0.41
2:K:53:LEU:HD12	2:K:54:THR:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:HD11	1:B:77:TYR:HE2	1.85	0.41
1:C:157:LEU:HB2	1:C:160:LEU:HD12	2.02	0.41
1:C:198:LEU:O	1:C:202:VAL:HG12	2.20	0.41
1:C:267:PRO:HG3	1:C:351:TYR:OH	2.20	0.41
1:E:17:LYS:HG3	1:E:21:GLN:NE2	2.35	0.41
1:F:296:ILE:HD13	1:F:312:VAL:HA	2.01	0.41
1:F:332:PHE:CE2	1:F:375:LEU:HB3	2.55	0.41
1:G:371:ASP:OD1	1:G:371:ASP:N	2.35	0.41
1:H:147:ARG:HE	1:H:150:GLU:HG2	1.84	0.41
1:H:166:SER:HA	1:H:184:VAL:O	2.20	0.41
1:H:170:PHE:CE1	1:H:180:ILE:HG12	2.55	0.41
1:I:30:ILE:HD12	1:I:33:GLN:HB2	2.02	0.41
1:I:184:VAL:HG13	1:I:223:PHE:HB2	2.01	0.41
1:I:241:LEU:HD23	1:I:244:ARG:HH11	1.85	0.41
2:A:9:ASN:OD1	2:A:10:VAL:N	2.54	0.41
2:A:33:HIS:O	2:A:37:THR:HG23	2.20	0.41
1:B:206:ILE:C	1:B:209:PRO:HD2	2.41	0.41
1:C:77:TYR:CE2	1:C:162:PRO:HB2	2.56	0.41
1:C:85:ASP:CG	1:C:88:SER:H	2.20	0.41
1:I:212:PRO:HB2	1:I:215:TRP:HB2	2.02	0.41
2:L:47:SER:CB	2:L:73:VAL:HB	2.50	0.41
2:A:130:VAL:HG22	2:A:147:ARG:HA	2.03	0.41
2:A:138:GLY:N	2:A:148:ARG:HH21	2.19	0.41
2:K:83:ASN:HA	2:K:86:ARG:HG2	2.03	0.41
2:J:14:LEU:CB	2:J:99:VAL:HG12	2.50	0.41
2:J:98:LEU:HA	2:J:98:LEU:HD13	1.87	0.41
1:C:157:LEU:HB3	1:C:159:TRP:CE2	2.56	0.41
1:D:52:VAL:O	1:D:94:ALA:N	2.43	0.41
1:D:327:LEU:HA	1:D:330:ARG:NE	2.31	0.41
1:E:161:ARG:HB2	1:E:188:GLN:HG2	2.01	0.41
1:G:180:ILE:N	1:G:215:TRP:HB3	2.35	0.41
1:H:46:LYS:CD	1:H:47:THR:H	2.32	0.41
1:H:246:ILE:HG12	1:H:261:ALA:HA	2.02	0.41
1:I:38:ARG:HB3	1:I:57:THR:OG1	2.20	0.41
1:I:161:ARG:HG3	1:I:189:HIS:C	2.41	0.41
2:A:57:TYR:CD2	2:K:122:ARG:HG2	2.56	0.41
1:B:146:GLN:HG3	1:B:357:TYR:CD1	2.55	0.41
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.82	0.41
1:B:276:TYR:OH	1:B:359:HIS:ND1	2.37	0.41
1:D:56:ILE:HG22	1:D:58:THR:HG22	2.03	0.41
1:D:92:LEU:HD13	1:D:92:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:MET:HE3	1:D:135:PRO:HD2	2.02	0.41
1:E:4:LEU:HD22	1:E:181:ASP:HB2	2.01	0.41
1:E:63:ASP:O	1:E:67:ILE:HD12	2.19	0.41
1:E:155:GLY:O	1:E:158:PRO:HD3	2.21	0.41
1:E:208:LYS:HB2	1:E:209:PRO:HD3	2.02	0.41
1:G:33:GLN:OE1	1:G:60:ALA:HB1	2.20	0.41
1:G:115:GLY:HA3	1:G:303:GLY:O	2.20	0.41
1:G:272:ARG:HG2	1:G:276:TYR:CE2	2.55	0.41
1:H:31:LEU:HA	1:H:34:ASP:O	2.20	0.41
1:H:157:LEU:HB3	1:H:159:TRP:NE1	2.36	0.41
1:H:272:ARG:HD3	1:H:351:TYR:CE1	2.55	0.41
2:L:86:ARG:NH1	2:L:114:GLY:O	2.52	0.41
2:K:2:ILE:HG13	2:K:3:PHE:N	2.30	0.41
2:K:15:VAL:HG13	2:K:98:LEU:HB2	2.03	0.41
2:J:30:ARG:CZ	2:J:34:MET:HE1	2.51	0.41
1:B:14:HIS:CG	1:B:15:PRO:HD2	2.56	0.41
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.85	0.41
1:D:76:GLY:C	1:D:78:VAL:HG13	2.41	0.41
1:D:204:GLU:HA	1:D:208:LYS:HG2	2.01	0.41
1:D:211:LEU:HD13	1:D:211:LEU:HA	1.79	0.41
1:E:223:PHE:HB3	1:E:226:PRO:HG3	2.02	0.41
1:F:207:ILE:HD13	1:F:222:PHE:CD2	2.56	0.41
1:H:334:ASP:OD1	1:H:339:GLY:HA3	2.20	0.41
1:I:2:LYS:HE2	1:I:171:GLN:HB3	2.03	0.41
1:I:223:PHE:O	1:I:224:ILE:HD13	2.21	0.41
2:L:31:HIS:CE1	2:L:69:LYS:HG2	2.56	0.41
2:A:109:LEU:HD22	2:A:123:LEU:HD11	2.03	0.41
2:K:112:ALA:HB1	2:K:117:GLY:O	2.21	0.41
2:J:96:CYS:HB3	2:J:111:TYR:CD1	2.56	0.41
1:B:110:ASP:HB3	1:B:113:GLU:CD	2.41	0.41
1:D:56:ILE:O	1:D:97:LYS:HA	2.21	0.41
1:E:69:ARG:NH1	1:E:89:CYS:O	2.51	0.41
1:E:318:GLU:OE1	1:E:322:SER:N	2.54	0.41
1:F:9:SER:HA	1:F:248:VAL:HG23	2.02	0.41
1:G:159:TRP:CZ3	1:G:160:LEU:HG	2.55	0.41
1:G:292:ASP:OD2	1:G:317:THR:HB	2.21	0.41
1:H:247:ILE:HG13	1:H:248:VAL:N	2.36	0.41
1:H:278:ALA:HA	1:H:281:VAL:HG22	2.03	0.41
1:H:382:LEU:H	1:H:382:LEU:HD23	1.84	0.41
2:A:92:TRP:HA	2:A:92:TRP:CE3	2.55	0.41
2:J:127:PHE:CE2	2:J:128:GLN:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:HIS:CD2	1:B:165:LYS:HE3	2.56	0.41
1:C:12:GLU:HB2	1:C:21:GLN:HE22	1.86	0.41
1:C:188:GLN:HG3	1:C:230:PHE:O	2.21	0.41
1:C:202:VAL:HG23	1:C:206:ILE:HD13	2.02	0.41
1:C:250:THR:OG1	1:C:251:TYR:N	2.54	0.41
1:D:31:LEU:HA	1:D:34:ASP:O	2.20	0.41
1:D:125:TYR:N	1:D:251:TYR:OH	2.45	0.41
1:D:137:PRO:HA	1:D:170:PHE:CZ	2.56	0.41
1:D:221:LYS:HB2	1:D:221:LYS:HE2	1.86	0.41
1:D:314:THR:HG21	1:D:318:GLU:HB3	2.03	0.41
1:D:370:THR:HG22	1:D:373:ALA:HB2	2.03	0.41
1:E:181:ASP:O	1:E:220:THR:HA	2.20	0.41
1:E:292:ASP:H	1:E:317:THR:HB	1.86	0.41
1:F:27:LEU:O	1:F:30:ILE:HG22	2.21	0.41
1:F:215:TRP:O	1:F:217:THR:HG23	2.20	0.41
1:F:257:HIS:CD2	1:F:259:GLY:N	2.88	0.41
1:F:300:TYR:O	1:G:167:GLN:NE2	2.54	0.41
1:F:346:LEU:O	1:F:348:HIS:N	2.51	0.41
1:G:28:ASP:OD2	1:G:351:TYR:N	2.54	0.41
1:G:71:THR:HA	1:G:74:GLU:OE1	2.21	0.41
1:G:139:THR:O	1:G:143:ARG:NE	2.41	0.41
1:G:204:GLU:O	1:G:209:PRO:HD3	2.20	0.41
1:G:250:THR:HG22	1:G:262:PHE:HE2	1.84	0.41
1:G:327:LEU:HA	1:G:330:ARG:HH21	1.86	0.41
1:G:361:GLY:N	1:G:368:GLU:OE2	2.54	0.41
1:H:114:GLN:HB2	1:H:338:TYR:CD1	2.55	0.41
1:I:46:LYS:CG	1:I:47:THR:H	2.34	0.41
1:I:183:VAL:O	1:I:222:PHE:HA	2.21	0.41
1:I:213:ALA:HA	1:I:216:LEU:HB3	2.02	0.41
1:I:284:ASN:ND2	1:I:370:THR:HA	2.36	0.41
1:I:325:LEU:HA	1:I:328:LEU:HG	2.03	0.41
2:A:128:GLN:CG	2:A:147:ARG:HD3	2.43	0.41
1:C:130:THR:HA	2:J:3:PHE:O	2.21	0.41
1:D:114:GLN:NE2	1:D:338:TYR:OH	2.53	0.41
1:E:15:PRO:O	1:E:18:ILE:HB	2.21	0.41
1:E:163:ASP:HB3	1:E:188:GLN:HB2	2.03	0.41
1:F:150:GLU:OE1	1:F:154:ASN:ND2	2.29	0.41
1:F:260:GLY:HA3	1:F:271:ASP:OD1	2.21	0.41
1:F:265:LYS:O	1:F:272:ARG:NH1	2.54	0.41
1:G:55:GLU:O	1:G:56:ILE:HD13	2.20	0.41
1:G:119:GLN:H	1:G:302:ILE:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:ARG:HH21	1:G:283:LYS:CE	2.34	0.41
1:H:142:HIS:CE1	1:H:248:VAL:HG22	2.56	0.41
1:I:5:PHE:CZ	1:I:254:MET:HB2	2.56	0.41
1:I:337:PRO:O	1:I:341:ILE:HG13	2.21	0.41
2:L:28:MET:O	2:L:32:ARG:HG3	2.21	0.41
2:J:4:THR:C	2:J:6:GLU:H	2.24	0.41
2:J:122:ARG:C	2:J:123:LEU:HD23	2.41	0.41
1:B:137:PRO:HA	1:B:170:PHE:CZ	2.56	0.40
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.78	0.40
1:B:346:LEU:O	1:B:348:HIS:N	2.52	0.40
1:E:16:ASP:OD1	1:E:240:GLY:HA2	2.20	0.40
1:E:318:GLU:OE2	1:E:322:SER:HB3	2.21	0.40
1:G:93:SER:OG	1:I:93:SER:O	2.20	0.40
1:G:245:LYS:HG3	1:G:248:VAL:HG21	2.04	0.40
2:L:77:ASP:HB3	2:L:80:GLN:H	1.86	0.40
2:J:12:TYR:HE1	2:J:78:LYS:HD2	1.84	0.40
2:J:131:PRO:HD2	2:J:148:ARG:NH2	2.34	0.40
1:C:112:LEU:HD12	1:C:336:ARG:NH1	2.36	0.40
1:C:344:LEU:HD23	1:C:344:LEU:HA	1.76	0.40
1:E:27:LEU:HD23	1:E:272:ARG:HH12	1.87	0.40
1:E:187:THR:N	1:E:225:ASN:OD1	2.42	0.40
1:F:239:CYS:SG	1:G:42:GLU:HG3	2.61	0.40
1:F:301:ALA:HB2	1:G:184:VAL:HG21	2.02	0.40
1:G:47:THR:H	1:G:47:THR:HG23	1.62	0.40
1:H:297:GLN:HB3	1:H:311:MET:HB3	2.02	0.40
1:H:300:TYR:O	1:I:167:GLN:NE2	2.43	0.40
1:I:290:LEU:HD23	1:I:290:LEU:HA	1.94	0.40
2:J:126:SER:O	2:J:149:TRP:HB2	2.21	0.40
2:J:148:ARG:HB2	2:J:150:GLN:HE22	1.85	0.40
1:B:4:LEU:CD2	1:B:171:GLN:HG2	2.51	0.40
1:B:58:THR:C	1:B:100:PRO:HG3	2.41	0.40
1:C:127:THR:O	1:C:133:LEU:HA	2.20	0.40
1:D:305:ALA:HB1	1:D:336:ARG:HE	1.86	0.40
1:D:362:ARG:HB2	1:D:365:PHE:CE2	2.56	0.40
1:E:31:LEU:HD22	1:E:349:PRO:N	2.37	0.40
1:E:136:ALA:O	1:E:139:THR:OG1	2.29	0.40
1:F:69:ARG:NH1	1:F:87:ASN:O	2.55	0.40
1:F:157:LEU:HD13	1:F:159:TRP:CZ2	2.56	0.40
1:F:372:LYS:HB3	1:F:372:LYS:HE3	1.87	0.40
1:G:117:GLY:O	1:G:302:ILE:HG13	2.21	0.40
1:G:328:LEU:HA	1:G:331:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:GLU:O	1:H:69:ARG:HG3	2.22	0.40
1:H:79:HIS:CD2	1:H:81:ASP:H	2.38	0.40
1:I:330:ARG:HB3	1:I:335:LEU:HD11	2.01	0.40
2:L:90:ASN:ND2	2:L:114:GLY:O	2.54	0.40
2:A:13:VAL:HG21	2:A:72:ARG:NH2	2.37	0.40
2:J:56:CYS:HA	2:J:66:THR:O	2.21	0.40
1:B:177:ILE:HD12	1:B:177:ILE:H	1.86	0.40
1:B:178:VAL:HG23	1:B:179:GLY:H	1.86	0.40
1:B:353:GLU:CD	1:B:364:HIS:HE2	2.25	0.40
1:C:247:ILE:HA	1:C:247:ILE:HD13	1.84	0.40
1:D:314:THR:O	1:D:317:THR:OG1	2.31	0.40
1:E:170:PHE:HB3	1:E:177:ILE:HG23	2.03	0.40
1:F:36:LYS:HA	1:F:36:LYS:HD3	1.91	0.40
1:F:112:LEU:HD22	1:F:339:GLY:HA2	2.03	0.40
1:F:203:MET:HA	1:F:207:ILE:HD12	2.03	0.40
1:H:364:HIS:O	1:H:369:LYS:NZ	2.55	0.40
1:I:132:VAL:CG1	1:I:361:GLY:HA2	2.51	0.40
2:A:53:LEU:HG	2:A:141:THR:C	2.41	0.40
2:A:128:GLN:HG3	2:A:147:ARG:NH1	2.32	0.40
2:K:23:CYS:SG	2:K:26:VAL:HG22	2.62	0.40
1:C:50:VAL:HG22	1:C:89:CYS:SG	2.61	0.40
1:C:241:LEU:HB2	1:C:244:ARG:HG3	2.03	0.40
1:D:347:LEU:O	1:D:348:HIS:ND1	2.55	0.40
1:E:46:LYS:CG	1:E:47:THR:H	2.29	0.40
1:E:144:LEU:HD11	1:E:211:LEU:HD21	2.03	0.40
1:E:343:MET:HG2	1:E:344:LEU:HG	2.02	0.40
1:F:18:ILE:HA	1:F:21:GLN:NE2	2.37	0.40
1:F:143:ARG:HH12	1:F:210:ILE:HD12	1.86	0.40
1:F:299:SER:OG	1:F:308:THR:OG1	2.37	0.40
1:I:84:PHE:CG	1:I:235:PRO:HG2	2.56	0.40
1:I:179:GLY:HA2	1:I:215:TRP:CG	2.55	0.40
2:L:128:GLN:HB3	2:L:147:ARG:NH1	2.35	0.40
2:A:140:PHE:HD1	2:A:147:ARG:O	2.04	0.40
2:K:94:GLN:NE2	2:K:95:ASP:H	2.19	0.40
2:J:130:VAL:HG23	2:J:148:ARG:NH1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	382/390 (98%)	354 (93%)	27 (7%)	1 (0%)	41	75
1	C	382/390 (98%)	358 (94%)	24 (6%)	0	100	100
1	D	381/390 (98%)	355 (93%)	26 (7%)	0	100	100
1	E	381/390 (98%)	356 (93%)	25 (7%)	0	100	100
1	F	382/390 (98%)	355 (93%)	26 (7%)	1 (0%)	41	75
1	G	381/390 (98%)	358 (94%)	23 (6%)	0	100	100
1	H	381/390 (98%)	368 (97%)	13 (3%)	0	100	100
1	I	381/390 (98%)	362 (95%)	19 (5%)	0	100	100
2	A	149/158 (94%)	119 (80%)	28 (19%)	2 (1%)	12	50
2	J	145/158 (92%)	121 (83%)	23 (16%)	1 (1%)	22	61
2	K	143/158 (90%)	121 (85%)	21 (15%)	1 (1%)	22	61
2	L	150/158 (95%)	124 (83%)	25 (17%)	1 (1%)	22	61
All	All	3638/3752 (97%)	3351 (92%)	280 (8%)	7 (0%)	50	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	10	VAL
2	J	10	VAL
2	A	10	VAL
1	B	108	ARG
1	F	98	GLN
2	A	9	ASN
2	K	5	LYS

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	B	312/318 (98%)	309 (99%)	3 (1%)	76	88
1	C	312/318 (98%)	311 (100%)	1 (0%)	92	97
1	D	311/318 (98%)	310 (100%)	1 (0%)	92	97
1	E	311/318 (98%)	309 (99%)	2 (1%)	86	94
1	F	312/318 (98%)	310 (99%)	2 (1%)	86	94
1	G	311/318 (98%)	309 (99%)	2 (1%)	86	94
1	H	311/318 (98%)	309 (99%)	2 (1%)	86	94
1	I	311/318 (98%)	311 (100%)	0	100	100
2	A	127/134 (95%)	126 (99%)	1 (1%)	81	91
2	J	125/134 (93%)	123 (98%)	2 (2%)	62	83
2	K	125/134 (93%)	121 (97%)	4 (3%)	39	70
2	L	128/134 (96%)	126 (98%)	2 (2%)	62	83
All	All	2996/3080 (97%)	2974 (99%)	22 (1%)	84	93

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

Mol	Chain	Res	Type
1	B	17	LYS
1	B	108	ARG
1	B	122	MET
1	C	122	MET
1	D	293	ARG
1	E	110	ASP
1	E	122	MET
1	F	36	LYS
1	F	122	MET
1	G	122	MET
1	G	143	ARG
1	H	266	ASP
1	H	336	ARG
2	L	56	CYS

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Mol	Chain	Res	Type
2	L	118	TYR
2	A	56	CYS
2	K	13	VAL
2	K	56	CYS
2	K	78	LYS
2	K	139	CYS
2	J	139	CYS
2	J	148	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	B	119	GLN
1	B	195	GLN
1	B	225	ASN
1	B	257	HIS
1	B	297	GLN
1	B	374	GLN
1	B	384	HIS
1	C	21	GLN
1	C	119	GLN
1	C	146	GLN
1	C	195	GLN
1	C	257	HIS
1	D	33	GLN
1	D	119	GLN
1	D	148	GLN
1	E	79	HIS
1	E	195	GLN
1	E	257	HIS
1	F	33	GLN
1	F	70	ASN
1	F	104	GLN
1	F	167	GLN
1	F	195	GLN
1	F	297	GLN
1	F	324	GLN
1	F	342	GLN
1	F	384	HIS
1	G	114	GLN
1	G	142	HIS

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Mol	Chain	Res	Type
1	G	146	GLN
1	G	171	GLN
1	G	195	GLN
1	G	225	ASN
1	G	257	HIS
1	G	297	GLN
1	G	374	GLN
1	H	21	GLN
1	H	79	HIS
1	H	87	ASN
1	H	103	ASN
1	H	104	GLN
1	H	114	GLN
1	H	142	HIS
1	H	148	GLN
1	H	167	GLN
1	H	297	GLN
1	I	33	GLN
1	I	98	GLN
1	I	119	GLN
1	I	171	GLN
1	I	189	HIS
1	I	284	ASN
1	I	297	GLN
1	I	324	GLN
1	I	342	GLN
1	I	359	HIS
2	L	94	GLN
2	L	152	GLN
2	A	21	ASN
2	A	33	HIS
2	A	152	GLN
2	K	31	HIS
2	K	94	GLN
2	K	103	GLN
2	K	128	GLN
2	K	137	GLN
2	K	150	GLN
2	J	90	ASN
2	J	105	HIS
2	J	150	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12809. 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 |
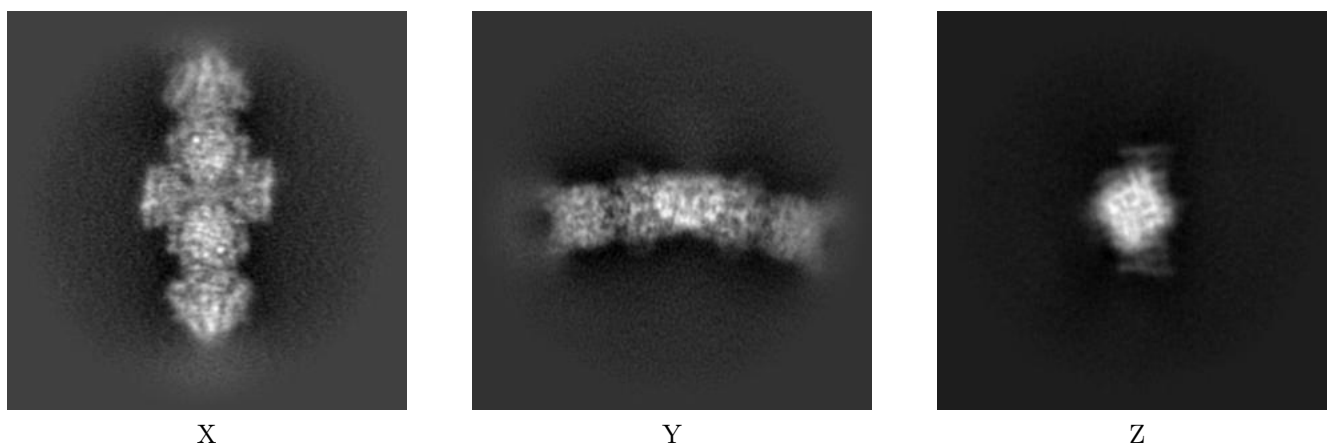
The images above show the map projected in three orthogonal directions.

6.2   Central slices (i)

6.2.1   Primary map

| X Index: 150 | Y Index: 150 | Z Index: 150 |
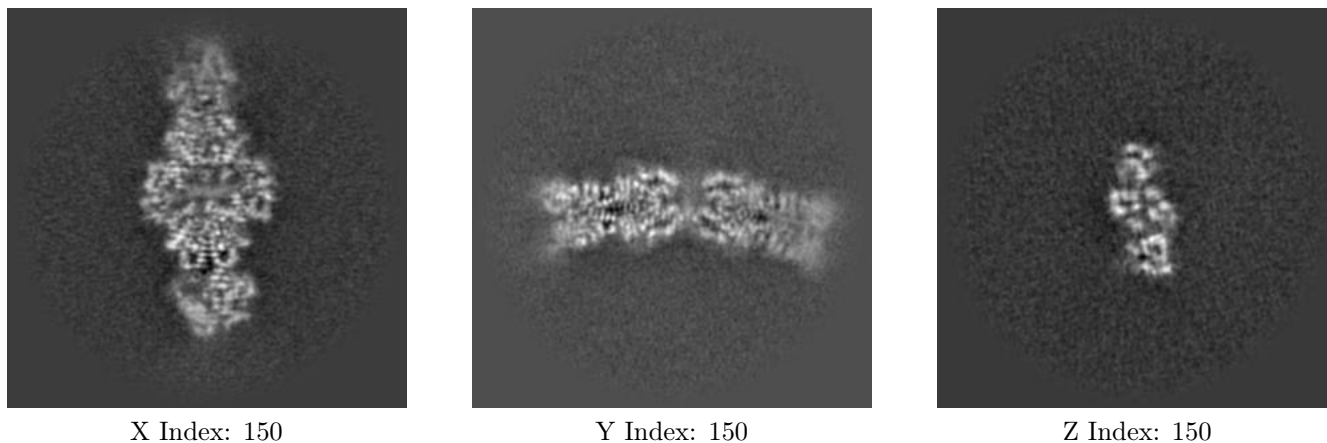
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
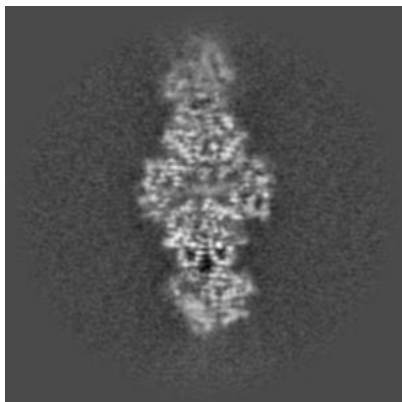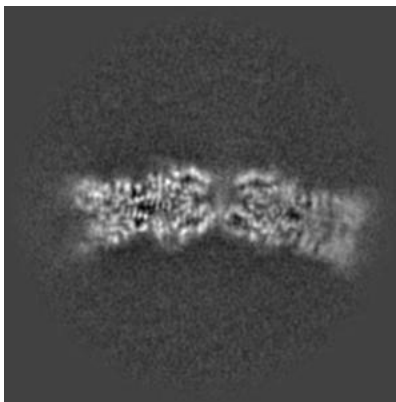
| X Index: 149 | Y Index: 149 | Z Index: 144 |
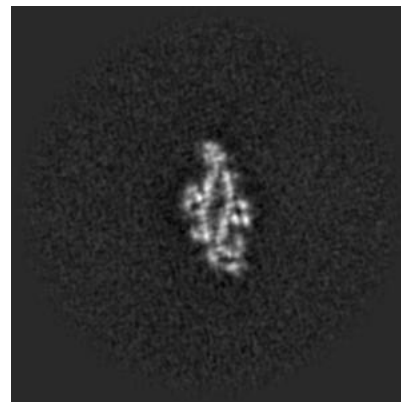
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

| X | Y | Z |
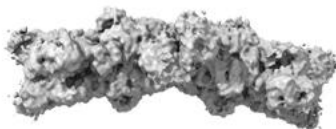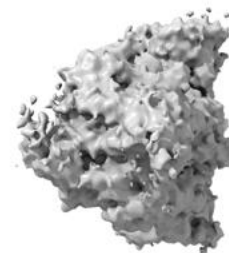
The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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6.5   Mask visualisation ⓘ

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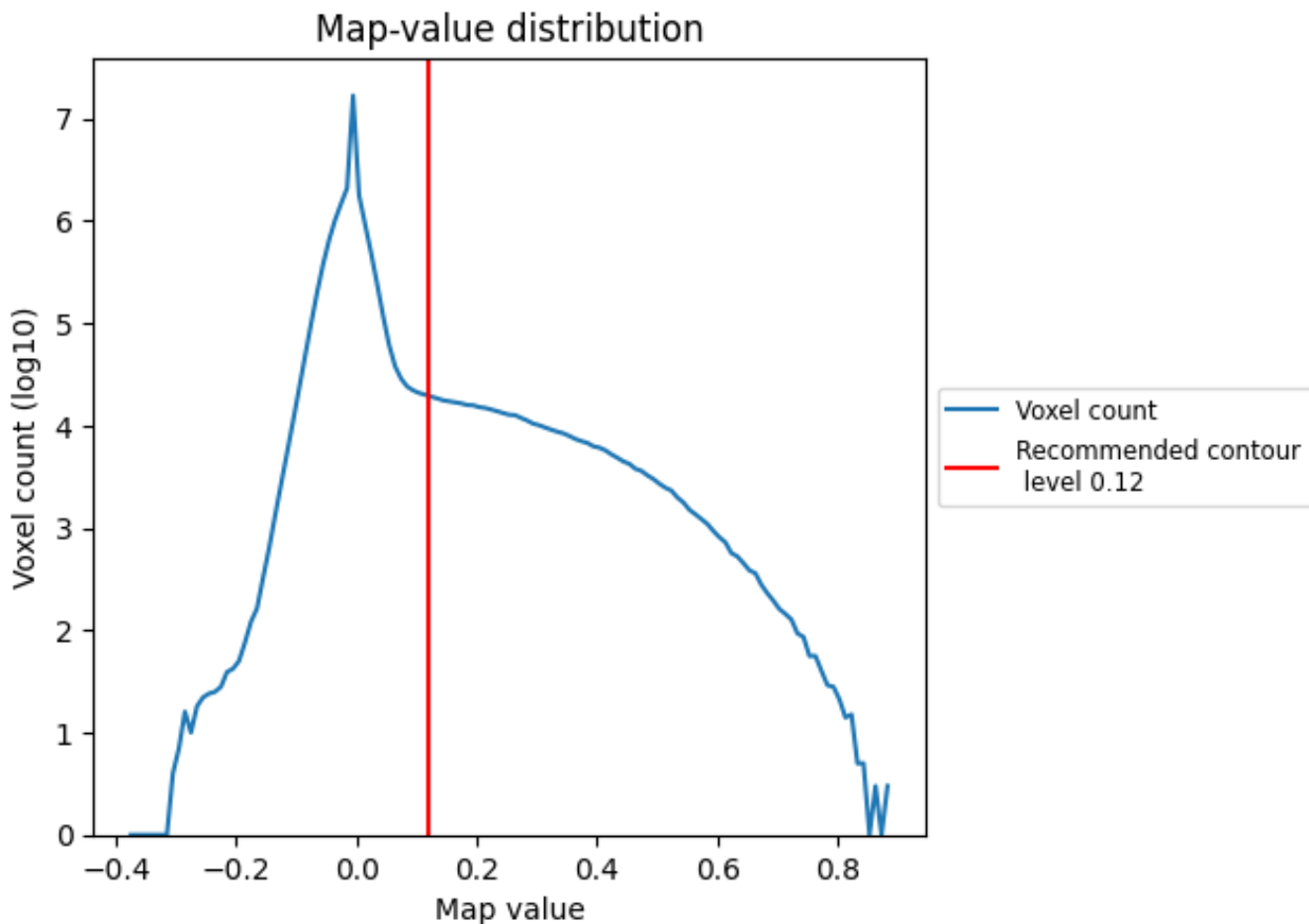
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
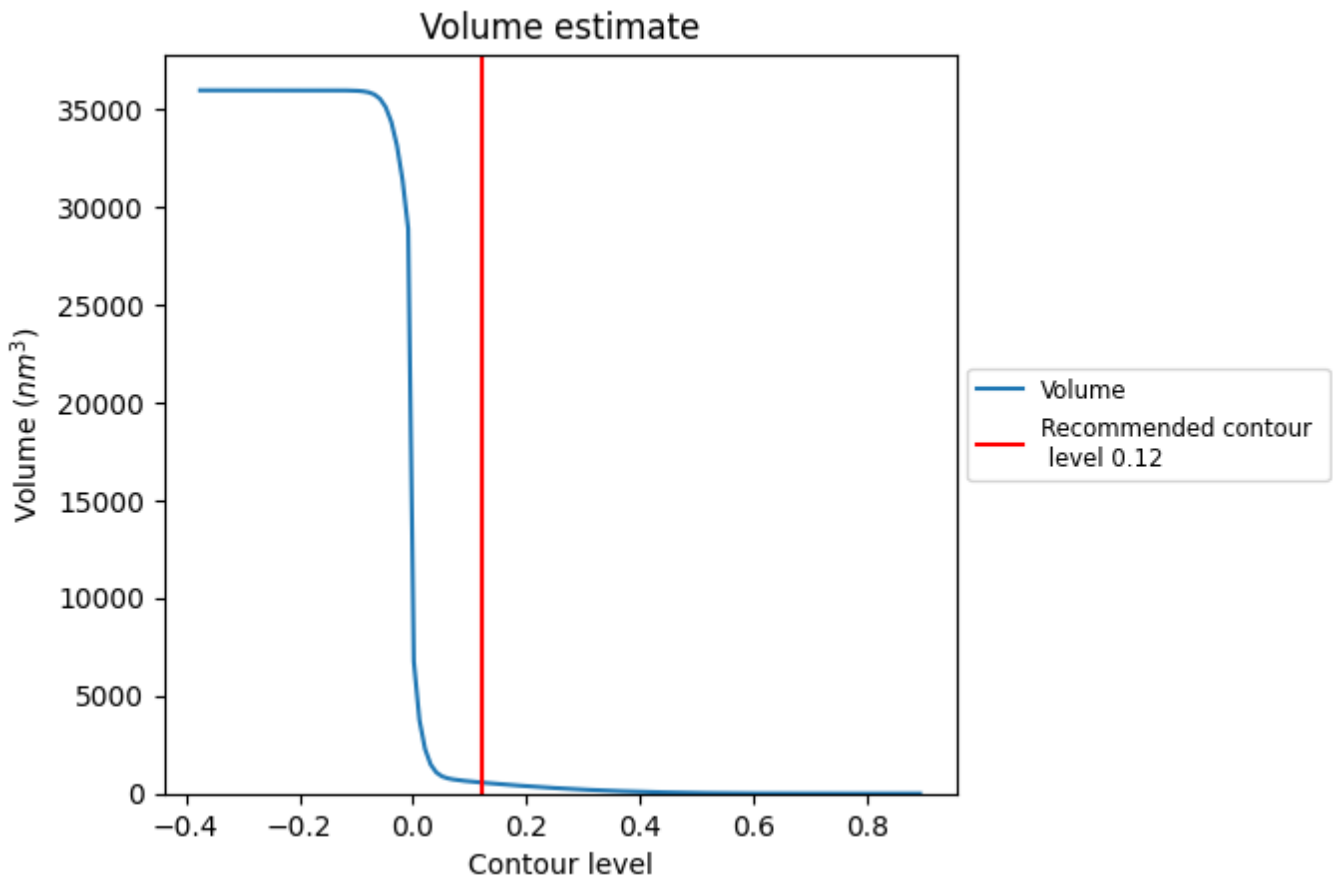
The volume at the recommended contour level is 565 nm^3; this corresponds to an approximate mass of 510 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ
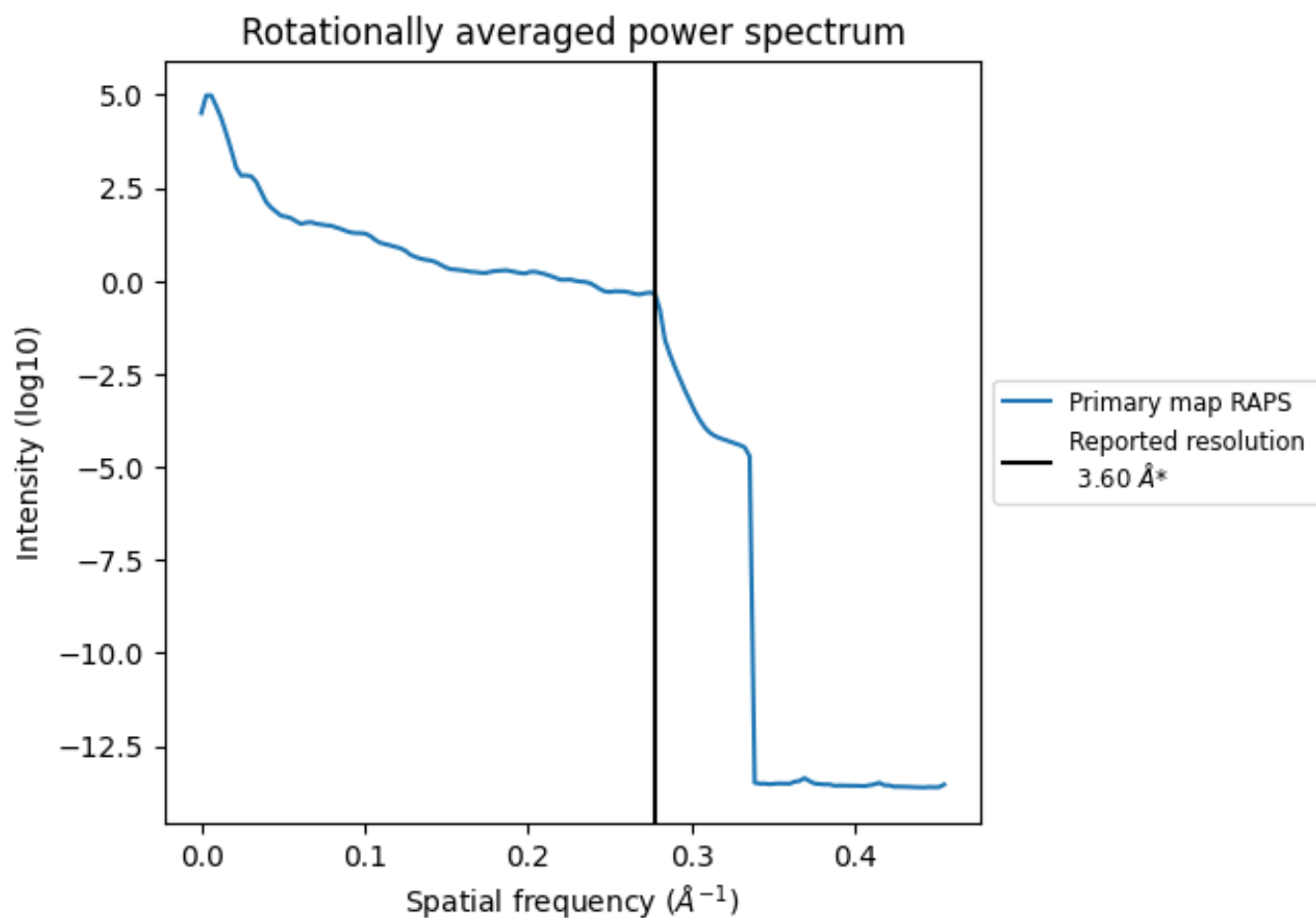
*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

8 Fourier-Shell correlation (i)

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

9   Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12809 and PDB model 7OCK. Per-residue inclusion information can be found in section 3 on page 7.

9.1   Map-model overlay (i)

X	Y	Z
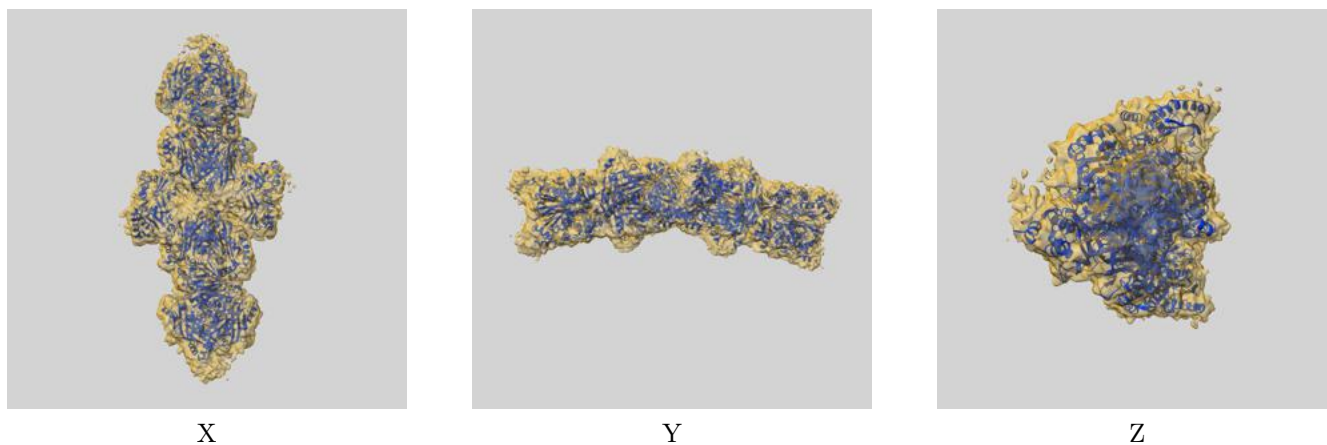
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion ⓘ
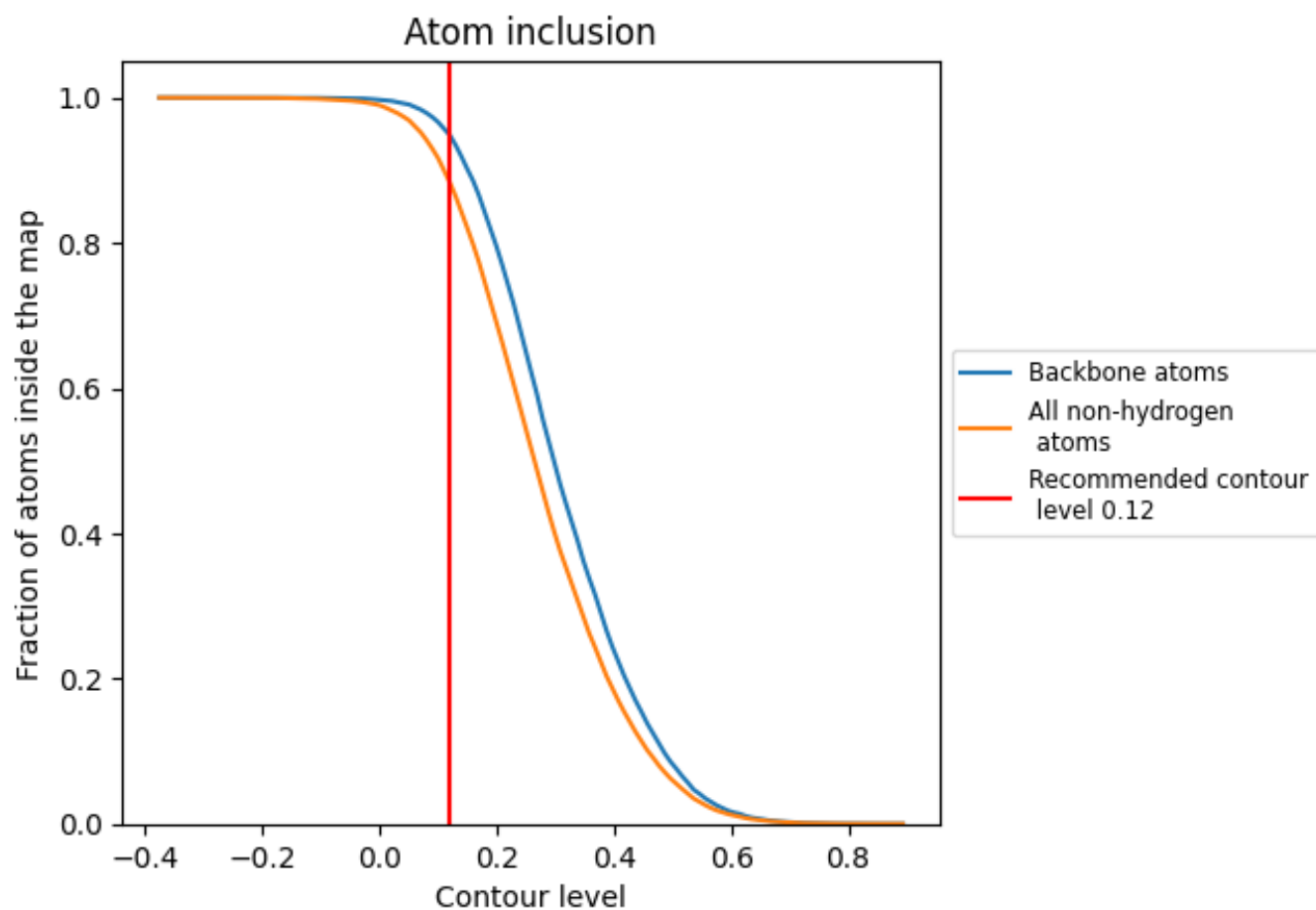
At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.