Full wwPDB EM Validation Report (i)

Mar 3, 2024 – 12:47 PM EST

PDB ID	:	5VY5
EMDB ID	:	EMD-8743
Title	:	Rabbit muscle aldolase using 200keV
Authors	:	Herzik Jr., M.A.; Wu, M.; Lander, G.C.
Deposited on	:	2017-05-24
Resolution	:	2.60 Å(reported)

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

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

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

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

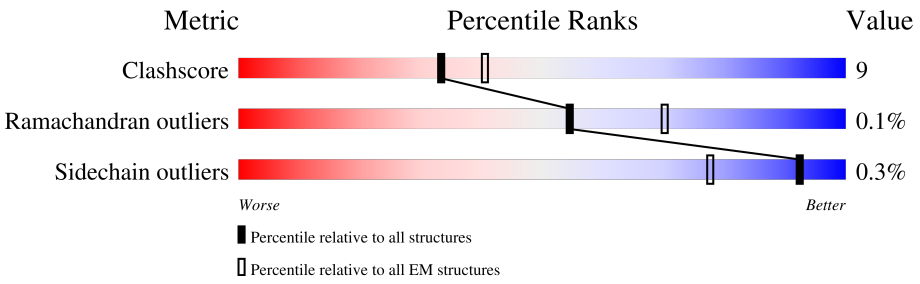
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	363	6% 72% 22% 6%
1	1-B	363	6% 72% 23% 6%
1	1-C	363	6% 73% 21% 6%
1	1-D	363	6% 72% 22% 6%
1	10-A	363	73% 21% 6%
1	10-B	363	73% 21% 6%
1	10-C	363	73% 21% 6%
1	10-D	363	73% 21% 6%

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Mol	Chain	Length	Quality of chain
1	2-A	363	76% 18% 6%
1	2-B	363	76% 18% 6%
1	2-C	363	76% 18% 6%
1	2-D	363	75% 19% 6%
1	3-A	363	74% 20% 6%
1	3-B	363	74% 20% 6%
1	3-C	363	75% 19% 6%
1	3-D	363	75% 20% 6%
1	4-A	363	74% 21% 6%
1	4-B	363	74% 21% 6%
1	4-C	363	74% 20% 6%
1	4-D	363	74% 20% 6%
1	5-A	363	75% 19% • 6%
1	5-B	363	75% 19% • 6%
1	5-C	363	75% 19% • 6%
1	5-D	363	75% 19% • 6%
1	6-A	363	72% 22% 6%
1	6-B	363	72% 23% 6%
1	6-C	363	71% 23% 6%
1	6-D	363	71% 23% 6%
1	7-A	363	73% 21% 6%
1	7-B	363	73% 22% 6%
1	7-C	363	73% 21% 6%
1	7-D	363	74% 21% 6%
1	8-A	363	77% 18% 6%

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Mol	Chain	Length	Quality of chain
1	8-B	363	77% 17% 6%
1	8-C	363	77% 17% 6%
1	8-D	363	77% 17% 6%
1	9-A	363	77% 18% 6%
1	9-B	363	77% 18% 6%
1	9-C	363	76% 18% 6%
1	9-D	363	76% 18% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 104720 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 Fructose-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1-B	343	2618	1647	465	495	11	0	0
1	2-B	343	2618	1647	465	495	11	0	0
1	3-B	343	2618	1647	465	495	11	0	0
1	4-B	343	2618	1647	465	495	11	0	0
1	5-B	343	2618	1647	465	495	11	0	0
1	6-B	343	2618	1647	465	495	11	0	0
1	7-B	343	2618	1647	465	495	11	0	0
1	8-B	343	2618	1647	465	495	11	0	0
1	9-B	343	2618	1647	465	495	11	0	0
1	10-B	343	2618	1647	465	495	11	0	0
1	1-A	343	2618	1647	465	495	11	0	0
1	2-A	343	2618	1647	465	495	11	0	0
1	3-A	343	2618	1647	465	495	11	0	0
1	4-A	343	2618	1647	465	495	11	0	0
1	5-A	343	2618	1647	465	495	11	0	0
1	6-A	343	2618	1647	465	495	11	0	0
1	7-A	343	2618	1647	465	495	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8-A	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	9-A	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	10-A	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	1-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	2-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	3-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	4-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	5-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	6-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	7-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	8-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	9-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	10-C	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	1-D	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	2-D	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	3-D	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	4-D	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	5-D	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	6-D	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	7-D	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	8-D	343	2618	1647	465	495	11	0	0

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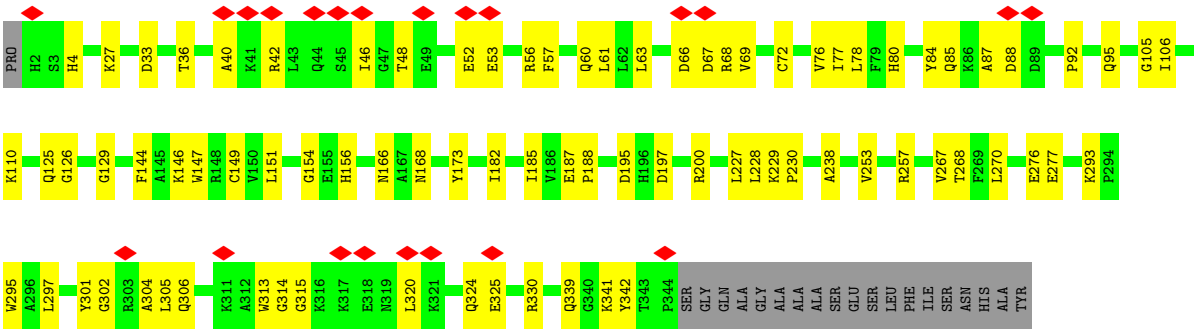
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	9-D	343	2618	1647	465	495	11	0	0
			Total	C	N	O	S		
1	10-D	343	2618	1647	465	495	11	0	0

3 Residue-property plots (i)

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

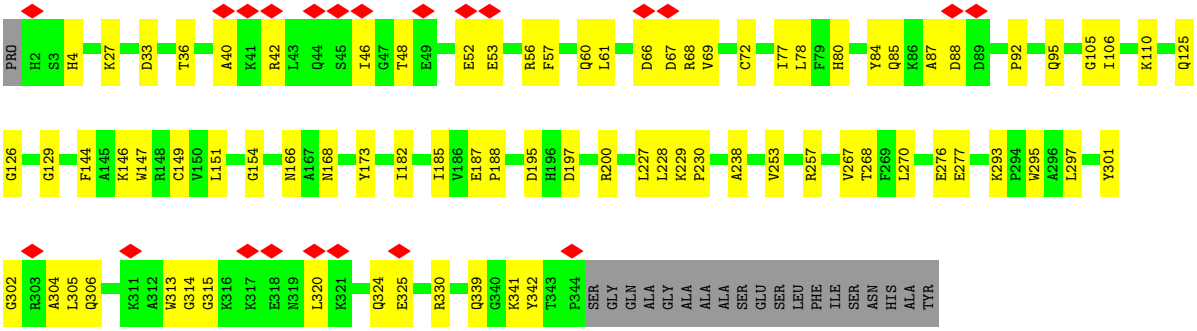
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 1-B:



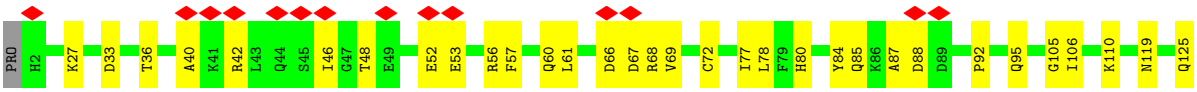
• Molecule 1: Fructose-bisphosphate aldolase A

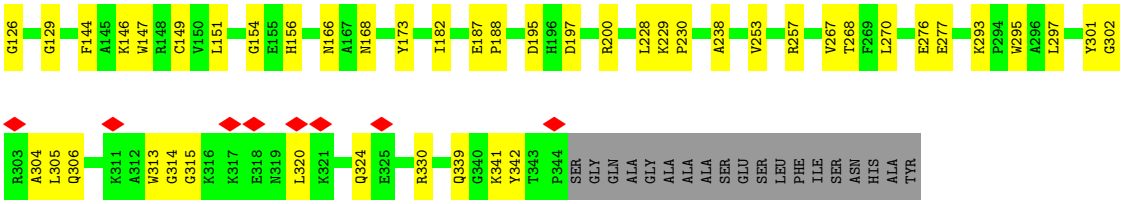
Chain 1-A:



• Molecule 1: Fructose-bisphosphate aldolase A

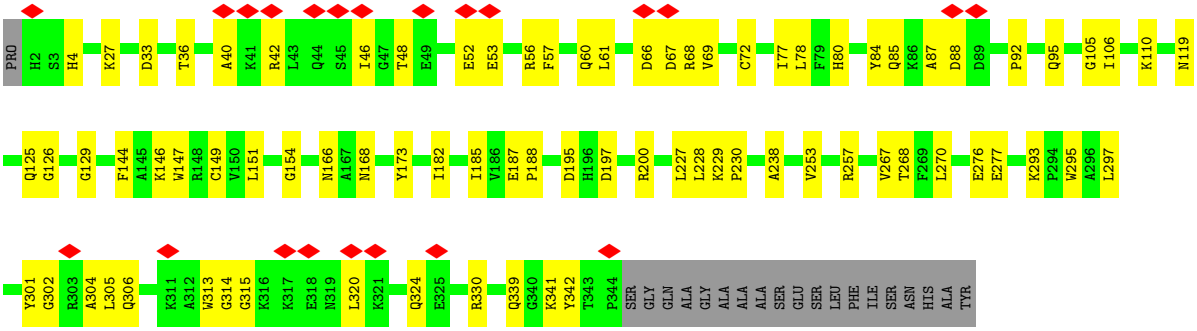
Chain 1-C:





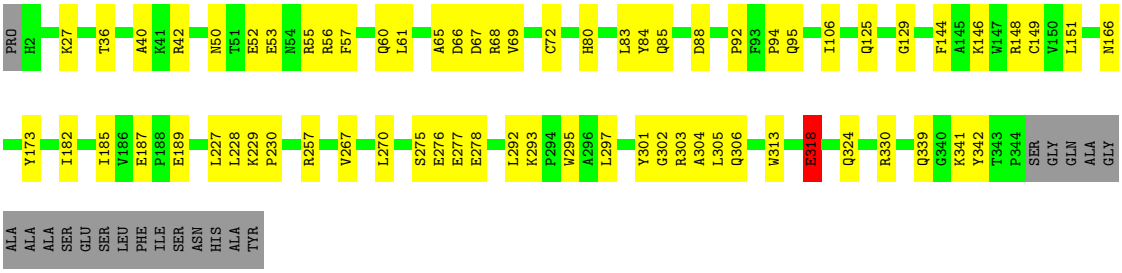
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 1-D:



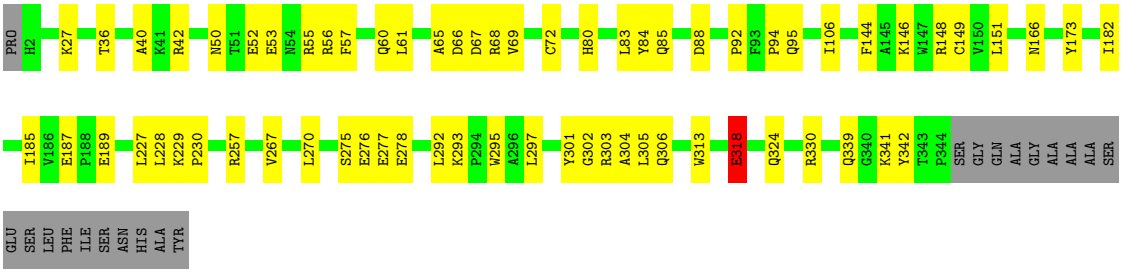
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 2-B:



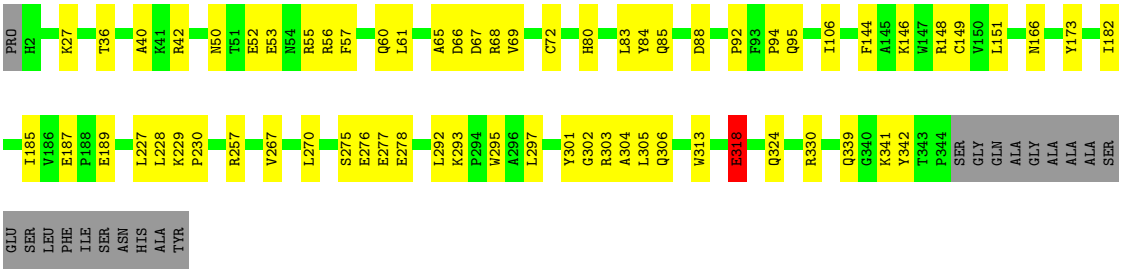
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 2-A:



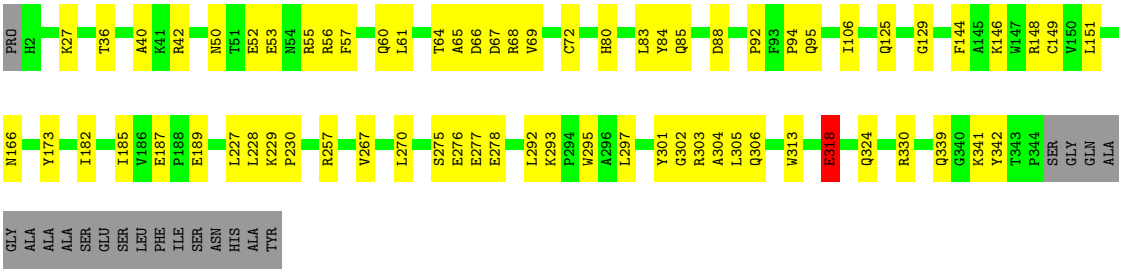
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 2-C:



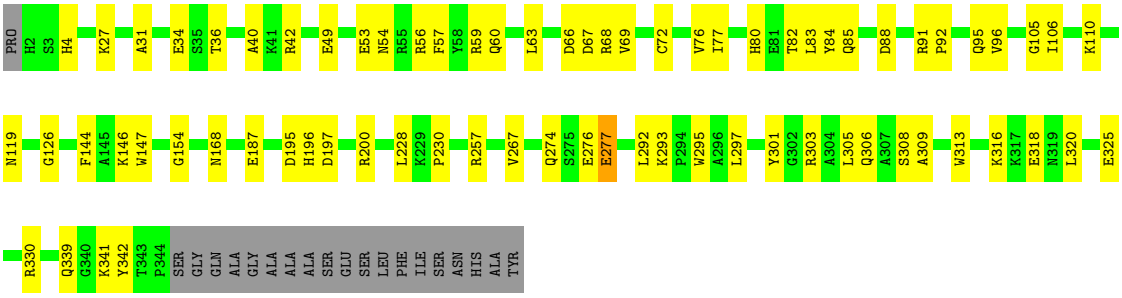
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 2-D:



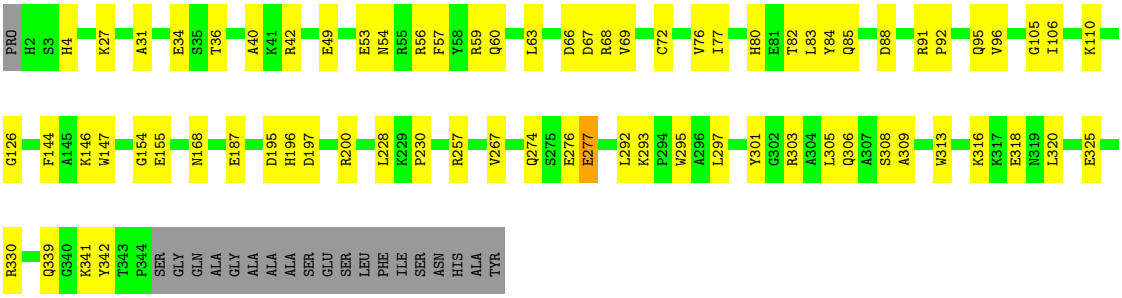
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 3-B:



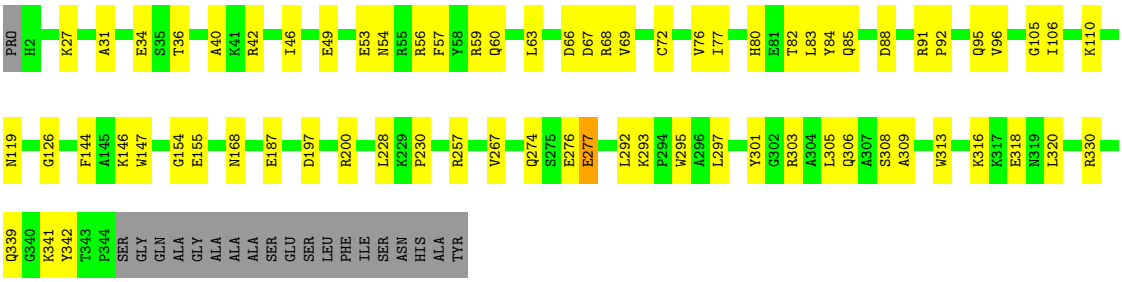
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 3-A:



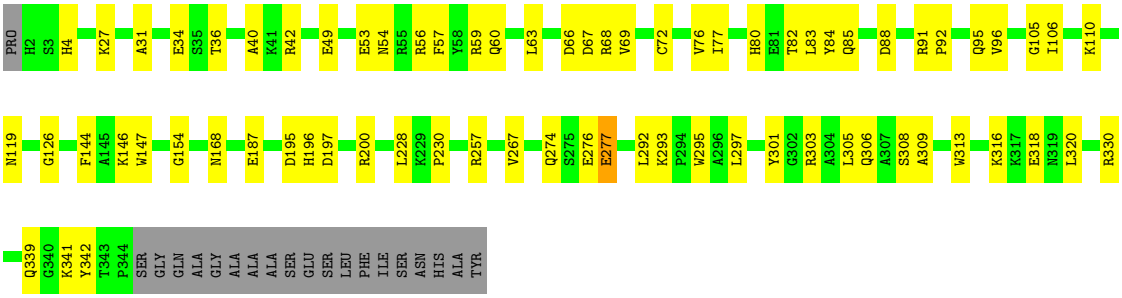
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 3-C:



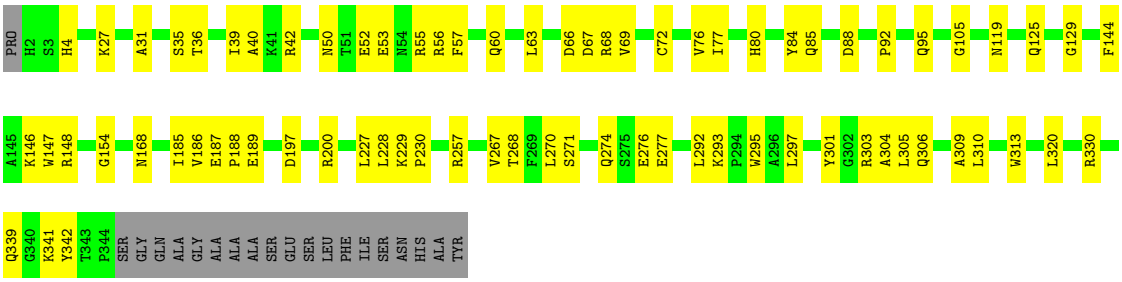
- Molecule 1: Fructose-bisphosphate aldolase A

Chain 3-D:



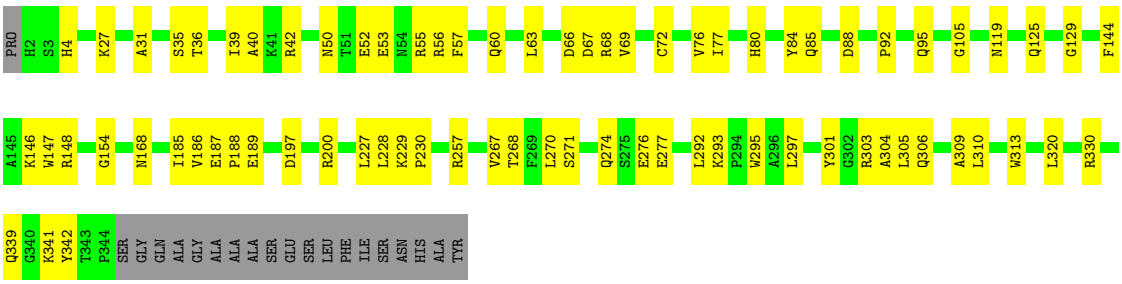
- Molecule 1: Fructose-bisphosphate aldolase A

Chain 4-B:



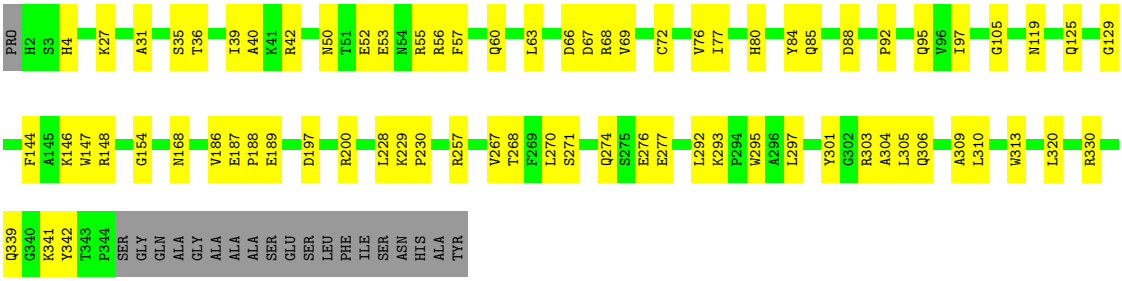
- Molecule 1: Fructose-bisphosphate aldolase A

Chain 4-A:



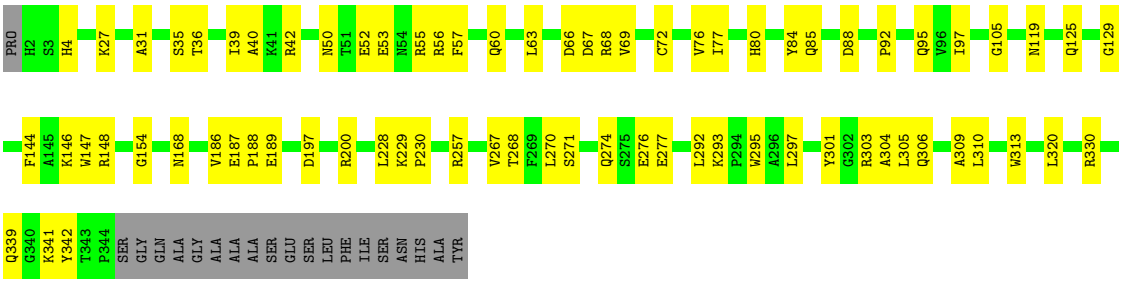
- Molecule 1: Fructose-bisphosphate aldolase A

Chain 4-C:



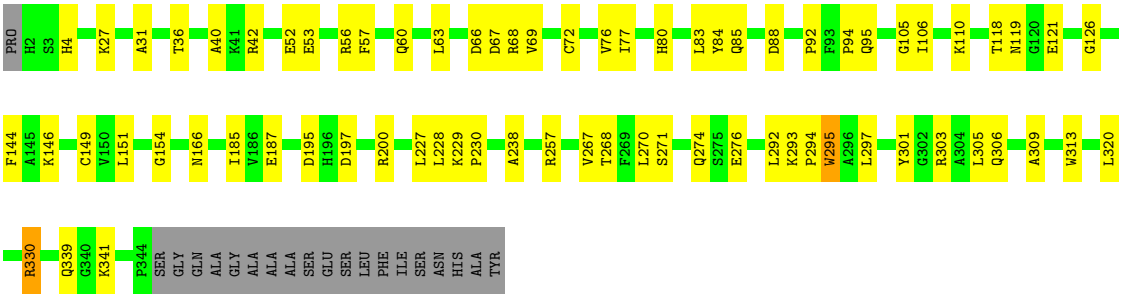
- Molecule 1: Fructose-bisphosphate aldolase A

Chain 4-D:



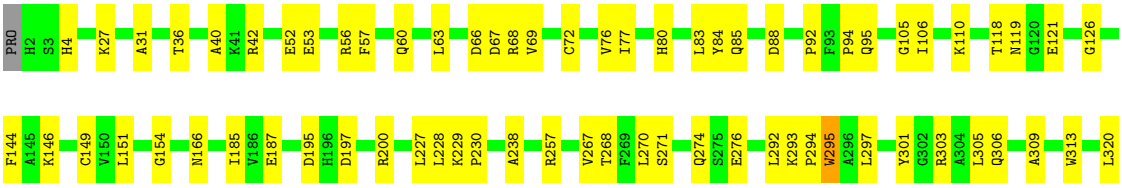
- Molecule 1: Fructose-bisphosphate aldolase A

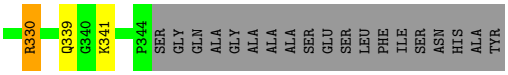
Chain 5-B:



- Molecule 1: Fructose-bisphosphate aldolase A

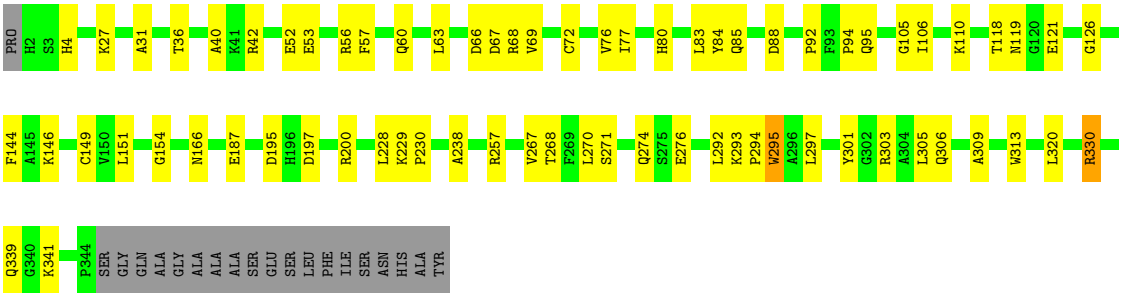
Chain 5-A:





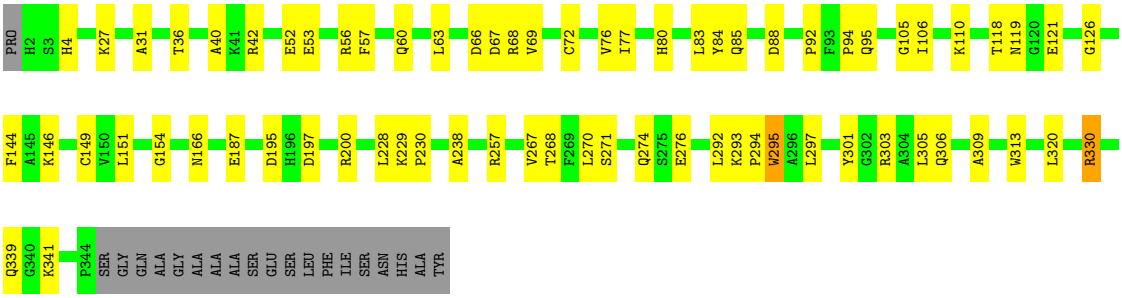
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 5-C:



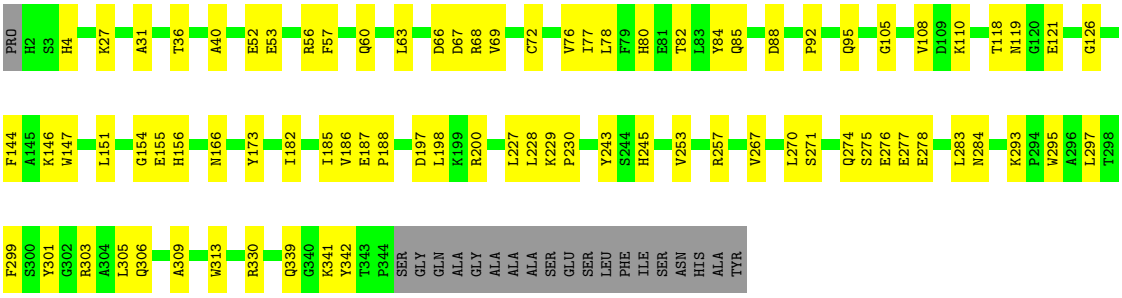
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 5-D:



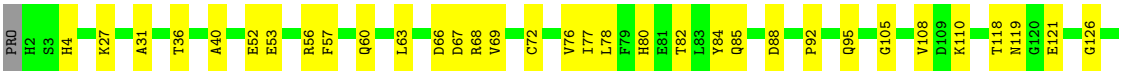
• Molecule 1: Fructose-bisphosphate aldolase A

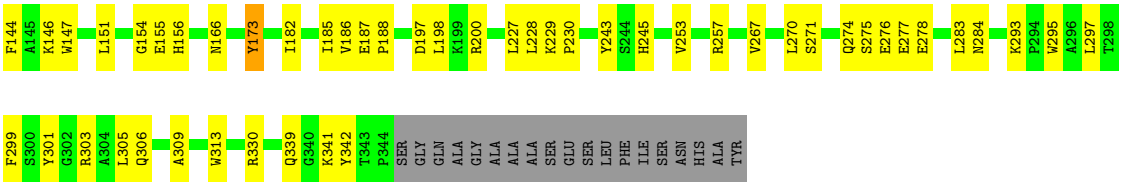
Chain 6-B:



• Molecule 1: Fructose-bisphosphate aldolase A

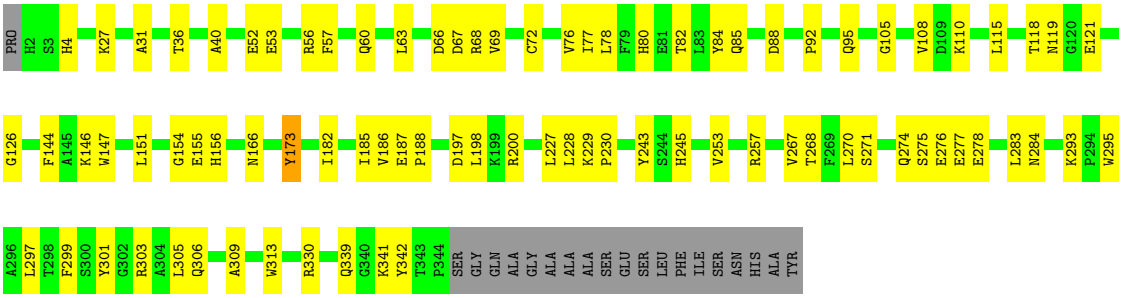
Chain 6-A:





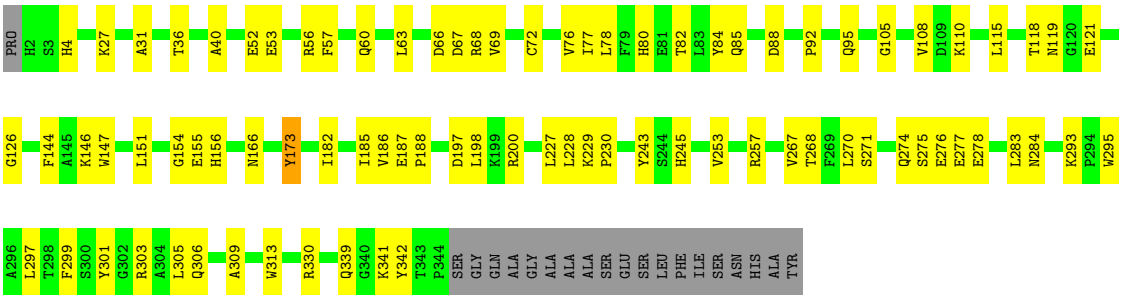
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 6-C:



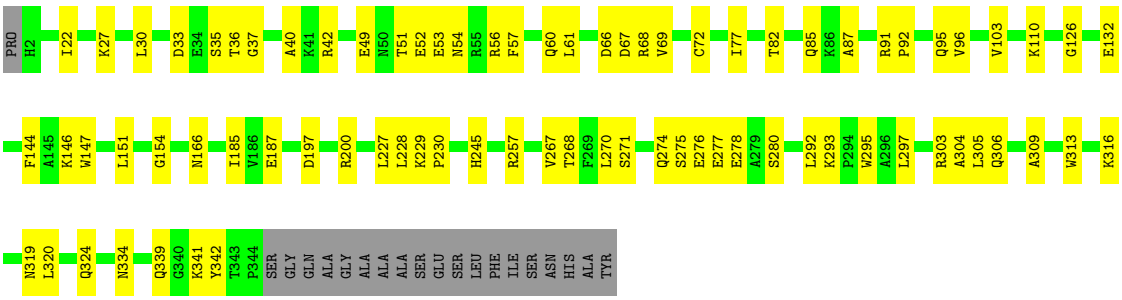
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 6-D:



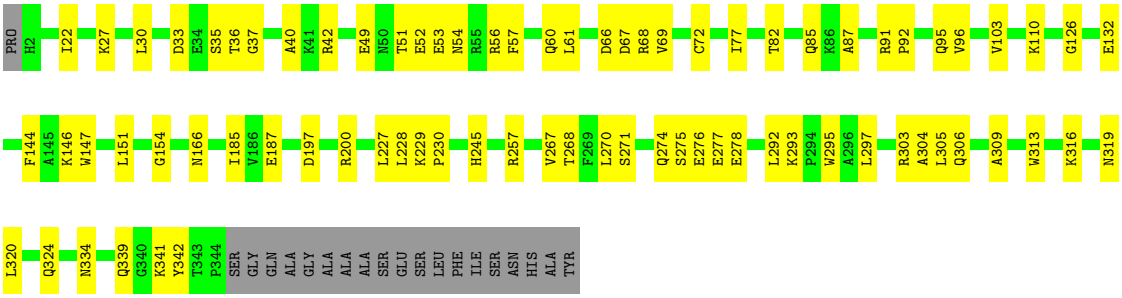
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 7-B:



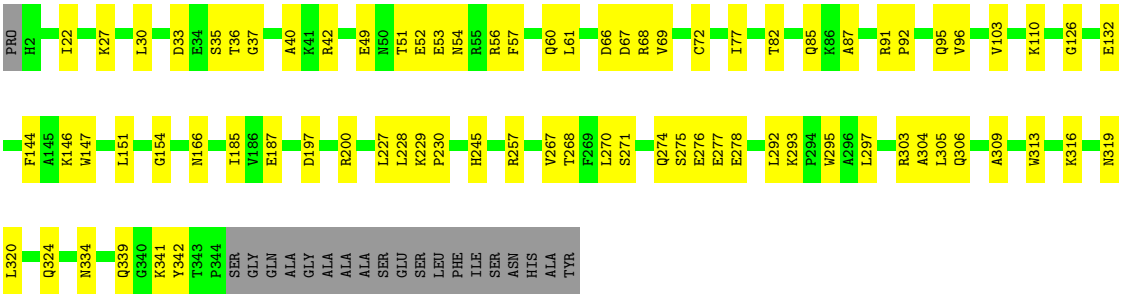
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 7-A:



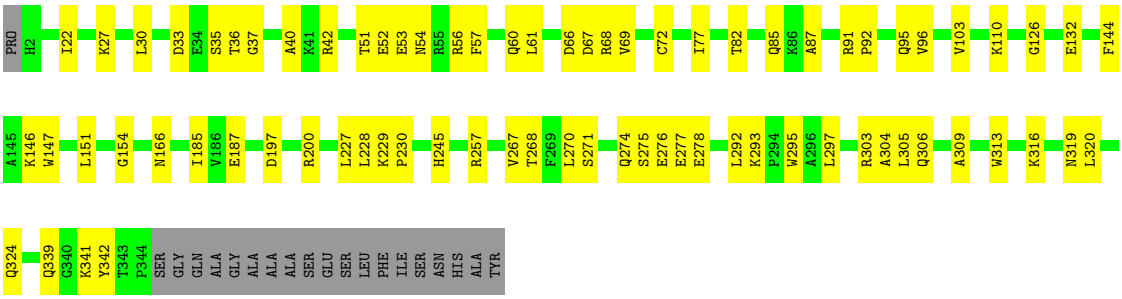
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 7-C:



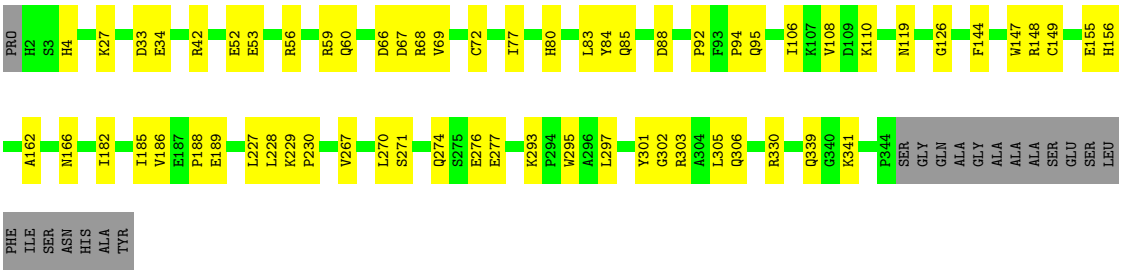
• Molecule 1: Fructose-bisphosphate aldolase A

Chain 7-D:



• Molecule 1: Fructose-bisphosphate aldolase A

Chain 8-B:



• Molecule 1: Fructose-bisphosphate aldolase A

Chain 8-A: 77% 18% 6%

PRO H2 S3 H4 K27 D33 E34 R42 E52 E53 R56 F57 Y58 R59 Q60 D66 D67 R68 V69 C72 I77 H80 L83 Y84 Q85 D88 P92 F93 P94 Q95 I106 K107 V108 D109 K110 N119 G126 F144 W147 R148 C149 E155

H156 A162 N166 I182 I185 V186 E187 P188 E189 L227 L228 K229 P230 V267 L270 S271 Q274 S275 E276 E277 K293 P294 W295 A296 L297 Y301 G302 R303 A304 L305 Q306 W313 R330 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA ALA ALA SER

GLU SER LEU PHE ILE SER ASN HIS ALA TYR

- Molecule 1: Fructose-bisphosphate aldolase A

Chain 8-C: 77% 17% 6%

PRO H2 S3 H4 K27 D33 E34 R42 E52 E53 R56 F57 Y58 R59 Q60 D66 D67 R68 V69 C72 I77 H80 L83 Y84 Q85 D88 P92 F93 P94 Q95 I106 K107 V108 D109 K110 N119 G126 F144 W147 R148 C149 E155

H156 A162 N166 I182 I185 E189 L227 L228 K229 P230 V267 L270 S271 Q274 S275 E276 E277 K293 P294 W295 A296 L297 Y301 G302 R303 A304 L305 Q306 W313 R330 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA ALA ALA SER GLU SER

LEU PHE ILE SER ASN HIS ALA TYR

- Molecule 1: Fructose-bisphosphate aldolase A

Chain 8-D: 77% 17% 6%

PRO H2 S3 H4 K27 D33 E34 R42 E52 E53 R56 F57 Y58 R59 Q60 D66 D67 R68 V69 C72 I77 H80 L83 Y84 Q85 D88 P92 F93 P94 Q95 I106 K107 V108 D109 K110 N119 G126 F144 W147 R148 C149 E155

H156 A162 N166 I182 I185 E189 L227 L228 K229 P230 V267 L270 S271 Q274 S275 E276 E277 K293 P294 W295 A296 L297 Y301 G302 R303 A304 L305 Q306 W313 R330 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA ALA ALA SER GLU SER

LEU PHE ILE SER ASN HIS ALA TYR

- Molecule 1: Fructose-bisphosphate aldolase A

Chain 9-B: 77% 18% 6%

PRO H2 S3 H4 K27 D33 R42 E53 R56 F57 Y58 R59 Q60 L61 A65 D66 D67 R68 V69 C72 I77 H80 E81 T82 L83 Y84 Q85 D88 P92 Q95 G105 I106 K110 T118 N119 G120 E121 Q125 G126 G129 L130 C134

F144 W147 R148 C149 A162 N166 I185 V186 E187 P188 D197 L227 L228 K229 P230 S271 S275 E276 E277 E278 A279 S280 Y301 G302 R303 Q306 A309 W313 Q324 E325 R330 N334 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA

ALA ALA SER GLU SER LEU PHE ILE SER ASN HIS ALA TYR

- Molecule 1: Fructose-bisphosphate aldolase A

Chain 9-A: 77% 18% 6%

PRO H2 S3 H4 K27 D33 R42 E53 R56 F57 Y58 R59 Q60 L61 A65 D66 D67 R68 V69 C72 I77 H80 E81 T82 L83 Y84 Q85 D88 P92 Q95 G105 I106 K110 T118 N119 G120 E121 G125 G126 G129 L130 C134

F144 W147 R148 C149 A162 N166 I185 V186 E187 P188 D197 L227 L228 K229 P230 S271 S275 E276 E277 E278 A279 S280 Y301 G302 R303 Q306 A309 W313 Q324 E325 R330 N334 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA

ALA ALA SER GLU SER LEU PHE ILE SER ASN HIS ALA TYR

• Molecule 1: Fructose-bisphosphate aldolase A

Chain 9-C: 76% 18% 6%

PRO H2 S3 H4 K27 D33 R42 E53 R56 F57 Q60 T64 A65 D66 D67 R68 V69 C72 I77 H80 E81 T82 L83 Y84 Q85 D88 P92 Q95 G105 I106 K110 T118 N119 G120 E121 G125 G126 G129 L130 C134

F144 W147 R148 C149 A162 N166 I185 V186 E187 P188 D197 L227 L228 K229 P230 R257 S271 Q274 S275 E276 E277 E278 A279 S280 L292 Y301 G302 R303 Q306 A309 W313 Q324 E325 R330 Q339 G340 K341 P344 SER GLY GLN ALA

GLY ALA ALA ALA SER GLU SER LEU PHE ILE SER ASN HIS ALA TYR

• Molecule 1: Fructose-bisphosphate aldolase A

Chain 9-D: 76% 18% 6%

PRO H2 S3 H4 K27 D33 R42 E53 R56 F57 Q60 T64 A65 D66 D67 R68 V69 C72 I77 H80 E81 T82 L83 Y84 Q85 D88 P92 Q95 G105 I106 K110 T118 N119 G120 E121 G125 G126 G129 L130 C134

F144 W147 R148 C149 A162 N166 I185 V186 E187 P188 D197 L227 L228 K229 P230 R257 S271 Q274 S275 E276 E277 E278 A279 S280 L292 Y301 G302 R303 Q306 A309 W313 Q324 E325 R330 Q339 G340 K341 P344 SER GLY GLN ALA

GLY ALA ALA ALA SER GLU SER LEU PHE ILE SER ASN HIS ALA TYR

• Molecule 1: Fructose-bisphosphate aldolase A

Chain 10-B: 73% 21% 6%

PRO H2 S3 H4 K27 A31 A32 D33 E34 S35 T36 A40 I46 G47 T48 E52 E53 R56 F57 Y58 R59 Q60 L63 T64 A65 D66 D67 R68 V69 C72 V76 I77 H80 Y84 Q85 D88 R91 P92 Q95 V96 G105 K110 T118

N119 G120 E121 G126 F144 A145 K146 W147 L151 G154 N166 A167 N168 I185 V186 E187 P188 D197 L198 K199 R200 L227 L228 K229 P230 Y243 S244 H245 V253 R257 V267 T268 F269 L270 E276 E277 E278 K293 L297 A304 L305 Q306 A307

W313 G314 G315 L320 R330 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA ALA ALA SER GLU SER LEU PHE ILE SER ASN HIS ALA TYR

• Molecule 1: Fructose-bisphosphate aldolase A

Chain 10-A: 73% 21% 6%

PRO H2 S3 H4 K27 A31 A32 D33 E34 S35 T36 A40 I46 G47 T48 E52 E53 R56 F57 Y58 R59 Q60 L63 T64 A65 D66 D67 R68 V69 C72 V76 I77 H80 Y84 Q85 D88 R91 P92 Q95 V96 G105 K110 T118

N119 G120 E121 G126 F144 A145 K146 W147 L151 G154 N166 A167 N168 I185 V186 E187 P188 D197 L198 K199 R200 L227 L228 K229 P230 Y243 S244 H245 V253 R257 V267 T268 F269 L270 E276 E277 E278 K293 L297 A304 L305 Q306 A307

W313 G314 G315 L320 R330 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA ALA ALA SER GLU SER LEU PHE ILE SER ASN HIS ALA TYR

- Molecule 1: Fructose-bisphosphate aldolase A

Chain 10-C: 73% 21% 6%

PRO H2 S3 H4 K27 A31 A32 D33 E34 S35 T36 A40 I46 G47 T48 E52 E53 R56 F57 Y58 R59 Q60 L63 T64 A65 D66 D67 R68 V69 C72 V76 I77 H80 Y84 Q85 D88 R91 P92 Q95 V96 G105 K110 T118

N119 G120 E121 G126 F144 A145 K146 W147 L151 G154 N166 A167 N168 I185 V186 E187 P188 D197 L198 K199 R200 L227 L228 K229 P230 Y243 S244 H245 V253 R257 V267 T268 F269 L270 E276 E277 E278 K293 L297 A304 L305 Q306 A307

W313 G314 G315 L320 R330 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA ALA ALA SER GLU SER LEU PHE ILE SER ASN HIS ALA TYR

- Molecule 1: Fructose-bisphosphate aldolase A

Chain 10-D: 73% 21% 6%

PRO H2 S3 H4 K27 A31 A32 D33 E34 S35 T36 A40 I46 G47 T48 E52 E53 R56 F57 Y58 R59 Q60 L63 T64 A65 D66 D67 R68 V69 C72 V76 I77 H80 Y84 Q85 D88 R91 P92 Q95 V96 G105 K110 T118

N119 G120 E121 G126 F144 A145 K146 W147 L151 G154 N166 A167 N168 I185 V186 E187 P188 D197 L198 K199 R200 L227 L228 K229 P230 Y243 S244 H245 V253 R257 V267 T268 F269 L270 E276 E277 E278 K293 L297 A304 L305 Q306 A307

W313 G314 G315 L320 R330 Q339 G340 K341 P344 SER GLY GLN ALA GLY ALA ALA ALA SER GLU SER LEU PHE ILE SER ASN HIS ALA TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	83910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	68	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.129	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	116.48, 116.48, 116.48	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.91, 0.91, 0.91	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1-A	0.52	0/2668	0.53	0/3616
1	1-B	0.52	0/2668	0.53	0/3616
1	1-C	0.52	0/2668	0.53	0/3616
1	1-D	0.52	0/2668	0.53	0/3616
1	2-A	0.53	0/2668	0.53	1/3616 (0.0%)
1	2-B	0.53	0/2668	0.53	1/3616 (0.0%)
1	2-C	0.53	0/2668	0.53	1/3616 (0.0%)
1	2-D	0.53	0/2668	0.53	1/3616 (0.0%)
1	3-A	0.53	0/2668	0.54	0/3616
1	3-B	0.53	0/2668	0.54	0/3616
1	3-C	0.53	0/2668	0.54	0/3616
1	3-D	0.53	0/2668	0.54	0/3616
1	4-A	0.53	0/2668	0.54	0/3616
1	4-B	0.53	0/2668	0.54	0/3616
1	4-C	0.53	0/2668	0.54	0/3616
1	4-D	0.53	0/2668	0.54	0/3616
1	5-A	0.53	0/2668	0.54	0/3616
1	5-B	0.53	0/2668	0.54	0/3616
1	5-C	0.53	0/2668	0.54	0/3616
1	5-D	0.53	0/2668	0.54	0/3616
1	6-A	0.51	0/2668	0.53	0/3616
1	6-B	0.51	0/2668	0.53	0/3616
1	6-C	0.51	0/2668	0.53	0/3616
1	6-D	0.51	0/2668	0.53	0/3616
1	7-A	0.54	0/2668	0.55	0/3616
1	7-B	0.54	0/2668	0.55	0/3616
1	7-C	0.54	0/2668	0.55	0/3616
1	7-D	0.54	0/2668	0.55	0/3616
1	8-A	0.52	0/2668	0.52	0/3616
1	8-B	0.52	0/2668	0.52	0/3616
1	8-C	0.52	0/2668	0.52	0/3616
1	8-D	0.52	0/2668	0.52	0/3616
1	9-A	0.53	0/2668	0.53	0/3616
1	9-B	0.53	0/2668	0.53	0/3616

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	9-C	0.53	0/2668	0.53	0/3616
1	9-D	0.53	0/2668	0.53	0/3616
1	10-A	0.53	0/2668	0.53	0/3616
1	10-B	0.53	0/2668	0.53	0/3616
1	10-C	0.53	0/2668	0.53	0/3616
1	10-D	0.53	0/2668	0.53	0/3616
All	All	0.53	0/106720	0.53	4/144640 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-C	318	GLU	CA-CB-CG	5.14	124.70	113.40
1	2-D	318	GLU	CA-CB-CG	5.14	124.70	113.40
1	2-A	318	GLU	CA-CB-CG	5.12	124.67	113.40
1	2-B	318	GLU	CA-CB-CG	5.12	124.66	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2618	0	2648	57	0
1	1-B	2618	0	2648	58	0
1	1-C	2618	0	2648	54	0
1	1-D	2618	0	2648	55	0
1	2-A	2618	0	2648	42	0
1	2-B	2618	0	2648	44	0
1	2-C	2618	0	2648	42	0
1	2-D	2618	0	2648	45	0
1	3-A	2618	0	2648	50	0
1	3-B	2618	0	2648	52	0
1	3-C	2618	0	2648	49	0
1	3-D	2618	0	2648	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-A	2618	0	2648	55	0
1	4-B	2618	0	2648	54	0
1	4-C	2618	0	2648	55	0
1	4-D	2618	0	2648	55	0
1	5-A	2618	0	2648	51	0
1	5-B	2618	0	2648	51	0
1	5-C	2618	0	2648	49	0
1	5-D	2618	0	2648	49	0
1	6-A	2618	0	2648	56	0
1	6-B	2618	0	2648	56	0
1	6-C	2618	0	2648	55	0
1	6-D	2618	0	2648	55	0
1	7-A	2618	0	2648	55	0
1	7-B	2618	0	2648	57	0
1	7-C	2618	0	2648	54	0
1	7-D	2618	0	2648	51	0
1	8-A	2618	0	2648	38	0
1	8-B	2618	0	2648	38	0
1	8-C	2618	0	2648	37	0
1	8-D	2618	0	2648	37	0
1	9-A	2618	0	2648	45	0
1	9-B	2618	0	2648	45	0
1	9-C	2618	0	2648	44	0
1	9-D	2618	0	2648	44	0
1	10-A	2618	0	2648	51	0
1	10-B	2618	0	2648	51	0
1	10-C	2618	0	2648	50	0
1	10-D	2618	0	2648	50	0
All	All	104720	0	105920	1921	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 9.

All (1921) 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:B:318:GLU:OE1	1:B:318:GLU:N	2.05	0.90
1:A:318:GLU:OE1	1:A:318:GLU:N	2.05	0.90
1:C:318:GLU:OE1	1:C:318:GLU:N	2.05	0.88
1:D:318:GLU:OE1	1:D:318:GLU:N	2.05	0.87
1:B:42:ARG:HH22	1:B:303:ARG:HB3	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HH22	1:A:303:ARG:HB3	1.43	0.83
1:D:42:ARG:HH22	1:D:303:ARG:HB3	1.43	0.83
1:C:42:ARG:HH22	1:C:303:ARG:HB3	1.43	0.82
1:B:77:ILE:HD11	1:B:146:LYS:HB2	1.62	0.80
1:A:77:ILE:HD11	1:A:146:LYS:HB2	1.62	0.80
1:C:77:ILE:HD11	1:C:146:LYS:HB2	1.63	0.80
1:D:77:ILE:HD11	1:D:146:LYS:HB2	1.62	0.80
1:B:36:THR:O	1:B:40:ALA:HB2	1.83	0.78
1:A:36:THR:O	1:A:40:ALA:HB2	1.83	0.78
1:B:36:THR:O	1:B:40:ALA:HB2	1.84	0.77
1:A:36:THR:O	1:A:40:ALA:HB2	1.84	0.77
1:C:36:THR:O	1:C:40:ALA:HB2	1.83	0.77
1:D:36:THR:O	1:D:40:ALA:HB2	1.83	0.77
1:C:42:ARG:HH22	1:C:303:ARG:HB3	1.48	0.77
1:D:42:ARG:HH22	1:D:303:ARG:HB3	1.48	0.77
1:D:36:THR:O	1:D:40:ALA:HB2	1.84	0.77
1:A:148:ARG:NH1	1:A:189:GLU:OE1	2.18	0.77
1:B:42:ARG:HH22	1:B:303:ARG:HB3	1.48	0.76
1:B:148:ARG:NH1	1:B:189:GLU:OE1	2.18	0.76
1:A:42:ARG:HH22	1:A:303:ARG:HB3	1.48	0.76
1:C:36:THR:O	1:C:40:ALA:HB2	1.84	0.76
1:D:148:ARG:NH1	1:D:189:GLU:OE1	2.18	0.76
1:C:148:ARG:NH1	1:C:189:GLU:OE1	2.18	0.76
1:C:197:ASP:OD1	1:C:243:TYR:OH	2.05	0.75
1:B:125:GLN:NE2	1:D:129:GLY:H	1.85	0.75
1:B:129:GLY:H	1:D:125:GLN:HE21	1.32	0.75
1:D:197:ASP:OD1	1:D:243:TYR:OH	2.05	0.75
1:B:129:GLY:H	1:D:125:GLN:NE2	1.85	0.74
1:B:125:GLN:HE21	1:D:129:GLY:H	1.32	0.74
1:D:42:ARG:HH22	1:D:303:ARG:HB3	1.51	0.74
1:C:42:ARG:HH22	1:C:303:ARG:HB3	1.51	0.74
1:B:197:ASP:OD1	1:B:243:TYR:OH	2.05	0.74
1:A:129:GLY:H	1:C:125:GLN:HE21	1.33	0.73
1:D:277:GLU:OE2	1:D:330:ARG:NH1	2.21	0.73
1:A:277:GLU:OE2	1:A:330:ARG:NH1	2.21	0.73
1:C:277:GLU:OE2	1:C:330:ARG:NH1	2.21	0.73
1:A:42:ARG:HH22	1:A:303:ARG:HB3	1.51	0.73
1:B:277:GLU:OE2	1:B:330:ARG:NH1	2.21	0.73
1:B:42:ARG:HH22	1:B:303:ARG:HB3	1.51	0.73
1:B:36:THR:O	1:B:40:ALA:HB2	1.88	0.72
1:A:36:THR:O	1:A:40:ALA:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLY:H	1:C:125:GLN:NE2	1.87	0.72
1:A:125:GLN:NE2	1:C:129:GLY:H	1.88	0.72
1:A:283:LEU:HD11	1:A:299:PHE:HB3	1.72	0.72
1:B:283:LEU:HD11	1:B:299:PHE:HB3	1.72	0.72
1:C:36:THR:O	1:C:40:ALA:HB2	1.88	0.72
1:D:36:THR:O	1:D:40:ALA:HB2	1.88	0.72
1:A:197:ASP:OD1	1:A:243:TYR:OH	2.05	0.72
1:A:125:GLN:HE21	1:C:129:GLY:H	1.36	0.71
1:D:283:LEU:HD11	1:D:299:PHE:HB3	1.72	0.71
1:C:283:LEU:HD11	1:C:299:PHE:HB3	1.72	0.71
1:A:129:GLY:H	1:C:125:GLN:NE2	1.88	0.71
1:D:65:ALA:HA	1:D:324:GLN:HE21	1.55	0.71
1:B:77:ILE:HD11	1:B:146:LYS:HB2	1.72	0.71
1:A:77:ILE:HD11	1:A:146:LYS:HB2	1.73	0.71
1:C:65:ALA:HA	1:C:324:GLN:HE21	1.55	0.71
1:A:125:GLN:HE21	1:C:129:GLY:H	1.38	0.71
1:A:125:GLN:HE21	1:C:129:GLY:H	1.37	0.70
1:B:65:ALA:HA	1:B:324:GLN:HE21	1.55	0.70
1:A:65:ALA:HA	1:A:324:GLN:HE21	1.55	0.70
1:B:60:GLN:NE2	1:B:88:ASP:H	1.90	0.70
1:B:125:GLN:HE21	1:D:129:GLY:H	1.38	0.70
1:A:60:GLN:NE2	1:A:88:ASP:H	1.90	0.70
1:C:77:ILE:HD11	1:C:146:LYS:HB2	1.72	0.70
1:A:129:GLY:H	1:C:125:GLN:HE21	1.36	0.70
1:B:129:GLY:H	1:D:125:GLN:HE21	1.37	0.70
1:D:77:ILE:HD11	1:D:146:LYS:HB2	1.73	0.70
1:D:60:GLN:NE2	1:D:88:ASP:H	1.90	0.69
1:B:129:GLY:H	1:D:125:GLN:NE2	1.90	0.69
1:B:66:ASP:OD2	1:B:68:ARG:NH1	2.25	0.69
1:A:66:ASP:OD2	1:A:68:ARG:NH1	2.25	0.69
1:C:60:GLN:NE2	1:C:88:ASP:H	1.90	0.69
1:C:66:ASP:OD2	1:C:68:ARG:NH1	2.25	0.69
1:B:125:GLN:NE2	1:D:129:GLY:H	1.91	0.69
1:A:129:GLY:H	1:C:125:GLN:NE2	1.91	0.69
1:D:66:ASP:OD2	1:D:68:ARG:NH1	2.25	0.69
1:A:125:GLN:NE2	1:C:129:GLY:H	1.91	0.69
1:B:318:GLU:H	1:B:318:GLU:CD	1.95	0.69
1:A:125:GLN:NE2	1:C:129:GLY:H	1.90	0.69
1:A:318:GLU:H	1:A:318:GLU:CD	1.95	0.69
1:B:129:GLY:H	1:D:125:GLN:NE2	1.90	0.69
1:A:129:GLY:H	1:C:125:GLN:HE21	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:GLN:O	1:D:309:ALA:N	2.21	0.69
1:B:105:GLY:HA2	1:B:144:PHE:O	1.93	0.68
1:A:105:GLY:HA2	1:A:144:PHE:O	1.93	0.68
1:C:306:GLN:O	1:C:309:ALA:N	2.21	0.68
1:A:306:GLN:O	1:A:309:ALA:N	2.22	0.68
1:B:306:GLN:O	1:B:309:ALA:N	2.21	0.68
1:B:125:GLN:HE21	1:D:129:GLY:H	1.39	0.68
1:B:125:GLN:NE2	1:D:129:GLY:H	1.91	0.68
1:D:105:GLY:HA2	1:D:144:PHE:O	1.93	0.68
1:B:306:GLN:O	1:B:309:ALA:N	2.26	0.68
1:C:105:GLY:HA2	1:C:144:PHE:O	1.93	0.68
1:A:306:GLN:O	1:A:309:ALA:N	2.26	0.68
1:C:306:GLN:O	1:C:309:ALA:N	2.27	0.68
1:D:306:GLN:O	1:D:309:ALA:N	2.27	0.68
1:C:274:GLN:O	1:C:303:ARG:NH2	2.27	0.67
1:D:274:GLN:O	1:D:303:ARG:NH2	2.27	0.67
1:C:276:GLU:O	1:C:330:ARG:NH2	2.27	0.67
1:D:276:GLU:O	1:D:330:ARG:NH2	2.27	0.67
1:B:274:GLN:O	1:B:303:ARG:NH2	2.27	0.67
1:A:36:THR:O	1:A:40:ALA:HB2	1.94	0.67
1:A:274:GLN:O	1:A:303:ARG:NH2	2.27	0.67
1:B:197:ASP:OD1	1:B:198:LEU:N	2.28	0.67
1:A:276:GLU:O	1:A:330:ARG:NH2	2.27	0.67
1:D:197:ASP:OD1	1:D:198:LEU:N	2.28	0.67
1:B:36:THR:O	1:B:40:ALA:HB2	1.94	0.67
1:B:129:GLY:H	1:D:125:GLN:HE21	1.39	0.67
1:B:276:GLU:O	1:B:330:ARG:NH2	2.27	0.67
1:A:197:ASP:OD1	1:A:198:LEU:N	2.28	0.67
1:C:197:ASP:OD1	1:C:198:LEU:N	2.28	0.67
1:B:276:GLU:O	1:B:330:ARG:NH2	2.28	0.67
1:A:276:GLU:O	1:A:330:ARG:NH2	2.28	0.67
1:B:197:ASP:OD1	1:B:243:TYR:OH	2.10	0.67
1:C:197:ASP:OD1	1:C:243:TYR:OH	2.10	0.67
1:A:197:ASP:OD1	1:A:243:TYR:OH	2.10	0.67
1:D:197:ASP:OD1	1:D:243:TYR:OH	2.10	0.67
1:B:306:GLN:O	1:B:309:ALA:N	2.27	0.66
1:D:36:THR:O	1:D:40:ALA:HB2	1.95	0.66
1:A:306:GLN:O	1:A:309:ALA:N	2.27	0.66
1:C:36:THR:O	1:C:40:ALA:HB2	1.95	0.66
1:A:274:GLN:O	1:A:303:ARG:NH2	2.29	0.66
1:A:274:GLN:O	1:A:303:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:O	1:B:303:ARG:NH2	2.29	0.66
1:B:274:GLN:O	1:B:303:ARG:NH2	2.29	0.66
1:C:276:GLU:O	1:C:330:ARG:NH2	2.28	0.66
1:D:276:GLU:O	1:D:330:ARG:NH2	2.28	0.66
1:D:36:THR:O	1:D:40:ALA:HB2	1.94	0.66
1:A:52:GLU:OE2	1:A:85:GLN:NE2	2.29	0.66
1:C:274:GLN:O	1:C:303:ARG:NH2	2.29	0.66
1:C:274:GLN:O	1:C:303:ARG:NH2	2.29	0.66
1:C:105:GLY:HA2	1:C:144:PHE:O	1.96	0.66
1:D:105:GLY:HA2	1:D:144:PHE:O	1.96	0.66
1:B:52:GLU:OE2	1:B:85:GLN:NE2	2.29	0.66
1:C:36:THR:O	1:C:40:ALA:HB2	1.94	0.66
1:D:274:GLN:O	1:D:303:ARG:NH2	2.29	0.66
1:D:274:GLN:O	1:D:303:ARG:NH2	2.29	0.66
1:C:306:GLN:O	1:C:309:ALA:N	2.27	0.65
1:A:36:THR:O	1:A:40:ALA:HB2	1.95	0.65
1:B:105:GLY:HA2	1:B:144:PHE:O	1.96	0.65
1:A:105:GLY:HA2	1:A:144:PHE:O	1.96	0.65
1:B:36:THR:O	1:B:40:ALA:HB2	1.95	0.65
1:C:52:GLU:OE2	1:C:85:GLN:NE2	2.29	0.65
1:D:306:GLN:O	1:D:309:ALA:N	2.27	0.65
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.29	0.65
1:C:197:ASP:OD1	1:C:198:LEU:N	2.30	0.65
1:D:197:ASP:OD1	1:D:198:LEU:N	2.30	0.65
1:C:66:ASP:OD2	1:C:68:ARG:NH1	2.30	0.65
1:D:66:ASP:OD2	1:D:68:ARG:NH1	2.30	0.65
1:C:52:GLU:OE2	1:C:85:GLN:NE2	2.30	0.65
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.30	0.65
1:A:276:GLU:O	1:A:330:ARG:NH2	2.30	0.65
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.30	0.65
1:B:276:GLU:O	1:B:330:ARG:NH2	2.30	0.65
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.30	0.65
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.30	0.65
1:B:66:ASP:OD2	1:B:68:ARG:NH1	2.30	0.64
1:A:66:ASP:OD2	1:A:68:ARG:NH1	2.30	0.64
1:C:318:GLU:H	1:C:318:GLU:CD	1.95	0.64
1:C:276:GLU:O	1:C:330:ARG:NH2	2.30	0.64
1:D:276:GLU:O	1:D:330:ARG:NH2	2.30	0.64
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.30	0.64
1:C:77:ILE:HD11	1:C:146:LYS:HB2	1.79	0.64
1:D:77:ILE:HD11	1:D:146:LYS:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ILE:HG12	1:B:103:VAL:HG21	1.80	0.64
1:C:277:GLU:OE2	1:C:342:TYR:OH	2.15	0.64
1:D:318:GLU:H	1:D:318:GLU:CD	1.95	0.64
1:C:276:GLU:HG2	1:C:330:ARG:HD2	1.79	0.64
1:D:277:GLU:OE2	1:D:342:TYR:OH	2.15	0.64
1:A:22:ILE:HG12	1:A:103:VAL:HG21	1.80	0.64
1:C:52:GLU:OE2	1:C:85:GLN:NE2	2.30	0.64
1:B:276:GLU:O	1:B:330:ARG:NH2	2.31	0.64
1:A:276:GLU:O	1:A:330:ARG:NH2	2.31	0.64
1:A:52:GLU:OE2	1:A:85:GLN:NE2	2.30	0.64
1:D:276:GLU:HG2	1:D:330:ARG:HD2	1.79	0.64
1:B:197:ASP:OD1	1:B:198:LEU:N	2.30	0.64
1:C:52:GLU:OE2	1:C:85:GLN:NE2	2.31	0.64
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.31	0.64
1:A:277:GLU:OE2	1:A:342:TYR:OH	2.15	0.64
1:A:77:ILE:HD11	1:A:146:LYS:HB2	1.79	0.64
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.30	0.64
1:B:277:GLU:OE2	1:B:342:TYR:OH	2.15	0.64
1:B:52:GLU:OE2	1:B:85:GLN:NE2	2.30	0.64
1:A:197:ASP:OD1	1:A:198:LEU:N	2.30	0.64
1:C:276:GLU:O	1:C:330:ARG:NH2	2.31	0.64
1:D:276:GLU:O	1:D:330:ARG:NH2	2.31	0.64
1:B:77:ILE:HD11	1:B:146:LYS:HB2	1.79	0.64
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.80	0.64
1:C:147:TRP:O	1:C:187:GLU:HB3	1.98	0.64
1:D:147:TRP:O	1:D:187:GLU:HB3	1.98	0.64
1:B:52:GLU:OE2	1:B:85:GLN:NE2	2.30	0.64
1:A:42:ARG:HH22	1:A:303:ARG:HB2	1.63	0.64
1:A:52:GLU:OE2	1:A:85:GLN:NE2	2.30	0.64
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.30	0.64
1:C:105:GLY:HA2	1:C:144:PHE:O	1.98	0.64
1:D:105:GLY:HA2	1:D:144:PHE:O	1.98	0.64
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.31	0.64
1:A:110:LYS:HD2	1:A:126:GLY:HA2	1.80	0.64
1:B:65:ALA:HA	1:B:324:GLN:NE2	2.13	0.64
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.30	0.64
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.31	0.63
1:B:276:GLU:HG2	1:B:330:ARG:HD2	1.79	0.63
1:B:42:ARG:HH22	1:B:303:ARG:HB2	1.64	0.63
1:A:65:ALA:HA	1:A:324:GLN:NE2	2.13	0.63
1:A:276:GLU:HG2	1:A:330:ARG:HD2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLY:O	1:B:200:ARG:NH2	2.31	0.63
1:A:154:GLY:O	1:A:200:ARG:NH2	2.31	0.63
1:D:110:LYS:HD2	1:D:126:GLY:HA2	1.80	0.63
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.30	0.63
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.30	0.63
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.32	0.63
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.32	0.63
1:C:110:LYS:HD2	1:C:126:GLY:HA2	1.80	0.63
1:C:65:ALA:HA	1:C:324:GLN:NE2	2.13	0.63
1:D:276:GLU:O	1:D:330:ARG:NH2	2.31	0.63
1:D:22:ILE:HG12	1:D:103:VAL:HG21	1.80	0.63
1:C:42:ARG:HH22	1:C:303:ARG:HB2	1.63	0.63
1:D:65:ALA:HA	1:D:324:GLN:NE2	2.13	0.63
1:B:105:GLY:HA2	1:B:144:PHE:O	1.98	0.63
1:A:52:GLU:OE2	1:A:85:GLN:NE2	2.31	0.63
1:C:276:GLU:O	1:C:330:ARG:NH2	2.31	0.63
1:B:52:GLU:OE2	1:B:85:GLN:NE2	2.25	0.63
1:C:22:ILE:HG12	1:C:103:VAL:HG21	1.80	0.63
1:D:42:ARG:HH22	1:D:303:ARG:HB2	1.63	0.63
1:B:52:GLU:OE2	1:B:85:GLN:NE2	2.31	0.63
1:C:65:ALA:HA	1:C:324:GLN:NE2	2.14	0.63
1:B:147:TRP:O	1:B:187:GLU:HB3	1.98	0.63
1:A:147:TRP:O	1:A:187:GLU:HB3	1.98	0.63
1:C:52:GLU:OE2	1:C:85:GLN:NE2	2.32	0.63
1:A:105:GLY:HA2	1:A:144:PHE:O	1.98	0.63
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.32	0.63
1:D:154:GLY:O	1:D:200:ARG:NH2	2.31	0.63
1:A:52:GLU:OE2	1:A:85:GLN:NE2	2.25	0.63
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.81	0.63
1:C:52:GLU:OE2	1:C:85:GLN:NE2	2.32	0.63
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.32	0.63
1:D:65:ALA:HA	1:D:324:GLN:NE2	2.14	0.63
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.31	0.63
1:C:154:GLY:O	1:C:200:ARG:NH2	2.31	0.63
1:D:110:LYS:HD2	1:D:126:GLY:HA2	1.81	0.63
1:A:110:LYS:HD2	1:A:126:GLY:HA2	1.81	0.63
1:B:276:GLU:O	1:B:330:ARG:NH2	2.31	0.62
1:A:276:GLU:O	1:A:330:ARG:NH2	2.31	0.62
1:C:36:THR:O	1:C:40:ALA:HB2	1.99	0.62
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.31	0.62
1:C:110:LYS:HD2	1:C:126:GLY:HA2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:THR:O	1:B:40:ALA:HB2	1.99	0.62
1:A:36:THR:O	1:A:40:ALA:HB2	1.99	0.62
1:D:36:THR:O	1:D:40:ALA:HB2	1.99	0.62
1:A:277:GLU:OE2	1:A:342:TYR:OH	2.17	0.62
1:A:110:LYS:HD2	1:A:126:GLY:HA2	1.81	0.62
1:B:277:GLU:OE2	1:B:342:TYR:OH	2.17	0.62
1:C:147:TRP:O	1:C:187:GLU:HB3	1.99	0.62
1:D:147:TRP:O	1:D:187:GLU:HB3	2.00	0.62
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.32	0.62
1:D:110:LYS:HD2	1:D:126:GLY:HA2	1.81	0.62
1:B:52:GLU:OE2	1:B:85:GLN:NE2	2.32	0.62
1:A:52:GLU:OE2	1:A:85:GLN:NE2	2.32	0.62
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.32	0.62
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.32	0.62
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.32	0.62
1:D:60:GLN:HE21	1:D:87:ALA:HA	1.64	0.62
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.81	0.62
1:A:52:GLU:OE2	1:A:85:GLN:NE2	2.32	0.62
1:C:60:GLN:HE21	1:C:87:ALA:HA	1.64	0.62
1:B:52:GLU:OE2	1:B:85:GLN:NE2	2.32	0.62
1:C:52:GLU:OE2	1:C:85:GLN:NE2	2.32	0.62
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.32	0.62
1:B:52:GLU:OE2	1:B:85:GLN:NE2	2.32	0.62
1:A:52:GLU:OE2	1:A:85:GLN:NE2	2.32	0.62
1:A:162:ALA:O	1:A:166:ASN:ND2	2.31	0.62
1:C:110:LYS:HD2	1:C:126:GLY:HA2	1.81	0.62
1:B:65:ALA:HA	1:B:324:GLN:NE2	2.14	0.62
1:A:65:ALA:HA	1:A:324:GLN:NE2	2.14	0.62
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.32	0.62
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.32	0.62
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.32	0.62
1:B:162:ALA:O	1:B:166:ASN:ND2	2.31	0.62
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.32	0.62
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.32	0.62
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.32	0.62
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.32	0.62
1:B:147:TRP:O	1:B:187:GLU:HB3	1.99	0.62
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.32	0.62
1:B:60:GLN:HE21	1:B:87:ALA:HA	1.64	0.62
1:B:48:THR:HG21	1:B:315:GLY:HA3	1.82	0.61
1:D:48:THR:HG21	1:D:315:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TRP:O	1:A:187:GLU:HB3	2.00	0.61
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.32	0.61
1:A:48:THR:HG21	1:A:315:GLY:HA3	1.82	0.61
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.32	0.61
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.32	0.61
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.32	0.61
1:C:275:SER:HB3	1:C:278:GLU:HG2	1.82	0.61
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.32	0.61
1:C:48:THR:HG21	1:C:315:GLY:HA3	1.82	0.61
1:C:105:GLY:HA2	1:C:144:PHE:O	2.00	0.61
1:D:105:GLY:HA2	1:D:144:PHE:O	2.00	0.61
1:A:60:GLN:HE21	1:A:87:ALA:HA	1.64	0.61
1:D:275:SER:HB3	1:D:278:GLU:HG2	1.82	0.61
1:A:105:GLY:HA2	1:A:144:PHE:O	2.00	0.61
1:B:105:GLY:HA2	1:B:144:PHE:O	2.00	0.61
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.33	0.61
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.32	0.61
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.33	0.61
1:A:277:GLU:OE2	1:A:342:TYR:OH	2.17	0.61
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.33	0.61
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.33	0.61
1:B:277:GLU:OE2	1:B:342:TYR:OH	2.17	0.61
1:C:295:TRP:HE1	1:C:297:LEU:HD21	1.66	0.61
1:D:295:TRP:HE1	1:D:297:LEU:HD21	1.66	0.61
1:B:53:GLU:OE2	1:B:56:ARG:NH2	2.33	0.60
1:A:53:GLU:OE2	1:A:56:ARG:NH2	2.33	0.60
1:C:277:GLU:OE2	1:C:342:TYR:OH	2.17	0.60
1:C:105:GLY:HA2	1:C:144:PHE:O	2.02	0.60
1:D:105:GLY:HA2	1:D:144:PHE:O	2.02	0.60
1:D:277:GLU:OE2	1:D:342:TYR:OH	2.17	0.60
1:D:257:ARG:NH1	1:D:292:LEU:O	2.35	0.60
1:B:295:TRP:HE1	1:B:297:LEU:HD21	1.66	0.60
1:C:53:GLU:OE2	1:C:56:ARG:NH2	2.33	0.60
1:C:257:ARG:NH1	1:C:292:LEU:O	2.35	0.59
1:B:105:GLY:HA2	1:B:144:PHE:O	2.02	0.59
1:A:105:GLY:HA2	1:A:144:PHE:O	2.02	0.59
1:C:277:GLU:OE2	1:C:342:TYR:OH	2.17	0.59
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.25	0.59
1:D:277:GLU:OE2	1:D:342:TYR:OH	2.17	0.59
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.66	0.59
1:B:275:SER:HB3	1:B:278:GLU:HG2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:SER:HB3	1:A:278:GLU:HG2	1.82	0.59
1:C:130:LEU:O	1:C:134:CYS:HB2	2.03	0.59
1:D:130:LEU:O	1:D:134:CYS:HB2	2.03	0.59
1:D:36:THR:O	1:D:40:ALA:HB2	2.02	0.59
1:D:53:GLU:OE2	1:D:56:ARG:NH2	2.33	0.59
1:C:52:GLU:OE2	1:C:85:GLN:NE2	2.25	0.59
1:C:36:THR:O	1:C:40:ALA:HB2	2.02	0.59
1:D:316:LYS:NZ	1:D:318:GLU:OE1	2.34	0.59
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.84	0.59
1:A:110:LYS:HD2	1:A:126:GLY:HA2	1.84	0.59
1:C:105:GLY:HA2	1:C:144:PHE:O	2.03	0.59
1:D:105:GLY:HA2	1:D:144:PHE:O	2.03	0.59
1:B:36:THR:O	1:B:40:ALA:HB2	2.02	0.59
1:C:316:LYS:NZ	1:C:318:GLU:OE1	2.34	0.59
1:A:36:THR:O	1:A:40:ALA:HB2	2.02	0.59
1:A:105:GLY:HA2	1:A:144:PHE:O	2.03	0.59
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.36	0.59
1:B:105:GLY:HA2	1:B:144:PHE:O	2.03	0.59
1:A:257:ARG:NH1	1:A:292:LEU:O	2.35	0.59
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.36	0.59
1:D:66:ASP:OD2	1:D:68:ARG:NE	2.36	0.59
1:B:257:ARG:NH1	1:B:292:LEU:O	2.35	0.58
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.36	0.58
1:C:277:GLU:OE2	1:C:342:TYR:OH	2.21	0.58
1:D:277:GLU:OE2	1:D:342:TYR:OH	2.21	0.58
1:B:229:LYS:HE2	1:B:270:LEU:HD21	1.85	0.58
1:A:130:LEU:O	1:A:134:CYS:HB2	2.03	0.58
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.86	0.58
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.86	0.58
1:B:130:LEU:O	1:B:134:CYS:HB2	2.03	0.58
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.37	0.58
1:D:83:LEU:HD22	1:D:106:ILE:HD12	1.86	0.58
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.86	0.58
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.37	0.58
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.86	0.58
1:A:229:LYS:HE2	1:A:270:LEU:HD21	1.85	0.58
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.86	0.58
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.86	0.58
1:C:83:LEU:HD22	1:C:106:ILE:HD12	1.86	0.58
1:D:66:ASP:OD2	1:D:68:ARG:NE	2.37	0.57
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.37	0.57
1:C:276:GLU:O	1:C:330:ARG:NH2	2.37	0.57
1:D:148:ARG:NE	1:D:189:GLU:OE2	2.37	0.57
1:D:276:GLU:O	1:D:330:ARG:NH2	2.37	0.57
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.86	0.57
1:C:148:ARG:NE	1:C:189:GLU:OE2	2.37	0.57
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.86	0.57
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.87	0.57
1:A:148:ARG:NE	1:A:189:GLU:OE2	2.37	0.57
1:A:277:GLU:OE2	1:A:342:TYR:OH	2.21	0.57
1:D:229:LYS:HE2	1:D:270:LEU:HD21	1.85	0.57
1:C:42:ARG:HH22	1:C:303:ARG:HB2	1.70	0.57
1:B:83:LEU:HD22	1:B:106:ILE:HD12	1.86	0.57
1:B:148:ARG:NE	1:B:189:GLU:OE2	2.37	0.57
1:B:277:GLU:OE2	1:B:342:TYR:OH	2.21	0.57
1:C:229:LYS:HE2	1:C:270:LEU:HD21	1.85	0.57
1:D:110:LYS:HD2	1:D:126:GLY:HA2	1.84	0.57
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.86	0.57
1:D:42:ARG:HH22	1:D:303:ARG:HB2	1.70	0.57
1:C:110:LYS:HD2	1:C:126:GLY:HA2	1.84	0.57
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.86	0.57
1:A:83:LEU:HD22	1:A:106:ILE:HD12	1.86	0.57
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.86	0.57
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.37	0.57
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.37	0.57
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.86	0.57
1:D:66:ASP:OD2	1:D:68:ARG:NE	2.37	0.57
1:A:147:TRP:O	1:A:187:GLU:HB3	2.05	0.57
1:A:276:GLU:O	1:A:330:ARG:NH2	2.37	0.56
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.37	0.56
1:D:105:GLY:HA2	1:D:144:PHE:O	2.05	0.56
1:B:306:GLN:O	1:B:309:ALA:N	2.31	0.56
1:B:147:TRP:O	1:B:187:GLU:HB3	2.05	0.56
1:B:105:GLY:HA2	1:B:144:PHE:O	2.05	0.56
1:C:105:GLY:HA2	1:C:144:PHE:O	2.05	0.56
1:C:229:LYS:HG2	1:C:270:LEU:HD12	1.87	0.56
1:D:229:LYS:HG2	1:D:270:LEU:HD12	1.87	0.56
1:B:33:ASP:HB3	1:B:77:ILE:HG22	1.88	0.56
1:A:33:ASP:HB3	1:A:77:ILE:HG22	1.88	0.56
1:B:276:GLU:O	1:B:330:ARG:NH2	2.38	0.56
1:B:316:LYS:NZ	1:B:318:GLU:OE1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLY:HA2	1:A:144:PHE:O	2.05	0.56
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.87	0.56
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.87	0.56
1:C:229:LYS:HG2	1:C:270:LEU:HD12	1.88	0.56
1:A:147:TRP:O	1:A:187:GLU:HB3	2.05	0.56
1:C:147:TRP:O	1:C:187:GLU:HB3	2.05	0.56
1:D:147:TRP:O	1:D:187:GLU:HB3	2.05	0.56
1:D:229:LYS:HG2	1:D:270:LEU:HD12	1.88	0.56
1:A:316:LYS:NZ	1:A:318:GLU:OE1	2.34	0.56
1:B:147:TRP:O	1:B:187:GLU:HB3	2.05	0.56
1:D:147:TRP:O	1:D:187:GLU:HB3	2.05	0.56
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.88	0.56
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.88	0.56
1:C:147:TRP:O	1:C:187:GLU:HB3	2.05	0.56
1:A:42:ARG:HH22	1:A:303:ARG:HB2	1.70	0.56
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.88	0.56
1:B:42:ARG:HH22	1:B:303:ARG:HB2	1.70	0.55
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.39	0.55
1:D:66:ASP:OD2	1:D:68:ARG:NE	2.39	0.55
1:C:295:TRP:HE1	1:C:297:LEU:HD21	1.71	0.55
1:D:295:TRP:HE1	1:D:297:LEU:HD21	1.72	0.55
1:B:229:LYS:HG2	1:B:270:LEU:HD12	1.88	0.55
1:A:229:LYS:HG2	1:A:270:LEU:HD12	1.88	0.55
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.88	0.55
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.39	0.55
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.39	0.55
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.89	0.55
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.39	0.55
1:C:66:ASP:OD1	1:C:67:ASP:N	2.40	0.55
1:D:66:ASP:OD1	1:D:67:ASP:N	2.40	0.55
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.89	0.55
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.39	0.55
1:C:162:ALA:O	1:C:166:ASN:ND2	2.31	0.55
1:B:60:GLN:HE21	1:B:87:ALA:HA	1.72	0.55
1:C:148:ARG:NE	1:C:189:GLU:OE2	2.40	0.55
1:B:295:TRP:HE1	1:B:297:LEU:HD21	1.72	0.55
1:D:66:ASP:OD2	1:D:68:ARG:NE	2.39	0.55
1:D:162:ALA:O	1:D:166:ASN:ND2	2.31	0.55
1:C:151:LEU:HD21	1:C:166:ASN:HD22	1.72	0.55
1:D:148:ARG:NE	1:D:189:GLU:OE2	2.40	0.55
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.39	0.55
1:B:271:SER:O	1:B:274:GLN:HG2	2.07	0.55
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.88	0.55
1:B:65:ALA:HA	1:B:324:GLN:HE21	1.72	0.55
1:D:151:LEU:HD21	1:D:166:ASN:HD22	1.72	0.55
1:C:151:LEU:HD21	1:C:166:ASN:HD22	1.72	0.55
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.89	0.55
1:D:151:LEU:HD21	1:D:166:ASN:HD22	1.72	0.55
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.89	0.55
1:C:295:TRP:HE1	1:C:297:LEU:HD21	1.72	0.55
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.40	0.55
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.40	0.55
1:A:271:SER:O	1:A:274:GLN:HG2	2.07	0.55
1:D:66:ASP:OD2	1:D:68:ARG:NE	2.40	0.55
1:A:60:GLN:HE21	1:A:87:ALA:HA	1.72	0.55
1:A:65:ALA:HA	1:A:324:GLN:HE21	1.72	0.55
1:D:295:TRP:HE1	1:D:297:LEU:HD21	1.72	0.55
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.88	0.55
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.89	0.55
1:D:295:TRP:HE1	1:D:297:LEU:HD21	1.72	0.55
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.40	0.55
1:B:295:TRP:HE1	1:B:297:LEU:HD21	1.72	0.55
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.72	0.55
1:B:151:LEU:HD21	1:B:166:ASN:HD22	1.72	0.55
1:A:151:LEU:HD21	1:A:166:ASN:HD22	1.72	0.55
1:A:229:LYS:HG2	1:A:270:LEU:HD12	1.88	0.55
1:C:295:TRP:HE1	1:C:297:LEU:HD21	1.73	0.55
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.88	0.55
1:B:66:ASP:OD1	1:B:67:ASP:N	2.40	0.54
1:B:151:LEU:HD21	1:B:166:ASN:HD22	1.72	0.54
1:A:66:ASP:OD1	1:A:67:ASP:N	2.40	0.54
1:B:229:LYS:HG2	1:B:270:LEU:HD12	1.88	0.54
1:A:330:ARG:NE	1:A:330:ARG:HA	2.23	0.54
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.89	0.54
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.88	0.54
1:C:60:GLN:HE21	1:C:87:ALA:HA	1.72	0.54
1:B:330:ARG:NE	1:B:330:ARG:HA	2.23	0.54
1:C:229:LYS:HG2	1:C:270:LEU:HD12	1.89	0.54
1:D:295:TRP:HE1	1:D:297:LEU:HD21	1.72	0.54
1:B:148:ARG:NE	1:B:189:GLU:OE2	2.40	0.54
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LYS:HG2	1:D:270:LEU:HD12	1.89	0.54
1:A:151:LEU:HD21	1:A:166:ASN:HD22	1.72	0.54
1:C:295:TRP:HE1	1:C:297:LEU:HD21	1.72	0.54
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.40	0.54
1:A:306:GLN:O	1:A:309:ALA:N	2.31	0.54
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.88	0.54
1:B:229:LYS:HG2	1:B:270:LEU:HD12	1.89	0.54
1:A:229:LYS:HG2	1:A:270:LEU:HD12	1.89	0.54
1:D:60:GLN:HE21	1:D:87:ALA:HA	1.72	0.54
1:A:148:ARG:NE	1:A:189:GLU:OE2	2.40	0.54
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.40	0.54
1:A:330:ARG:HA	1:A:330:ARG:HE	1.73	0.54
1:B:33:ASP:HB3	1:B:77:ILE:HG22	1.89	0.54
1:B:151:LEU:HD21	1:B:166:ASN:HD22	1.73	0.54
1:A:151:LEU:HD21	1:A:166:ASN:HD22	1.73	0.54
1:B:77:ILE:HD13	1:B:146:LYS:HD2	1.89	0.54
1:B:66:ASP:OD1	1:B:67:ASP:N	2.41	0.54
1:A:66:ASP:OD1	1:A:67:ASP:N	2.41	0.54
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.90	0.54
1:B:330:ARG:HA	1:B:330:ARG:HE	1.73	0.54
1:D:66:ASP:OD2	1:D:68:ARG:NE	2.40	0.54
1:D:149:CYS:SG	1:D:166:ASN:HB3	2.48	0.54
1:C:151:LEU:HD21	1:C:166:ASN:HD22	1.73	0.54
1:D:151:LEU:HD21	1:D:166:ASN:HD22	1.73	0.54
1:A:77:ILE:HD13	1:A:146:LYS:HD2	1.89	0.54
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.90	0.54
1:B:66:ASP:OD1	1:B:67:ASP:N	2.41	0.54
1:A:33:ASP:HB3	1:A:77:ILE:HG22	1.89	0.54
1:C:149:CYS:SG	1:C:166:ASN:HB3	2.48	0.54
1:B:295:TRP:HE1	1:B:297:LEU:HD21	1.72	0.54
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.40	0.54
1:A:66:ASP:OD1	1:A:67:ASP:N	2.41	0.54
1:C:271:SER:O	1:C:274:GLN:HG2	2.07	0.54
1:D:271:SER:O	1:D:274:GLN:HG2	2.07	0.54
1:B:66:ASP:OD1	1:B:67:ASP:N	2.41	0.54
1:A:66:ASP:OD1	1:A:67:ASP:N	2.41	0.54
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.72	0.54
1:B:271:SER:O	1:B:274:GLN:HG2	2.08	0.54
1:A:271:SER:O	1:A:274:GLN:HG2	2.08	0.54
1:B:118:THR:HG21	1:B:121:GLU:HB2	1.90	0.54
1:A:197:ASP:N	1:A:197:ASP:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLN:HE22	1:B:88:ASP:H	1.55	0.54
1:A:60:GLN:HE22	1:A:88:ASP:H	1.55	0.54
1:C:60:GLN:HE22	1:C:88:ASP:H	1.55	0.54
1:D:60:GLN:HE22	1:D:88:ASP:H	1.56	0.54
1:A:118:THR:HG21	1:A:121:GLU:HB2	1.90	0.54
1:C:149:CYS:SG	1:C:166:ASN:HB3	2.48	0.54
1:D:149:CYS:SG	1:D:166:ASN:HB3	2.49	0.54
1:B:197:ASP:N	1:B:197:ASP:OD1	2.41	0.54
1:D:118:THR:HG21	1:D:121:GLU:HB2	1.89	0.54
1:B:295:TRP:HE1	1:B:297:LEU:HD21	1.72	0.53
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.72	0.53
1:C:118:THR:HG21	1:C:121:GLU:HB2	1.89	0.53
1:A:48:THR:HG21	1:A:315:GLY:HA3	1.90	0.53
1:C:77:ILE:HD13	1:C:146:LYS:HD2	1.89	0.53
1:D:77:ILE:HD13	1:D:146:LYS:HD2	1.89	0.53
1:C:65:ALA:HA	1:C:324:GLN:HE21	1.72	0.53
1:A:66:ASP:OD1	1:A:67:ASP:N	2.42	0.53
1:B:66:ASP:OD1	1:B:67:ASP:N	2.42	0.53
1:D:151:LEU:HD21	1:D:166:ASN:HD22	1.73	0.53
1:B:48:THR:HG21	1:B:315:GLY:HA3	1.90	0.53
1:D:110:LYS:HD2	1:D:126:GLY:HA2	1.91	0.53
1:D:330:ARG:NE	1:D:330:ARG:HA	2.23	0.53
1:B:66:ASP:OD1	1:B:67:ASP:N	2.42	0.53
1:A:149:CYS:SG	1:A:166:ASN:HB3	2.48	0.53
1:D:65:ALA:HA	1:D:324:GLN:HE21	1.72	0.53
1:A:257:ARG:NH1	1:A:292:LEU:O	2.42	0.53
1:C:110:LYS:HD2	1:C:126:GLY:HA2	1.91	0.53
1:D:118:THR:HG21	1:D:121:GLU:HB2	1.90	0.53
1:A:66:ASP:OD1	1:A:67:ASP:N	2.42	0.53
1:B:149:CYS:SG	1:B:166:ASN:HB3	2.49	0.53
1:C:118:THR:HG21	1:C:121:GLU:HB2	1.89	0.53
1:D:118:THR:HG21	1:D:121:GLU:HB2	1.89	0.53
1:B:197:ASP:N	1:B:197:ASP:OD1	2.42	0.53
1:B:257:ARG:NH1	1:B:292:LEU:O	2.42	0.53
1:C:66:ASP:OD1	1:C:67:ASP:N	2.41	0.53
1:C:118:THR:HG21	1:C:121:GLU:HB2	1.90	0.53
1:C:330:ARG:HA	1:C:330:ARG:HE	1.73	0.53
1:C:330:ARG:HA	1:C:330:ARG:NE	2.23	0.53
1:D:330:ARG:HA	1:D:330:ARG:HE	1.73	0.53
1:A:151:LEU:HD21	1:A:166:ASN:HD22	1.73	0.53
1:C:151:LEU:HD21	1:C:166:ASN:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:HE	1:B:96:VAL:HG22	1.74	0.53
1:A:197:ASP:N	1:A:197:ASP:OD1	2.42	0.53
1:B:66:ASP:OD1	1:B:67:ASP:N	2.42	0.53
1:A:275:SER:HB3	1:A:278:GLU:HG2	1.91	0.53
1:B:118:THR:HG21	1:B:121:GLU:HB2	1.89	0.53
1:C:197:ASP:N	1:C:197:ASP:OD1	2.41	0.53
1:B:118:THR:HG21	1:B:121:GLU:HB2	1.89	0.53
1:D:66:ASP:OD1	1:D:67:ASP:N	2.41	0.53
1:D:257:ARG:NH1	1:D:292:LEU:O	2.42	0.53
1:A:66:ASP:OD1	1:A:67:ASP:N	2.42	0.53
1:C:42:ARG:HH22	1:C:303:ARG:HB2	1.74	0.53
1:D:42:ARG:HH22	1:D:303:ARG:HB2	1.74	0.53
1:B:151:LEU:HD21	1:B:166:ASN:HD22	1.73	0.53
1:B:275:SER:HB3	1:B:278:GLU:HG2	1.91	0.53
1:A:118:THR:HG21	1:A:121:GLU:HB2	1.89	0.53
1:A:149:CYS:SG	1:A:166:ASN:HB3	2.48	0.53
1:A:118:THR:HG21	1:A:121:GLU:HB2	1.89	0.53
1:C:48:THR:HG21	1:C:315:GLY:HA3	1.90	0.53
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.90	0.53
1:A:91:ARG:HE	1:A:96:VAL:HG22	1.74	0.53
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.90	0.53
1:D:197:ASP:OD1	1:D:197:ASP:N	2.41	0.53
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.90	0.53
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.90	0.53
1:D:118:THR:HG21	1:D:121:GLU:HB2	1.90	0.53
1:D:257:ARG:NH1	1:D:292:LEU:O	2.42	0.53
1:A:253:VAL:O	1:A:257:ARG:HG2	2.09	0.53
1:D:48:THR:HG21	1:D:315:GLY:HA3	1.90	0.53
1:B:146:LYS:HE2	1:B:187:GLU:OE1	2.09	0.52
1:C:257:ARG:NH1	1:C:292:LEU:O	2.42	0.52
1:C:77:ILE:CD1	1:C:146:LYS:HB2	2.39	0.52
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.90	0.52
1:D:77:ILE:CD1	1:D:146:LYS:HB2	2.39	0.52
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.90	0.52
1:C:118:THR:HG21	1:C:121:GLU:HB2	1.90	0.52
1:C:275:SER:HB3	1:C:278:GLU:HG2	1.91	0.52
1:C:257:ARG:NH1	1:C:292:LEU:O	2.42	0.52
1:C:155:GLU:HG2	1:C:156:HIS:CD2	2.44	0.52
1:B:149:CYS:SG	1:B:166:ASN:HB3	2.48	0.52
1:B:253:VAL:O	1:B:257:ARG:HG2	2.09	0.52
1:A:146:LYS:HE2	1:A:187:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:HG21	1:B:121:GLU:HB2	1.90	0.52
1:A:257:ARG:NH1	1:A:292:LEU:O	2.42	0.52
1:C:66:ASP:OD1	1:C:67:ASP:N	2.41	0.52
1:D:66:ASP:OD1	1:D:67:ASP:N	2.41	0.52
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.91	0.52
1:D:155:GLU:HG2	1:D:156:HIS:CD2	2.44	0.52
1:B:31:ALA:HA	1:B:77:ILE:HG22	1.92	0.52
1:A:31:ALA:HA	1:A:77:ILE:HG22	1.92	0.52
1:B:257:ARG:NH1	1:B:292:LEU:O	2.42	0.52
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.91	0.52
1:C:66:ASP:OD1	1:C:67:ASP:N	2.41	0.52
1:D:66:ASP:OD1	1:D:67:ASP:N	2.41	0.52
1:D:271:SER:O	1:D:274:GLN:HG2	2.08	0.52
1:C:66:ASP:OD1	1:C:67:ASP:N	2.42	0.52
1:A:118:THR:HG21	1:A:121:GLU:HB2	1.90	0.52
1:D:275:SER:HB3	1:D:278:GLU:HG2	1.91	0.52
1:C:305:LEU:HD23	1:C:330:ARG:HG3	1.92	0.52
1:D:66:ASP:OD1	1:D:67:ASP:N	2.42	0.52
1:C:66:ASP:OD1	1:C:67:ASP:N	2.42	0.52
1:B:151:LEU:HD21	1:B:166:ASN:HD22	1.75	0.52
1:C:110:LYS:HD2	1:C:126:GLY:HA2	1.92	0.52
1:B:155:GLU:HG2	1:B:156:HIS:CD2	2.44	0.52
1:D:305:LEU:HD23	1:D:330:ARG:HG3	1.92	0.52
1:B:168:ASN:HD22	1:D:168:ASN:HD22	1.56	0.52
1:C:271:SER:O	1:C:274:GLN:HG2	2.08	0.52
1:A:151:LEU:HD21	1:A:166:ASN:HD22	1.75	0.52
1:D:110:LYS:HD2	1:D:126:GLY:HA2	1.92	0.52
1:B:66:ASP:OD1	1:B:67:ASP:N	2.43	0.52
1:A:66:ASP:OD1	1:A:67:ASP:N	2.43	0.52
1:A:155:GLU:HG2	1:A:156:HIS:CD2	2.44	0.52
1:B:280:SER:OG	1:B:330:ARG:NH2	2.43	0.52
1:A:280:SER:OG	1:A:330:ARG:NH2	2.43	0.52
1:A:66:ASP:OD1	1:A:67:ASP:N	2.43	0.52
1:A:91:ARG:HE	1:A:96:VAL:HG22	1.75	0.52
1:C:91:ARG:HE	1:C:96:VAL:HG22	1.74	0.52
1:B:77:ILE:HD11	1:B:146:LYS:CB	2.36	0.52
1:D:66:ASP:OD1	1:D:67:ASP:N	2.42	0.52
1:B:66:ASP:OD1	1:B:67:ASP:N	2.43	0.52
1:C:245:HIS:HE1	1:C:278:GLU:OE1	1.93	0.52
1:C:253:VAL:O	1:C:257:ARG:HG2	2.09	0.52
1:D:253:VAL:O	1:D:257:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HH22	1:B:303:ARG:HB2	1.74	0.52
1:D:151:LEU:HD21	1:D:166:ASN:HD22	1.75	0.52
1:B:91:ARG:HE	1:B:96:VAL:HG22	1.75	0.52
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.91	0.52
1:A:110:LYS:HD2	1:A:126:GLY:HA2	1.91	0.52
1:D:91:ARG:HE	1:D:96:VAL:HG22	1.74	0.52
1:A:77:ILE:HD11	1:A:146:LYS:CB	2.36	0.52
1:B:186:VAL:HG12	1:B:188:PRO:HD3	1.92	0.52
1:A:186:VAL:HG12	1:A:188:PRO:HD3	1.92	0.52
1:C:151:LEU:HD21	1:C:166:ASN:HD22	1.75	0.52
1:B:245:HIS:HE1	1:B:278:GLU:OE1	1.93	0.52
1:D:245:HIS:HE1	1:D:278:GLU:OE1	1.93	0.52
1:B:151:LEU:HD21	1:B:166:ASN:HD22	1.75	0.52
1:B:77:ILE:CD1	1:B:146:LYS:HB2	2.39	0.52
1:D:31:ALA:HA	1:D:77:ILE:HG22	1.92	0.52
1:D:68:ARG:NH2	1:D:325:GLU:OE1	2.38	0.52
1:A:245:HIS:HE1	1:A:278:GLU:OE1	1.93	0.52
1:A:151:LEU:HD21	1:A:166:ASN:HD22	1.75	0.51
1:A:77:ILE:CD1	1:A:146:LYS:HB2	2.39	0.51
1:C:66:ASP:OD1	1:C:67:ASP:N	2.42	0.51
1:C:31:ALA:HA	1:C:77:ILE:HG22	1.92	0.51
1:B:33:ASP:HB3	1:B:77:ILE:HG22	1.91	0.51
1:A:42:ARG:HH22	1:A:303:ARG:HB2	1.74	0.51
1:D:36:THR:O	1:D:40:ALA:CB	2.57	0.51
1:C:42:ARG:NH2	1:C:303:ARG:HB3	2.24	0.51
1:A:33:ASP:HB3	1:A:77:ILE:HG22	1.91	0.51
1:D:66:ASP:OD1	1:D:67:ASP:N	2.43	0.51
1:D:66:ASP:OD1	1:D:67:ASP:N	2.42	0.51
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.46	0.51
1:C:36:THR:O	1:C:40:ALA:CB	2.57	0.51
1:B:245:HIS:HE1	1:B:278:GLU:OE1	1.93	0.51
1:B:168:ASN:HD22	1:D:168:ASN:HD22	1.57	0.51
1:D:151:LEU:HD21	1:D:166:ASN:HD22	1.75	0.51
1:A:83:LEU:HD22	1:A:106:ILE:HD12	1.92	0.51
1:A:245:HIS:HE1	1:A:278:GLU:OE1	1.93	0.51
1:D:42:ARG:NH2	1:D:303:ARG:HB3	2.24	0.51
1:C:68:ARG:NH2	1:C:325:GLU:OE1	2.38	0.51
1:C:280:SER:OG	1:C:330:ARG:NH2	2.43	0.51
1:C:66:ASP:OD1	1:C:67:ASP:N	2.43	0.51
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.14	0.51
1:B:50:ASN:OD1	1:B:55:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:LEU:HD22	1:D:106:ILE:HD12	1.92	0.51
1:D:280:SER:OG	1:D:330:ARG:NH2	2.43	0.51
1:C:60:GLN:HE22	1:C:88:ASP:CG	2.14	0.51
1:C:146:LYS:HE2	1:C:187:GLU:OE1	2.09	0.51
1:A:50:ASN:OD1	1:A:55:ARG:NH1	2.43	0.51
1:B:83:LEU:HD22	1:B:106:ILE:HD12	1.92	0.51
1:C:83:LEU:HD22	1:C:106:ILE:HD12	1.92	0.51
1:B:305:LEU:HD23	1:B:330:ARG:HG3	1.92	0.51
1:A:305:LEU:HD23	1:A:330:ARG:HG3	1.92	0.51
1:C:151:LEU:HD21	1:C:166:ASN:HD22	1.75	0.51
1:B:295:TRP:HE1	1:B:297:LEU:HD21	1.76	0.51
1:C:197:ASP:N	1:C:197:ASP:OD1	2.42	0.51
1:D:197:ASP:OD1	1:D:197:ASP:N	2.42	0.51
1:B:149:CYS:SG	1:B:166:ASN:HB3	2.51	0.51
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.14	0.51
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.14	0.51
1:C:186:VAL:HG12	1:C:188:PRO:HD3	1.92	0.51
1:C:66:ASP:OD1	1:C:67:ASP:N	2.43	0.51
1:D:66:ASP:OD1	1:D:67:ASP:N	2.43	0.51
1:C:66:ASP:OD1	1:C:67:ASP:N	2.44	0.51
1:D:66:ASP:OD1	1:D:67:ASP:N	2.44	0.51
1:D:146:LYS:HE2	1:D:187:GLU:OE1	2.09	0.51
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.76	0.51
1:C:295:TRP:HE1	1:C:297:LEU:HD21	1.76	0.51
1:D:295:TRP:HE1	1:D:297:LEU:HD21	1.76	0.51
1:A:149:CYS:SG	1:A:166:ASN:HB3	2.51	0.51
1:C:60:GLN:HE22	1:C:88:ASP:CG	2.14	0.51
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.14	0.51
1:D:186:VAL:HG12	1:D:188:PRO:HD3	1.92	0.51
1:C:60:GLN:HE22	1:C:88:ASP:CG	2.14	0.51
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.14	0.51
1:B:83:LEU:HD22	1:B:106:ILE:HD12	1.93	0.51
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.14	0.51
1:C:110:LYS:HD2	1:C:126:GLY:HA2	1.93	0.51
1:C:229:LYS:HG2	1:C:270:LEU:HD12	1.93	0.51
1:D:229:LYS:HG2	1:D:270:LEU:HD12	1.93	0.51
1:C:149:CYS:SG	1:C:166:ASN:HB3	2.51	0.51
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.76	0.51
1:C:60:GLN:HE22	1:C:88:ASP:CG	2.14	0.51
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.14	0.51
1:B:33:ASP:HB3	1:B:77:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD22	1:A:106:ILE:HD12	1.93	0.51
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.14	0.51
1:D:110:LYS:HD2	1:D:126:GLY:HA2	1.93	0.50
1:C:50:ASN:OD1	1:C:55:ARG:NH1	2.43	0.50
1:D:149:CYS:SG	1:D:166:ASN:HB3	2.51	0.50
1:C:245:HIS:HE1	1:C:278:GLU:OE1	1.93	0.50
1:B:66:ASP:OD1	1:B:67:ASP:N	2.44	0.50
1:A:33:ASP:HB3	1:A:77:ILE:HG22	1.93	0.50
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.93	0.50
1:C:91:ARG:HE	1:C:96:VAL:HG22	1.75	0.50
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.14	0.50
1:D:50:ASN:OD1	1:D:55:ARG:NH1	2.43	0.50
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.92	0.50
1:A:110:LYS:HD2	1:A:126:GLY:HA2	1.92	0.50
1:D:245:HIS:HE1	1:D:278:GLU:OE1	1.93	0.50
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.93	0.50
1:C:83:LEU:HD22	1:C:106:ILE:HD12	1.93	0.50
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.14	0.50
1:B:229:LYS:HG2	1:B:270:LEU:HD12	1.93	0.50
1:C:60:GLN:HE22	1:C:88:ASP:CG	2.14	0.50
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.76	0.50
1:B:91:ARG:HE	1:B:96:VAL:HG22	1.77	0.50
1:B:154:GLY:O	1:B:200:ARG:NH2	2.44	0.50
1:C:276:GLU:HG3	1:C:304:ALA:O	2.11	0.50
1:D:276:GLU:HG3	1:D:304:ALA:O	2.11	0.50
1:A:66:ASP:OD1	1:A:67:ASP:N	2.44	0.50
1:D:83:LEU:HD22	1:D:106:ILE:HD12	1.93	0.50
1:A:229:LYS:HG2	1:A:270:LEU:HD12	1.93	0.50
1:A:306:GLN:O	1:A:309:ALA:N	2.45	0.50
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.15	0.50
1:A:91:ARG:HE	1:A:96:VAL:HG22	1.77	0.50
1:A:154:GLY:O	1:A:200:ARG:NH2	2.44	0.50
1:D:91:ARG:HE	1:D:96:VAL:HG22	1.75	0.50
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.77	0.50
1:C:295:TRP:HE1	1:C:297:LEU:HD21	1.77	0.50
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.15	0.50
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.14	0.50
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.14	0.50
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.59	0.50
1:B:295:TRP:HE1	1:B:297:LEU:HD21	1.77	0.50
1:D:42:ARG:NH1	1:D:306:GLN:HE21	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:TRP:HE1	1:D:297:LEU:HD21	1.77	0.50
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.15	0.50
1:C:60:GLN:HE22	1:C:88:ASP:CG	2.15	0.50
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.15	0.50
1:C:36:THR:O	1:C:40:ALA:CB	2.58	0.50
1:D:36:THR:O	1:D:40:ALA:CB	2.58	0.50
1:C:306:GLN:O	1:C:309:ALA:N	2.31	0.50
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.14	0.50
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.14	0.50
1:B:34:GLU:O	1:B:59:ARG:NH2	2.45	0.50
1:C:42:ARG:NH1	1:C:306:GLN:HE21	2.10	0.50
1:D:42:ARG:HH22	1:D:306:GLN:HG3	1.77	0.50
1:C:146:LYS:HE3	1:C:187:GLU:OE1	2.12	0.50
1:B:68:ARG:NH2	1:B:325:GLU:OE1	2.38	0.50
1:C:60:GLN:HE22	1:C:88:ASP:CG	2.15	0.50
1:A:34:GLU:O	1:A:59:ARG:NH2	2.45	0.50
1:B:42:ARG:NH1	1:B:306:GLN:HE21	2.10	0.50
1:A:42:ARG:NH1	1:A:306:GLN:HE21	2.10	0.50
1:C:42:ARG:HH22	1:C:306:GLN:HG3	1.77	0.50
1:B:50:ASN:OD1	1:B:55:ARG:NH1	2.45	0.50
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.59	0.50
1:C:306:GLN:O	1:C:309:ALA:N	2.45	0.50
1:D:146:LYS:HE3	1:D:187:GLU:OE1	2.12	0.50
1:A:276:GLU:HG3	1:A:304:ALA:O	2.11	0.50
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.60	0.50
1:B:36:THR:O	1:B:40:ALA:CB	2.57	0.50
1:B:306:GLN:O	1:B:309:ALA:N	2.45	0.50
1:A:146:LYS:HE3	1:A:187:GLU:OE1	2.12	0.50
1:A:257:ARG:NH1	1:A:292:LEU:O	2.45	0.50
1:C:257:ARG:NH1	1:C:292:LEU:O	2.45	0.50
1:D:257:ARG:NH1	1:D:292:LEU:O	2.45	0.50
1:D:306:GLN:O	1:D:309:ALA:N	2.45	0.50
1:A:50:ASN:OD1	1:A:55:ARG:NH1	2.45	0.49
1:B:34:GLU:O	1:B:59:ARG:NH2	2.45	0.49
1:A:34:GLU:O	1:A:59:ARG:NH2	2.45	0.49
1:B:257:ARG:NH1	1:B:292:LEU:O	2.45	0.49
1:B:276:GLU:HG3	1:B:304:ALA:O	2.11	0.49
1:D:306:GLN:O	1:D:309:ALA:N	2.31	0.49
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.15	0.49
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.59	0.49
1:B:146:LYS:HE3	1:B:187:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:O	1:A:40:ALA:CB	2.57	0.49
1:D:316:LYS:HE2	1:D:319:ASN:HD21	1.77	0.49
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.15	0.49
1:A:68:ARG:NH2	1:A:325:GLU:OE1	2.38	0.49
1:C:34:GLU:O	1:C:59:ARG:NH2	2.45	0.49
1:D:34:GLU:O	1:D:59:ARG:NH2	2.45	0.49
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.77	0.49
1:C:34:GLU:O	1:C:59:ARG:NH2	2.45	0.49
1:D:34:GLU:O	1:D:59:ARG:NH2	2.46	0.49
1:D:257:ARG:NH1	1:D:292:LEU:O	2.45	0.49
1:B:77:ILE:CD1	1:B:146:LYS:HB2	2.40	0.49
1:A:77:ILE:CD1	1:A:146:LYS:HB2	2.40	0.49
1:A:31:ALA:HA	1:A:77:ILE:CG2	2.43	0.49
1:C:31:ALA:HA	1:C:77:ILE:CG2	2.42	0.49
1:C:229:LYS:HD3	1:C:270:LEU:HD21	1.94	0.49
1:D:31:ALA:HA	1:D:77:ILE:CG2	2.42	0.49
1:D:229:LYS:HD3	1:D:270:LEU:HD21	1.95	0.49
1:C:154:GLY:O	1:C:200:ARG:NH2	2.44	0.49
1:D:154:GLY:O	1:D:200:ARG:NH2	2.44	0.49
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.15	0.49
1:C:257:ARG:NH1	1:C:292:LEU:O	2.45	0.49
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.59	0.49
1:A:168:ASN:HD22	1:C:168:ASN:HD22	1.59	0.49
1:B:31:ALA:HA	1:B:77:ILE:CG2	2.43	0.49
1:B:31:ALA:HA	1:B:77:ILE:CG2	2.42	0.49
1:A:31:ALA:HA	1:A:77:ILE:CG2	2.42	0.49
1:C:316:LYS:HE2	1:C:319:ASN:HD21	1.77	0.49
1:C:83:LEU:HD22	1:C:106:ILE:HD12	1.94	0.49
1:C:185:ILE:HG12	1:C:227:LEU:HB2	1.95	0.49
1:A:316:LYS:HE2	1:A:319:ASN:HD21	1.77	0.49
1:D:83:LEU:HD22	1:D:106:ILE:HD12	1.94	0.49
1:A:168:ASN:HD22	1:C:168:ASN:HD22	1.59	0.49
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.93	0.49
1:A:110:LYS:HD2	1:A:126:GLY:HA2	1.92	0.49
1:C:275:SER:HB3	1:C:278:GLU:HG2	1.94	0.49
1:D:185:ILE:HG12	1:D:227:LEU:HB2	1.95	0.49
1:B:146:LYS:HE2	1:B:187:GLU:OE1	2.13	0.49
1:B:316:LYS:HE2	1:B:319:ASN:HD21	1.77	0.49
1:B:83:LEU:HD22	1:B:106:ILE:HD12	1.94	0.49
1:A:257:ARG:NH1	1:A:292:LEU:O	2.45	0.49
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:SER:HB3	1:D:278:GLU:HG2	1.94	0.49
1:A:83:LEU:HD22	1:A:106:ILE:HD12	1.94	0.49
1:D:229:LYS:HD3	1:D:270:LEU:HD21	1.95	0.49
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.77	0.49
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.95	0.49
1:B:257:ARG:NH1	1:B:292:LEU:O	2.45	0.49
1:A:185:ILE:HG12	1:A:227:LEU:HB2	1.95	0.49
1:C:50:ASN:OD1	1:C:55:ARG:NH1	2.45	0.49
1:D:83:LEU:HD22	1:D:106:ILE:HD12	1.95	0.49
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.60	0.49
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.77	0.49
1:B:229:LYS:HD3	1:B:270:LEU:HD21	1.94	0.49
1:B:56:ARG:HB2	1:B:85:GLN:HE21	1.78	0.49
1:A:146:LYS:HE2	1:A:187:GLU:OE1	2.13	0.49
1:C:91:ARG:HE	1:C:96:VAL:HG22	1.77	0.49
1:C:146:LYS:HE2	1:C:187:GLU:OE1	2.13	0.49
1:D:146:LYS:HE2	1:D:187:GLU:OE1	2.13	0.49
1:C:229:LYS:HD3	1:C:270:LEU:HD21	1.95	0.49
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.95	0.49
1:B:42:ARG:HH22	1:B:306:GLN:HG3	1.77	0.49
1:A:42:ARG:HH22	1:A:306:GLN:HG3	1.77	0.49
1:B:185:ILE:HG12	1:B:227:LEU:HB2	1.95	0.49
1:D:50:ASN:OD1	1:D:55:ARG:NH1	2.45	0.49
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.59	0.49
1:C:83:LEU:HD22	1:C:106:ILE:HD12	1.95	0.49
1:C:31:ALA:HA	1:C:77:ILE:CG2	2.43	0.49
1:D:31:ALA:HA	1:D:77:ILE:CG2	2.43	0.49
1:D:91:ARG:HE	1:D:96:VAL:HG22	1.77	0.49
1:C:229:LYS:HG2	1:C:270:LEU:HD12	1.95	0.48
1:A:275:SER:HB3	1:A:278:GLU:HG2	1.94	0.48
1:B:83:LEU:HD22	1:B:106:ILE:HD12	1.95	0.48
1:A:83:LEU:HD22	1:A:106:ILE:HD12	1.95	0.48
1:C:31:ALA:HA	1:C:77:ILE:CG2	2.43	0.48
1:D:31:ALA:HA	1:D:77:ILE:CG2	2.43	0.48
1:C:77:ILE:HD11	1:C:146:LYS:CB	2.36	0.48
1:A:229:LYS:HD3	1:A:270:LEU:HD21	1.95	0.48
1:C:245:HIS:HE1	1:C:278:GLU:OE1	1.96	0.48
1:D:245:HIS:HE1	1:D:278:GLU:OE1	1.96	0.48
1:A:56:ARG:HB2	1:A:85:GLN:HE21	1.78	0.48
1:A:306:GLN:O	1:A:309:ALA:N	2.46	0.48
1:C:66:ASP:O	1:C:69:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.95	0.48
1:A:56:ARG:HB2	1:A:85:GLN:HE21	1.78	0.48
1:A:168:ASN:HD22	1:C:168:ASN:HD22	1.60	0.48
1:C:36:THR:O	1:C:40:ALA:CB	2.60	0.48
1:D:36:THR:O	1:D:40:ALA:CB	2.60	0.48
1:C:294:PRO:HG2	1:C:295:TRP:CE2	2.48	0.48
1:D:77:ILE:HD11	1:D:146:LYS:CB	2.36	0.48
1:B:306:GLN:O	1:B:309:ALA:N	2.46	0.48
1:A:42:ARG:NH2	1:A:303:ARG:HB3	2.22	0.48
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.95	0.48
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.95	0.48
1:B:168:ASN:HD22	1:D:168:ASN:HD22	1.60	0.48
1:D:229:LYS:HG2	1:D:270:LEU:HD12	1.95	0.48
1:B:275:SER:HB3	1:B:278:GLU:HG2	1.94	0.48
1:C:146:LYS:HE3	1:C:187:GLU:OE1	2.14	0.48
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.96	0.48
1:D:146:LYS:HE3	1:D:187:GLU:OE1	2.14	0.48
1:B:56:ARG:HB2	1:B:85:GLN:HE21	1.79	0.48
1:B:42:ARG:NH2	1:B:303:ARG:HB3	2.22	0.48
1:C:306:GLN:O	1:C:309:ALA:N	2.46	0.48
1:D:306:GLN:O	1:D:309:ALA:N	2.46	0.48
1:D:66:ASP:O	1:D:69:VAL:HG22	2.14	0.48
1:C:77:ILE:CD1	1:C:146:LYS:HB2	2.40	0.48
1:B:31:ALA:HA	1:B:77:ILE:CG2	2.43	0.48
1:A:294:PRO:HG2	1:A:295:TRP:CE2	2.48	0.48
1:D:294:PRO:HG2	1:D:295:TRP:CE2	2.48	0.48
1:B:245:HIS:HE1	1:B:278:GLU:OE1	1.96	0.48
1:C:185:ILE:HG12	1:C:227:LEU:HB2	1.95	0.48
1:D:185:ILE:HG12	1:D:227:LEU:HB2	1.95	0.48
1:A:168:ASN:HD22	1:C:168:ASN:HD22	1.60	0.48
1:A:229:LYS:HG2	1:A:270:LEU:HD12	1.95	0.48
1:C:77:ILE:HD11	1:C:146:LYS:CB	2.43	0.48
1:D:77:ILE:CD1	1:D:146:LYS:HB2	2.40	0.48
1:A:31:ALA:HA	1:A:77:ILE:CG2	2.44	0.48
1:B:294:PRO:HG2	1:B:295:TRP:CE2	2.48	0.48
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.49	0.48
1:B:229:LYS:HG2	1:B:270:LEU:HD12	1.95	0.48
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.78	0.48
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.78	0.48
1:C:56:ARG:HB2	1:C:85:GLN:HE21	1.78	0.48
1:D:77:ILE:HD11	1:D:146:LYS:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:HIS:HE1	1:A:278:GLU:OE1	1.96	0.48
1:A:57:PHE:CZ	1:A:320:LEU:HD12	2.49	0.48
1:A:185:ILE:HG12	1:A:227:LEU:HB2	1.95	0.48
1:D:56:ARG:HB2	1:D:85:GLN:HE21	1.79	0.48
1:B:168:ASN:HD22	1:D:168:ASN:HD22	1.60	0.48
1:A:186:VAL:HG12	1:A:188:PRO:HD3	1.95	0.48
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.78	0.48
1:B:185:ILE:HG12	1:B:227:LEU:HB2	1.95	0.48
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.78	0.48
1:A:66:ASP:O	1:A:69:VAL:HG22	2.14	0.48
1:B:61:LEU:HD11	1:B:324:GLN:HB2	1.95	0.48
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.96	0.48
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.49	0.48
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.32	0.48
1:B:229:LYS:HD3	1:B:270:LEU:HD21	1.95	0.48
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	0.48
1:A:61:LEU:HD11	1:A:324:GLN:HB2	1.95	0.48
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.96	0.48
1:B:186:VAL:HG12	1:B:188:PRO:HD3	1.96	0.48
1:C:186:VAL:HG12	1:C:188:PRO:HD3	1.95	0.48
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.32	0.48
1:A:103:VAL:HG23	1:A:144:PHE:HE2	1.79	0.48
1:A:229:LYS:HD3	1:A:270:LEU:HD21	1.95	0.48
1:B:66:ASP:O	1:B:69:VAL:HG22	2.13	0.48
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.49	0.48
1:B:103:VAL:HG23	1:B:144:PHE:HE2	1.79	0.48
1:D:103:VAL:HG23	1:D:144:PHE:HE2	1.79	0.48
1:A:66:ASP:O	1:A:69:VAL:HG22	2.13	0.48
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.32	0.47
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.60	0.47
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.60	0.47
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.96	0.47
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.96	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.13	0.47
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.59	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.14	0.47
1:D:186:VAL:HG12	1:D:188:PRO:HD3	1.96	0.47
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.32	0.47
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.49	0.47
1:C:103:VAL:HG23	1:C:144:PHE:HE2	1.79	0.47
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PHE:CZ	1:D:320:LEU:HD12	2.49	0.47
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.96	0.47
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.96	0.47
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.97	0.47
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.45	0.47
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.60	0.47
1:C:56:ARG:HB2	1:C:85:GLN:HE21	1.78	0.47
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.45	0.47
1:D:66:ASP:O	1:D:69:VAL:HG22	2.13	0.47
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.45	0.47
1:B:146:LYS:HE3	1:B:187:GLU:OE1	2.14	0.47
1:D:66:ASP:O	1:D:69:VAL:HG22	2.14	0.47
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.61	0.47
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.61	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.14	0.47
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.97	0.47
1:D:66:ASP:O	1:D:69:VAL:HG22	2.14	0.47
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.79	0.47
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.79	0.47
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.97	0.47
1:C:78:LEU:O	1:C:106:ILE:HA	2.15	0.47
1:D:78:LEU:O	1:D:106:ILE:HA	2.15	0.47
1:A:146:LYS:HE3	1:A:187:GLU:OE1	2.14	0.47
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.97	0.47
1:D:56:ARG:HB2	1:D:85:GLN:HE21	1.78	0.47
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.45	0.47
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.50	0.47
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.48	0.47
1:D:66:ASP:OD2	1:D:68:ARG:NE	2.48	0.47
1:B:77:ILE:HD11	1:B:146:LYS:CB	2.43	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	0.47
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.97	0.47
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.45	0.47
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.63	0.47
1:C:82:THR:HA	1:C:85:GLN:HG2	1.96	0.47
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.63	0.47
1:D:82:THR:HA	1:D:85:GLN:HG2	1.96	0.47
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.45	0.47
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.45	0.47
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.97	0.47
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.79	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	0.47
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.18	0.47
1:B:277:GLU:OE2	1:B:342:TYR:OH	2.32	0.47
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.18	0.47
1:A:77:ILE:HD11	1:A:146:LYS:CB	2.43	0.47
1:A:277:GLU:OE2	1:A:342:TYR:OH	2.32	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.15	0.47
1:A:66:ASP:O	1:A:69:VAL:HG22	2.14	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	0.47
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.97	0.47
1:A:66:ASP:O	1:A:69:VAL:HG22	2.14	0.47
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.97	0.47
1:D:66:ASP:O	1:D:69:VAL:HG22	2.14	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.14	0.47
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.48	0.47
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.97	0.47
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.48	0.47
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.97	0.47
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.97	0.47
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.97	0.47
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.32	0.47
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.33	0.47
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.32	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.15	0.47
1:A:66:ASP:O	1:A:69:VAL:HG22	2.14	0.47
1:C:61:LEU:HD11	1:C:324:GLN:HB2	1.95	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.14	0.47
1:C:60:GLN:HE22	1:C:88:ASP:CG	2.18	0.47
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.18	0.47
1:D:66:ASP:O	1:D:69:VAL:HG22	2.15	0.47
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.63	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.14	0.47
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.97	0.47
1:D:66:ASP:O	1:D:69:VAL:HG22	2.14	0.47
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.78	0.47
1:A:36:THR:O	1:A:40:ALA:CB	2.63	0.47
1:B:36:THR:O	1:B:40:ALA:CB	2.60	0.47
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.63	0.47
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.32	0.47
1:B:276:GLU:OE2	1:B:307:ALA:HB3	2.15	0.47
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.33	0.47
1:C:60:GLN:O	1:C:64:THR:OG1	2.25	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.15	0.47
1:D:66:ASP:O	1:D:69:VAL:HG22	2.15	0.47
1:B:36:THR:O	1:B:40:ALA:CB	2.63	0.47
1:D:61:LEU:HD11	1:D:324:GLN:HB2	1.95	0.47
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.61	0.47
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.63	0.47
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.45	0.47
1:A:49:GLU:O	1:A:54:ASN:ND2	2.39	0.47
1:A:66:ASP:O	1:A:69:VAL:HG22	2.14	0.47
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.45	0.47
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.97	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	0.47
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.45	0.47
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.32	0.47
1:A:276:GLU:OE2	1:A:307:ALA:HB3	2.15	0.47
1:A:66:ASP:O	1:A:69:VAL:HG22	2.15	0.46
1:C:149:CYS:SG	1:C:166:ASN:HB3	2.55	0.46
1:D:66:ASP:O	1:D:69:VAL:HG22	2.14	0.46
1:C:301:TYR:HB2	1:C:305:LEU:HG	1.97	0.46
1:D:301:TYR:HB2	1:D:305:LEU:HG	1.98	0.46
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.61	0.46
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.63	0.46
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.15	0.46
1:A:66:ASP:O	1:A:69:VAL:HG22	2.14	0.46
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.45	0.46
1:D:149:CYS:SG	1:D:166:ASN:HB3	2.56	0.46
1:A:36:THR:O	1:A:40:ALA:CB	2.60	0.46
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.15	0.46
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.32	0.46
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.32	0.46
1:A:82:THR:HA	1:A:85:GLN:HG2	1.96	0.46
1:B:149:CYS:SG	1:B:166:ASN:HB3	2.55	0.46
1:A:149:CYS:SG	1:A:166:ASN:HB3	2.55	0.46
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.15	0.46
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.16	0.46
1:B:82:THR:HA	1:B:85:GLN:HG2	1.96	0.46
1:D:60:GLN:O	1:D:64:THR:OG1	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ASP:HB3	1:C:238:ALA:HB3	1.98	0.46
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.80	0.46
1:C:66:ASP:O	1:C:69:VAL:HG22	2.15	0.46
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.46	0.46
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.51	0.46
1:B:68:ARG:NH2	1:B:325:GLU:OE1	2.38	0.46
1:D:195:ASP:HB3	1:D:238:ALA:HB3	1.98	0.46
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.46	0.46
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.46	0.46
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.80	0.46
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.98	0.46
1:D:66:ASP:O	1:D:69:VAL:HG22	2.15	0.46
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.15	0.46
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.46	0.46
1:B:49:GLU:O	1:B:54:ASN:ND2	2.39	0.46
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.15	0.46
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.63	0.46
1:A:68:ARG:NH2	1:A:325:GLU:OE1	2.38	0.46
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.16	0.46
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.15	0.46
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.62	0.46
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.51	0.46
1:C:144:PHE:HA	1:C:182:ILE:HG23	1.98	0.46
1:D:144:PHE:HA	1:D:182:ILE:HG23	1.98	0.46
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.98	0.46
1:D:31:ALA:HA	1:D:77:ILE:CG2	2.45	0.46
1:B:66:ASP:O	1:B:69:VAL:HG22	2.15	0.46
1:D:301:TYR:HB2	1:D:305:LEU:HG	1.98	0.46
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.79	0.46
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.79	0.46
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.16	0.46
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.16	0.46
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.98	0.46
1:B:301:TYR:HB2	1:B:305:LEU:HG	1.98	0.46
1:A:31:ALA:HA	1:A:77:ILE:CG2	2.45	0.46
1:A:66:ASP:O	1:A:69:VAL:HG22	2.15	0.46
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.98	0.46
1:A:301:TYR:HB2	1:A:305:LEU:HG	1.97	0.46
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.16	0.46
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.16	0.46
1:A:66:ASP:O	1:A:69:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:TYR:HB2	1:C:305:LEU:HG	1.98	0.46
1:A:78:LEU:O	1:A:106:ILE:HA	2.15	0.46
1:C:149:CYS:SG	1:C:188:PRO:HA	2.56	0.46
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.16	0.46
1:B:31:ALA:HA	1:B:77:ILE:CG2	2.45	0.46
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.64	0.46
1:B:66:ASP:O	1:B:69:VAL:HG22	2.15	0.46
1:C:31:ALA:HA	1:C:77:ILE:CG2	2.46	0.46
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.16	0.46
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.16	0.46
1:B:61:LEU:HA	1:B:324:GLN:HE21	1.81	0.46
1:B:78:LEU:O	1:B:106:ILE:HA	2.15	0.46
1:D:149:CYS:SG	1:D:188:PRO:HA	2.56	0.46
1:C:42:ARG:HH22	1:C:303:ARG:HB2	1.81	0.46
1:D:42:ARG:HH22	1:D:303:ARG:HB2	1.81	0.46
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.64	0.46
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.51	0.46
1:D:57:PHE:CZ	1:D:320:LEU:HD12	2.51	0.46
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.16	0.46
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.16	0.46
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.46	0.46
1:C:301:TYR:HB2	1:C:305:LEU:HG	1.98	0.45
1:B:42:ARG:HH22	1:B:303:ARG:HB2	1.81	0.45
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.16	0.45
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.16	0.45
1:B:36:THR:O	1:B:40:ALA:CB	2.58	0.45
1:A:36:THR:O	1:A:40:ALA:CB	2.58	0.45
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.34	0.45
1:A:35:SER:OG	1:A:36:THR:N	2.49	0.45
1:C:276:GLU:OE2	1:C:307:ALA:HB3	2.16	0.45
1:D:276:GLU:OE2	1:D:307:ALA:HB3	2.15	0.45
1:A:61:LEU:HA	1:A:324:GLN:HE21	1.81	0.45
1:A:42:ARG:HH22	1:A:303:ARG:HB2	1.81	0.45
1:A:229:LYS:HE2	1:A:270:LEU:CD2	2.45	0.45
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.16	0.45
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.34	0.45
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.46	0.45
1:C:271:SER:O	1:C:274:GLN:HG2	2.17	0.45
1:D:271:SER:O	1:D:274:GLN:HG2	2.17	0.45
1:B:35:SER:OG	1:B:36:THR:N	2.49	0.45
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.17	0.45
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.65	0.45
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.65	0.45
1:D:61:LEU:HA	1:D:324:GLN:HE21	1.81	0.45
1:D:301:TYR:HB2	1:D:305:LEU:HG	1.98	0.45
1:B:229:LYS:HE2	1:B:270:LEU:CD2	2.45	0.45
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.46	0.45
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.52	0.45
1:C:42:ARG:NH2	1:C:303:ARG:HB3	2.24	0.45
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.34	0.45
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.34	0.45
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.52	0.45
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.65	0.45
1:B:149:CYS:SG	1:B:188:PRO:HA	2.56	0.45
1:B:301:TYR:HB2	1:B:305:LEU:HG	1.98	0.45
1:A:149:CYS:SG	1:A:188:PRO:HA	2.56	0.45
1:C:61:LEU:HA	1:C:324:GLN:HE21	1.81	0.45
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.46	0.45
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.80	0.45
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.64	0.45
1:D:147:TRP:O	1:D:187:GLU:HB3	2.16	0.45
1:B:301:TYR:HB2	1:B:305:LEU:HG	1.98	0.45
1:A:301:TYR:HB2	1:A:305:LEU:HG	1.98	0.45
1:C:197:ASP:N	1:C:197:ASP:OD1	2.49	0.45
1:A:46:ILE:CG1	1:A:314:GLY:HA2	2.47	0.45
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.17	0.45
1:A:119:ASN:HB2	1:C:4:HIS:CD2	2.52	0.45
1:D:197:ASP:OD1	1:D:197:ASP:N	2.49	0.45
1:D:162:ALA:O	1:D:166:ASN:ND2	2.39	0.45
1:B:46:ILE:CG1	1:B:314:GLY:HA2	2.47	0.45
1:A:301:TYR:HB2	1:A:305:LEU:HG	1.98	0.45
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.51	0.45
1:B:82:THR:HA	1:B:85:GLN:HG2	1.99	0.45
1:A:147:TRP:O	1:A:187:GLU:HB3	2.16	0.45
1:C:147:TRP:O	1:C:187:GLU:HB3	2.16	0.45
1:D:42:ARG:NH2	1:D:303:ARG:HB3	2.24	0.45
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.17	0.45
1:B:280:SER:OG	1:B:334:ASN:OD1	2.23	0.45
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.52	0.45
1:A:280:SER:OG	1:A:334:ASN:OD1	2.24	0.45
1:C:42:ARG:NH2	1:C:303:ARG:HB3	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.17	0.45
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.17	0.45
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.17	0.45
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.17	0.45
1:C:36:THR:O	1:C:40:ALA:CB	2.63	0.45
1:D:36:THR:O	1:D:40:ALA:CB	2.63	0.45
1:A:57:PHE:CZ	1:A:320:LEU:HD12	2.51	0.45
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.17	0.45
1:A:63:LEU:HD21	1:A:76:VAL:HG11	1.99	0.45
1:A:162:ALA:O	1:A:166:ASN:ND2	2.39	0.45
1:C:34:GLU:O	1:C:59:ARG:NH2	2.50	0.45
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.17	0.45
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.31	0.45
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.31	0.45
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.65	0.45
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.17	0.45
1:B:154:GLY:O	1:B:200:ARG:NH2	2.50	0.45
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.17	0.45
1:A:144:PHE:HA	1:A:182:ILE:HG23	1.98	0.45
1:B:147:TRP:O	1:B:187:GLU:HB3	2.16	0.45
1:A:82:THR:HA	1:A:85:GLN:HG2	1.99	0.45
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.17	0.45
1:B:63:LEU:HD21	1:B:76:VAL:HG11	1.99	0.45
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.17	0.45
1:D:34:GLU:O	1:D:59:ARG:NH2	2.50	0.45
1:D:92:PRO:HD2	1:D:95:GLN:OE1	2.17	0.45
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.17	0.45
1:C:105:GLY:CA	1:C:144:PHE:O	2.65	0.45
1:D:105:GLY:CA	1:D:144:PHE:O	2.65	0.45
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.17	0.45
1:C:46:ILE:CG1	1:C:314:GLY:HA2	2.47	0.45
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.65	0.45
1:B:144:PHE:HA	1:B:182:ILE:HG23	1.98	0.45
1:C:271:SER:O	1:C:274:GLN:HG2	2.17	0.45
1:D:271:SER:O	1:D:274:GLN:HG2	2.17	0.45
1:B:271:SER:O	1:B:274:GLN:HG2	2.17	0.45
1:A:271:SER:O	1:A:274:GLN:HG2	2.17	0.45
1:C:61:LEU:HA	1:C:324:GLN:HE21	1.82	0.45
1:B:34:GLU:O	1:B:59:ARG:NH2	2.50	0.45
1:A:119:ASN:HB2	1:C:4:HIS:CD2	2.52	0.45
1:D:42:ARG:NH2	1:D:303:ARG:HB3	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.17	0.45
1:A:33:ASP:OD2	1:A:146:LYS:HE2	2.17	0.45
1:D:46:ILE:CG1	1:D:314:GLY:HA2	2.47	0.45
1:A:154:GLY:O	1:A:200:ARG:NH2	2.50	0.44
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.31	0.44
1:D:229:LYS:HE2	1:D:270:LEU:CD2	2.45	0.44
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.31	0.44
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.17	0.44
1:A:271:SER:O	1:A:274:GLN:HG2	2.17	0.44
1:B:284:ASN:ND2	1:B:342:TYR:O	2.50	0.44
1:A:284:ASN:ND2	1:A:342:TYR:O	2.50	0.44
1:C:63:LEU:HD21	1:C:76:VAL:HG11	1.99	0.44
1:B:185:ILE:HG12	1:B:227:LEU:HB2	1.99	0.44
1:A:61:LEU:HA	1:A:324:GLN:HE21	1.82	0.44
1:A:185:ILE:HG12	1:A:227:LEU:HB2	1.99	0.44
1:C:35:SER:OG	1:C:36:THR:N	2.49	0.44
1:D:61:LEU:HA	1:D:324:GLN:HE21	1.82	0.44
1:B:162:ALA:O	1:B:166:ASN:ND2	2.39	0.44
1:A:34:GLU:O	1:A:59:ARG:NH2	2.50	0.44
1:C:162:ALA:O	1:C:166:ASN:ND2	2.39	0.44
1:C:229:LYS:HE2	1:C:270:LEU:CD2	2.45	0.44
1:D:60:GLN:O	1:D:64:THR:OG1	2.26	0.44
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.17	0.44
1:B:271:SER:O	1:B:274:GLN:HG2	2.17	0.44
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.32	0.44
1:C:284:ASN:ND2	1:C:342:TYR:O	2.50	0.44
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.32	0.44
1:D:284:ASN:ND2	1:D:342:TYR:O	2.50	0.44
1:B:61:LEU:HA	1:B:324:GLN:HE21	1.82	0.44
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.31	0.44
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.31	0.44
1:B:33:ASP:OD2	1:B:146:LYS:HE2	2.17	0.44
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.47	0.44
1:A:229:LYS:HG2	1:A:270:LEU:CD1	2.47	0.44
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.52	0.44
1:D:57:PHE:CZ	1:D:320:LEU:HD12	2.52	0.44
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.48	0.44
1:B:195:ASP:HB3	1:B:238:ALA:HB3	1.98	0.44
1:A:195:ASP:HB3	1:A:238:ALA:HB3	1.98	0.44
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.31	0.44
1:C:49:GLU:O	1:C:54:ASN:ND2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LEU:HD21	1:D:76:VAL:HG11	1.99	0.44
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.32	0.44
1:C:60:GLN:O	1:C:64:THR:OG1	2.29	0.44
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.52	0.44
1:A:57:PHE:CZ	1:A:320:LEU:HD12	2.52	0.44
1:A:119:ASN:HB2	1:C:4:HIS:CD2	2.53	0.44
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.48	0.44
1:A:4:HIS:CD2	1:C:156:HIS:HE2	2.35	0.44
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.65	0.44
1:D:154:GLY:O	1:D:200:ARG:NH2	2.50	0.44
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.31	0.44
1:C:277:GLU:OE2	1:C:342:TYR:OH	2.32	0.44
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.31	0.44
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.31	0.44
1:B:63:LEU:HD21	1:B:76:VAL:HG11	1.99	0.44
1:B:154:GLY:O	1:B:200:ARG:NH2	2.51	0.44
1:A:63:LEU:HD21	1:A:76:VAL:HG11	1.99	0.44
1:A:154:GLY:O	1:A:200:ARG:NH2	2.51	0.44
1:B:42:ARG:NH2	1:B:303:ARG:HB3	2.24	0.44
1:A:42:ARG:NH2	1:A:303:ARG:HB3	2.24	0.44
1:C:185:ILE:HG12	1:C:227:LEU:HB2	1.99	0.44
1:D:185:ILE:HG12	1:D:227:LEU:HB2	1.99	0.44
1:C:276:GLU:O	1:C:277:GLU:HB3	2.18	0.44
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.32	0.44
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.53	0.44
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.64	0.44
1:D:277:GLU:OE2	1:D:342:TYR:OH	2.32	0.44
1:B:197:ASP:OD1	1:B:197:ASP:N	2.51	0.44
1:A:197:ASP:OD1	1:A:197:ASP:N	2.51	0.44
1:C:63:LEU:HD21	1:C:76:VAL:HG11	1.99	0.44
1:D:155:GLU:HG2	1:D:156:HIS:N	2.32	0.44
1:D:276:GLU:O	1:D:277:GLU:HB3	2.18	0.44
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.32	0.44
1:C:154:GLY:O	1:C:200:ARG:NH2	2.50	0.44
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.65	0.44
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.32	0.44
1:A:229:LYS:HG2	1:A:270:LEU:CD1	2.48	0.44
1:D:301:TYR:HB3	1:D:304:ALA:HB3	2.00	0.44
1:C:155:GLU:HG2	1:C:156:HIS:N	2.32	0.44
1:A:276:GLU:O	1:A:277:GLU:HB3	2.18	0.44
1:A:105:GLY:CA	1:A:144:PHE:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.64	0.44
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.48	0.44
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.32	0.44
1:C:301:TYR:HB3	1:C:304:ALA:HB3	2.00	0.44
1:D:63:LEU:HD21	1:D:76:VAL:HG11	2.00	0.44
1:B:276:GLU:O	1:B:277:GLU:HB3	2.18	0.44
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.32	0.44
1:D:60:GLN:O	1:D:64:THR:OG1	2.29	0.44
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.47	0.44
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.33	0.44
1:A:147:TRP:O	1:A:187:GLU:HB3	2.18	0.44
1:D:301:TYR:HB2	1:D:305:LEU:HG	1.99	0.44
1:D:82:THR:HA	1:D:85:GLN:HG2	1.99	0.44
1:B:77:ILE:HD11	1:B:146:LYS:CB	2.47	0.44
1:A:77:ILE:HD11	1:A:146:LYS:CB	2.47	0.44
1:C:82:THR:HA	1:C:85:GLN:HG2	1.99	0.44
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.36	0.44
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.32	0.44
1:C:46:ILE:HG13	1:C:314:GLY:HA2	2.00	0.44
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.32	0.44
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.32	0.44
1:B:147:TRP:O	1:B:187:GLU:HB3	2.18	0.44
1:C:82:THR:HA	1:C:85:GLN:HG2	1.99	0.44
1:D:49:GLU:O	1:D:54:ASN:ND2	2.43	0.44
1:B:82:THR:HA	1:B:85:GLN:HG2	1.99	0.44
1:B:105:GLY:CA	1:B:144:PHE:O	2.65	0.44
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.48	0.44
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.33	0.44
1:B:197:ASP:OD1	1:B:197:ASP:N	2.51	0.43
1:C:301:TYR:HB2	1:C:305:LEU:HG	2.00	0.43
1:B:27:LYS:HA	1:B:72:CYS:O	2.18	0.43
1:C:27:LYS:HA	1:C:72:CYS:O	2.18	0.43
1:D:27:LYS:HA	1:D:72:CYS:O	2.17	0.43
1:C:197:ASP:N	1:C:197:ASP:OD1	2.51	0.43
1:B:229:LYS:HG3	1:B:268:THR:O	2.18	0.43
1:D:35:SER:OG	1:D:36:THR:N	2.49	0.43
1:D:82:THR:HA	1:D:85:GLN:HG2	1.99	0.43
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.36	0.43
1:A:277:GLU:OE2	1:A:330:ARG:NH2	2.50	0.43
1:D:46:ILE:HG13	1:D:314:GLY:HA2	2.00	0.43
1:A:197:ASP:OD1	1:A:197:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ILE:HD11	1:C:314:GLY:N	2.33	0.43
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.54	0.43
1:D:46:ILE:HD11	1:D:314:GLY:N	2.33	0.43
1:D:57:PHE:CZ	1:D:320:LEU:HD12	2.54	0.43
1:B:63:LEU:HD21	1:B:76:VAL:HG11	2.00	0.43
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.53	0.43
1:D:197:ASP:OD1	1:D:197:ASP:N	2.51	0.43
1:C:154:GLY:O	1:C:200:ARG:NH2	2.51	0.43
1:D:154:GLY:O	1:D:200:ARG:NH2	2.51	0.43
1:A:229:LYS:HG3	1:A:268:THR:O	2.18	0.43
1:C:27:LYS:HA	1:C:72:CYS:O	2.18	0.43
1:B:301:TYR:HB2	1:B:305:LEU:HG	1.99	0.43
1:A:301:TYR:HB2	1:A:305:LEU:HG	1.99	0.43
1:A:63:LEU:HD21	1:A:76:VAL:HG11	2.00	0.43
1:C:63:LEU:HD21	1:C:76:VAL:HG11	2.00	0.43
1:D:63:LEU:HD21	1:D:76:VAL:HG11	2.00	0.43
1:B:78:LEU:HD22	1:B:82:THR:HG21	2.01	0.43
1:B:155:GLU:HG2	1:B:156:HIS:N	2.32	0.43
1:A:78:LEU:HD22	1:A:82:THR:HG21	2.00	0.43
1:A:155:GLU:HG2	1:A:156:HIS:N	2.32	0.43
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.48	0.43
1:A:82:THR:HA	1:A:85:GLN:HG2	1.99	0.43
1:B:46:ILE:HG13	1:B:314:GLY:HA2	2.00	0.43
1:B:277:GLU:OE2	1:B:330:ARG:NH2	2.50	0.43
1:A:46:ILE:HG13	1:A:314:GLY:HA2	2.00	0.43
1:C:229:LYS:HG2	1:C:270:LEU:CD1	2.47	0.43
1:B:46:ILE:HD11	1:B:314:GLY:N	2.33	0.43
1:A:46:ILE:HD11	1:A:314:GLY:N	2.33	0.43
1:C:147:TRP:O	1:C:187:GLU:HB3	2.18	0.43
1:D:144:PHE:HA	1:D:182:ILE:HG23	2.01	0.43
1:A:27:LYS:HA	1:A:72:CYS:O	2.18	0.43
1:A:229:LYS:HG2	1:A:270:LEU:CD1	2.48	0.43
1:D:27:LYS:HA	1:D:72:CYS:O	2.18	0.43
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.36	0.43
1:C:27:LYS:HA	1:C:72:CYS:O	2.18	0.43
1:D:229:LYS:HG2	1:D:270:LEU:CD1	2.47	0.43
1:A:57:PHE:CZ	1:A:320:LEU:HD12	2.54	0.43
1:C:144:PHE:HA	1:C:182:ILE:HG23	2.01	0.43
1:C:197:ASP:N	1:C:197:ASP:OD1	2.51	0.43
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.32	0.43
1:D:147:TRP:O	1:D:187:GLU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ILE:HD12	1:C:46:ILE:HA	1.90	0.43
1:C:63:LEU:HD21	1:C:76:VAL:HG11	2.00	0.43
1:D:229:LYS:HG2	1:D:270:LEU:CD1	2.48	0.43
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.32	0.43
1:B:42:ARG:HH12	1:B:303:ARG:HB3	1.83	0.43
1:C:229:LYS:HG2	1:C:270:LEU:CD1	2.48	0.43
1:C:305:LEU:HD23	1:C:330:ARG:HG3	2.01	0.43
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.36	0.43
1:D:27:LYS:HA	1:D:72:CYS:O	2.18	0.43
1:D:33:ASP:OD2	1:D:146:LYS:HE2	2.17	0.43
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.54	0.43
1:D:197:ASP:OD1	1:D:197:ASP:N	2.52	0.43
1:B:63:LEU:HD21	1:B:76:VAL:HG11	2.00	0.43
1:A:63:LEU:HD21	1:A:76:VAL:HG11	2.00	0.43
1:C:229:LYS:HG2	1:C:270:LEU:CD1	2.48	0.43
1:D:63:LEU:HD21	1:D:76:VAL:HG11	2.00	0.43
1:B:197:ASP:N	1:B:197:ASP:OD1	2.52	0.43
1:B:197:ASP:OD1	1:B:197:ASP:N	2.49	0.43
1:A:197:ASP:OD1	1:A:197:ASP:N	2.49	0.43
1:D:305:LEU:HD23	1:D:330:ARG:HG3	2.01	0.43
1:C:31:ALA:HA	1:C:77:ILE:CG2	2.48	0.43
1:C:33:ASP:OD2	1:C:146:LYS:HE2	2.17	0.43
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.33	0.43
1:A:197:ASP:N	1:A:197:ASP:OD1	2.52	0.43
1:C:229:LYS:HG2	1:C:270:LEU:CD1	2.49	0.43
1:D:229:LYS:HG2	1:D:270:LEU:CD1	2.49	0.43
1:A:42:ARG:HH12	1:A:303:ARG:HB3	1.83	0.43
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.83	0.43
1:C:229:LYS:HG3	1:C:268:THR:O	2.18	0.43
1:D:229:LYS:HG2	1:D:270:LEU:CD1	2.48	0.43
1:D:229:LYS:HG3	1:D:268:THR:O	2.18	0.43
1:B:229:LYS:HG3	1:B:268:THR:O	2.19	0.43
1:D:31:ALA:HA	1:D:77:ILE:CG2	2.48	0.43
1:B:42:ARG:HH12	1:B:303:ARG:HG3	1.84	0.43
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.54	0.43
1:B:293:LYS:HD2	1:B:297:LEU:HD11	2.01	0.43
1:A:293:LYS:HD2	1:A:297:LEU:HD11	2.01	0.43
1:D:83:LEU:HD12	1:D:94:PRO:HG3	2.00	0.43
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.01	0.43
1:A:147:TRP:O	1:A:187:GLU:HB3	2.19	0.43
1:C:271:SER:O	1:C:274:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:SER:O	1:D:274:GLN:HG2	2.19	0.43
1:C:144:PHE:HA	1:C:182:ILE:HG23	2.01	0.43
1:C:105:GLY:CA	1:C:144:PHE:O	2.67	0.43
1:D:36:THR:O	1:D:40:ALA:HB2	2.19	0.43
1:D:105:GLY:CA	1:D:144:PHE:O	2.67	0.43
1:B:144:PHE:HA	1:B:182:ILE:HG23	2.01	0.43
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.32	0.43
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.37	0.43
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.34	0.43
1:A:42:ARG:HH12	1:A:303:ARG:HG3	1.84	0.43
1:A:146:LYS:HG2	1:A:147:TRP:N	2.34	0.43
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.34	0.43
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.34	0.43
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.34	0.43
1:B:154:GLY:O	1:B:200:ARG:NH2	2.52	0.43
1:B:301:TYR:HB3	1:B:304:ALA:HB3	2.00	0.43
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.37	0.43
1:D:57:PHE:CZ	1:D:320:LEU:HD12	2.54	0.43
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.37	0.43
1:C:83:LEU:HD12	1:C:94:PRO:HG3	2.00	0.43
1:B:275:SER:HB3	1:B:278:GLU:CG	2.49	0.43
1:B:147:TRP:O	1:B:187:GLU:HB3	2.19	0.43
1:D:77:ILE:HD13	1:D:144:PHE:HE1	1.83	0.43
1:A:229:LYS:HG3	1:A:268:THR:O	2.19	0.43
1:C:36:THR:O	1:C:40:ALA:HB2	2.19	0.43
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.33	0.43
1:A:144:PHE:HA	1:A:182:ILE:HG23	2.01	0.43
1:D:302:GLY:O	1:D:306:GLN:HG2	2.19	0.43
1:B:146:LYS:HG2	1:B:147:TRP:N	2.34	0.43
1:A:57:PHE:HZ	1:A:320:LEU:HD12	1.84	0.43
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.54	0.43
1:B:228:LEU:HG	1:B:230:PRO:HD3	2.01	0.43
1:A:42:ARG:NH2	1:A:303:ARG:HB3	2.24	0.43
1:A:154:GLY:O	1:A:200:ARG:NH2	2.52	0.43
1:A:228:LEU:HG	1:A:230:PRO:HD3	2.01	0.43
1:C:197:ASP:N	1:C:197:ASP:OD1	2.52	0.43
1:A:185:ILE:HG12	1:A:227:LEU:HB2	2.01	0.43
1:A:275:SER:HB3	1:A:278:GLU:CG	2.49	0.43
1:B:77:ILE:HD13	1:B:144:PHE:HE1	1.83	0.43
1:C:42:ARG:HH12	1:C:303:ARG:HB3	1.83	0.43
1:C:77:ILE:HD13	1:C:144:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ARG:HH12	1:D:303:ARG:HB3	1.83	0.43
1:D:144:PHE:HA	1:D:182:ILE:HG23	2.01	0.43
1:D:277:GLU:OE2	1:D:330:ARG:NH2	2.50	0.43
1:C:302:GLY:O	1:C:306:GLN:HG2	2.19	0.42
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.84	0.42
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.37	0.42
1:B:57:PHE:HZ	1:B:320:LEU:HD12	1.84	0.42
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.54	0.42
1:A:306:GLN:O	1:A:308:SER:N	2.52	0.42
1:A:57:PHE:CZ	1:A:320:LEU:HD12	2.54	0.42
1:A:301:TYR:HB3	1:A:304:ALA:HB3	2.00	0.42
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.54	0.42
1:A:57:PHE:CZ	1:A:320:LEU:HD12	2.54	0.42
1:A:229:LYS:HG2	1:A:270:LEU:CD1	2.49	0.42
1:D:197:ASP:OD1	1:D:197:ASP:N	2.52	0.42
1:C:275:SER:HB3	1:C:278:GLU:CG	2.48	0.42
1:D:185:ILE:HG12	1:D:227:LEU:HB2	2.01	0.42
1:B:30:LEU:HD13	1:B:305:LEU:HD23	2.01	0.42
1:A:30:LEU:HD13	1:A:305:LEU:HD23	2.01	0.42
1:A:185:ILE:HG12	1:A:227:LEU:HB2	2.01	0.42
1:B:154:GLY:O	1:B:200:ARG:NH2	2.52	0.42
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.84	0.42
1:A:302:GLY:O	1:A:306:GLN:HG2	2.19	0.42
1:B:306:GLN:O	1:B:308:SER:N	2.53	0.42
1:A:277:GLU:HA	1:A:277:GLU:OE1	2.19	0.42
1:B:42:ARG:NH2	1:B:303:ARG:HB3	2.24	0.42
1:A:119:ASN:HB2	1:C:4:HIS:CD2	2.55	0.42
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.49	0.42
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.53	0.42
1:C:185:ILE:HG12	1:C:227:LEU:HB2	2.01	0.42
1:D:275:SER:HB3	1:D:278:GLU:CG	2.49	0.42
1:B:27:LYS:HA	1:B:72:CYS:O	2.18	0.42
1:C:147:TRP:O	1:C:187:GLU:HB3	2.19	0.42
1:B:302:GLY:O	1:B:306:GLN:HG2	2.19	0.42
1:A:302:GLY:O	1:A:306:GLN:HG2	2.19	0.42
1:A:305:LEU:HD23	1:A:330:ARG:HG3	2.01	0.42
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.01	0.42
1:B:31:ALA:HA	1:B:77:ILE:CG2	2.48	0.42
1:A:31:ALA:HA	1:A:77:ILE:CG2	2.48	0.42
1:A:154:GLY:O	1:A:200:ARG:NH2	2.52	0.42
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLY:O	1:B:306:GLN:HG2	2.19	0.42
1:C:302:GLY:O	1:C:306:GLN:HG2	2.19	0.42
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.36	0.42
1:D:302:GLY:O	1:D:306:GLN:HG2	2.19	0.42
1:B:277:GLU:HA	1:B:277:GLU:OE1	2.19	0.42
1:C:146:LYS:HG2	1:C:147:TRP:N	2.34	0.42
1:D:146:LYS:HG2	1:D:147:TRP:N	2.34	0.42
1:C:228:LEU:HG	1:C:230:PRO:HD3	2.01	0.42
1:D:293:LYS:HD2	1:D:297:LEU:HD11	2.01	0.42
1:B:271:SER:O	1:B:274:GLN:HG2	2.19	0.42
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.35	0.42
1:A:77:ILE:HD13	1:A:144:PHE:HE1	1.83	0.42
1:A:271:SER:O	1:A:274:GLN:HG2	2.19	0.42
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.35	0.42
1:B:305:LEU:HD23	1:B:330:ARG:HG3	2.01	0.42
1:B:66:ASP:OD2	1:B:68:ARG:HG3	2.18	0.42
1:C:277:GLU:OE2	1:C:330:ARG:NH2	2.50	0.42
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.54	0.42
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.37	0.42
1:B:302:GLY:O	1:B:306:GLN:HG2	2.19	0.42
1:C:27:LYS:HA	1:C:72:CYS:O	2.19	0.42
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.37	0.42
1:D:83:LEU:HD12	1:D:94:PRO:HG3	2.00	0.42
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.54	0.42
1:B:228:LEU:HG	1:B:230:PRO:HD3	2.02	0.42
1:C:293:LYS:HD2	1:C:297:LEU:HD11	2.01	0.42
1:A:27:LYS:HA	1:A:72:CYS:O	2.18	0.42
1:D:147:TRP:O	1:D:187:GLU:HB3	2.19	0.42
1:C:229:LYS:HG3	1:C:268:THR:O	2.19	0.42
1:C:276:GLU:HG2	1:C:304:ALA:O	2.19	0.42
1:D:229:LYS:HG3	1:D:268:THR:O	2.19	0.42
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.50	0.42
1:A:229:LYS:HG2	1:A:270:LEU:CD1	2.50	0.42
1:D:27:LYS:HA	1:D:72:CYS:O	2.19	0.42
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.55	0.42
1:C:154:GLY:O	1:C:200:ARG:NH2	2.52	0.42
1:D:77:ILE:HD11	1:D:146:LYS:CB	2.47	0.42
1:D:228:LEU:HG	1:D:230:PRO:HD3	2.01	0.42
1:A:83:LEU:HD12	1:A:94:PRO:HG3	2.00	0.42
1:A:228:LEU:HG	1:A:230:PRO:HD3	2.02	0.42
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.35	0.42
1:D:185:ILE:HG12	1:D:227:LEU:HB2	2.01	0.42
1:A:27:LYS:HA	1:A:72:CYS:O	2.18	0.42
1:A:66:ASP:OD2	1:A:68:ARG:HG3	2.18	0.42
1:C:66:ASP:OD2	1:C:68:ARG:HG3	2.18	0.42
1:D:276:GLU:HG2	1:D:304:ALA:O	2.19	0.42
1:A:302:GLY:O	1:A:306:GLN:HG2	2.19	0.42
1:C:83:LEU:HD12	1:C:94:PRO:HG3	2.00	0.42
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.84	0.42
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.84	0.42
1:D:31:ALA:HA	1:D:77:ILE:HG23	2.02	0.42
1:B:83:LEU:HD12	1:B:94:PRO:HG3	2.00	0.42
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.54	0.42
1:B:253:VAL:O	1:B:257:ARG:HG3	2.20	0.42
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.84	0.42
1:C:301:TYR:HB2	1:C:305:LEU:HG	2.02	0.42
1:D:301:TYR:HB2	1:D:305:LEU:HG	2.02	0.42
1:C:51:THR:HG23	1:C:54:ASN:H	1.85	0.42
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.85	0.42
1:D:302:GLY:O	1:D:306:GLN:HG2	2.19	0.42
1:B:36:THR:O	1:B:40:ALA:CB	2.68	0.42
1:B:276:GLU:HG3	1:B:304:ALA:O	2.20	0.42
1:A:36:THR:O	1:A:40:ALA:CB	2.67	0.42
1:A:276:GLU:HG3	1:A:304:ALA:O	2.20	0.42
1:C:27:LYS:HA	1:C:72:CYS:O	2.19	0.42
1:C:31:ALA:HA	1:C:77:ILE:HG23	2.02	0.42
1:D:154:GLY:O	1:D:200:ARG:NH2	2.52	0.42
1:C:228:LEU:HG	1:C:230:PRO:HD3	2.02	0.42
1:D:57:PHE:CZ	1:D:320:LEU:HD12	2.54	0.42
1:A:253:VAL:O	1:A:257:ARG:HG3	2.20	0.42
1:D:51:THR:HG23	1:D:54:ASN:H	1.85	0.42
1:A:119:ASN:HB2	1:C:4:HIS:CD2	2.54	0.42
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.85	0.42
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.68	0.42
1:C:302:GLY:O	1:C:306:GLN:HG2	2.19	0.42
1:C:185:ILE:HG12	1:C:227:LEU:HB2	2.01	0.42
1:B:27:LYS:HA	1:B:72:CYS:O	2.18	0.42
1:A:105:GLY:CA	1:A:144:PHE:O	2.67	0.42
1:D:66:ASP:OD2	1:D:68:ARG:HG3	2.18	0.42
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.38	0.42
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.37	0.42
1:C:77:ILE:HD11	1:C:146:LYS:CB	2.47	0.42
1:B:77:ILE:CD1	1:B:146:LYS:HB2	2.50	0.42
1:A:77:ILE:CD1	1:A:146:LYS:HB2	2.50	0.42
1:C:301:TYR:HB2	1:C:305:LEU:HG	2.02	0.42
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.68	0.42
1:D:301:TYR:HB2	1:D:305:LEU:HG	2.02	0.42
1:B:105:GLY:CA	1:B:144:PHE:O	2.67	0.42
1:A:276:GLU:HG2	1:A:304:ALA:O	2.19	0.42
1:C:154:GLY:O	1:C:200:ARG:NH2	2.52	0.42
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.38	0.42
1:C:306:GLN:O	1:C:308:SER:N	2.52	0.42
1:D:42:ARG:HH12	1:D:303:ARG:HG3	1.84	0.42
1:B:31:ALA:HA	1:B:77:ILE:HG23	2.02	0.42
1:B:229:LYS:HG3	1:B:268:THR:O	2.20	0.42
1:A:229:LYS:HG3	1:A:268:THR:O	2.20	0.42
1:D:27:LYS:HA	1:D:72:CYS:O	2.20	0.42
1:D:228:LEU:HG	1:D:230:PRO:HD3	2.02	0.42
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.84	0.42
1:B:276:GLU:HG2	1:B:304:ALA:O	2.19	0.42
1:D:154:GLY:O	1:D:200:ARG:NH2	2.52	0.42
1:B:253:VAL:O	1:B:257:ARG:HG3	2.20	0.42
1:B:27:LYS:HA	1:B:72:CYS:O	2.19	0.42
1:A:27:LYS:HA	1:A:72:CYS:O	2.19	0.42
1:C:57:PHE:HZ	1:C:320:LEU:HD12	1.84	0.42
1:C:277:GLU:HA	1:C:277:GLU:OE1	2.19	0.42
1:D:57:PHE:HZ	1:D:320:LEU:HD12	1.84	0.42
1:D:306:GLN:O	1:D:308:SER:N	2.52	0.42
1:A:31:ALA:HA	1:A:77:ILE:HG23	2.02	0.42
1:C:144:PHE:HA	1:C:182:ILE:HG23	2.02	0.42
1:D:144:PHE:HA	1:D:182:ILE:HG23	2.02	0.42
1:B:51:THR:HG23	1:B:54:ASN:H	1.85	0.42
1:B:110:LYS:CE	1:B:126:GLY:HA2	2.50	0.42
1:C:27:LYS:HA	1:C:72:CYS:O	2.20	0.42
1:B:63:LEU:HD21	1:B:76:VAL:HG11	2.02	0.42
1:A:63:LEU:HD21	1:A:76:VAL:HG11	2.02	0.42
1:A:253:VAL:O	1:A:257:ARG:HG3	2.20	0.41
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.85	0.41
1:C:42:ARG:HH12	1:C:303:ARG:HG3	1.84	0.41
1:D:277:GLU:HA	1:D:277:GLU:OE1	2.19	0.41
1:D:78:LEU:HD22	1:D:82:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:SER:HB3	1:B:278:GLU:HG2	2.02	0.41
1:A:51:THR:HG23	1:A:54:ASN:H	1.85	0.41
1:A:275:SER:HB3	1:A:278:GLU:HG2	2.02	0.41
1:A:110:LYS:CE	1:A:126:GLY:HA2	2.50	0.41
1:D:27:LYS:HA	1:D:72:CYS:O	2.20	0.41
1:B:118:THR:CG2	1:B:121:GLU:HB2	2.50	0.41
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.50	0.41
1:C:27:LYS:HA	1:C:72:CYS:O	2.20	0.41
1:A:36:THR:O	1:A:40:ALA:HB2	2.19	0.41
1:B:83:LEU:HD12	1:B:94:PRO:HG3	2.00	0.41
1:A:83:LEU:HD12	1:A:94:PRO:HG3	2.00	0.41
1:B:68:ARG:NH2	1:B:325:GLU:OE1	2.40	0.41
1:C:27:LYS:HA	1:C:72:CYS:O	2.20	0.41
1:D:27:LYS:HA	1:D:72:CYS:O	2.20	0.41
1:D:77:ILE:HD11	1:D:146:LYS:HB2	2.02	0.41
1:B:132:GLU:OE1	1:B:132:GLU:N	2.53	0.41
1:A:144:PHE:HA	1:A:182:ILE:HG23	2.01	0.41
1:B:36:THR:O	1:B:40:ALA:HB2	2.19	0.41
1:C:301:TYR:HB2	1:C:305:LEU:HG	2.03	0.41
1:B:77:ILE:CD1	1:B:146:LYS:HB2	2.41	0.41
1:A:77:ILE:CD1	1:A:146:LYS:HB2	2.41	0.41
1:B:301:TYR:HB2	1:B:305:LEU:HG	2.02	0.41
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.55	0.41
1:A:144:PHE:HA	1:A:182:ILE:HG23	2.02	0.41
1:C:27:LYS:HA	1:C:72:CYS:O	2.20	0.41
1:C:77:ILE:HD11	1:C:146:LYS:HB2	2.02	0.41
1:C:78:LEU:HD22	1:C:82:THR:HG21	2.01	0.41
1:B:22:ILE:HG12	1:B:103:VAL:CG2	2.48	0.41
1:A:132:GLU:OE1	1:A:132:GLU:N	2.53	0.41
1:C:30:LEU:HD13	1:C:305:LEU:HD23	2.01	0.41
1:C:132:GLU:OE1	1:C:132:GLU:N	2.53	0.41
1:D:30:LEU:HD13	1:D:305:LEU:HD23	2.01	0.41
1:D:132:GLU:OE1	1:D:132:GLU:N	2.53	0.41
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.55	0.41
1:C:83:LEU:HD12	1:C:94:PRO:HG3	2.01	0.41
1:D:83:LEU:HD12	1:D:94:PRO:HG3	2.01	0.41
1:D:27:LYS:HA	1:D:72:CYS:O	2.20	0.41
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.37	0.41
1:A:276:GLU:HG3	1:A:304:ALA:O	2.21	0.41
1:B:168:ASN:HD22	1:D:168:ASN:ND2	2.18	0.41
1:A:68:ARG:NH2	1:A:325:GLU:OE1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:TYR:HB2	1:D:305:LEU:HG	2.03	0.41
1:C:339:GLN:HB3	1:C:341:LYS:HZ3	1.84	0.41
1:A:155:GLU:HG2	1:A:156:HIS:CD2	2.56	0.41
1:A:22:ILE:HG12	1:A:103:VAL:CG2	2.49	0.41
1:B:144:PHE:HA	1:B:182:ILE:HG23	2.01	0.41
1:B:301:TYR:HB2	1:B:305:LEU:HG	2.02	0.41
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.55	0.41
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.85	0.41
1:C:27:LYS:HA	1:C:72:CYS:O	2.21	0.41
1:A:49:GLU:O	1:A:54:ASN:ND2	2.43	0.41
1:C:80:HIS:CE1	1:C:84:TYR:HE2	2.38	0.41
1:C:42:ARG:HD3	1:C:310:LEU:HD11	2.03	0.41
1:C:229:LYS:HG3	1:C:268:THR:O	2.20	0.41
1:D:42:ARG:HD3	1:D:310:LEU:HD11	2.03	0.41
1:D:229:LYS:HG3	1:D:268:THR:O	2.20	0.41
1:C:195:ASP:HB3	1:C:238:ALA:HB3	2.03	0.41
1:D:195:ASP:HB3	1:D:238:ALA:HB3	2.03	0.41
1:B:155:GLU:HG2	1:B:156:HIS:CD2	2.56	0.41
1:A:77:ILE:HD13	1:A:77:ILE:HG21	1.88	0.41
1:A:301:TYR:HB2	1:A:305:LEU:HG	2.02	0.41
1:C:77:ILE:CD1	1:C:146:LYS:HB2	2.50	0.41
1:C:108:VAL:HG23	1:C:147:TRP:HE3	1.86	0.41
1:D:77:ILE:CD1	1:D:146:LYS:HB2	2.50	0.41
1:D:108:VAL:HG23	1:D:147:TRP:HE3	1.86	0.41
1:D:275:SER:HB3	1:D:278:GLU:HG2	2.02	0.41
1:A:301:TYR:HB2	1:A:305:LEU:HG	2.02	0.41
1:C:110:LYS:CE	1:C:126:GLY:HA2	2.50	0.41
1:D:27:LYS:HA	1:D:72:CYS:O	2.21	0.41
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.38	0.41
1:B:276:GLU:HG3	1:B:304:ALA:O	2.21	0.41
1:B:77:ILE:HD13	1:B:77:ILE:HG21	1.88	0.41
1:B:144:PHE:HA	1:B:182:ILE:HG23	2.02	0.41
1:C:253:VAL:O	1:C:257:ARG:HG3	2.20	0.41
1:D:27:LYS:HA	1:D:72:CYS:O	2.20	0.41
1:D:253:VAL:O	1:D:257:ARG:HG3	2.20	0.41
1:C:275:SER:HB3	1:C:278:GLU:HG2	2.02	0.41
1:D:110:LYS:CE	1:D:126:GLY:HA2	2.50	0.41
1:B:271:SER:HB3	1:B:301:TYR:CD1	2.56	0.41
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.85	0.41
1:A:271:SER:HB3	1:A:301:TYR:CD1	2.56	0.41
1:A:60:GLN:O	1:A:64:THR:OG1	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.38	0.41
1:B:27:LYS:HA	1:B:72:CYS:O	2.19	0.41
1:B:301:TYR:HB2	1:B:305:LEU:HG	2.03	0.41
1:A:27:LYS:HA	1:A:72:CYS:O	2.19	0.41
1:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.84	0.41
1:A:119:ASN:HB2	1:C:4:HIS:CD2	2.54	0.41
1:A:27:LYS:HA	1:A:72:CYS:O	2.20	0.41
1:D:229:LYS:HG2	1:D:270:LEU:CD1	2.50	0.41
1:B:125:GLN:NE2	1:D:129:GLY:H	2.19	0.41
1:B:35:SER:O	1:B:39:ILE:HG22	2.21	0.41
1:A:35:SER:O	1:A:39:ILE:HG22	2.21	0.41
1:A:301:TYR:HB2	1:A:305:LEU:HG	2.03	0.41
1:C:105:GLY:CA	1:C:144:PHE:O	2.69	0.41
1:B:27:LYS:HA	1:B:72:CYS:O	2.20	0.41
1:B:118:THR:CG2	1:B:121:GLU:HB2	2.50	0.41
1:B:156:HIS:HE2	1:D:4:HIS:CD2	2.39	0.41
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.03	0.41
1:C:229:LYS:HG2	1:C:270:LEU:CD1	2.50	0.41
1:C:229:LYS:HG3	1:C:268:THR:O	2.21	0.41
1:B:49:GLU:O	1:B:54:ASN:ND2	2.43	0.41
1:B:195:ASP:O	1:B:196:HIS:ND1	2.54	0.41
1:A:195:ASP:O	1:A:196:HIS:ND1	2.54	0.41
1:D:105:GLY:CA	1:D:144:PHE:O	2.69	0.41
1:B:118:THR:CG2	1:B:121:GLU:HB2	2.51	0.41
1:B:229:LYS:HG3	1:B:268:THR:O	2.21	0.41
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.51	0.41
1:A:229:LYS:HG3	1:A:268:THR:O	2.21	0.41
1:C:339:GLN:HB3	1:C:341:LYS:NZ	2.36	0.41
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.55	0.41
1:B:77:ILE:HD11	1:B:146:LYS:HB2	2.02	0.41
1:A:77:ILE:HD11	1:A:146:LYS:HB2	2.02	0.41
1:D:155:GLU:HG2	1:D:156:HIS:CD2	2.56	0.41
1:B:83:LEU:HD12	1:B:94:PRO:HG3	2.01	0.41
1:B:108:VAL:HG23	1:B:147:TRP:HE3	1.86	0.41
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.55	0.41
1:A:83:LEU:HD12	1:A:94:PRO:HG3	2.01	0.41
1:A:108:VAL:HG23	1:A:147:TRP:HE3	1.86	0.41
1:C:108:VAL:HG23	1:C:147:TRP:HE3	1.86	0.41
1:C:257:ARG:NH1	1:C:292:LEU:O	2.53	0.41
1:C:271:SER:HB3	1:C:301:TYR:CD1	2.56	0.41
1:D:257:ARG:NH1	1:D:292:LEU:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:SER:HB3	1:D:301:TYR:CD1	2.56	0.41
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.03	0.41
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.86	0.41
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.50	0.41
1:A:185:ILE:HG12	1:A:227:LEU:HB2	2.03	0.41
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.86	0.41
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.56	0.41
1:B:229:LYS:HG3	1:B:268:THR:O	2.21	0.41
1:A:185:ILE:HG12	1:A:227:LEU:HB2	2.03	0.41
1:C:253:VAL:O	1:C:257:ARG:HG3	2.20	0.41
1:D:253:VAL:O	1:D:257:ARG:HG3	2.20	0.41
1:B:77:ILE:HD13	1:B:77:ILE:HG21	1.85	0.41
1:B:42:ARG:HD3	1:B:310:LEU:HD11	2.03	0.41
1:C:35:SER:O	1:C:39:ILE:HG22	2.21	0.41
1:D:35:SER:O	1:D:39:ILE:HG22	2.21	0.41
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.36	0.41
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.36	0.41
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.36	0.41
1:B:118:THR:CG2	1:B:121:GLU:HB2	2.50	0.41
1:C:147:TRP:HB2	1:C:173:TYR:CZ	2.56	0.41
1:C:155:GLU:HG2	1:C:156:HIS:CD2	2.56	0.41
1:C:37:GLY:O	1:C:40:ALA:HB3	2.21	0.41
1:D:37:GLY:O	1:D:40:ALA:HB3	2.21	0.41
1:A:27:LYS:HA	1:A:72:CYS:O	2.20	0.41
1:C:63:LEU:HD21	1:C:76:VAL:HG11	2.02	0.41
1:D:63:LEU:HD21	1:D:76:VAL:HG11	2.02	0.41
1:A:229:LYS:HG3	1:A:268:THR:O	2.21	0.40
1:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.86	0.40
1:D:229:LYS:HG3	1:D:268:THR:O	2.21	0.40
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.51	0.40
1:B:27:LYS:HA	1:B:72:CYS:O	2.20	0.40
1:B:108:VAL:HG23	1:B:147:TRP:HE3	1.86	0.40
1:D:147:TRP:HB2	1:D:173:TYR:CZ	2.56	0.40
1:B:37:GLY:O	1:B:40:ALA:HB3	2.21	0.40
1:A:37:GLY:O	1:A:40:ALA:HB3	2.21	0.40
1:B:57:PHE:HZ	1:B:320:LEU:HD12	1.85	0.40
1:B:60:GLN:O	1:B:64:THR:OG1	2.25	0.40
1:D:185:ILE:HG12	1:D:227:LEU:HB2	2.03	0.40
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.56	0.40
1:A:77:ILE:HG21	1:A:77:ILE:HD13	1.85	0.40
1:A:42:ARG:HD3	1:A:310:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.51	0.40
1:C:63:LEU:HD22	1:C:97:ILE:HG12	2.03	0.40
1:B:27:LYS:HA	1:B:72:CYS:O	2.20	0.40
1:A:27:LYS:HA	1:A:72:CYS:O	2.20	0.40
1:A:27:LYS:HA	1:A:72:CYS:O	2.20	0.40
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.51	0.40
1:B:57:PHE:HE2	1:B:313:TRP:NE1	2.19	0.40
1:D:108:VAL:HG23	1:D:147:TRP:HE3	1.86	0.40
1:B:27:LYS:HA	1:B:72:CYS:O	2.20	0.40
1:A:57:PHE:HZ	1:A:320:LEU:HD12	1.85	0.40
1:A:27:LYS:HA	1:A:72:CYS:O	2.21	0.40
1:D:276:GLU:HG3	1:D:304:ALA:O	2.20	0.40
1:B:154:GLY:O	1:B:200:ARG:NH2	2.54	0.40
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.51	0.40
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.04	0.40
1:A:77:ILE:HD13	1:A:77:ILE:HG21	1.87	0.40
1:A:185:ILE:HG12	1:A:227:LEU:HB2	2.03	0.40
1:D:63:LEU:HD22	1:D:97:ILE:HG12	2.03	0.40
1:C:229:LYS:HG3	1:C:268:THR:O	2.21	0.40
1:D:115:LEU:O	1:D:118:THR:HG22	2.22	0.40
1:D:229:LYS:HG3	1:D:268:THR:O	2.22	0.40
1:B:280:SER:OG	1:B:334:ASN:OD1	2.27	0.40
1:A:57:PHE:HE2	1:A:313:TRP:NE1	2.19	0.40
1:B:186:VAL:HG12	1:B:188:PRO:HD3	2.04	0.40
1:A:130:LEU:O	1:A:134:CYS:CB	2.68	0.40
1:C:57:PHE:HZ	1:C:320:LEU:HD12	1.85	0.40
1:C:185:ILE:HG12	1:C:227:LEU:HB2	2.03	0.40
1:D:57:PHE:HZ	1:D:320:LEU:HD12	1.85	0.40
1:B:27:LYS:HA	1:B:72:CYS:O	2.21	0.40
1:B:63:LEU:HD21	1:B:76:VAL:HG11	2.03	0.40
1:C:276:GLU:HG3	1:C:304:ALA:O	2.20	0.40
1:B:129:GLY:H	1:D:125:GLN:NE2	2.19	0.40
1:D:276:GLU:HG3	1:D:304:ALA:O	2.21	0.40
1:A:154:GLY:O	1:A:200:ARG:NH2	2.54	0.40
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.51	0.40
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.51	0.40
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.51	0.40
1:B:195:ASP:HB3	1:B:238:ALA:HB3	2.02	0.40
1:A:185:ILE:HG12	1:A:227:LEU:HB2	2.04	0.40
1:D:229:LYS:HG3	1:D:268:THR:O	2.21	0.40
1:B:147:TRP:HB2	1:B:173:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LYS:HD3	1:B:270:LEU:CD2	2.52	0.40
1:A:108:VAL:HG23	1:A:147:TRP:HE3	1.86	0.40
1:A:147:TRP:HB2	1:A:173:TYR:CZ	2.56	0.40
1:A:229:LYS:HD3	1:A:270:LEU:CD2	2.52	0.40
1:C:229:LYS:HG3	1:C:268:THR:O	2.22	0.40
1:B:103:VAL:HG23	1:B:144:PHE:CE2	2.57	0.40
1:B:305:LEU:HD13	1:B:334:ASN:HD22	1.85	0.40
1:C:49:GLU:O	1:C:54:ASN:ND2	2.39	0.40
1:C:305:LEU:HD13	1:C:334:ASN:HD22	1.85	0.40
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.68	0.40
1:A:186:VAL:HG12	1:A:188:PRO:HD3	2.04	0.40
1:B:130:LEU:O	1:B:134:CYS:CB	2.69	0.40
1:C:271:SER:O	1:C:274:GLN:HG2	2.22	0.40
1:D:185:ILE:HG12	1:D:227:LEU:HB2	2.03	0.40
1:C:276:GLU:HG3	1:C:304:ALA:O	2.21	0.40
1:C:154:GLY:O	1:C:200:ARG:NH2	2.54	0.40
1:D:154:GLY:O	1:D:200:ARG:NH2	2.54	0.40
1:D:195:ASP:O	1:D:196:HIS:ND1	2.54	0.40
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.51	0.40
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.51	0.40
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.04	0.40
1:A:195:ASP:HB3	1:A:238:ALA:HB3	2.03	0.40
1:C:115:LEU:O	1:C:118:THR:HG22	2.22	0.40
1:A:305:LEU:HD13	1:A:334:ASN:HD22	1.85	0.40
1:C:103:VAL:HG23	1:C:144:PHE:CE2	2.57	0.40
1:D:103:VAL:HG23	1:D:144:PHE:CE2	2.57	0.40
1:B:229:LYS:HD3	1:B:270:LEU:CD2	2.52	0.40
1:B:58:TYR:O	1:B:61:LEU:HB3	2.22	0.40
1:A:58:TYR:O	1:A:61:LEU:HB3	2.22	0.40
1:D:271:SER:O	1:D:274:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	341/363 (94%)	331 (97%)	10 (3%)	0	100	100
1	1-B	341/363 (94%)	331 (97%)	10 (3%)	0	100	100
1	1-C	341/363 (94%)	331 (97%)	10 (3%)	0	100	100
1	1-D	341/363 (94%)	331 (97%)	10 (3%)	0	100	100
1	2-A	341/363 (94%)	332 (97%)	9 (3%)	0	100	100
1	2-B	341/363 (94%)	332 (97%)	9 (3%)	0	100	100
1	2-C	341/363 (94%)	332 (97%)	9 (3%)	0	100	100
1	2-D	341/363 (94%)	332 (97%)	9 (3%)	0	100	100
1	3-A	341/363 (94%)	332 (97%)	8 (2%)	1 (0%)	41	64
1	3-B	341/363 (94%)	332 (97%)	9 (3%)	0	100	100
1	3-C	341/363 (94%)	332 (97%)	8 (2%)	1 (0%)	41	64
1	3-D	341/363 (94%)	332 (97%)	9 (3%)	0	100	100
1	4-A	341/363 (94%)	333 (98%)	8 (2%)	0	100	100
1	4-B	341/363 (94%)	333 (98%)	8 (2%)	0	100	100
1	4-C	341/363 (94%)	333 (98%)	8 (2%)	0	100	100
1	4-D	341/363 (94%)	333 (98%)	8 (2%)	0	100	100
1	5-A	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	5-B	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	5-C	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	5-D	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	6-A	341/363 (94%)	334 (98%)	7 (2%)	0	100	100
1	6-B	341/363 (94%)	334 (98%)	7 (2%)	0	100	100
1	6-C	341/363 (94%)	334 (98%)	7 (2%)	0	100	100
1	6-D	341/363 (94%)	334 (98%)	7 (2%)	0	100	100
1	7-A	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	7-B	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	7-C	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	7-D	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	8-A	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	8-B	341/363 (94%)	330 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-C	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	8-D	341/363 (94%)	330 (97%)	11 (3%)	0	100	100
1	9-A	341/363 (94%)	333 (98%)	7 (2%)	1 (0%)	41	64
1	9-B	341/363 (94%)	333 (98%)	7 (2%)	1 (0%)	41	64
1	9-C	341/363 (94%)	333 (98%)	7 (2%)	1 (0%)	41	64
1	9-D	341/363 (94%)	333 (98%)	7 (2%)	1 (0%)	41	64
1	10-A	341/363 (94%)	329 (96%)	11 (3%)	1 (0%)	41	64
1	10-B	341/363 (94%)	329 (96%)	11 (3%)	1 (0%)	41	64
1	10-C	341/363 (94%)	329 (96%)	11 (3%)	1 (0%)	41	64
1	10-D	341/363 (94%)	329 (96%)	11 (3%)	1 (0%)	41	64
All	All	13640/14520 (94%)	13256 (97%)	374 (3%)	10 (0%)	54	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3-A	155	GLU
1	3-C	155	GLU
1	9-B	188	PRO
1	9-A	188	PRO
1	9-C	188	PRO
1	9-D	188	PRO
1	10-B	188	PRO
1	10-A	188	PRO
1	10-C	188	PRO
1	10-D	188	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	1-B	278/291 (96%)	277 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-C	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	1-D	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	2-A	278/291 (96%)	276 (99%)	2 (1%)	84	94
1	2-B	278/291 (96%)	276 (99%)	2 (1%)	84	94
1	2-C	278/291 (96%)	276 (99%)	2 (1%)	84	94
1	2-D	278/291 (96%)	276 (99%)	2 (1%)	84	94
1	3-A	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	3-B	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	3-C	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	3-D	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	4-A	278/291 (96%)	278 (100%)	0	100	100
1	4-B	278/291 (96%)	278 (100%)	0	100	100
1	4-C	278/291 (96%)	278 (100%)	0	100	100
1	4-D	278/291 (96%)	278 (100%)	0	100	100
1	5-A	278/291 (96%)	276 (99%)	2 (1%)	84	94
1	5-B	278/291 (96%)	276 (99%)	2 (1%)	84	94
1	5-C	278/291 (96%)	276 (99%)	2 (1%)	84	94
1	5-D	278/291 (96%)	276 (99%)	2 (1%)	84	94
1	6-A	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	6-B	278/291 (96%)	278 (100%)	0	100	100
1	6-C	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	6-D	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	7-A	278/291 (96%)	278 (100%)	0	100	100
1	7-B	278/291 (96%)	278 (100%)	0	100	100
1	7-C	278/291 (96%)	278 (100%)	0	100	100
1	7-D	278/291 (96%)	278 (100%)	0	100	100
1	8-A	278/291 (96%)	278 (100%)	0	100	100
1	8-B	278/291 (96%)	278 (100%)	0	100	100
1	8-C	278/291 (96%)	278 (100%)	0	100	100
1	8-D	278/291 (96%)	278 (100%)	0	100	100
1	9-A	278/291 (96%)	277 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9-B	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	9-C	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	9-D	278/291 (96%)	277 (100%)	1 (0%)	91	97
1	10-A	278/291 (96%)	278 (100%)	0	100	100
1	10-B	278/291 (96%)	278 (100%)	0	100	100
1	10-C	278/291 (96%)	278 (100%)	0	100	100
1	10-D	278/291 (96%)	278 (100%)	0	100	100
All	All	11120/11640 (96%)	11089 (100%)	31 (0%)	92	98

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-B	173	TYR
1	1-A	173	TYR
1	1-C	173	TYR
1	1-D	173	TYR
1	2-B	173	TYR
1	2-B	318	GLU
1	2-A	173	TYR
1	2-A	318	GLU
1	2-C	173	TYR
1	2-C	318	GLU
1	2-D	173	TYR
1	2-D	318	GLU
1	3-B	277	GLU
1	3-A	277	GLU
1	3-C	277	GLU
1	3-D	277	GLU
1	5-B	295	TRP
1	5-B	330	ARG
1	5-A	295	TRP
1	5-A	330	ARG
1	5-C	295	TRP
1	5-C	330	ARG
1	5-D	295	TRP
1	5-D	330	ARG
1	6-A	173	TYR
1	6-C	173	TYR
1	6-D	173	TYR
1	9-B	277	GLU

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Mol	Chain	Res	Type
1	9-A	277	GLU
1	9-C	277	GLU
1	9-D	277	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-B	60	GLN
1	1-B	125	GLN
1	1-B	168	ASN
1	1-B	306	GLN
1	1-B	324	GLN
1	1-A	60	GLN
1	1-A	125	GLN
1	1-A	168	ASN
1	1-A	306	GLN
1	1-A	324	GLN
1	1-C	60	GLN
1	1-C	125	GLN
1	1-C	306	GLN
1	1-C	324	GLN
1	1-D	60	GLN
1	1-D	125	GLN
1	1-D	306	GLN
1	1-D	324	GLN
1	2-A	4	HIS
1	2-D	125	GLN
1	3-B	168	ASN
1	3-B	274	GLN
1	3-A	168	ASN
1	3-A	274	GLN
1	3-C	274	GLN
1	3-D	274	GLN
1	4-B	125	GLN
1	4-B	168	ASN
1	4-B	180	ASN
1	4-A	125	GLN
1	4-A	168	ASN
1	4-A	180	ASN
1	4-C	60	GLN
1	4-C	125	GLN
1	4-C	180	ASN

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Mol	Chain	Res	Type
1	4-D	60	GLN
1	4-D	125	GLN
1	4-D	180	ASN
1	6-B	156	HIS
1	6-B	245	HIS
1	6-A	156	HIS
1	6-A	245	HIS
1	6-C	156	HIS
1	6-C	245	HIS
1	6-D	156	HIS
1	6-D	245	HIS
1	7-B	60	GLN
1	7-B	319	ASN
1	7-B	324	GLN
1	7-A	60	GLN
1	7-A	324	GLN
1	7-C	60	GLN
1	7-C	324	GLN
1	7-D	60	GLN
1	7-D	324	GLN
1	8-B	4	HIS
1	8-B	80	HIS
1	8-B	156	HIS
1	8-A	4	HIS
1	8-A	80	HIS
1	8-A	156	HIS
1	8-C	4	HIS
1	8-C	80	HIS
1	8-C	156	HIS
1	8-D	4	HIS
1	8-D	80	HIS
1	8-D	156	HIS
1	9-B	60	GLN
1	9-B	125	GLN
1	9-A	60	GLN
1	9-A	125	GLN
1	9-C	60	GLN
1	9-C	125	GLN
1	9-D	60	GLN
1	9-D	125	GLN
1	10-B	168	ASN
1	10-B	324	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-A	324	GLN
1	10-C	168	ASN
1	10-C	324	GLN
1	10-D	324	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

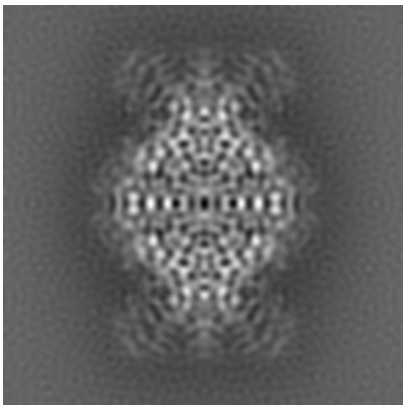
6 Map visualisation (i)

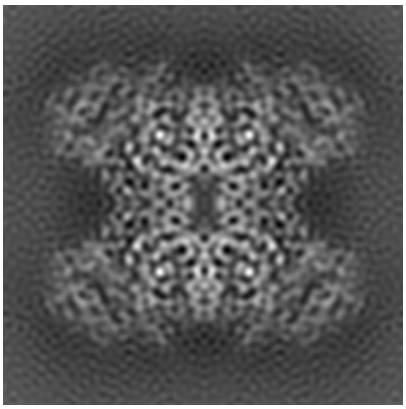
This section contains visualisations of the EMDB entry EMD-8743. These allow visual inspection of the internal detail of the map and identification of artifacts.

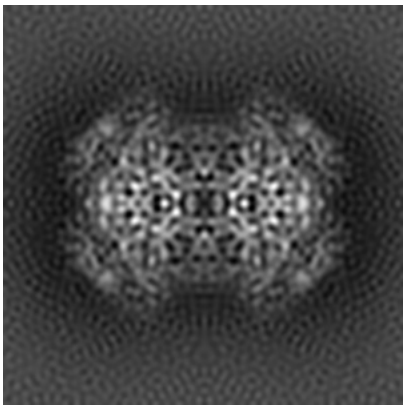
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

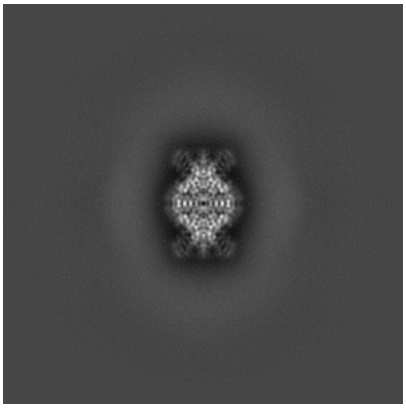
6.1.1 Primary map

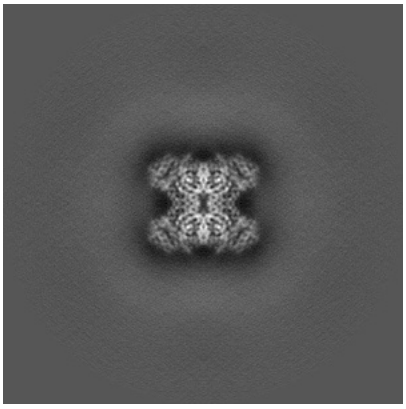

X

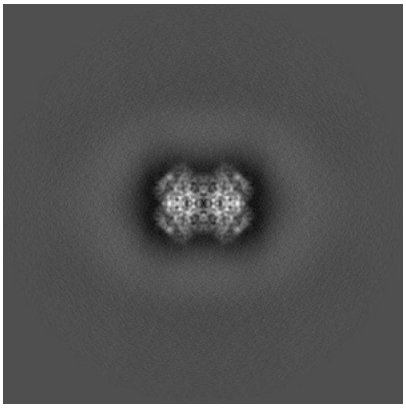

Y


Z

6.1.2 Raw map


X

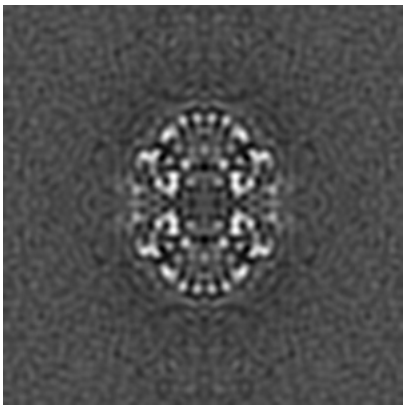

Y

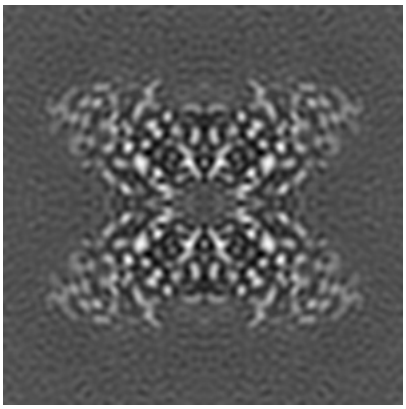

Z

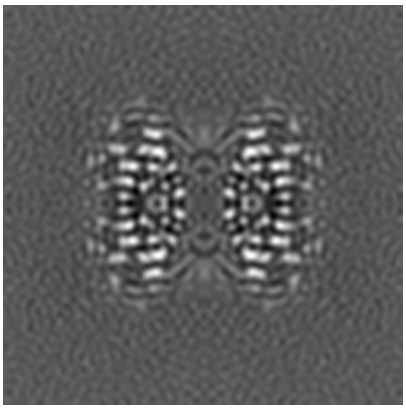
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

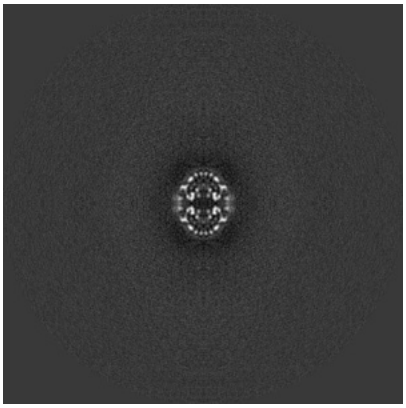
6.2.1 Primary map

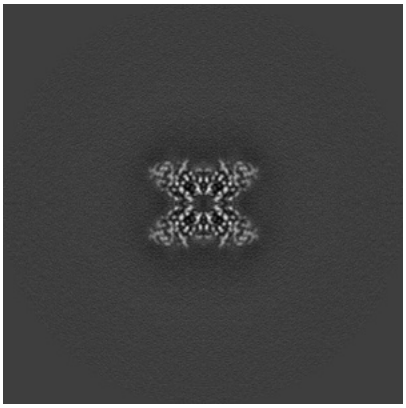

X Index: 64

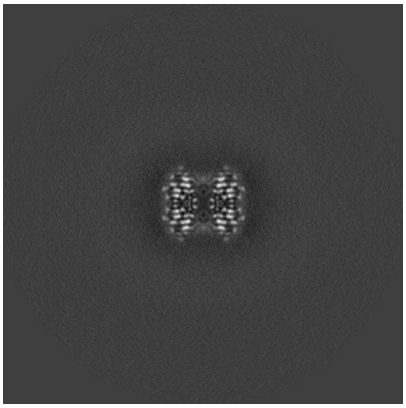

Y Index: 64


Z Index: 64

6.2.2 Raw map


X Index: 184

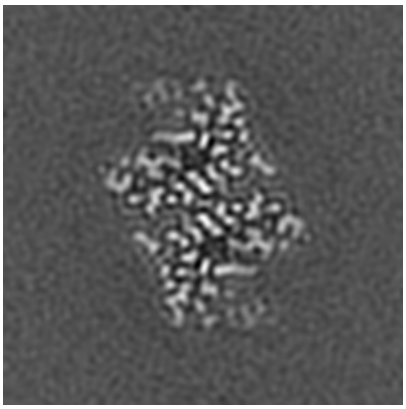

Y Index: 184

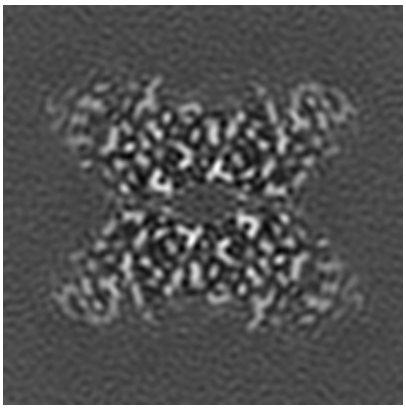

Z Index: 184

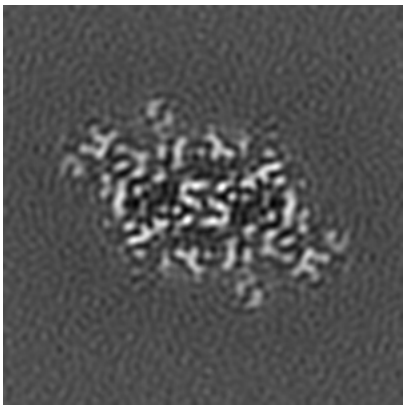
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

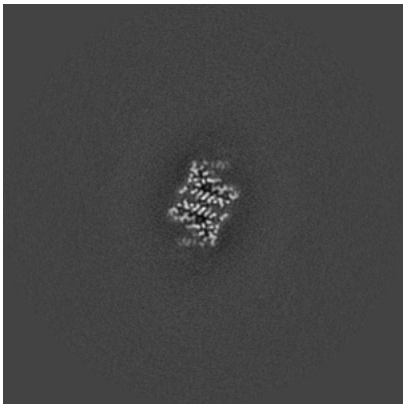
6.3.1 Primary map

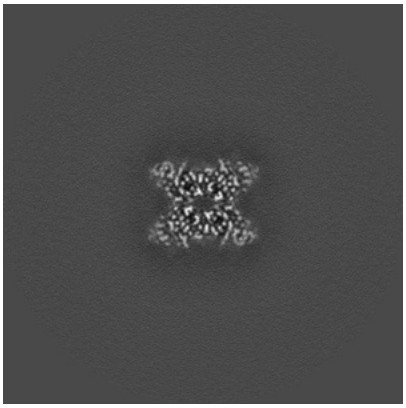

X Index: 77

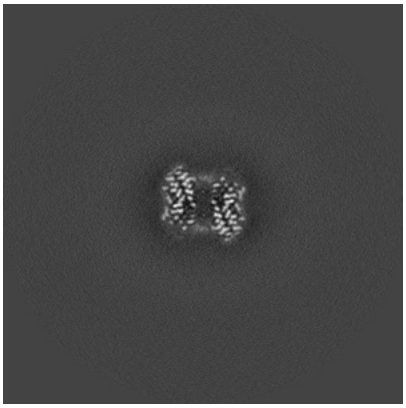

Y Index: 65


Z Index: 76

6.3.2 Raw map


X Index: 171

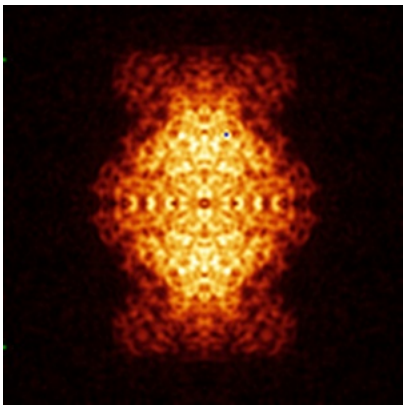

Y Index: 183

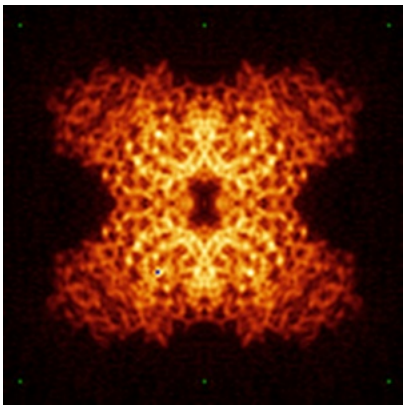

Z Index: 186

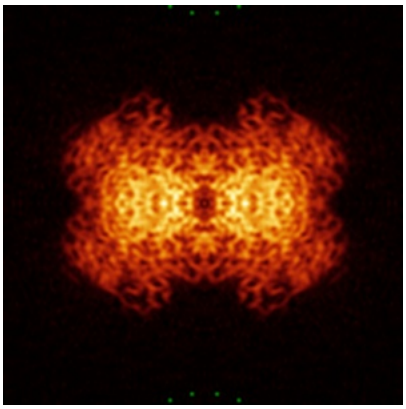
The images above show the largest variance slices of the map in three orthogonal directions.

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

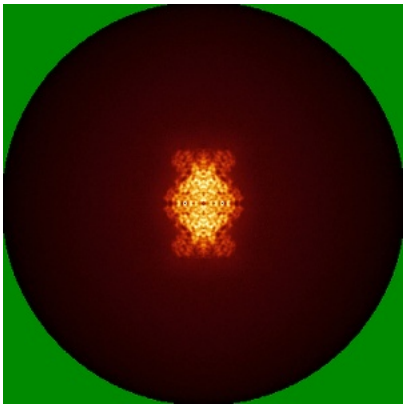
6.4.1 Primary map

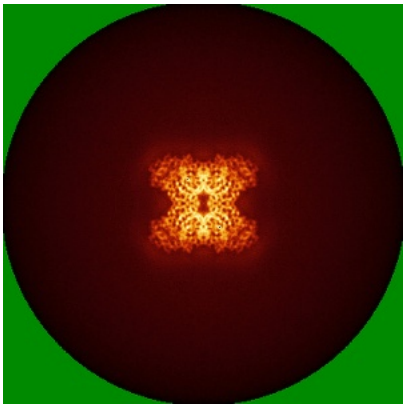

X

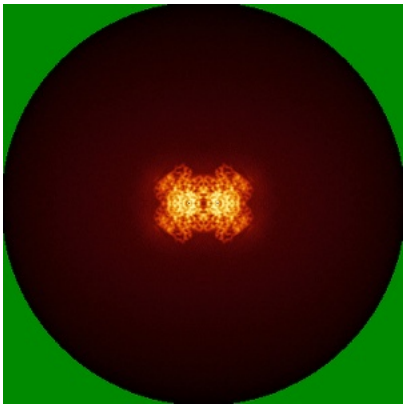

Y


Z

6.4.2 Raw map


X

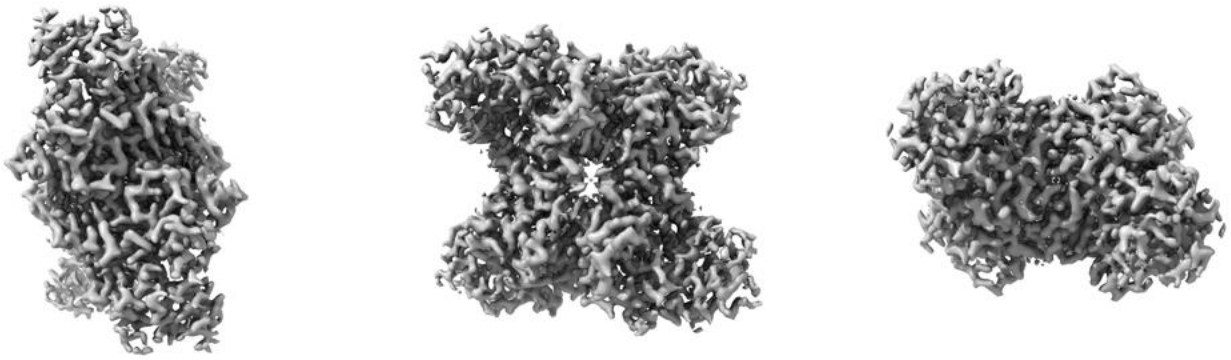

Y


Z

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

6.5 Orthogonal surface views (i)

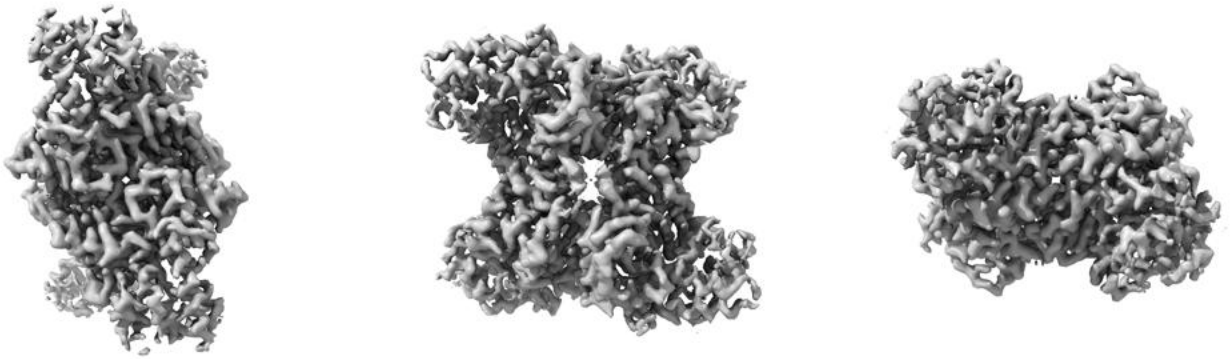
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

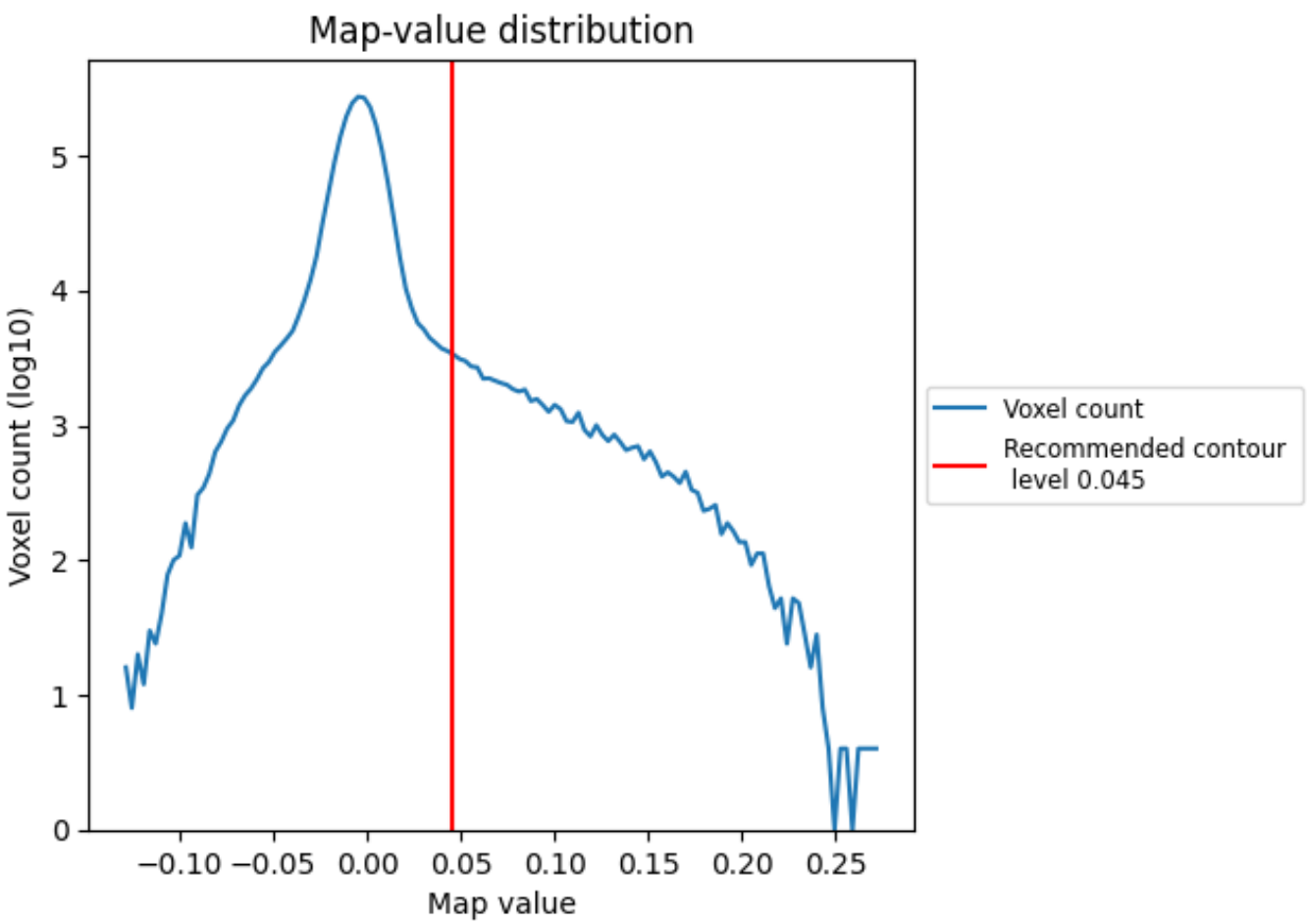
6.6 Mask visualisation (i)

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

7 Map analysis (i)

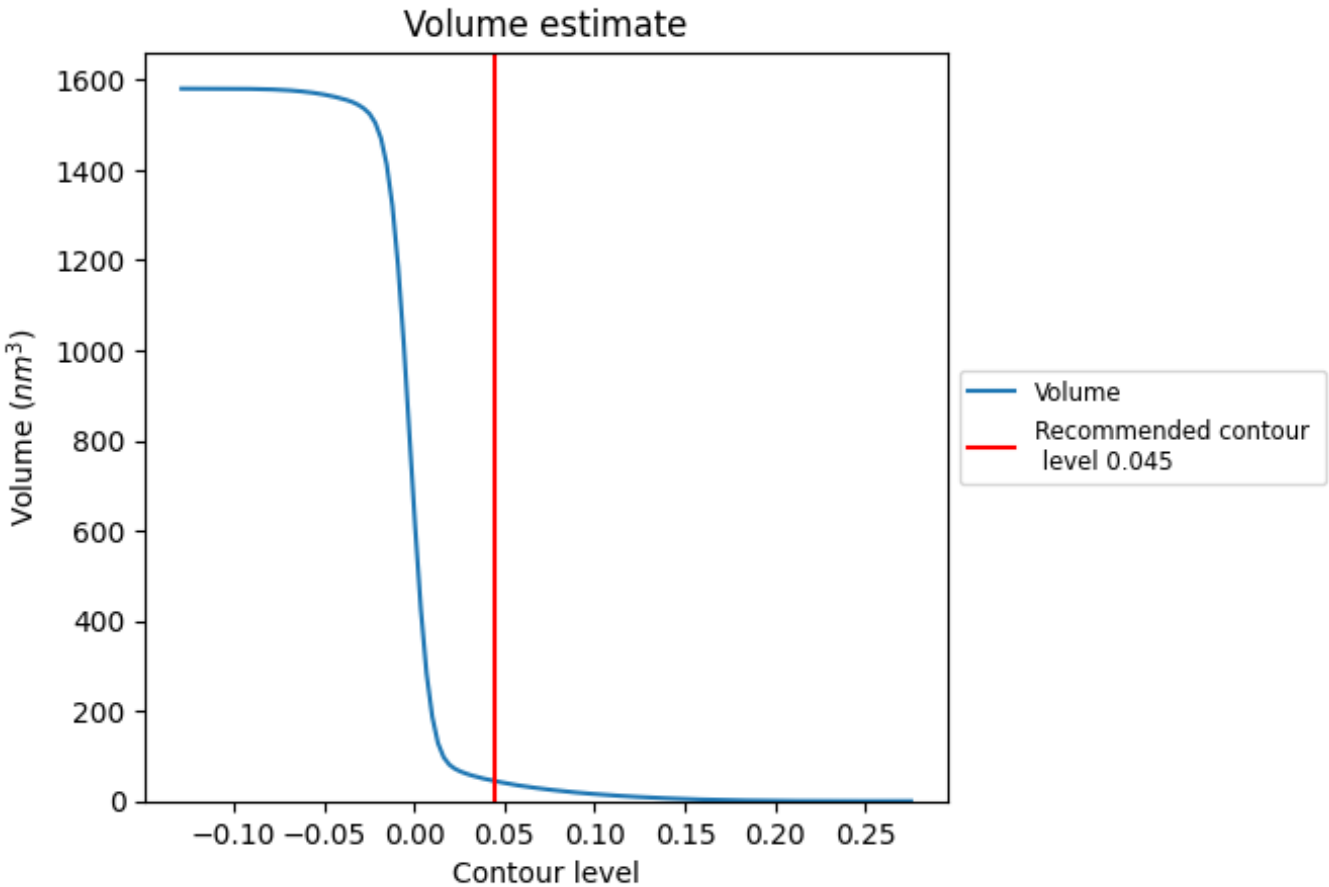
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

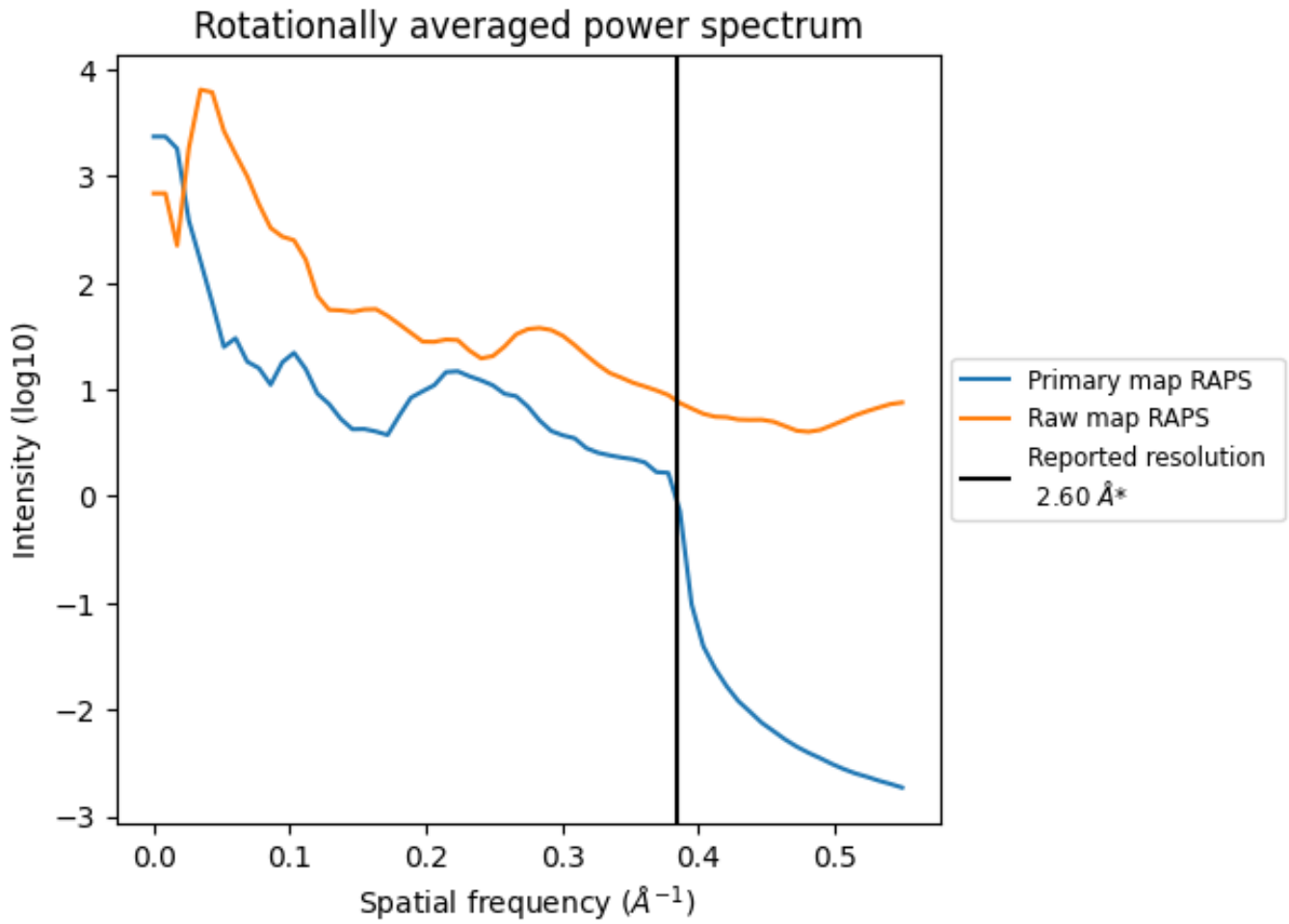
7.2 Volume estimate (i)



The volume at the recommended contour level is 44 nm^3; this corresponds to an approximate mass of 40 kDa.

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

7.3 Rotationally averaged power spectrum (i)

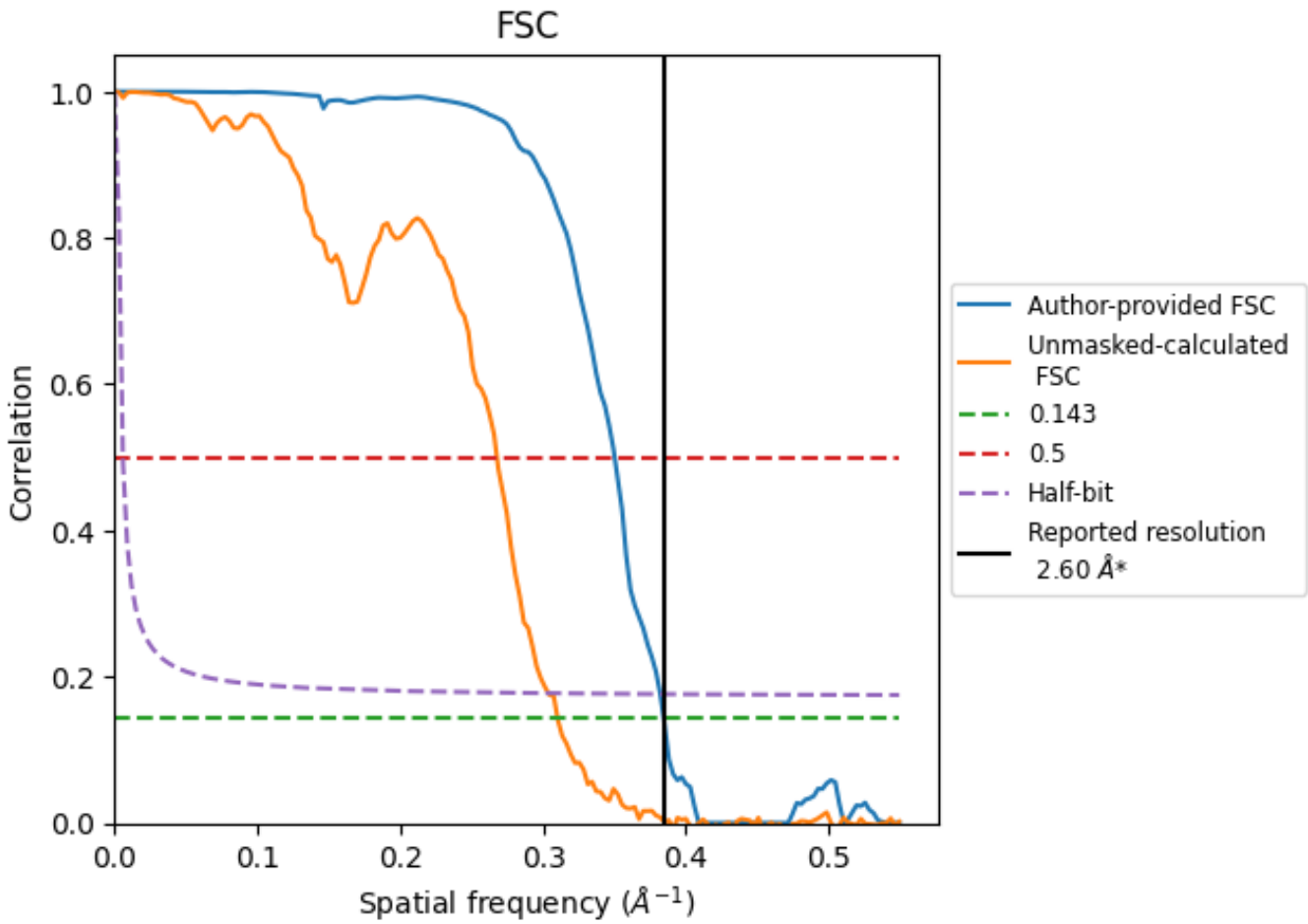


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

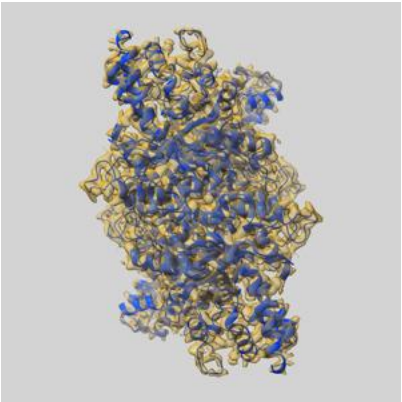
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	2.86	2.62
Unmasked-calculated*	3.22	3.74	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.6 by more than 10 %

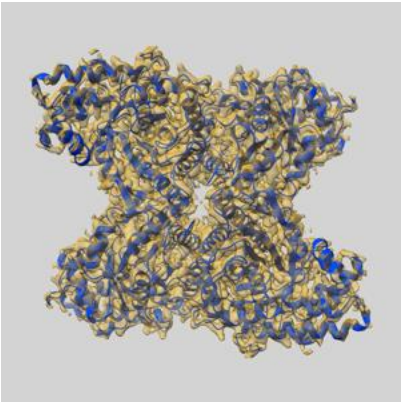
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8743 and PDB model 5VY5. Per-residue inclusion information can be found in section 3 on page 8.

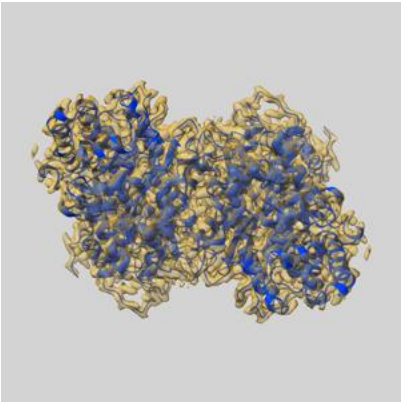
9.1 Map-model overlay (i)



X



Y



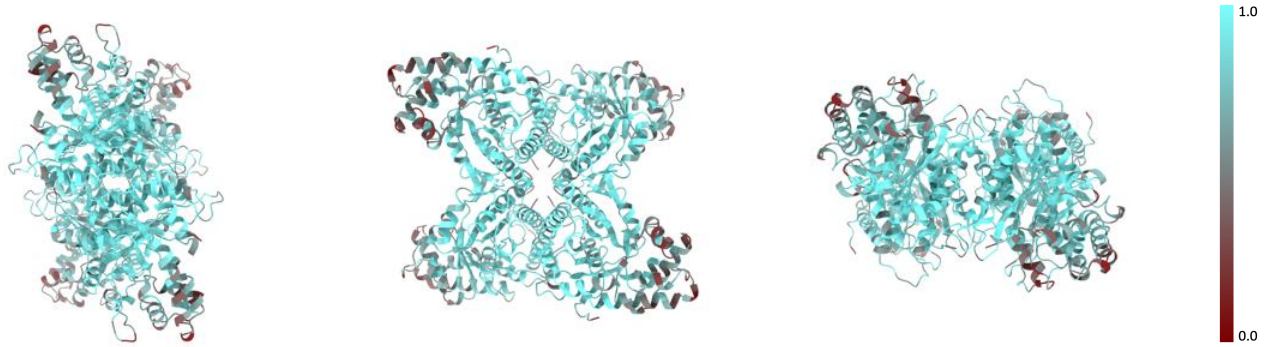
Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

This section was not generated.

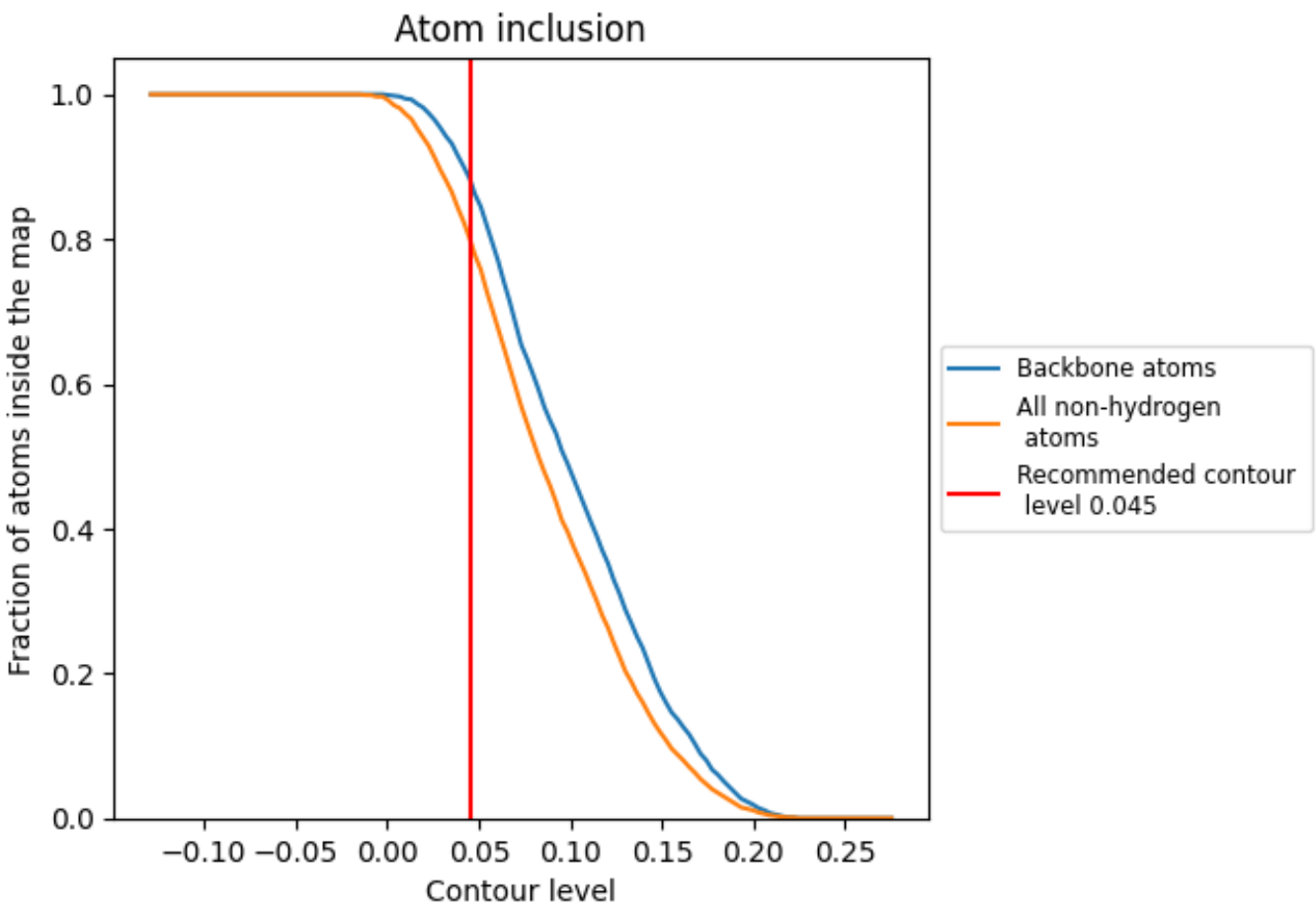
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8010
A	0.8000
B	0.8010
C	0.8010
D	0.8000