



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Nov 6, 2017 – 03:29 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 : unknown
Resolution : 2.60 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

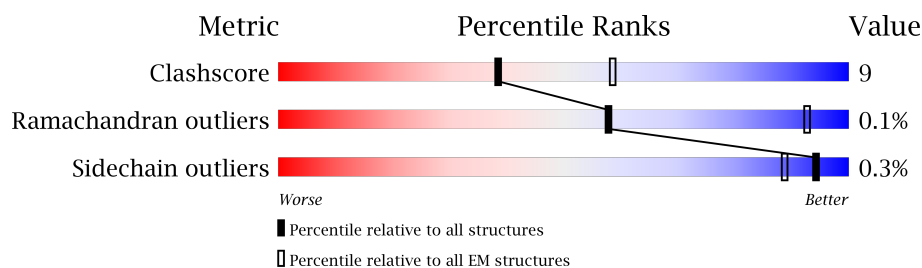
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.
















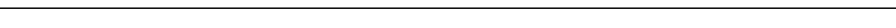











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1-A	363	
1	1-B	363	
1	1-C	363	
1	1-D	363	
1	10-A	363	
1	10-B	363	
1	10-C	363	
1	10-D	363	
1	2-A	363	

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Mol	Chain	Length	Quality of chain
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%
1	8-B	363	 77%17%6%

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Mol	Chain	Length	Quality of chain
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

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

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

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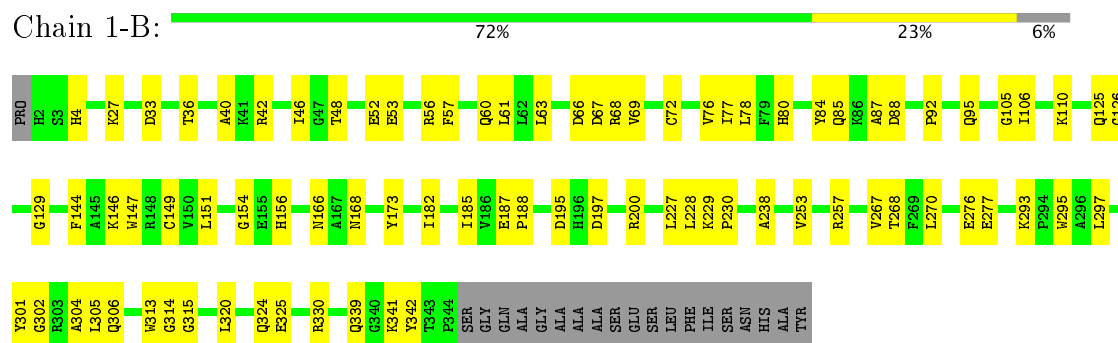
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	9-D	343	Total	C	N	O	S	0	0
			2618	1647	465	495	11		
1	10-D	343	Total	C	N	O	S	0	0
			2618	1647	465	495	11		

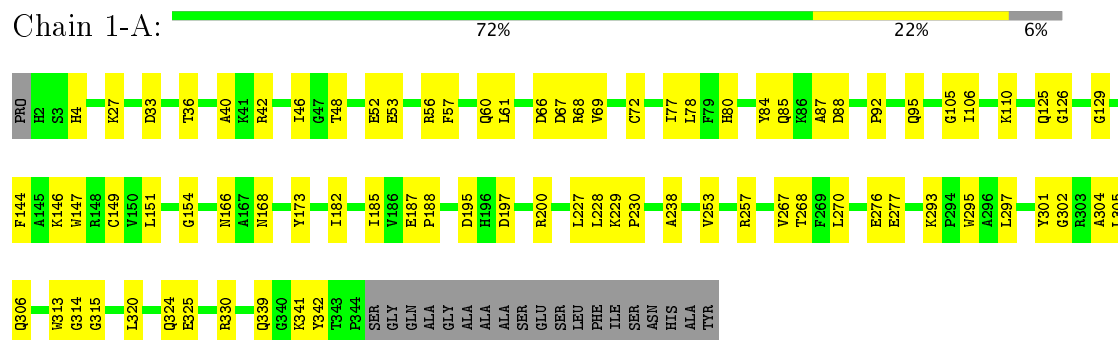
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

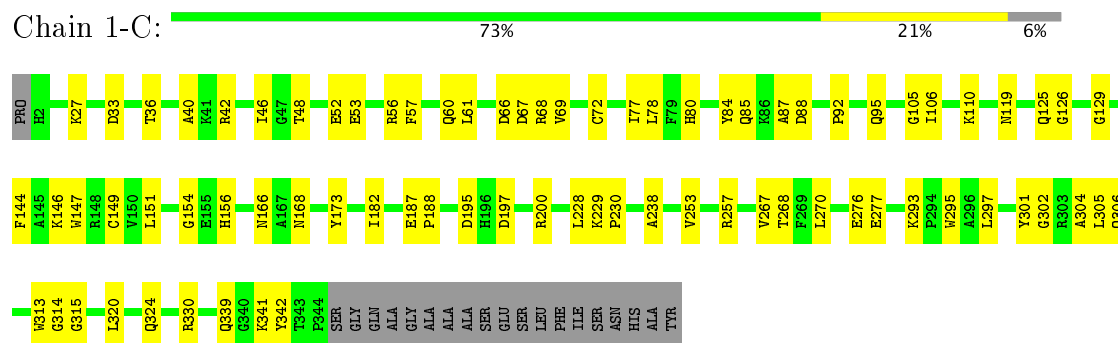
• Molecule 1: Fructose-bisphosphate aldolase A



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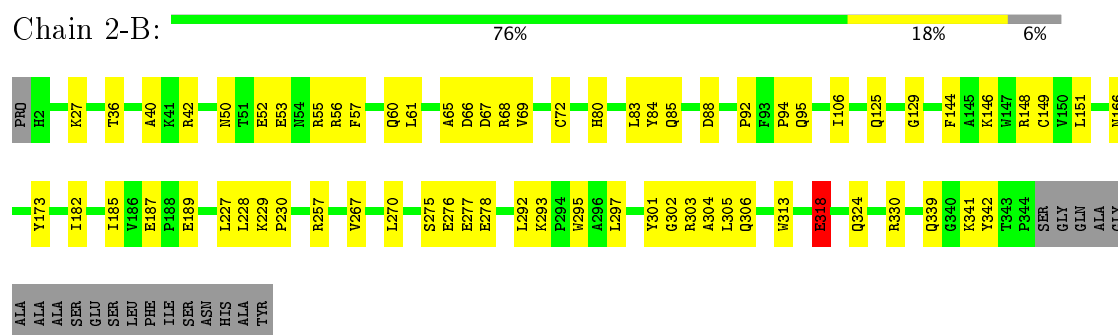
• Molecule 1: Fructose-bisphosphate aldolase A



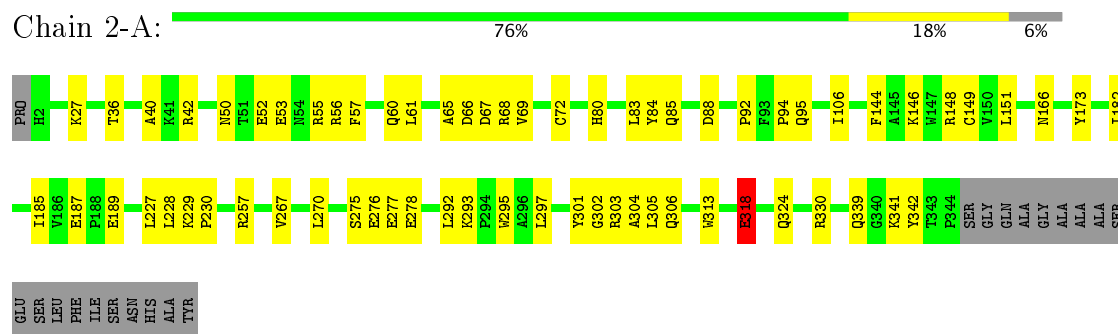
• Molecule 1: Fructose-bisphosphate aldolase A



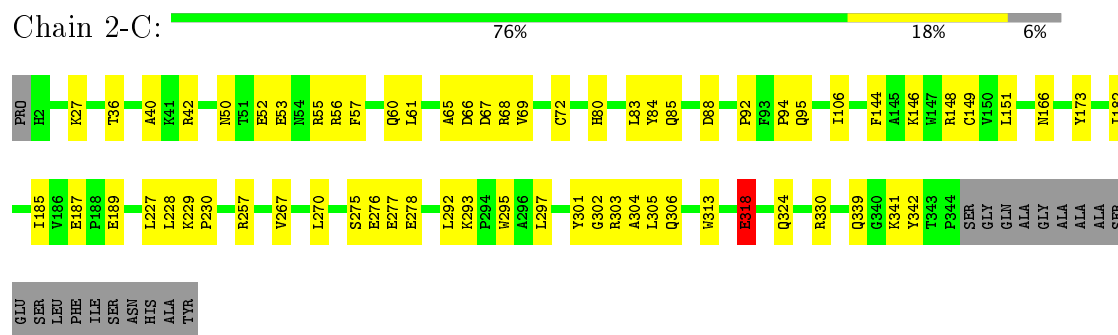
- Molecule 1: Fructose-bisphosphate aldolase A



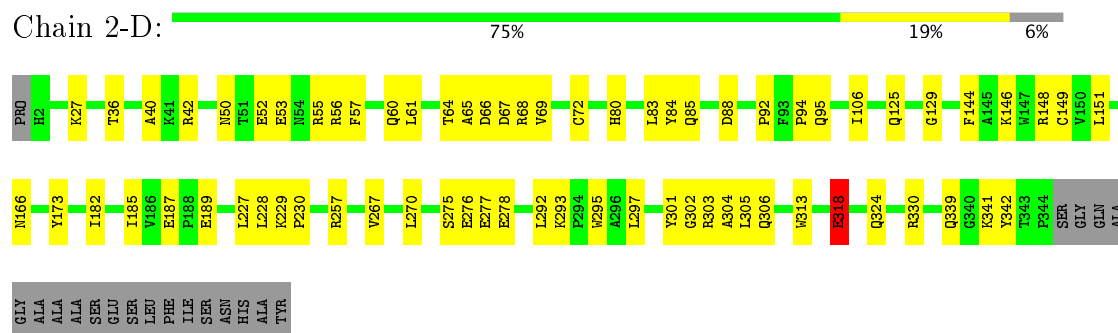
- Molecule 1: Fructose-bisphosphate aldolase A



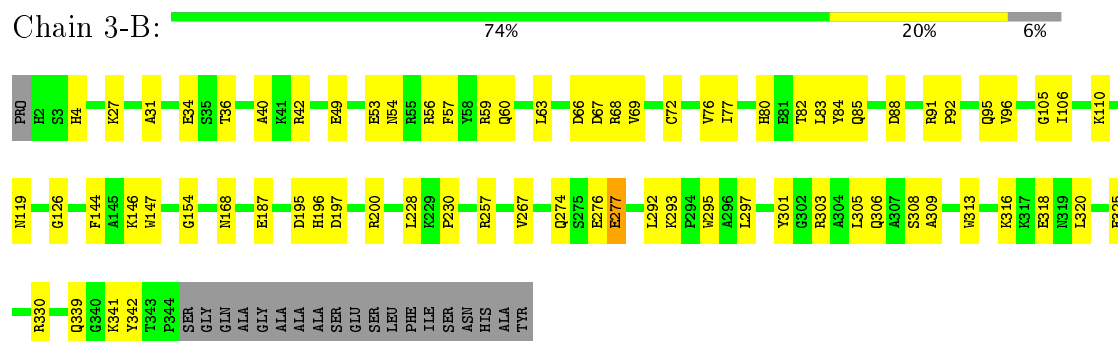
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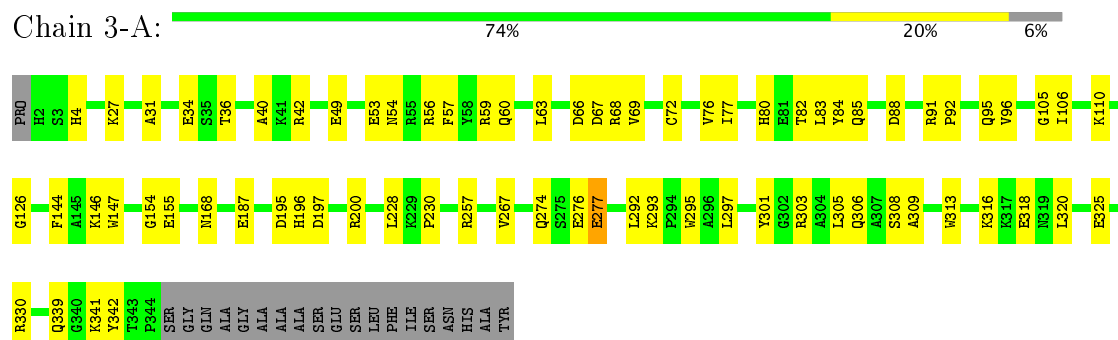
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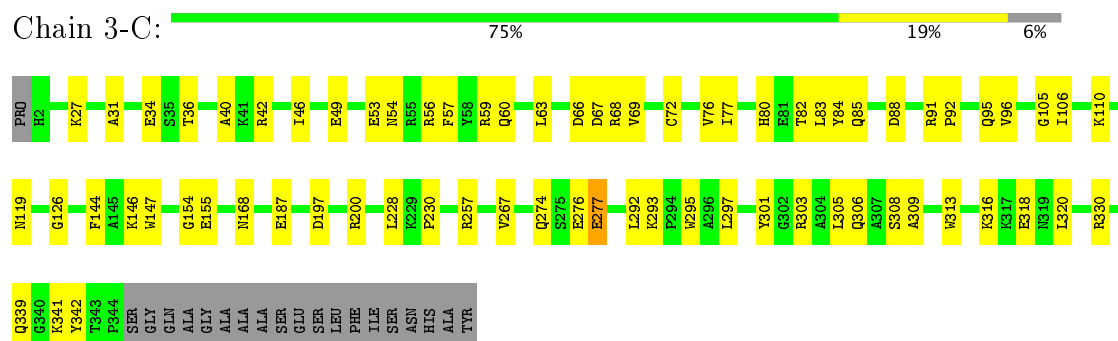
- Molecule 1: Fructose-bisphosphate aldolase A



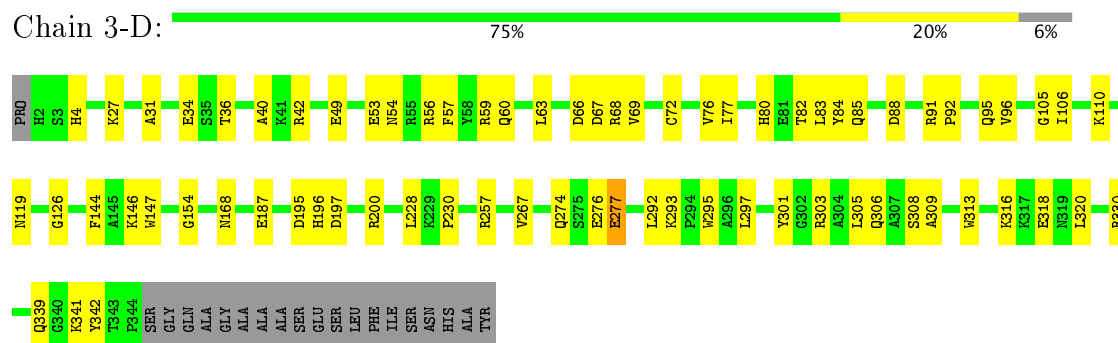
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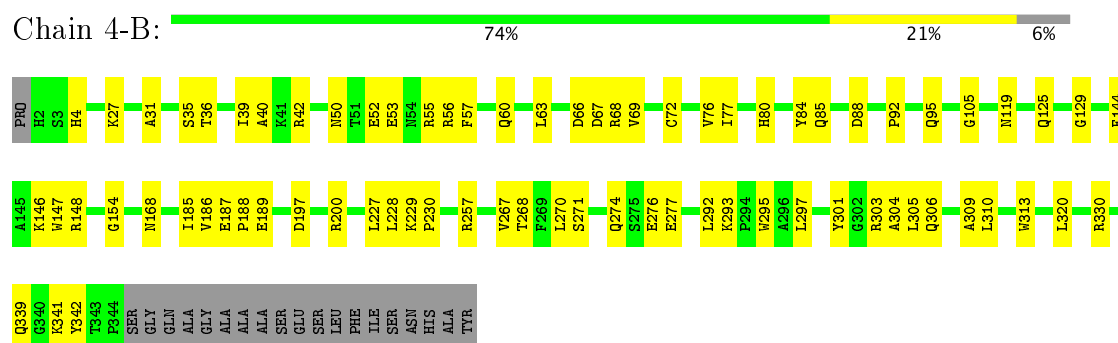
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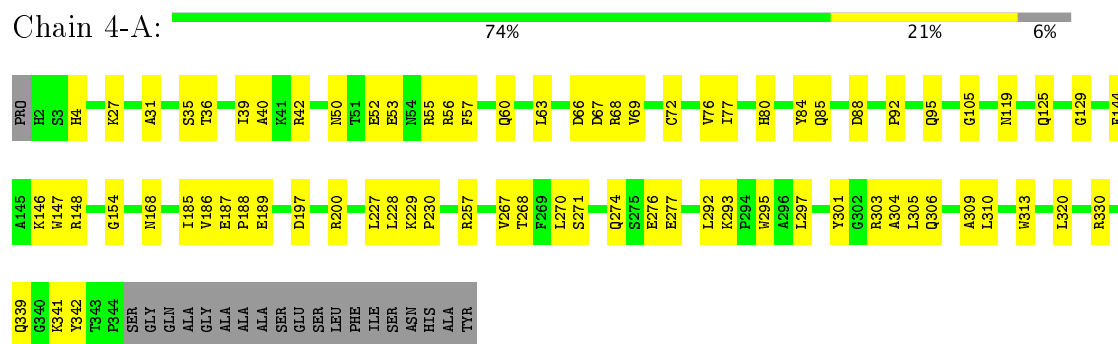
- Molecule 1: Fructose-bisphosphate aldolase A



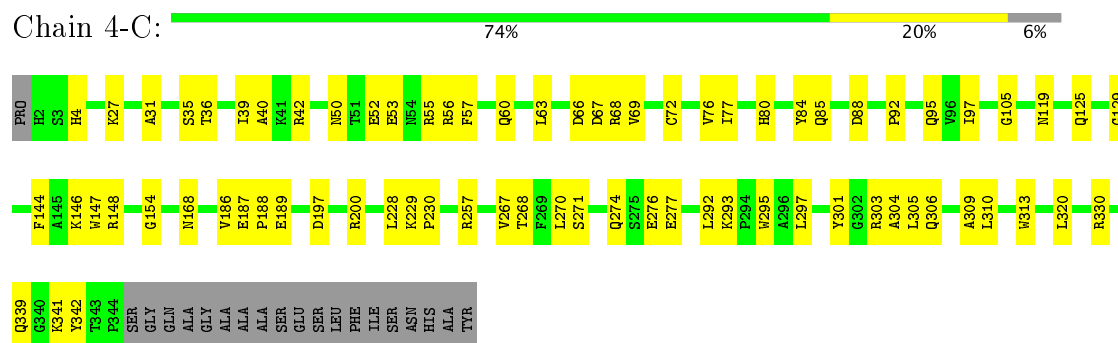
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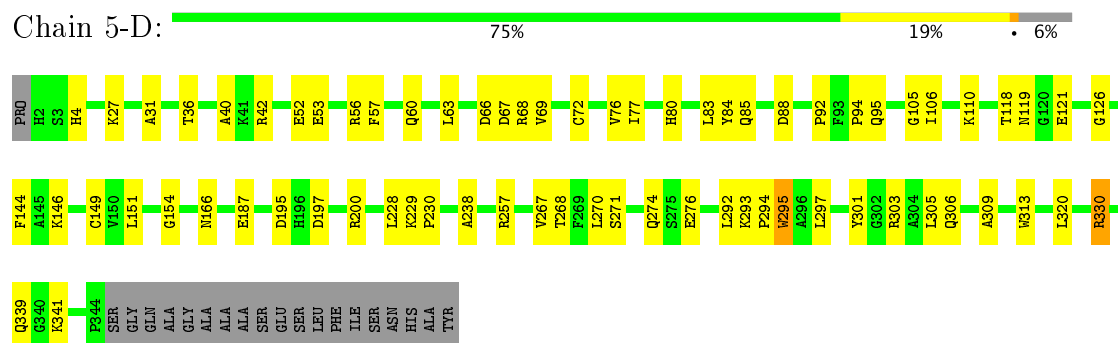
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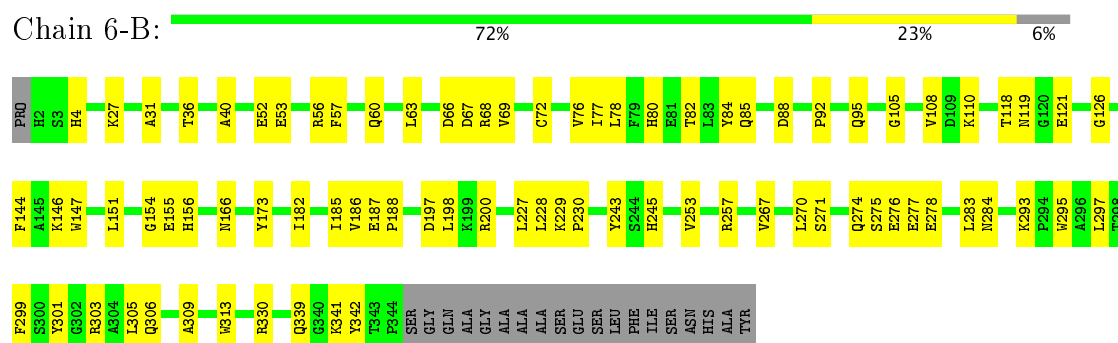
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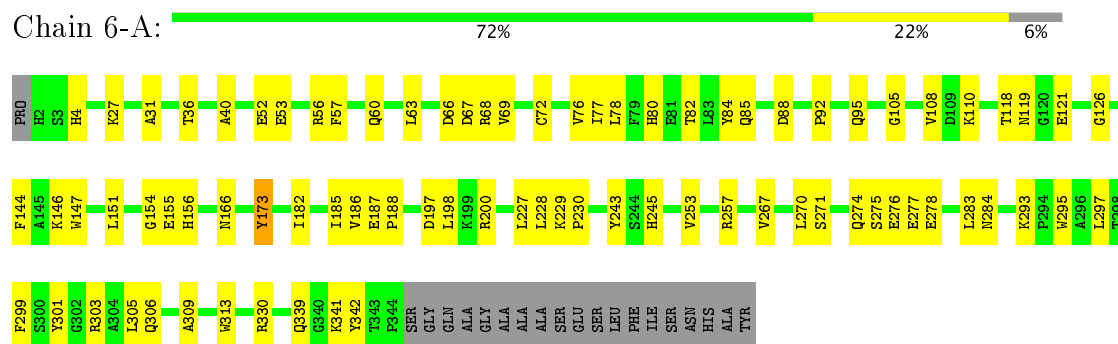
- Molecule 1: Fructose-bisphosphate aldolase A



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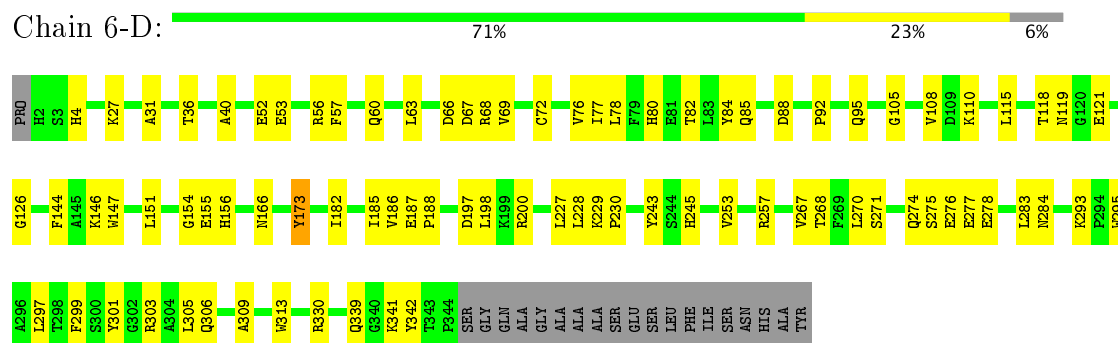
- Molecule 1: Fructose-bisphosphate aldolase A



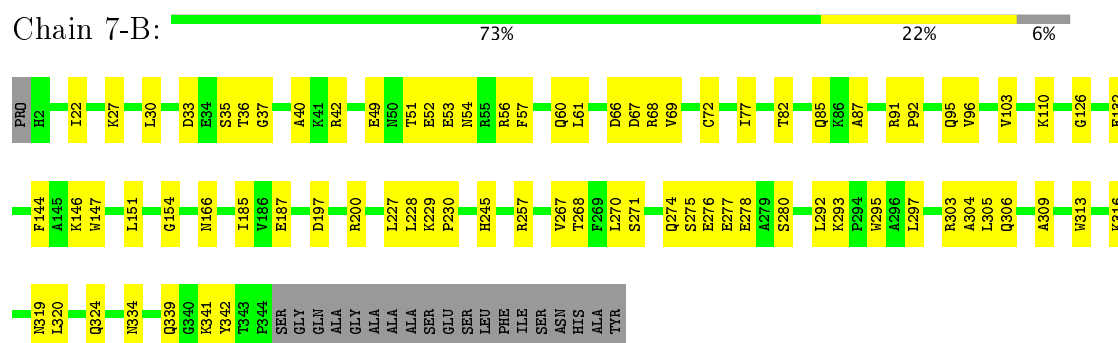
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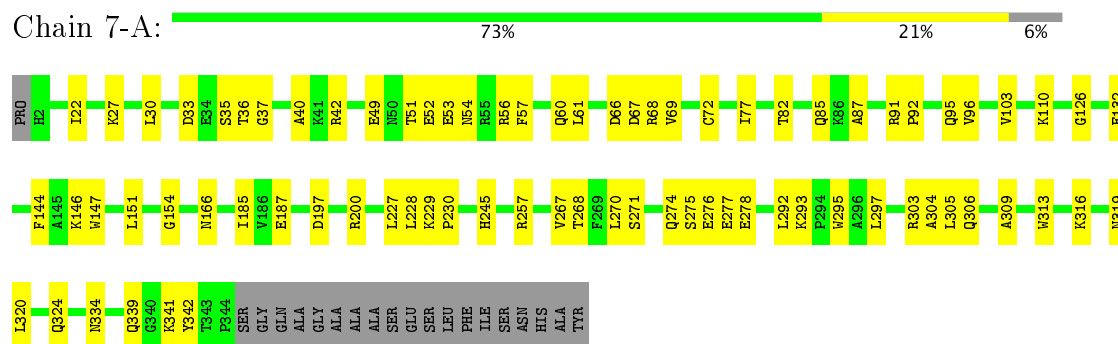
- Molecule 1: Fructose-bisphosphate aldolase A



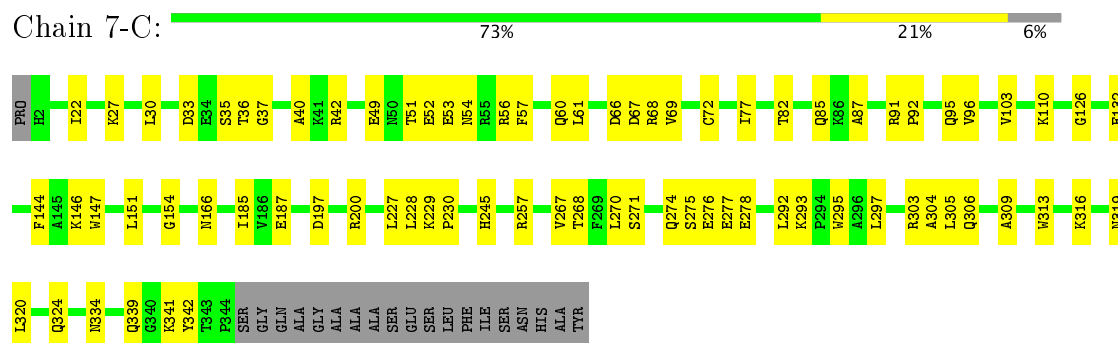
- Molecule 1: Fructose-bisphosphate aldolase A



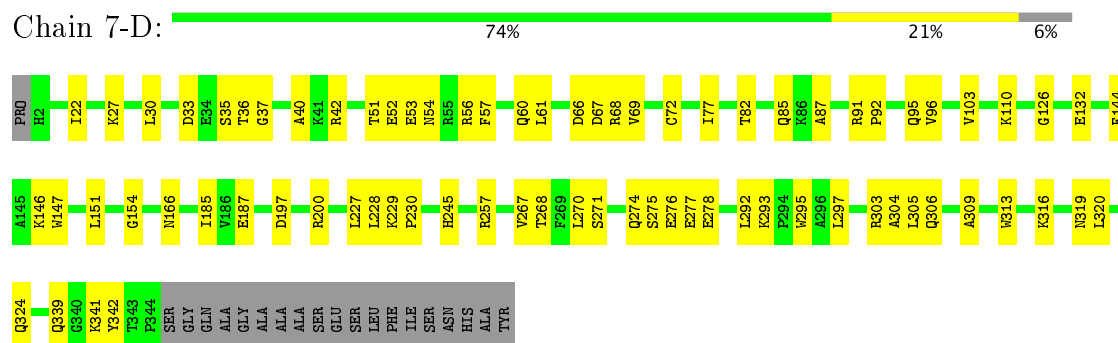
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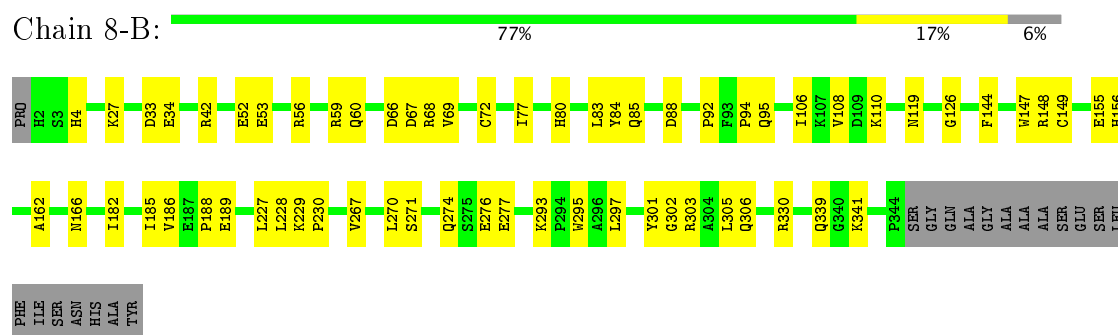
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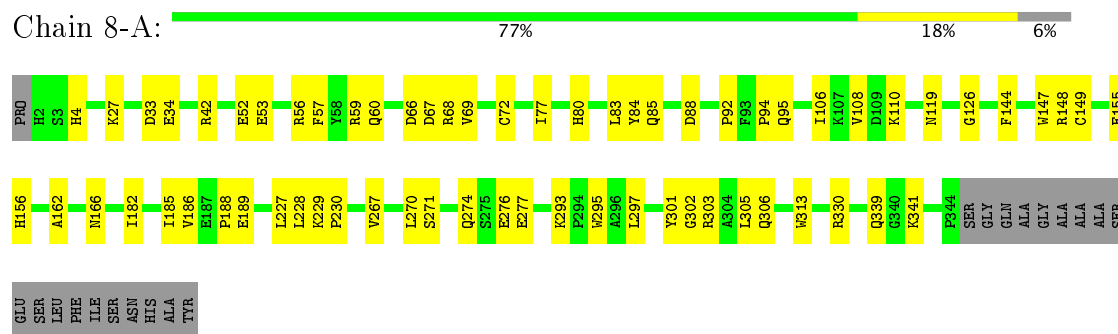
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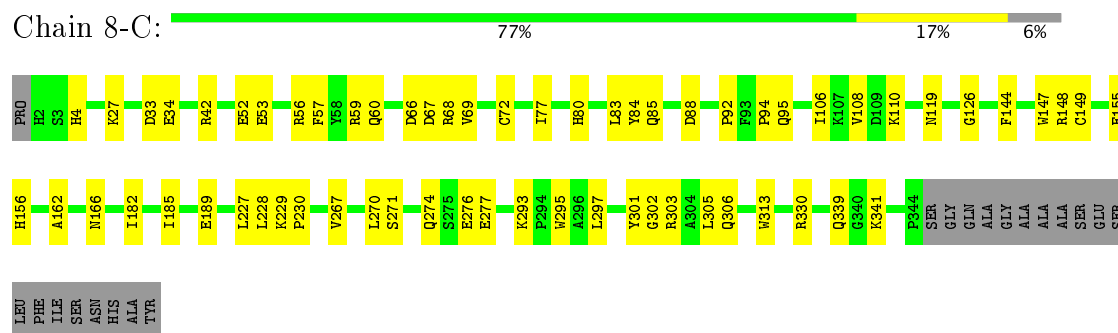
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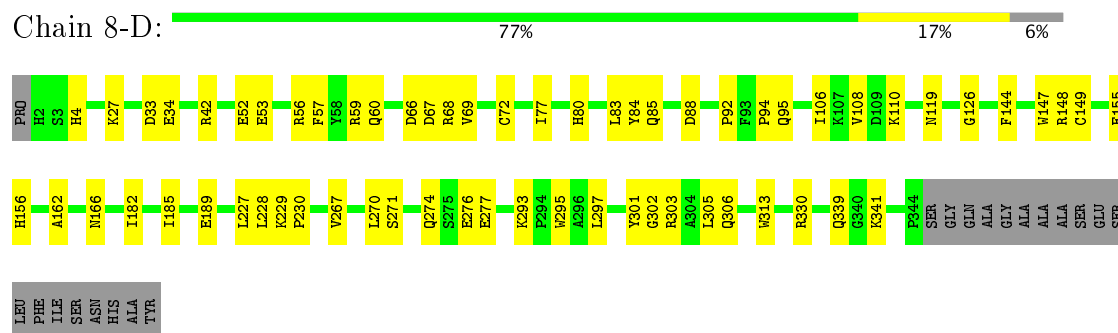
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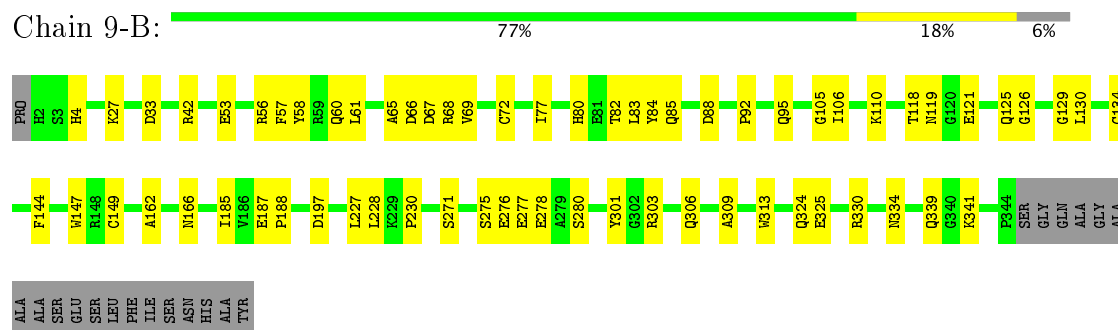
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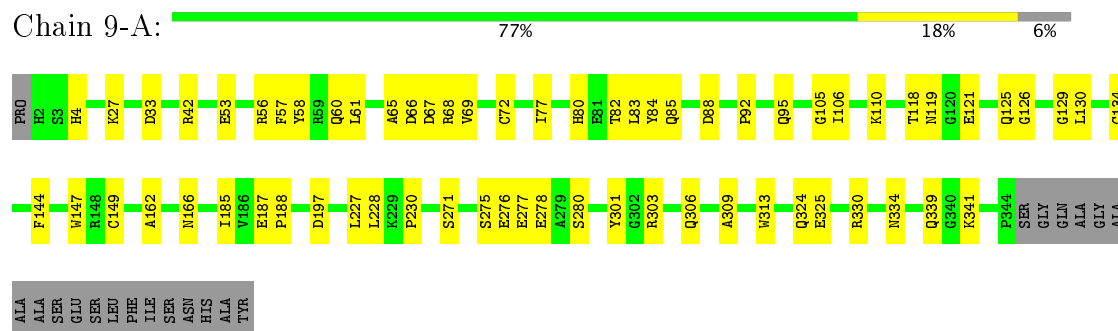
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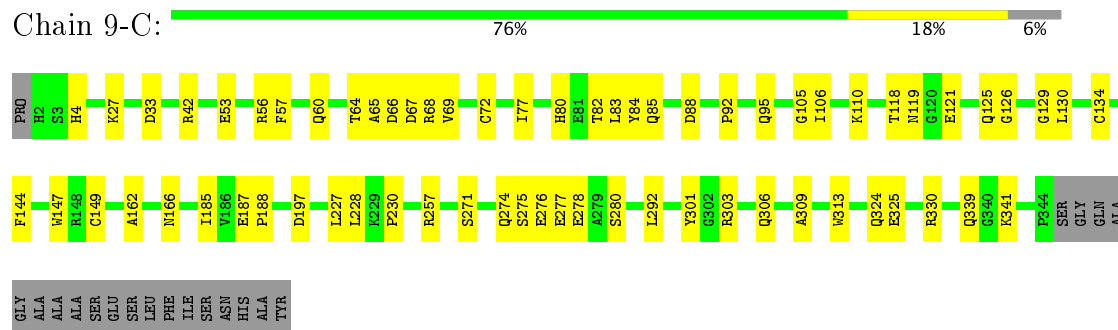
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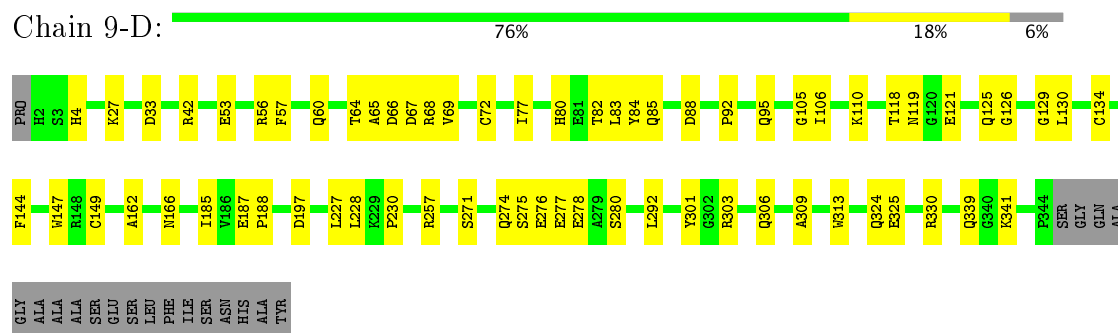
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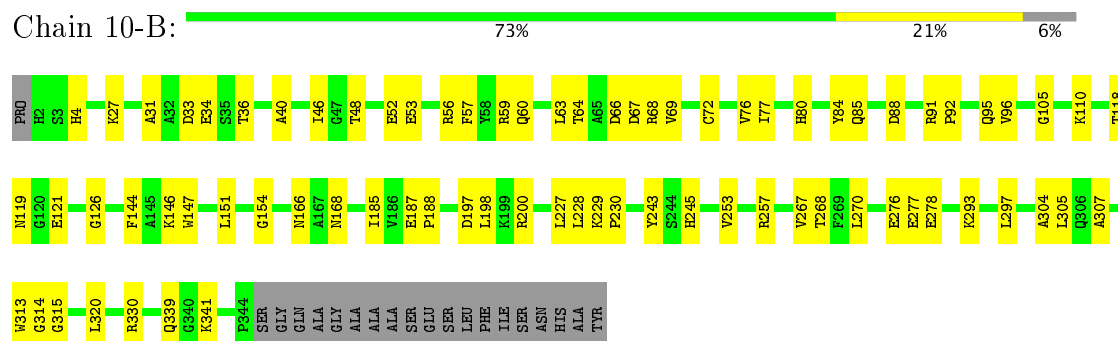
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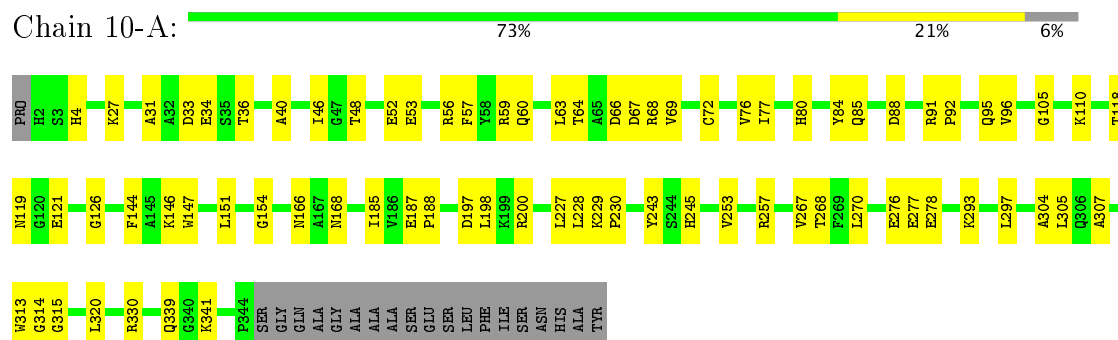
- Molecule 1: Fructose-bisphosphate aldolase A



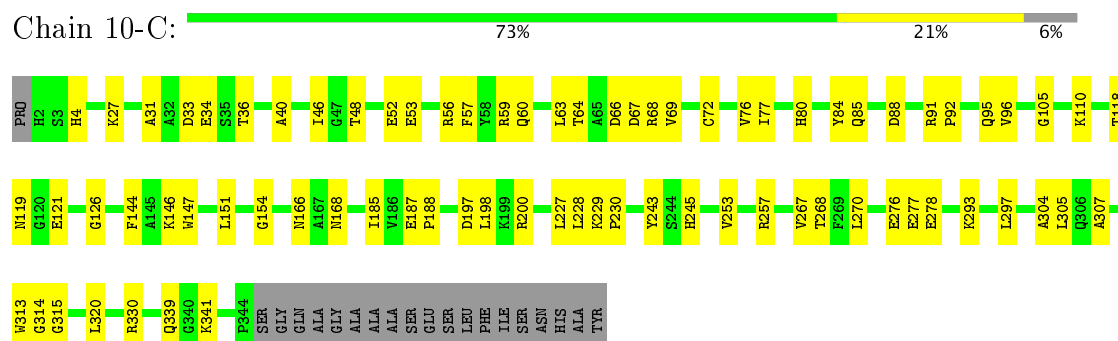
- Molecule 1: Fructose-bisphosphate aldolase A



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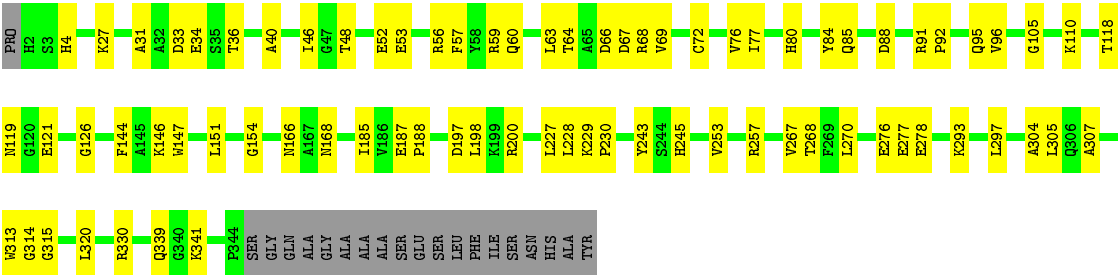


- Molecule 1: Fructose-bisphosphate aldolase A



- Molecule 1: Fructose-bisphosphate aldolase A

Chain 10-D: 73% 21% 6%



4 Experimental information

Property	Value	Source
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 ($e^-/\text{\AA}^2$)	68	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
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	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
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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
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
1	9-C	0.53	0/2668	0.53	0/3616
1	9-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(°)	Ideal(°)
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 ⓘ

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HH22	1:B: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:A:36:THR:O	1:A:40:ALA:HB2	1.83	0.78
1:B:36:THR:O	1:B: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:129:GLY:H	1:D:125:GLN:HE21	1.32	0.75
1:B:125:GLN:NE2	1:D:129:GLY:H	1.85	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:A:77:ILE:HD11	1:A:146:LYS:HB2	1.73	0.71
1:B:77:ILE:HD11	1:B:146:LYS:HB2	1.72	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:A:66:ASP:OD2	1:A:68:ARG:NH1	2.25	0.69
1:B:66:ASP:OD2	1:B: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:CD	1:A:318:GLU:H	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:A:105:GLY:HA2	1:A:144:PHE:O	1.93	0.68
1:B:105:GLY:HA2	1:B: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:A:276:GLU:O	1:A:330:ARG:NH2	2.27	0.67
1:B:197:ASP:OD1	1:B:198:LEU:N	2.28	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:A:197:ASP:OD1	1:A:198:LEU:N	2.28	0.67
1:B:276:GLU:O	1:B:330:ARG:NH2	2.27	0.67
1:C:197:ASP:OD1	1:C:198:LEU:N	2.28	0.67
1:A:276:GLU:O	1:A:330:ARG:NH2	2.28	0.67
1:B:276:GLU:O	1:B: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:A:105:GLY:HA2	1:A:144:PHE:O	1.96	0.65
1:B:105:GLY:HA2	1:B: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:A:66:ASP:OD2	1:A:68:ARG:NH1	2.30	0.64
1:B:66:ASP:OD2	1:B: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:CD	1:D:318:GLU:H	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:A:276:GLU:O	1:A:330:ARG:NH2	2.31	0.64
1:B:276:GLU:O	1:B: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: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:B:52:GLU:OE2	1:B: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:A:154:GLY:O	1:A:200:ARG:NH2	2.31	0.63
1:B:154:GLY:O	1:B: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:A:53:GLU:OE2	1:A:56:ARG:NH2	2.32	0.63
1:B:53:GLU:OE2	1:B: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:A:52:GLU:OE2	1:A:85:GLN:NE2	2.31	0.63
1:B:105:GLY:HA2	1:B:144:PHE:O	1.98	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:A:147:TRP:O	1:A:187:GLU:HB3	1.98	0.63
1:B:147:TRP:O	1:B: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:154:GLY:O	1:D:200:ARG:NH2	2.31	0.63
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.32	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:A:276:GLU:O	1:A:330:ARG:NH2	2.31	0.62
1:B:276:GLU:O	1:B: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:A:36:THR:O	1:A:40:ALA:HB2	1.99	0.62
1:B:36:THR:O	1:B: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:A:52:GLU:OE2	1:A:85:GLN:NE2	2.32	0.62
1:B:52:GLU:OE2	1:B: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:A:65:ALA:HA	1:A:324:GLN:NE2	2.14	0.62
1:B:65:ALA:HA	1:B: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:A:53:GLU:OE2	1:A:56:ARG:NH2	2.32	0.62
1:B:147:TRP:O	1:B:187:GLU:HB3	1.99	0.62
1:B:53:GLU:OE2	1:B: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:A:53:GLU:OE2	1:A:56:ARG:NH2	2.32	0.61
1:B:53:GLU:OE2	1:B: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:A:53:GLU:OE2	1:A:56:ARG:NH2	2.33	0.60
1:B:53:GLU:OE2	1:B: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:A:105:GLY:HA2	1:A:144:PHE:O	2.02	0.59
1:B:105:GLY:HA2	1:B:144:PHE:O	2.02	0.59
1:C:277:GLU:OE2	1:C:342:TYR:OH	2.17	0.59
1:D:277:GLU:OE2	1:D:342:TYR:OH	2.17	0.59
1:D:52:GLU:OE2	1:D:85:GLN:NE2	2.25	0.59
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.66	0.59
1:A:275:SER:HB3	1:A:278:GLU:HG2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:SER:HB3	1:B: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:A:110:LYS:HD2	1:A:126:GLY:HA2	1.84	0.59
1:B:110:LYS:HD2	1:B: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:105:GLY:HA2	1:A:144:PHE:O	2.03	0.59
1:A:36:THR:O	1:A:40:ALA:HB2	2.02	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:A:267:VAL:HB	1:A:297:LEU:HD23	1.86	0.58
1:B:267:VAL:HB	1:B: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:A:229:LYS:HE2	1:A:270:LEU:HD21	1.85	0.58
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.86	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:A:267:VAL:HB	1:A:297:LEU:HD23	1.87	0.57
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.86	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: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:B:83:LEU:HD22	1:B:106:ILE:HD12	1.86	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:A:66:ASP:OD2	1:A:68:ARG:NE	2.37	0.57
1:B:66:ASP:OD2	1:B: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:A:33:ASP:HB3	1:A:77:ILE:HG22	1.88	0.56
1:B:33:ASP:HB3	1:B: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:A:267:VAL:HB	1:A:297:LEU:HD23	1.88	0.56
1:B:267:VAL:HB	1:B: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:A:229:LYS:HG2	1:A:270:LEU:HD12	1.88	0.55
1:B:229:LYS:HG2	1:B: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:A:271:SER:O	1:A:274:GLN:HG2	2.07	0.55
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.40	0.55
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.40	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:295:TRP:HE1	1:D:297:LEU:HD21	1.72	0.55
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.89	0.55
1:C:66:ASP:OD2	1:C:68:ARG:NE	2.40	0.55
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.72	0.55
1:B:295:TRP:HE1	1:B:297:LEU:HD21	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:B:151:LEU:HD21	1:B:166:ASN:HD22	1.72	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:A:66:ASP:OD1	1:A:67:ASP:N	2.40	0.54
1:B:151:LEU:HD21	1:B:166:ASN:HD22	1.72	0.54
1:B:66:ASP:OD1	1:B:67:ASP:N	2.40	0.54
1:A:330:ARG:HA	1:A:330:ARG:NE	2.23	0.54
1:B:229:LYS:HG2	1:B:270:LEU:HD12	1.88	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:A:229:LYS:HG2	1:A:270:LEU:HD12	1.89	0.54
1:B:229:LYS:HG2	1:B: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:330:ARG:HE	1:A:330:ARG:HA	1.73	0.54
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.40	0.54
1:B:33:ASP:HB3	1:B:77:ILE:HG22	1.89	0.54
1:A:151:LEU:HD21	1:A:166:ASN:HD22	1.73	0.54
1:B:151:LEU:HD21	1:B:166:ASN:HD22	1.73	0.54
1:B:77:ILE:HD13	1:B:146:LYS:HD2	1.89	0.54
1:A:66:ASP:OD1	1:A:67:ASP:N	2.41	0.54
1:B:66:ASP:OD1	1:B: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:HE	1:B:330:ARG:HA	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:A:33:ASP:HB3	1:A:77:ILE:HG22	1.89	0.54
1:B:66:ASP:OD1	1:B:67:ASP:N	2.41	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:A:66:ASP:OD1	1:A:67:ASP:N	2.41	0.54
1:B:66:ASP:OD1	1:B:67:ASP:N	2.41	0.54
1:A:295:TRP:HE1	1:A:297:LEU:HD21	1.72	0.54
1:A:271:SER:O	1:A:274:GLN:HG2	2.08	0.54
1:B:271:SER:O	1:B: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:A:60:GLN:HE22	1:A:88:ASP:H	1.55	0.54
1:B:60:GLN:HE22	1:B: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:A:295:TRP:HE1	1:A:297:LEU:HD21	1.72	0.53
1:B:295:TRP:HE1	1:B: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:A:197:ASP:N	1:A:197:ASP:OD1	2.42	0.53
1:B:91:ARG:HE	1:B:96:VAL:HG22	1.74	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:257:ARG:NH1	1:D:292:LEU:O	2.42	0.53
1:D:66:ASP:OD1	1:D:67:ASP:N	2.41	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:A:91:ARG:HE	1:A:96:VAL:HG22	1.74	0.53
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.90	0.53
1:C:267:VAL:HB	1:C:297:LEU:HD23	1.90	0.53
1:D:197:ASP:N	1:D:197:ASP:OD1	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:267:VAL:HB	1:C:297:LEU:HD23	1.90	0.52
1:C:77:ILE:CD1	1:C:146:LYS:HB2	2.39	0.52
1:D:267:VAL:HB	1:D:297:LEU:HD23	1.90	0.52
1:D:77:ILE:CD1	1:D:146:LYS:HB2	2.39	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:155:GLU:HG2	1:D:156:HIS:CD2	2.44	0.52
1:D:33:ASP:HB3	1:D:77:ILE:HG22	1.91	0.52
1:A:31:ALA:HA	1:A:77:ILE:HG22	1.92	0.52
1:B:31:ALA:HA	1:B: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:A:155:GLU:HG2	1:A:156:HIS:CD2	2.44	0.52
1:A:66:ASP:OD1	1:A:67:ASP:N	2.43	0.52
1:B:66:ASP:OD1	1:B:67:ASP:N	2.43	0.52
1:A:280:SER:OG	1:A:330:ARG:NH2	2.43	0.52
1:B:280:SER:OG	1:B: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:253:VAL:O	1:C:257:ARG:HG2	2.09	0.52
1:C:245:HIS:HE1	1:C:278:GLU:OE1	1.93	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:A:110:LYS:HD2	1:A:126:GLY:HA2	1.91	0.52
1:B:110:LYS:HD2	1:B: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:A:186:VAL:HG12	1:A:188:PRO:HD3	1.92	0.52
1:B:186:VAL:HG12	1:B: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:280:SER:OG	1:C:330:ARG:NH2	2.43	0.51
1:C:68:ARG:NH2	1:C:325:GLU:OE1	2.38	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:A:305:LEU:HD23	1:A:330:ARG:HG3	1.92	0.51
1:B:305:LEU:HD23	1:B: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:OD1	1:C:197:ASP:N	2.42	0.51
1:D:197:ASP:N	1:D:197:ASP:OD1	2.42	0.51
1:B:149:CYS:SG	1:B:166:ASN:HB3	2.51	0.51
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.14	0.51
1:B:60:GLN:HE22	1:B: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:186:VAL:HG12	1:D:188:PRO:HD3	1.92	0.51
1:D:60:GLN:HE22	1:D:88:ASP:CG	2.14	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:A:83:LEU:HD22	1:A:106:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASP:HB3	1:B:77:ILE:HG22	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:A:33:ASP:HB3	1:A:77:ILE:HG22	1.93	0.50
1:B:66:ASP:OD1	1:B:67:ASP:N	2.44	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:A:110:LYS:HD2	1:A:126:GLY:HA2	1.92	0.50
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.92	0.50
1:D:245:HIS:HE1	1:D:278:GLU:OE1	1.93	0.50
1:C:83:LEU:HD22	1:C:106:ILE:HD12	1.93	0.50
1:C:33:ASP:HB3	1:C:77:ILE:HG22	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:154:GLY:O	1:B:200:ARG:NH2	2.44	0.50
1:B:91:ARG:HE	1:B:96:VAL:HG22	1.77	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:154:GLY:O	1:A:200:ARG:NH2	2.44	0.50
1:A:91:ARG:HE	1:A:96:VAL:HG22	1.77	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:A:60:GLN:HE22	1:A:88:ASP:CG	2.14	0.50
1:B:60:GLN:HE22	1:B: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:295:TRP:HE1	1:D:297:LEU:HD21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ARG:NH1	1:D:306:GLN:HE21	2.10	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:A:60:GLN:HE22	1:A:88:ASP:CG	2.14	0.50
1:B:60:GLN:HE22	1:B: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:A:42:ARG:NH1	1:A:306:GLN:HE21	2.10	0.50
1:B:42:ARG:NH1	1:B:306:GLN:HE21	2.10	0.50
1:C:42:ARG:HH22	1:C:306:GLN:HG3	1.77	0.50
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.59	0.50
1:B:50:ASN:OD1	1:B:55:ARG:NH1	2.45	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: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:B:306:GLN:O	1:B:309:ALA:N	2.45	0.50
1:B:36:THR:O	1:B:40:ALA:CB	2.57	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:A:34:GLU:O	1:A:59:ARG:NH2	2.45	0.49
1:B:34:GLU:O	1:B: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:A:36:THR:O	1:A:40:ALA:CB	2.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LYS:HE3	1:B:187:GLU:OE1	2.12	0.49
1:D:316:LYS:HE2	1:D:319:ASN:HD21	1.77	0.49
1:A:68:ARG:NH2	1:A:325:GLU:OE1	2.38	0.49
1:A:60:GLN:HE22	1:A:88:ASP:CG	2.15	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:A:77:ILE:CD1	1:A:146:LYS:HB2	2.40	0.49
1:B:77:ILE:CD1	1:B:146:LYS:HB2	2.40	0.49
1:A:31:ALA:HA	1:A:77:ILE:CG2	2.43	0.49
1:C:229:LYS:HD3	1:C:270:LEU:HD21	1.94	0.49
1:C:31:ALA:HA	1:C:77:ILE:CG2	2.42	0.49
1:D:229:LYS:HD3	1:D:270:LEU:HD21	1.95	0.49
1:D:31:ALA:HA	1:D:77:ILE:CG2	2.42	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:A:31:ALA:HA	1:A:77:ILE:CG2	2.42	0.49
1:B:31:ALA:HA	1:B: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:A:110:LYS:HD2	1:A:126:GLY:HA2	1.92	0.49
1:B:110:LYS:HD2	1:B:126:GLY:HA2	1.93	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:A:185:ILE:HG12	1:A:227:LEU:HB2	1.95	0.49
1:B:257:ARG:NH1	1:B:292:LEU:O	2.45	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:A:146:LYS:HE2	1:A:187:GLU:OE1	2.13	0.49
1:B:56:ARG:HB2	1:B:85:GLN:HE21	1.78	0.49
1:C:146:LYS:HE2	1:C:187:GLU:OE1	2.13	0.49
1:C:91:ARG:HE	1:C:96:VAL:HG22	1.77	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:A:42:ARG:HH22	1:A:306:GLN:HG3	1.77	0.49
1:B:42:ARG:HH22	1:B:306:GLN:HG3	1.77	0.49
1:B:185:ILE:HG12	1:B:227:LEU:HB2	1.95	0.49
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.59	0.49
1:D:50:ASN:OD1	1:D:55:ARG:NH1	2.45	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:A:83:LEU:HD22	1:A:106:ILE:HD12	1.95	0.48
1:B:83:LEU:HD22	1:B: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:A:42:ARG:NH2	1:A:303:ARG:HB3	2.22	0.48
1:B:306:GLN:O	1:B:309:ALA:N	2.46	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:229:LYS:HG2	1:A:270:LEU:HD12	1.95	0.48
1:A:168:ASN:HD22	1:C:168:ASN:HD22	1.60	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: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:168:ASN:HD22	1:D:168:ASN:HD22	1.60	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:228:LEU:HG	1:B:230:PRO:HD3	1.96	0.48
1:B:61:LEU:HD11	1:B:324:GLN:HB2	1.95	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:228:LEU:HG	1:A:230:PRO:HD3	1.96	0.48
1:A:61:LEU:HD11	1:A:324:GLN:HB2	1.95	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:A:57:PHE:HE2	1:A:313:TRP:HE1	1.60	0.47
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.60	0.47
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.96	0.47
1:B:228:LEU:HG	1:B: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: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
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.49	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:228:LEU:HG	1:C:230:PRO:HD3	1.97	0.47
1:C:66:ASP:O	1:C:69:VAL:HG22	2.14	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:D:339:GLN:HB3	1:D:341:LYS:HZ3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.97	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	0.47
1:A:277:GLU:OE2	1:A: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:B:277:GLU:OE2	1:B:342:TYR:OH	2.32	0.47
1:B:60:GLN:HE22	1:B:88:ASP:CG	2.18	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:228:LEU:HG	1:B:230:PRO:HD3	1.97	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	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:A:228:LEU:HG	1:A:230:PRO:HD3	1.97	0.47
1:A:66:ASP:OD2	1:A:68:ARG:NE	2.48	0.47
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.97	0.47
1:B:66:ASP:OD2	1:B:68:ARG:NE	2.48	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:A:80:HIS:CE1	1:A:84:TYR:HE2	2.33	0.47
1:B:276:GLU:OE2	1:B:307:ALA:HB3	2.15	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:A:293:LYS:HD2	1:A: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:B:293:LYS:HD2	1:B:297:LEU:CD1	2.45	0.47
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.97	0.47
1:A:80:HIS:CE1	1:A:84:TYR:HE2	2.32	0.47
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.45	0.47
1:B:66:ASP:O	1:B:69:VAL:HG22	2.14	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:293:LYS:HD2	1:A:297:LEU:CD1	2.45	0.46
1:A:66:ASP:O	1:A:69:VAL:HG22	2.14	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:A:149:CYS:SG	1:A:166:ASN:HB3	2.55	0.46
1:B:149:CYS:SG	1:B:166:ASN:HB3	2.55	0.46
1:A:92:PRO:HD2	1:A:95:GLN:OE1	2.16	0.46
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.15	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:293:LYS:HD2	1:C:297:LEU:CD1	2.46	0.46
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.15	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:A:92:PRO:HD2	1:A:95:GLN:OE1	2.16	0.46
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.16	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: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: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: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:78:LEU:O	1:B:106:ILE:HA	2.15	0.46
1:B:61:LEU:HA	1:B:324:GLN:HE21	1.81	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: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:B:36:THR:O	1:B:40:ALA:CB	2.58	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:229:LYS:HE2	1:A:270:LEU:CD2	2.45	0.45
1:A:42:ARG:HH22	1:A:303:ARG:HB2	1.81	0.45
1:B:92:PRO:HD2	1:B:95:GLN:OE1	2.16	0.45
1:B:293:LYS:HD2	1:B:297:LEU:CD1	2.46	0.45
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.34	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:A:92:PRO:HD2	1:A:95:GLN:OE1	2.17	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:57:PHE:HE2	1:A:313:TRP:HE1	1.65	0.45
1:B:57:PHE:HE2	1:B:313:TRP:HE1	1.65	0.45
1:D:301:TYR:HB2	1:D:305:LEU:HG	1.98	0.45
1:D:61:LEU:HA	1:D:324:GLN:HE21	1.81	0.45
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.46	0.45
1:B:229:LYS:HE2	1:B:270:LEU:CD2	2.45	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:A:149:CYS:SG	1:A:188:PRO:HA	2.56	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: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:A:301:TYR:HB2	1:A:305:LEU:HG	1.98	0.45
1:B:301:TYR:HB2	1:B:305:LEU:HG	1.98	0.45
1:C:197:ASP:OD1	1:C:197:ASP:N	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:N	1:D:197:ASP:OD1	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:A:147:TRP:O	1:A:187:GLU:HB3	2.16	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: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:A:280:SER:OG	1:A:334:ASN:OD1	2.24	0.45
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.52	0.45
1:B:280:SER:OG	1:B:334:ASN:OD1	2.23	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:339:GLN:HB3	1:C:341:LYS:NZ	2.31	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: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:A:82:THR:HA	1:A:85:GLN:HG2	1.99	0.45
1:B:147:TRP:O	1:B:187:GLU:HB3	2.16	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:105:GLY:CA	1:C:144:PHE:O	2.65	0.45
1:C:92:PRO:HD2	1:C:95:GLN:OE1	2.17	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:A:271:SER:O	1:A:274:GLN:HG2	2.17	0.45
1:B:271:SER:O	1:B: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:A:33:ASP:OD2	1:A:146:LYS:HE2	2.17	0.45
1:B:92:PRO:HD2	1:B:95:GLN:OE1	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:A:284:ASN:ND2	1:A:342:TYR:O	2.50	0.44
1:B:284:ASN:ND2	1:B:342:TYR:O	2.50	0.44
1:C:63:LEU:HD21	1:C:76:VAL:HG11	1.99	0.44
1:A:185:ILE:HG12	1:A:227:LEU:HB2	1.99	0.44
1:A:61:LEU:HA	1:A:324:GLN:HE21	1.82	0.44
1:B:185:ILE:HG12	1:B: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:A:34:GLU:O	1:A:59:ARG:NH2	2.50	0.44
1:B:162:ALA:O	1:B:166:ASN:ND2	2.39	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:A:339:GLN:HB3	1:A:341:LYS:NZ	2.31	0.44
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.31	0.44
1:A:229:LYS:HG2	1:A:270:LEU:CD1	2.47	0.44
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.47	0.44
1:B:33:ASP:OD2	1:B:146:LYS:HE2	2.17	0.44
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.52	0.44
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.48	0.44
1:D:57:PHE:CZ	1:D:320:LEU:HD12	2.52	0.44
1:A:195:ASP:HB3	1:A:238:ALA:HB3	1.98	0.44
1:B:195:ASP:HB3	1:B: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:339:GLN:HB3	1:D:341:LYS:NZ	2.32	0.44
1:D:63:LEU:HD21	1:D:76:VAL:HG11	1.99	0.44
1:C:60:GLN:O	1:C:64:THR:OG1	2.29	0.44
1:A:57:PHE:CZ	1:A:320:LEU:HD12	2.52	0.44
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.52	0.44
1:C:293:LYS:HD2	1:C:297:LEU:CD1	2.48	0.44
1:A:119:ASN:HB2	1:C:4:HIS:CD2	2.53	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:A:154:GLY:O	1:A:200:ARG:NH2	2.51	0.44
1:A:63:LEU:HD21	1:A:76:VAL:HG11	1.99	0.44
1:B:154:GLY:O	1:B:200:ARG:NH2	2.51	0.44
1:B:63:LEU:HD21	1:B:76:VAL:HG11	1.99	0.44
1:A:42:ARG:NH2	1:A:303:ARG:HB3	2.24	0.44
1:B:42:ARG:NH2	1:B: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:277:GLU:OE2	1:D:342:TYR:OH	2.32	0.44
1:D:57:PHE:HE2	1:D:313:TRP:HE1	1.64	0.44
1:A:197:ASP:OD1	1:A:197:ASP:N	2.51	0.44
1:B:197:ASP:OD1	1:B: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:A:229:LYS:HG2	1:A:270:LEU:CD1	2.48	0.44
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.32	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:A:339:GLN:HB3	1:A:341:LYS:NZ	2.32	0.44
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.48	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:A:77:ILE:HD11	1:A:146:LYS:CB	2.47	0.44
1:B:77:ILE:HD11	1:B:146:LYS:CB	2.47	0.44
1:C:82:THR:HA	1:C:85:GLN:HG2	1.99	0.44
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.32	0.44
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.36	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:N	1:B:197:ASP:OD1	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:OD1	1:C:197:ASP:N	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:N	1:A:197:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:PHE:CZ	1:C:320:LEU:HD12	2.54	0.43
1:C:46:ILE:HD11	1:C:314:GLY:N	2.33	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:N	1:D:197:ASP:OD1	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:A:301:TYR:HB2	1:A:305:LEU:HG	1.99	0.43
1:B:301:TYR:HB2	1:B: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:A:155:GLU:HG2	1:A:156:HIS:N	2.32	0.43
1:A:78:LEU:HD22	1:A:82:THR:HG21	2.00	0.43
1:B:155:GLU:HG2	1:B:156:HIS:N	2.32	0.43
1:B:78:LEU:HD22	1:B:82:THR:HG21	2.01	0.43
1:A:82:THR:HA	1:A:85:GLN:HG2	1.99	0.43
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.48	0.43
1:A:46:ILE:HG13	1:A:314:GLY:HA2	2.00	0.43
1:B:277:GLU:OE2	1:B:330:ARG:NH2	2.50	0.43
1:B:46:ILE:HG13	1:B:314:GLY:HA2	2.00	0.43
1:C:229:LYS:HG2	1:C:270:LEU:CD1	2.47	0.43
1:A:46:ILE:HD11	1:A:314:GLY:N	2.33	0.43
1:B:46:ILE:HD11	1:B: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:OD1	1:C:197:ASP:N	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:33:ASP:OD2	1:D:146:LYS:HE2	2.17	0.43
1:D:27:LYS:HA	1:D:72:CYS:O	2.18	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:A:63:LEU:HD21	1:A:76:VAL:HG11	2.00	0.43
1:B:63:LEU:HD21	1:B: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:A:197:ASP:N	1:A:197:ASP:OD1	2.49	0.43
1:B:197:ASP:N	1:B:197:ASP:OD1	2.49	0.43
1:D:305:LEU:HD23	1:D:330:ARG:HG3	2.01	0.43
1:C:33:ASP:OD2	1:C:146:LYS:HE2	2.17	0.43
1:C:31:ALA:HA	1:C:77:ILE:CG2	2.48	0.43
1:D:339:GLN:HB3	1:D:341:LYS:NZ	2.33	0.43
1:A:197:ASP:OD1	1:A:197:ASP:N	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:A:293:LYS:HD2	1:A:297:LEU:HD11	2.01	0.43
1:B:293:LYS:HD2	1:B: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:105:GLY:CA	1:D:144:PHE:O	2.67	0.43
1:D:36:THR:O	1:D:40:ALA:HB2	2.19	0.43
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.32	0.43
1:B:144:PHE:HA	1:B:182:ILE:HG23	2.01	0.43
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.37	0.43
1:A:146:LYS:HG2	1:A:147:TRP:N	2.34	0.43
1:A:42:ARG:HH12	1:A:303:ARG:HG3	1.84	0.43
1:A:339:GLN:HB3	1:A:341:LYS:NZ	2.34	0.43
1:B:339:GLN:HB3	1:B: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:A:144:PHE:HA	1:A:182:ILE:HG23	2.01	0.43
1:B:339:GLN:HB3	1:B:341:LYS:NZ	2.33	0.43
1:D:302:GLY:O	1:D:306:GLN:HG2	2.19	0.43
1:A:57:PHE:HZ	1:A:320:LEU:HD12	1.84	0.43
1:B:146:LYS:HG2	1:B:147:TRP:N	2.34	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:A:42:ARG:NH2	1:A:303:ARG:HB3	2.24	0.43
1:B:228:LEU:HG	1:B:230:PRO:HD3	2.01	0.43
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.54	0.43
1:C:197:ASP:OD1	1:C:197:ASP:N	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:77:ILE:HD13	1:C:144:PHE:HE1	1.83	0.43
1:C:42:ARG:HH12	1:C:303:ARG:HB3	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:A:80:HIS:CE1	1:A:84:TYR:HE2	2.37	0.42
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.84	0.42
1:A:306:GLN:O	1:A:308:SER:N	2.52	0.42
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.54	0.42
1:B:57:PHE:HZ	1:B:320:LEU:HD12	1.84	0.42
1:A:301:TYR:HB3	1:A:304:ALA:HB3	2.00	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:A:57:PHE:CZ	1:A:320:LEU:HD12	2.54	0.42
1:B:57:PHE:CZ	1:B:320:LEU:HD12	2.54	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:A:30:LEU:HD13	1:A:305:LEU:HD23	2.01	0.42
1:B:30:LEU:HD13	1:B: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:A:302:GLY:O	1:A:306:GLN:HG2	2.19	0.42
1:B:339:GLN:HB3	1:B:341:LYS:HZ3	1.84	0.42
1:A:277:GLU:HA	1:A:277:GLU:OE1	2.19	0.42
1:B:306:GLN:O	1:B:308:SER:N	2.53	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: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:119:ASN:HB2	1:D:4:HIS:CD2	2.53	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: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:302:GLY:O	1:B:306:GLN:HG2	2.19	0.42
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.01	0.42
1:A:154:GLY:O	1:A:200:ARG:NH2	2.52	0.42
1:A:31:ALA:HA	1:A:77:ILE:CG2	2.48	0.42
1:B:31:ALA:HA	1:B:77:ILE:CG2	2.48	0.42
1:B:302:GLY:O	1:B:306:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.37	0.42
1:C:302:GLY:O	1:C:306:GLN:HG2	2.19	0.42
1:D:302:GLY:O	1:D:306:GLN:HG2	2.19	0.42
1:D:80:HIS:CE1	1:D:84:TYR:HE2	2.36	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: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:A:77:ILE:HD13	1:A:144:PHE:HE1	1.83	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: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:80:HIS:CE1	1:A:84:TYR:HE2	2.37	0.42
1:A:4:HIS:CD2	1:C:119:ASN:HB2	2.54	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:A:229:LYS:HG2	1:A:270:LEU:CD1	2.50	0.42
1:B:229:LYS:HG2	1:B:270:LEU:CD1	2.50	0.42
1:D:27:LYS:HA	1:D:72:CYS:O	2.19	0.42
1:C:154:GLY:O	1:C:200:ARG:NH2	2.52	0.42
1:D:228:LEU:HG	1:D:230:PRO:HD3	2.01	0.42
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.55	0.42
1:D:77:ILE:HD11	1:D:146:LYS:CB	2.47	0.42
1:A:228:LEU:HG	1:A:230:PRO:HD3	2.02	0.42
1:A:83:LEU:HD12	1:A:94:PRO:HG3	2.00	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:66:ASP:OD2	1:A:68:ARG:HG3	2.18	0.42
1:A:27:LYS:HA	1:A:72:CYS:O	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:A:339:GLN:HB3	1:A:341:LYS:HZ3	1.84	0.42
1:B:339:GLN:HB3	1:B: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:A:276:GLU:HG3	1:A:304:ALA:O	2.20	0.42
1:A:36:THR:O	1:A:40:ALA:CB	2.67	0.42
1:B:276:GLU:HG3	1:B:304:ALA:O	2.20	0.42
1:B:36:THR:O	1:B:40:ALA:CB	2.68	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:339:GLN:HB3	1:A:341:LYS:HZ3	1.85	0.42
1:C:302:GLY:O	1:C:306:GLN:HG2	2.19	0.42
1:A:119:ASN:HB2	1:C:4:HIS:CD2	2.54	0.42
1:C:57:PHE:HE2	1:C:313:TRP:HE1	1.68	0.42
1:C:185:ILE:HG12	1:C:227:LEU:HB2	2.01	0.42
1:A:105:GLY:CA	1:A:144:PHE:O	2.67	0.42
1:B:27:LYS:HA	1:B:72:CYS:O	2.18	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:A:80:HIS:CE1	1:A:84:TYR:HE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:CE1	1:B:84:TYR:HE2	2.37	0.42
1:C:77:ILE:HD11	1:C:146:LYS:CB	2.47	0.42
1:A:77:ILE:CD1	1:A:146:LYS:HB2	2.50	0.42
1:B:77:ILE:CD1	1:B:146:LYS:HB2	2.50	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:D:57:PHE:HE2	1:D:313:TRP:HE1	1.68	0.42
1:A:276:GLU:HG2	1:A:304:ALA:O	2.19	0.42
1:B:105:GLY:CA	1:B:144:PHE:O	2.67	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:A:229:LYS:HG3	1:A:268:THR:O	2.20	0.42
1:B:229:LYS:HG3	1:B:268:THR:O	2.20	0.42
1:B:31:ALA:HA	1:B:77:ILE:HG23	2.02	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:A:27:LYS:HA	1:A:72:CYS:O	2.19	0.42
1:B:27:LYS:HA	1:B:72:CYS:O	2.19	0.42
1:C:277:GLU:OE1	1:C:277:GLU:HA	2.19	0.42
1:C:57:PHE:HZ	1:C:320:LEU:HD12	1.84	0.42
1:D:306:GLN:O	1:D:308:SER:N	2.52	0.42
1:D:57:PHE:HZ	1:D:320:LEU:HD12	1.84	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:A:63:LEU:HD21	1:A:76:VAL:HG11	2.02	0.42
1:B:63:LEU:HD21	1:B: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:OE1	1:D:277:GLU:HA	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:A:275:SER:HB3	1:A:278:GLU:HG2	2.02	0.41
1:A:51:THR:HG23	1:A:54:ASN:H	1.85	0.41
1:B:275:SER:HB3	1:B: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:A:118:THR:CG2	1:A:121:GLU:HB2	2.50	0.41
1:B:118:THR:CG2	1:B: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:A:83:LEU:HD12	1:A:94:PRO:HG3	2.00	0.41
1:B:83:LEU:HD12	1:B: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:N	1:B:132:GLU:OE1	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:A:77:ILE:CD1	1:A:146:LYS:HB2	2.41	0.41
1:B:77:ILE:CD1	1:B:146:LYS:HB2	2.41	0.41
1:A:144:PHE:HA	1:A:182:ILE:HG23	2.02	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: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:A:132:GLU:N	1:A:132:GLU:OE1	2.53	0.41
1:B:22:ILE:HG12	1:B:103:VAL:CG2	2.48	0.41
1:C:132:GLU:OE1	1:C:132:GLU:N	2.53	0.41
1:C:30:LEU:HD13	1:C:305:LEU:HD23	2.01	0.41
1:D:132:GLU:N	1:D:132:GLU:OE1	2.53	0.41
1:D:30:LEU:HD13	1:D:305:LEU:HD23	2.01	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:A:68:ARG:NH2	1:A:325:GLU:OE1	2.40	0.41
1:B:168:ASN:HD22	1:D:168:ASN:ND2	2.18	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:A:4:HIS:CD2	1:C:119:ASN:HB2	2.55	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: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:229:LYS:HG3	1:C:268:THR:O	2.20	0.41
1:C:42:ARG:HD3	1:C:310:LEU:HD11	2.03	0.41
1:D:229:LYS:HG3	1:D:268:THR:O	2.20	0.41
1:D:42:ARG:HD3	1:D:310:LEU:HD11	2.03	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:A:301:TYR:HB2	1:A:305:LEU:HG	2.02	0.41
1:A:77:ILE:HD13	1:A:77:ILE:HG21	1.88	0.41
1:B:155:GLU:HG2	1:B:156:HIS:CD2	2.56	0.41
1:C:108:VAL:HG23	1:C:147:TRP:HE3	1.86	0.41
1:C:77:ILE:CD1	1:C:146:LYS:HB2	2.50	0.41
1:D:108:VAL:HG23	1:D:147:TRP:HE3	1.86	0.41
1:D:77:ILE:CD1	1:D:146:LYS:HB2	2.50	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:144:PHE:HA	1:B:182:ILE:HG23	2.02	0.41
1:B:77:ILE:HD13	1:B:77:ILE:HG21	1.88	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:D:27:LYS:HA	1:D:72:CYS:O	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:A:271:SER:HB3	1:A:301:TYR:CD1	2.56	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: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:A:27:LYS:HA	1:A:72:CYS:O	2.19	0.41
1:B:301:TYR:HB2	1:B:305:LEU:HG	2.03	0.41
1:B:27:LYS:HA	1:B: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:A:301:TYR:HB2	1:A:305:LEU:HG	2.03	0.41
1:A:35:SER:O	1:A:39:ILE:HG22	2.21	0.41
1:B:35:SER:O	1:B:39:ILE:HG22	2.21	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:A:195:ASP:O	1:A:196:HIS:ND1	2.54	0.41
1:B:195:ASP:O	1:B:196:HIS:ND1	2.54	0.41
1:B:49:GLU:O	1:B:54:ASN:ND2	2.43	0.41
1:D:105:GLY:CA	1:D:144:PHE:O	2.69	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: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:C:339:GLN:HB3	1:C:341:LYS:NZ	2.36	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:B:4:HIS:CD2	1:D:119:ASN:HB2	2.55	0.41
1:D:155:GLU:HG2	1:D:156:HIS:CD2	2.56	0.41
1:B:119:ASN:HB2	1:D:4:HIS:CD2	2.55	0.41
1:B:83:LEU:HD12	1:B:94:PRO:HG3	2.01	0.41
1:A:108:VAL:HG23	1:A:147:TRP:HE3	1.86	0.41
1:A:83:LEU:HD12	1:A:94:PRO:HG3	2.01	0.41
1:B:108:VAL:HG23	1:B:147:TRP:HE3	1.86	0.41
1:C:108:VAL:HG23	1:C:147:TRP:HE3	1.86	0.41
1:C:271:SER:HB3	1:C:301:TYR:CD1	2.56	0.41
1:C:257:ARG:NH1	1:C:292:LEU:O	2.53	0.41
1:D:271:SER:HB3	1:D:301:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ARG:NH1	1:D:292:LEU:O	2.53	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: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:185:ILE:HG12	1:A:227:LEU:HB2	2.03	0.41
1:B:229:LYS:HG3	1:B:268:THR:O	2.21	0.41
1:C:253:VAL:O	1:C:257:ARG:HG3	2.20	0.41
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.56	0.41
1:D:253:VAL:O	1:D:257:ARG:HG3	2.20	0.41
1:B:77:ILE:HG21	1:B:77:ILE:HD13	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:A:339:GLN:HB3	1:A:341:LYS:NZ	2.36	0.41
1:B:339:GLN:HB3	1:B: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:155:GLU:HG2	1:C:156:HIS:CD2	2.56	0.41
1:C:147:TRP:HB2	1:C:173:TYR:CZ	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:108:VAL:HG23	1:B:147:TRP:HE3	1.86	0.40
1:B:27:LYS:HA	1:B:72:CYS:O	2.20	0.40
1:D:147:TRP:HB2	1:D:173:TYR:CZ	2.56	0.40
1:A:37:GLY:O	1:A:40:ALA:HB3	2.21	0.40
1:B:37:GLY:O	1:B: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:A:77:ILE:HG21	1:A:77:ILE:HD13	1.85	0.40
1:B:4:HIS:CD2	1:D:119:ASN:HB2	2.56	0.40
1:A:293:LYS:HD2	1:A:297:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HD3	1:A:310:LEU:HD11	2.03	0.40
1:C:63:LEU:HD22	1:C:97:ILE:HG12	2.03	0.40
1:A:27:LYS:HA	1:A:72:CYS:O	2.20	0.40
1:B:27:LYS:HA	1:B:72:CYS:O	2.20	0.40
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.51	0.40
1:A:27:LYS:HA	1:A:72:CYS:O	2.20	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:A:185:ILE:HG12	1:A:227:LEU:HB2	2.03	0.40
1:A:77:ILE:HD13	1:A:77:ILE:HG21	1.87	0.40
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.04	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:A:57:PHE:HE2	1:A:313:TRP:NE1	2.19	0.40
1:B:280:SER:OG	1:B:334:ASN:OD1	2.27	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:185:ILE:HG12	1:C:227:LEU:HB2	2.03	0.40
1:C:57:PHE:HZ	1:C:320:LEU:HD12	1.85	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:A:185:ILE:HG12	1:A:227:LEU:HB2	2.04	0.40
1:B:195:ASP:HB3	1:B:238:ALA:HB3	2.02	0.40
1:D:229:LYS:HG3	1:D:268:THR:O	2.21	0.40
1:A:108:VAL:HG23	1:A:147:TRP:HE3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:147:TRP:HB2	1:B:173:TYR:CZ	2.56	0.40
1:B:229:LYS:HD3	1:B: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:305:LEU:HD13	1:C:334:ASN:HD22	1.85	0.40
1:C:49:GLU:O	1:C:54:ASN:ND2	2.39	0.40
1:A:186:VAL:HG12	1:A:188:PRO:HD3	2.04	0.40
1:A:57:PHE:HE2	1:A:313:TRP:HE1	1.68	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:A:195:ASP:HB3	1:A:238:ALA:HB3	2.03	0.40
1:B:185:ILE:HG12	1:B:227:LEU:HB2	2.04	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:A:58:TYR:O	1:A:61:LEU:HB3	2.22	0.40
1:B:58:TYR:O	1:B: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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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%)	44	70
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%)	44	70
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%)	44	70
1	9-B	341/363 (94%)	333 (98%)	7 (2%)	1 (0%)	44	70
1	9-C	341/363 (94%)	333 (98%)	7 (2%)	1 (0%)	44	70
1	9-D	341/363 (94%)	333 (98%)	7 (2%)	1 (0%)	44	70
1	10-A	341/363 (94%)	329 (96%)	11 (3%)	1 (0%)	44	70
1	10-B	341/363 (94%)	329 (96%)	11 (3%)	1 (0%)	44	70
1	10-C	341/363 (94%)	329 (96%)	11 (3%)	1 (0%)	44	70
1	10-D	341/363 (94%)	329 (96%)	11 (3%)	1 (0%)	44	70
All	All	13640/14520 (94%)	13256 (97%)	374 (3%)	10 (0%)	58	79

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 ⓘ

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%)	93	98
1	1-B	278/291 (96%)	277 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-C	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	1-D	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	2-A	278/291 (96%)	276 (99%)	2 (1%)	87	96
1	2-B	278/291 (96%)	276 (99%)	2 (1%)	87	96
1	2-C	278/291 (96%)	276 (99%)	2 (1%)	87	96
1	2-D	278/291 (96%)	276 (99%)	2 (1%)	87	96
1	3-A	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	3-B	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	3-C	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	3-D	278/291 (96%)	277 (100%)	1 (0%)	93	98
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%)	87	96
1	5-B	278/291 (96%)	276 (99%)	2 (1%)	87	96
1	5-C	278/291 (96%)	276 (99%)	2 (1%)	87	96
1	5-D	278/291 (96%)	276 (99%)	2 (1%)	87	96
1	6-A	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	6-B	278/291 (96%)	278 (100%)	0	100	100
1	6-C	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	6-D	278/291 (96%)	277 (100%)	1 (0%)	93	98
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%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9-B	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	9-C	278/291 (96%)	277 (100%)	1 (0%)	93	98
1	9-D	278/291 (96%)	277 (100%)	1 (0%)	93	98
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%)	94	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

Some 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

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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 carbohydrates 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.