



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:53 am BST

PDB ID : 2Q41  
Title : Ensemble refinement of the protein crystal structure of spermidine synthase from *Arabidopsis thaliana* gene At1g23820  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

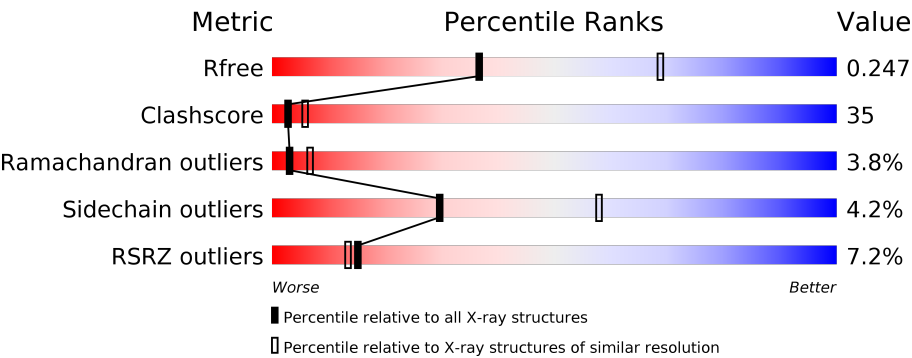
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	334	<div><div>7%</div><div><div></div><div>40%</div><div>43%</div><div>•</div><div>13%</div></div></div>
1	1-B	334	<div><div>3%</div><div><div></div><div>47%</div><div>36%</div><div>•</div><div>15%</div></div></div>
1	1-C	334	<div><div>11%</div><div><div></div><div>40%</div><div>43%</div><div>•</div><div>13%</div></div></div>
1	1-D	334	<div><div>4%</div><div><div></div><div>43%</div><div>38%</div><div>•</div><div>15%</div></div></div>
1	2-A	334	<div><div>7%</div><div><div></div><div>35%</div><div>48%</div><div>•</div><div>13%</div></div></div>
1	2-B	334	<div><div>3%</div><div><div></div><div>39%</div><div>43%</div><div>•</div><div>15%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	2-C	334	
1	2-D	334	
1	3-A	334	
1	3-B	334	
1	3-C	334	
1	3-D	334	
1	4-A	334	
1	4-B	334	
1	4-C	334	
1	4-D	334	
1	5-A	334	
1	5-B	334	
1	5-C	334	
1	5-D	334	
1	6-A	334	
1	6-B	334	
1	6-C	334	
1	6-D	334	
1	7-A	334	
1	7-B	334	
1	7-C	334	
1	7-D	334	
1	8-A	334	
1	8-B	334	
1	8-C	334	

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Mol	Chain	Length	Quality of chain
1	8-D	334	<div><div></div><div>4%</div><div>40%</div><div>41%</div><div>•</div><div>15%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 75520 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Spermidine synthase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	2-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	3-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	4-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	5-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	6-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	7-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	8-A	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	1-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	2-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	3-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	4-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	5-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	6-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	7-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	8-B	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	2-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	3-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	4-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	5-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	6-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	7-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	8-C	290	Total	C	N	O	S	Se	0	0	0
			2234	1433	361	426	7	7			
1	1-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	2-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	3-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	4-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	5-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	6-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	7-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			
1	8-D	285	Total	C	N	O	S	Se	0	0	0
			2198	1417	354	412	8	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9ZUB3
A	26	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	51	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	54	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	149	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	155	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	242	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
A	278	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	1	SER	-	EXPRESSION TAG	UNP Q9ZUB3
B	26	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	51	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	54	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	109	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	149	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	155	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	242	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
B	278	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	1	SER	-	EXPRESSION TAG	UNP Q9ZUB3
C	26	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	51	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	54	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	109	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	149	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	155	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	242	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
C	278	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	1	SER	-	EXPRESSION TAG	UNP Q9ZUB3
D	26	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	51	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	54	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	109	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	149	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	155	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	242	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3
D	278	MSE	MET	MODIFIED RESIDUE	UNP Q9ZUB3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	130	Total O 130 130	0	0
2	2-A	137	Total O 137 137	0	0
2	3-A	135	Total O 135 135	0	0
2	4-A	134	Total O 134 134	0	0
2	5-A	134	Total O 134 134	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-A	135	Total 135	O 135	0	0
2	7-A	128	Total 128	O 128	0	0
2	8-A	135	Total 135	O 135	0	0
2	1-B	177	Total 177	O 177	0	0
2	2-B	179	Total 179	O 179	0	0
2	3-B	175	Total 175	O 175	0	0
2	4-B	173	Total 173	O 173	0	0
2	5-B	171	Total 171	O 171	0	0
2	6-B	176	Total 176	O 176	0	0
2	7-B	177	Total 177	O 177	0	0
2	8-B	173	Total 173	O 173	0	0
2	1-C	135	Total 135	O 135	0	0
2	2-C	129	Total 129	O 129	0	0
2	3-C	132	Total 132	O 132	0	0
2	4-C	135	Total 135	O 135	0	0
2	5-C	138	Total 138	O 138	0	0
2	6-C	132	Total 132	O 132	0	0
2	7-C	133	Total 133	O 133	0	0
2	8-C	133	Total 133	O 133	0	0
2	1-D	134	Total 134	O 134	0	0
2	2-D	131	Total 131	O 131	0	0

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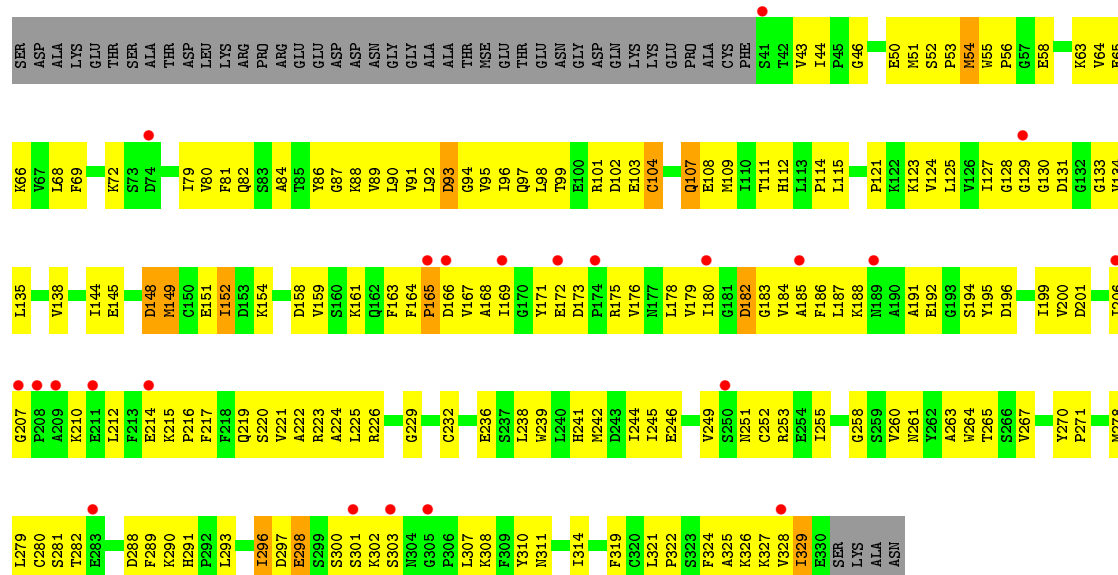


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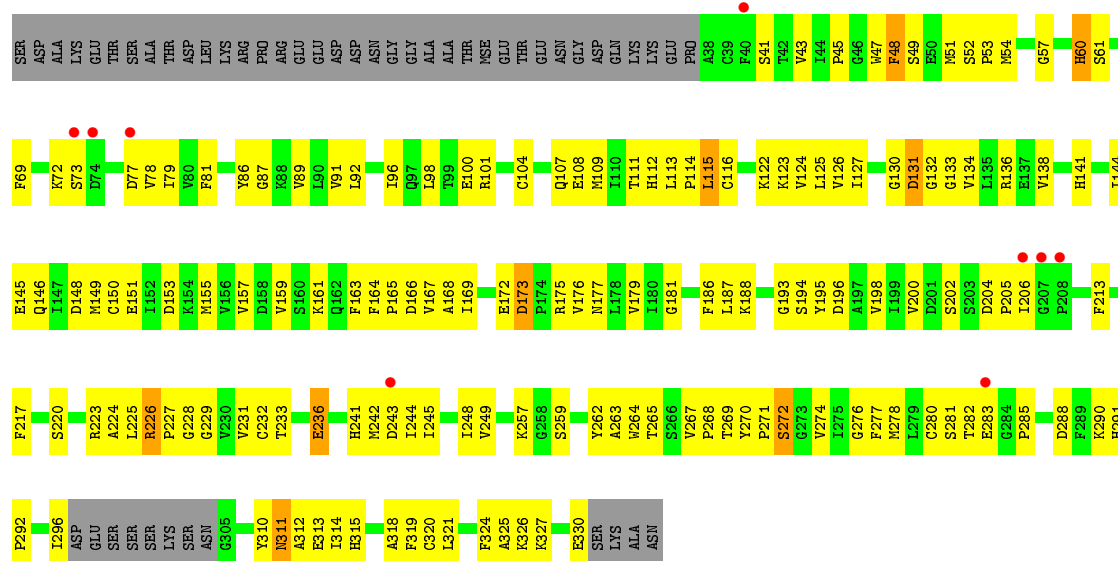
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-D	134	Total 134	O 134	0	0
2	4-D	134	Total 134	O 134	0	0
2	5-D	133	Total 133	O 133	0	0
2	6-D	133	Total 133	O 133	0	0
2	7-D	138	Total 138	O 138	0	0
2	8-D	135	Total 135	O 135	0	0



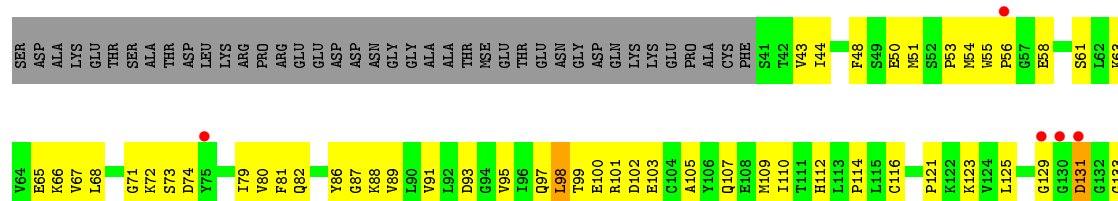
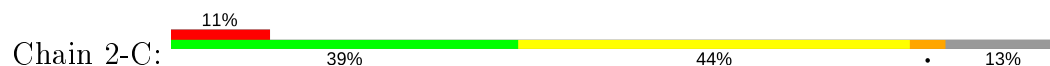


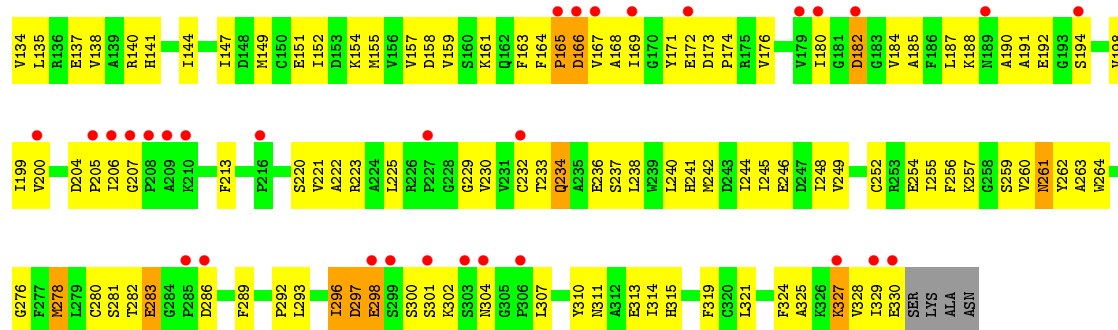


• Molecule 1: Spermidine synthase 1

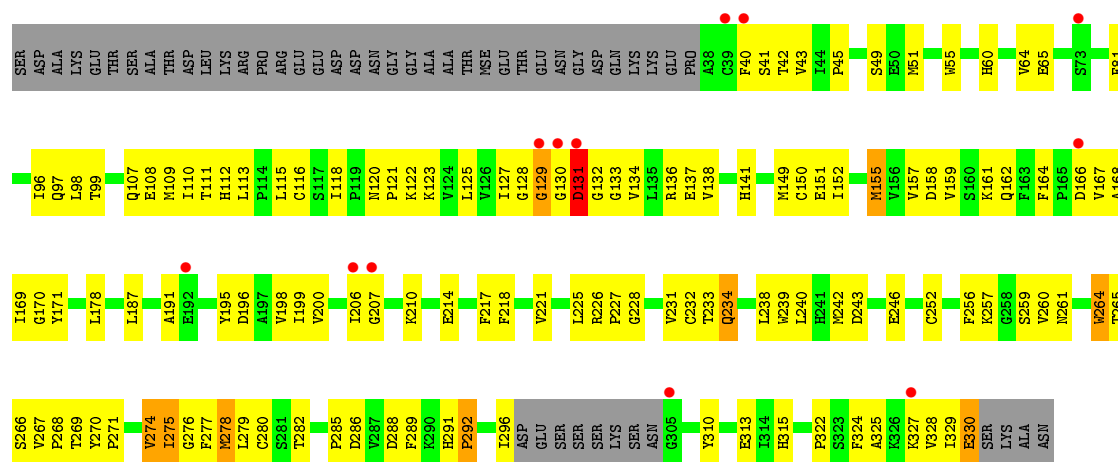


• Molecule 1: Spermidine synthase 1

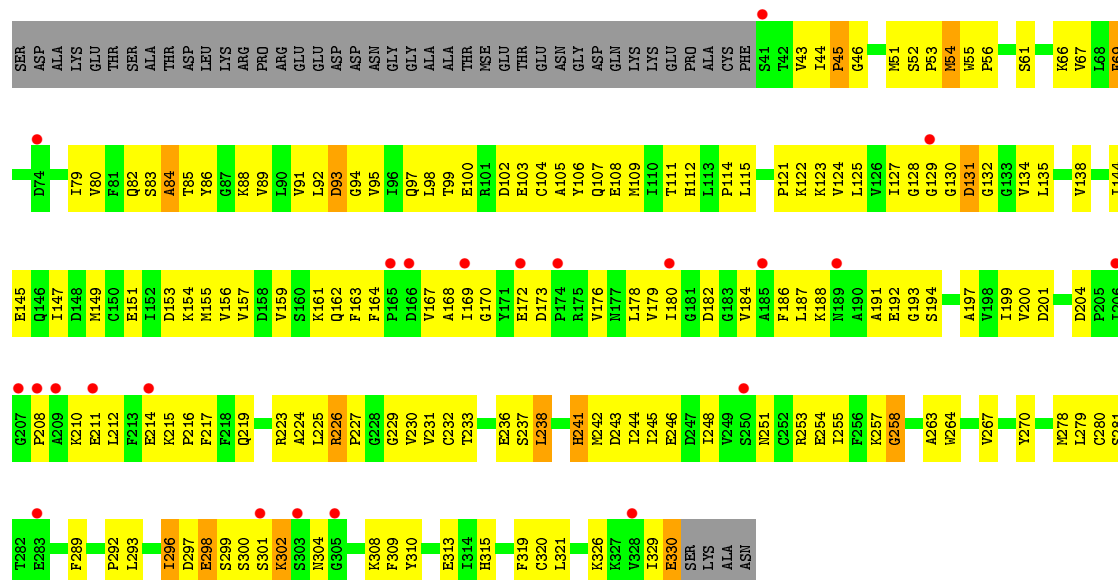




• Molecule 1: Spermidine synthase 1



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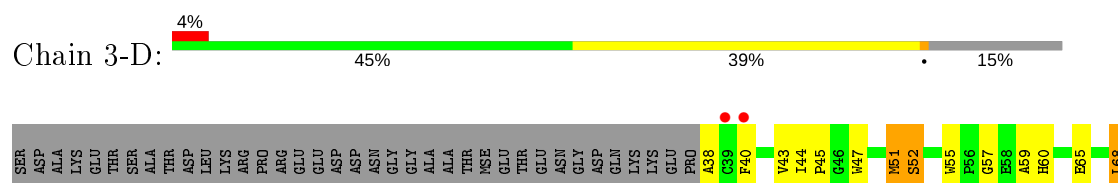
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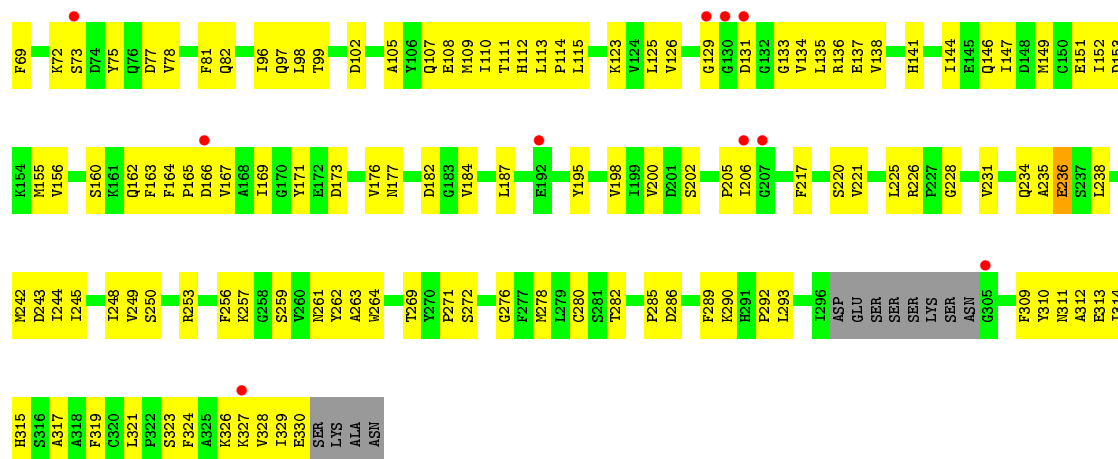


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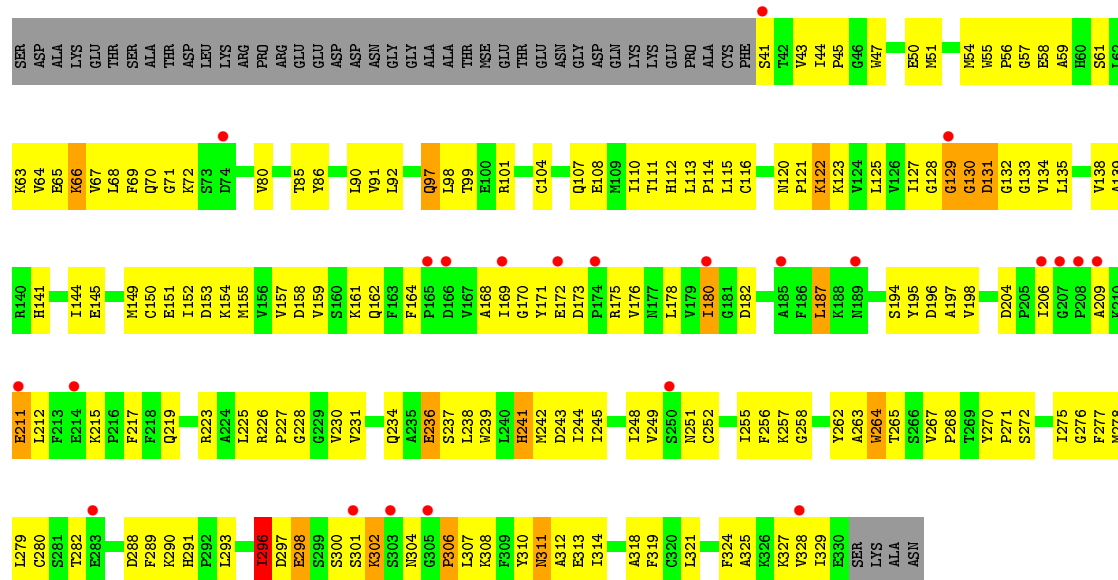


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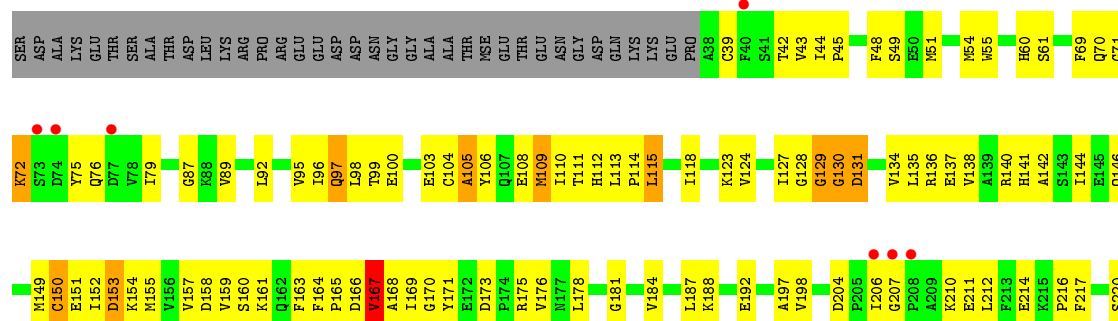
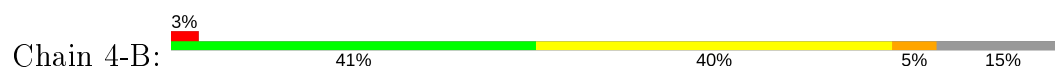


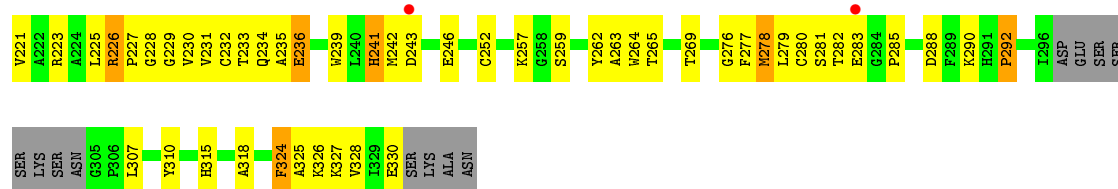


• Molecule 1: Spermidine synthase 1

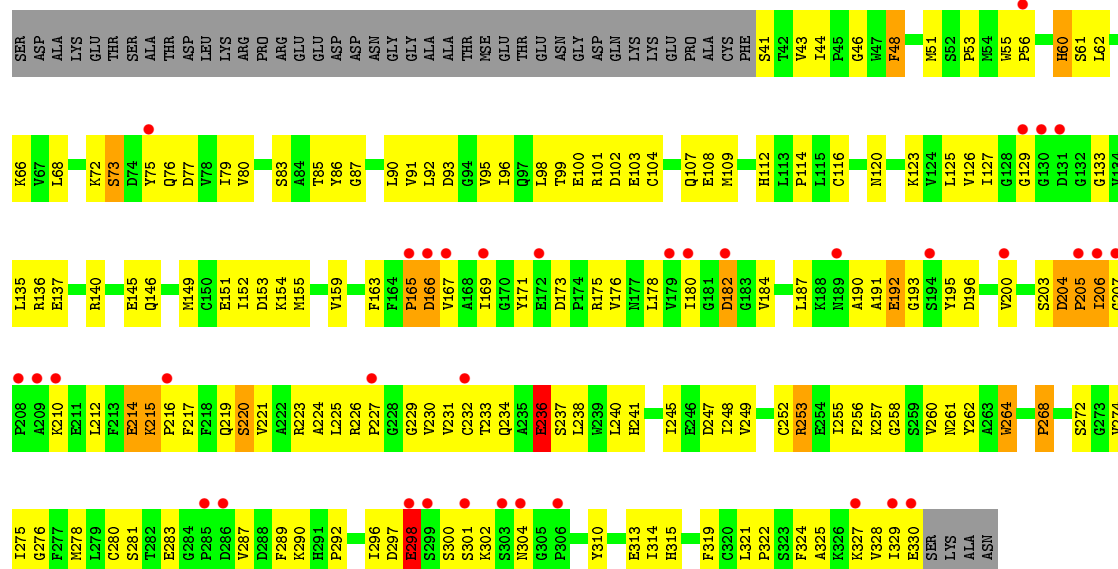


• Molecule 1: Spermidine synthase 1

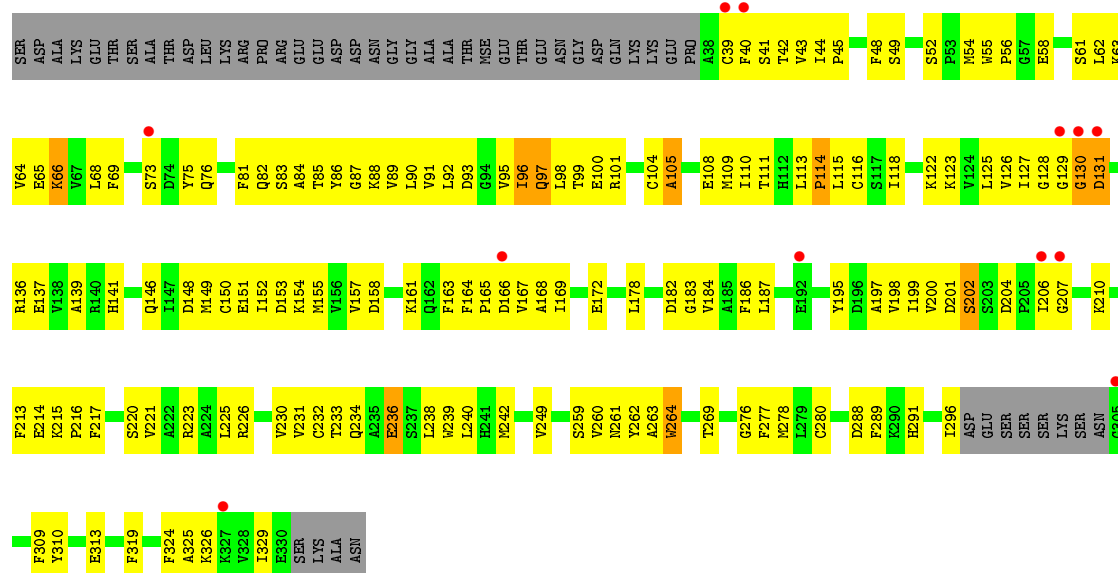
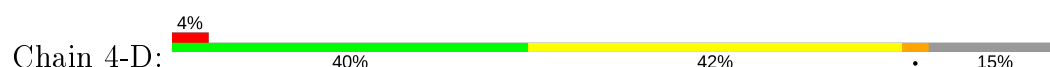




• Molecule 1: Spermidine synthase 1



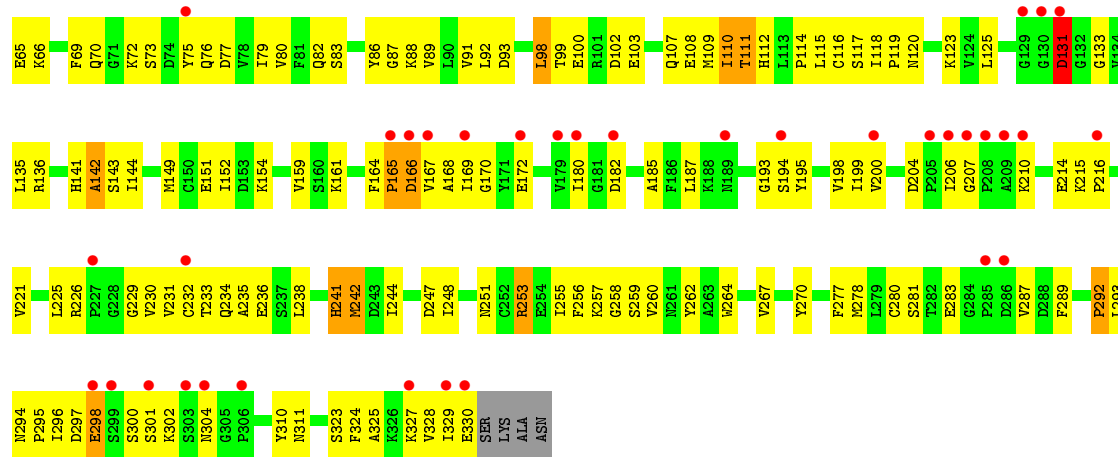
• Molecule 1: Spermidine synthase 1



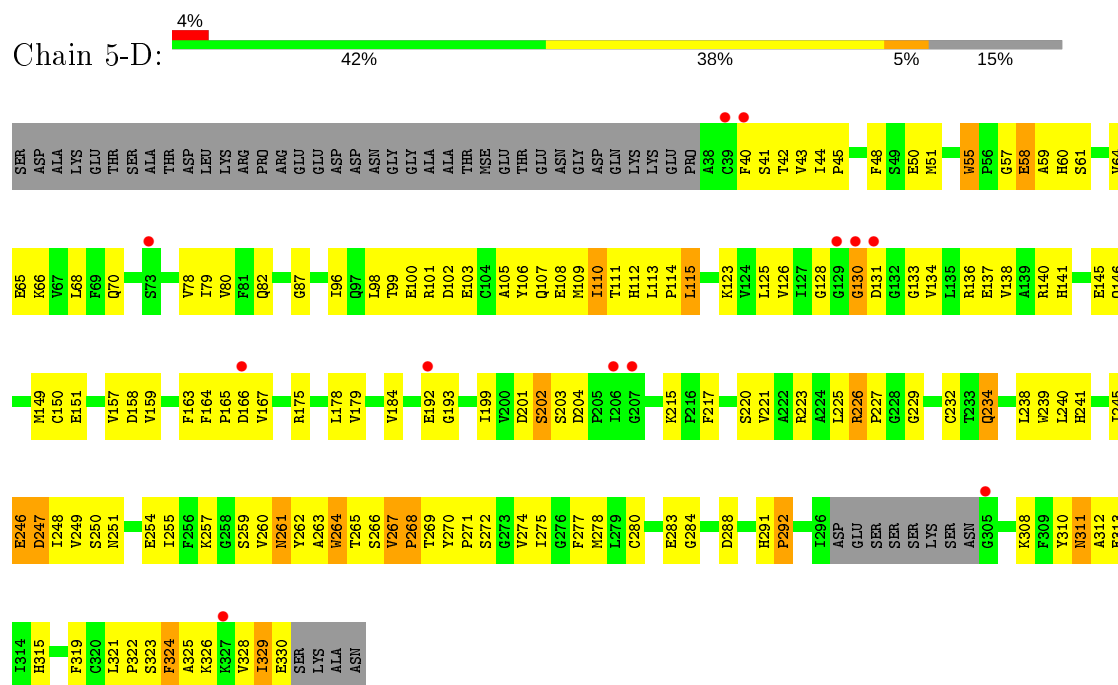
• Molecule 1: Spermidine synthase 1



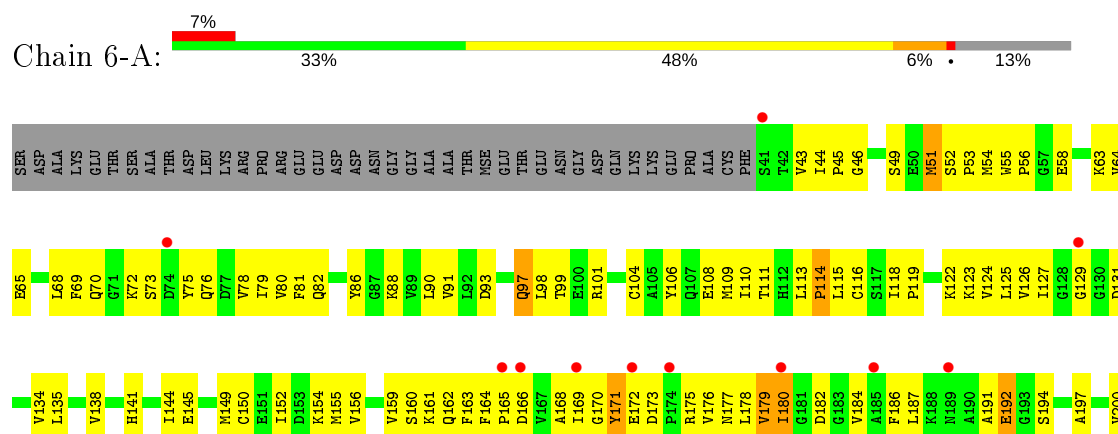


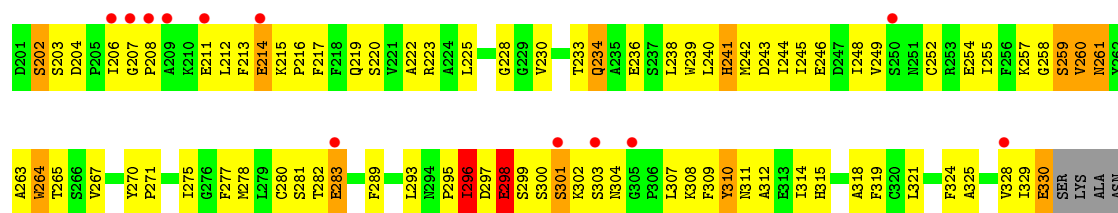


• Molecule 1: Spermidine synthase 1

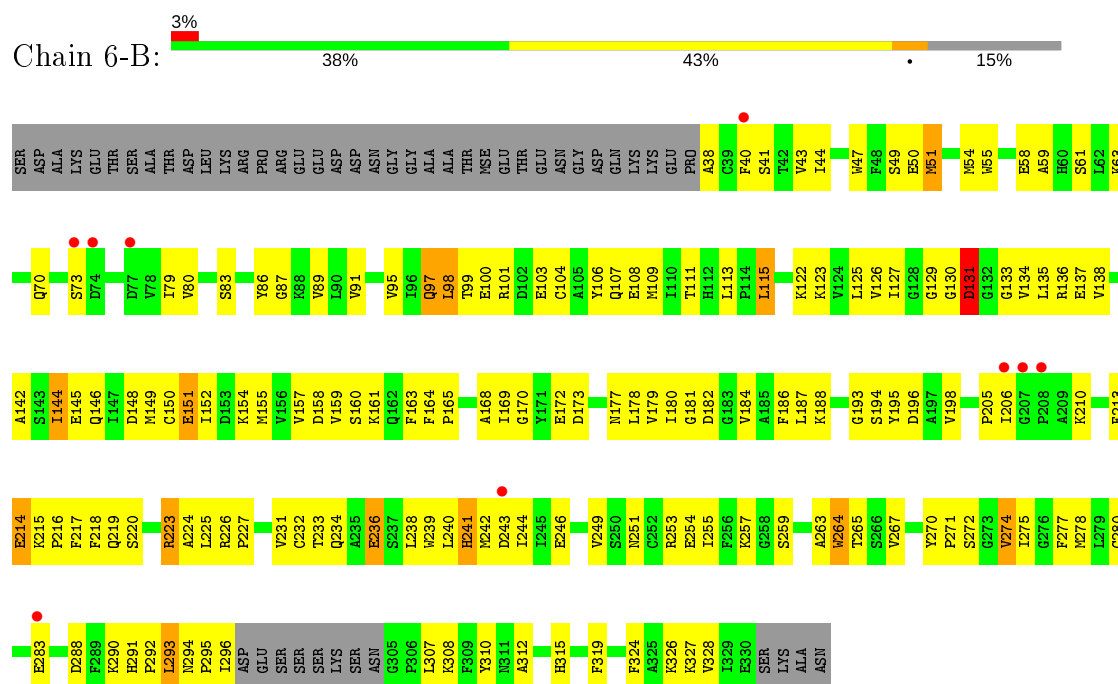


• Molecule 1: Spermidine synthase 1

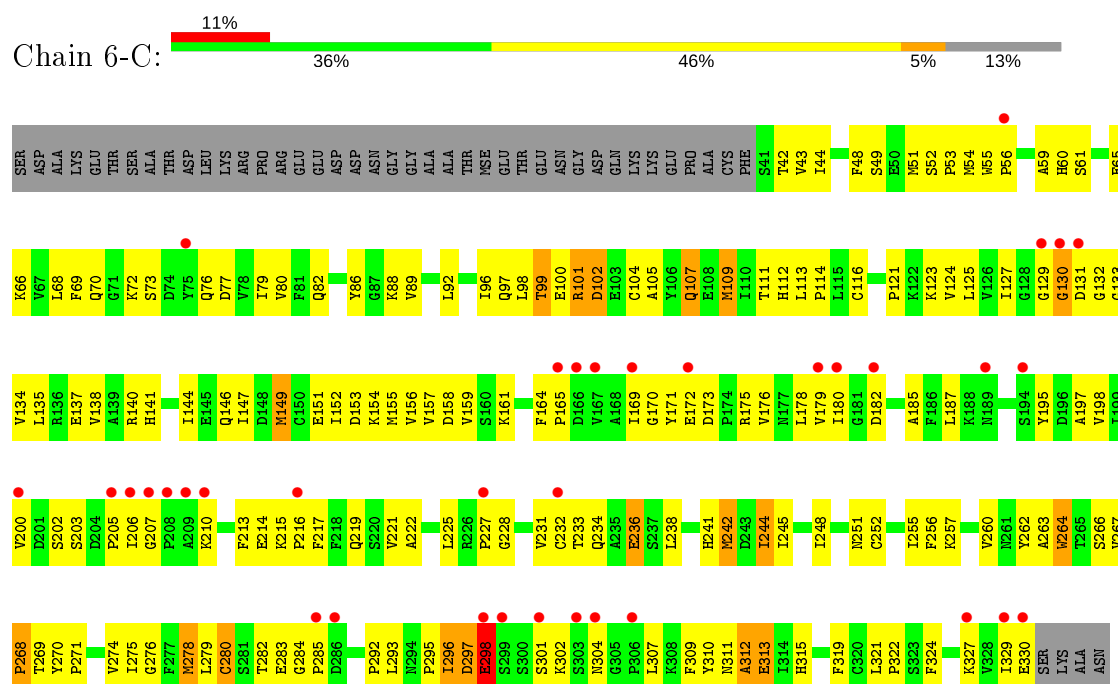




- Molecule 1: Spermidine synthase 1



- Molecule 1: Spermidine synthase 1



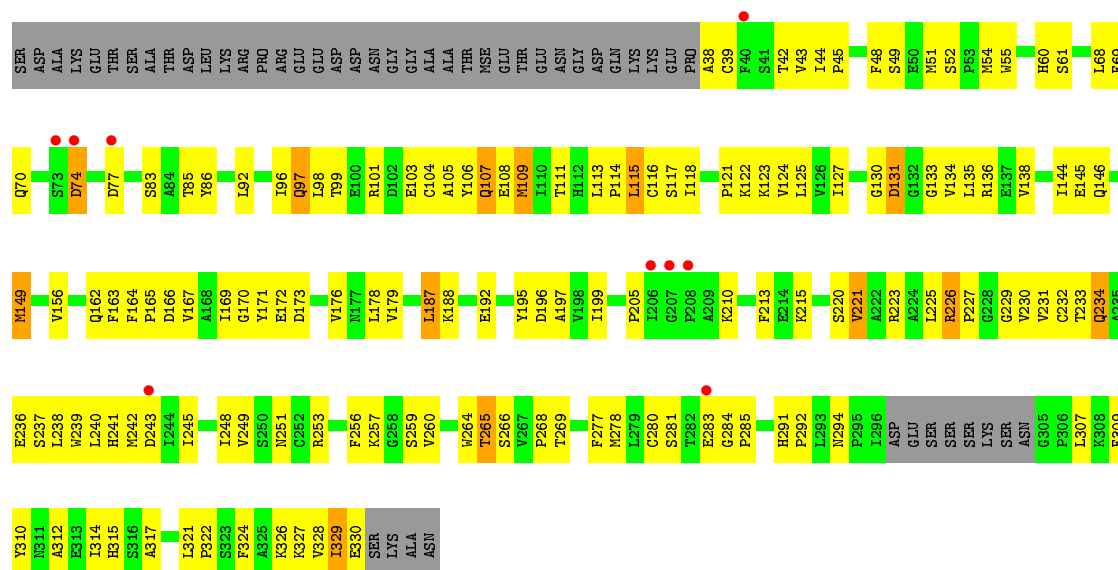
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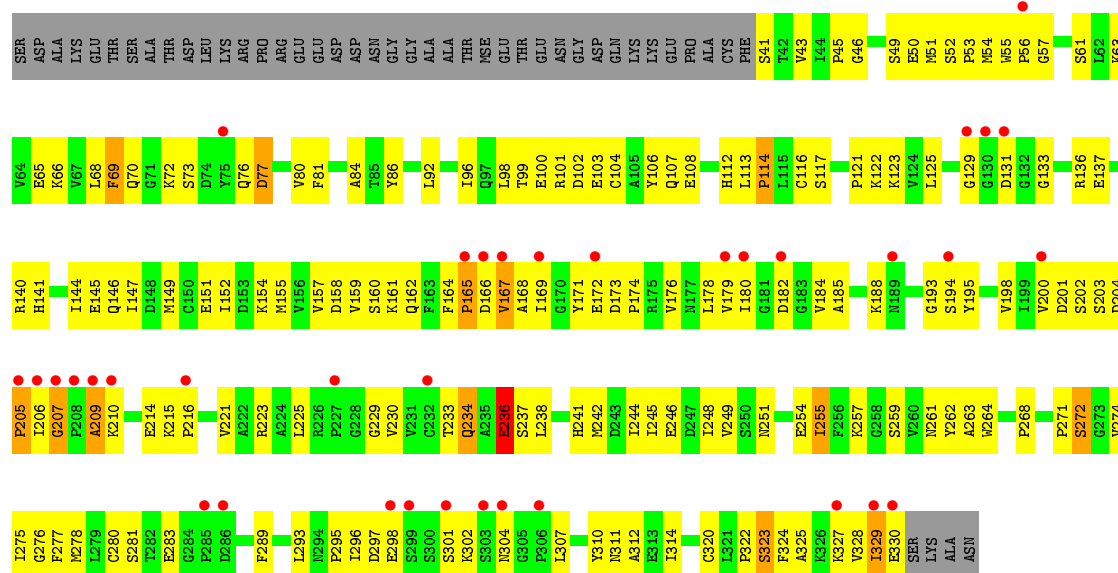
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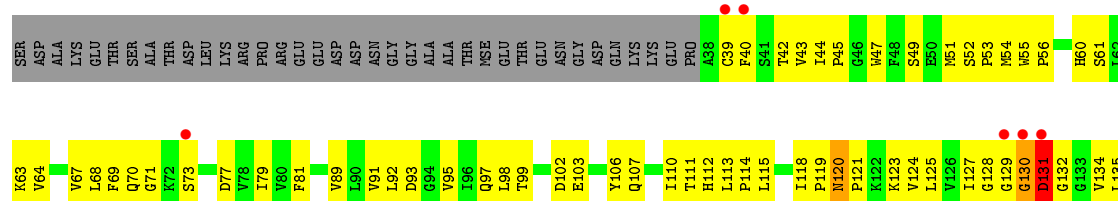
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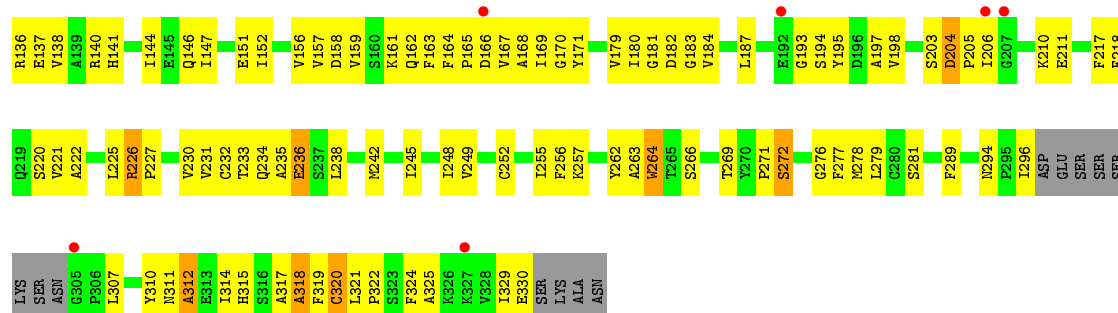


- Molecule 1: Spermidine synthase 1

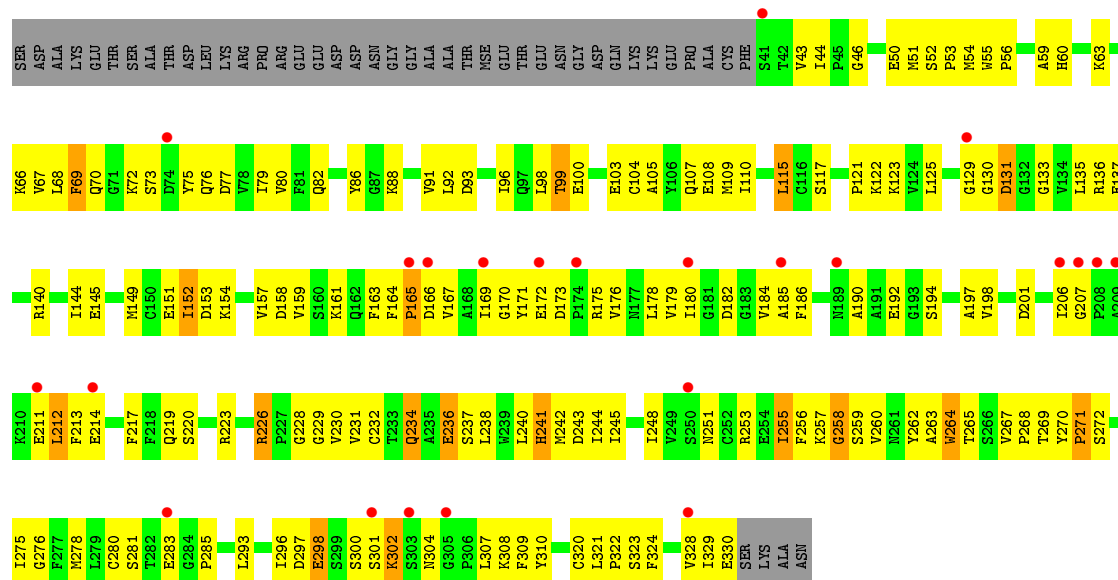


- Molecule 1: Spermidine synthase 1

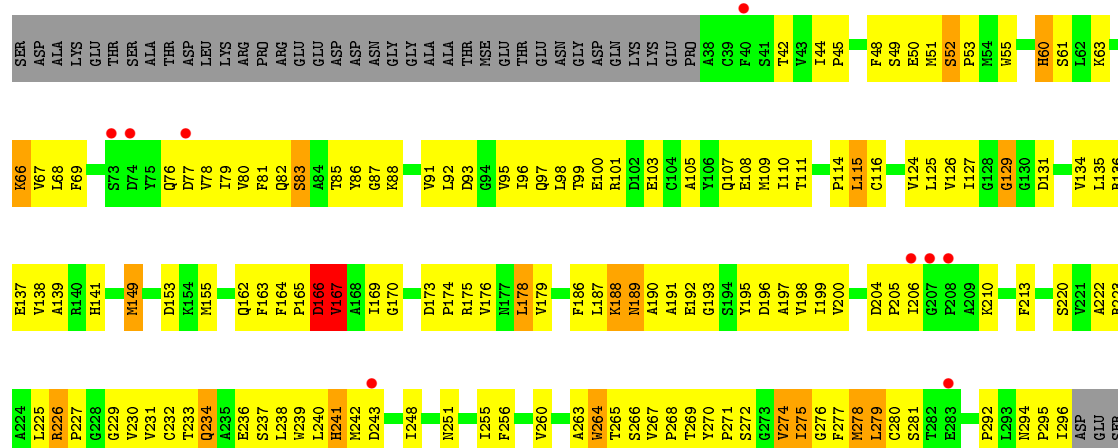


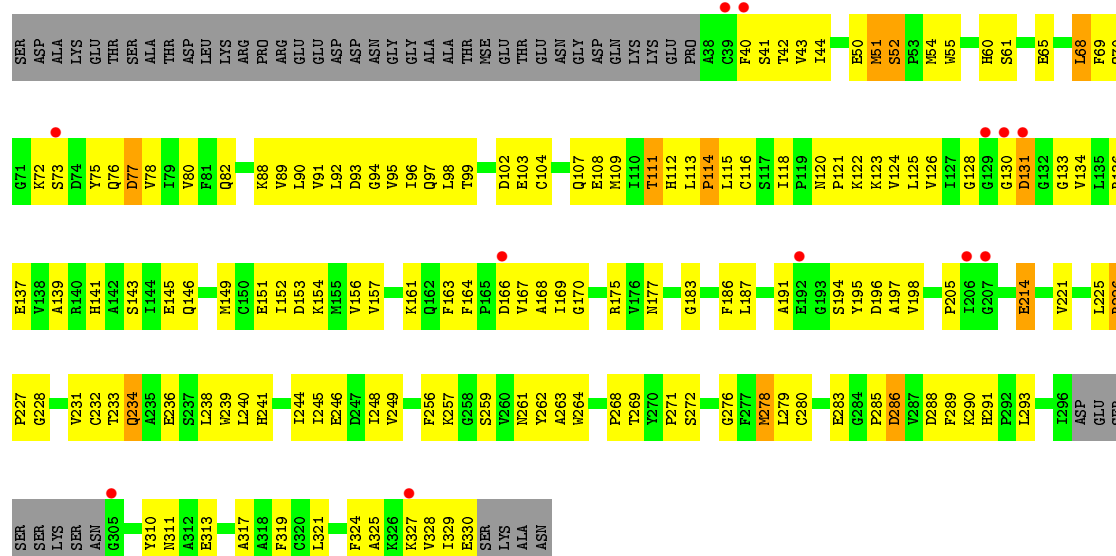


• Molecule 1: Spermidine synthase 1



• Molecule 1: Spermidine synthase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.81Å 95.21Å 89.16Å 90.00° 104.96° 90.00°	Depositor
Resolution (Å)	26.29 – 2.70 26.28 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.5 (26.29-2.70) 94.0 (26.28-2.66)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.164 , 0.249 0.167 , 0.247	Depositor DCC
$R_{free}$ test set	3788 reflections (9.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	75520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1-A	0.37	0/2282	0.61	0/3089
1	1-B	0.39	0/2246	0.61	0/3040
1	1-C	0.37	0/2282	0.62	0/3089
1	1-D	0.39	0/2246	0.61	0/3040
1	2-A	0.36	0/2282	0.60	0/3089
1	2-B	0.39	0/2246	0.62	0/3040
1	2-C	0.37	0/2282	0.62	0/3089
1	2-D	0.39	0/2246	0.62	0/3040
1	3-A	0.37	0/2282	0.61	0/3089
1	3-B	0.40	0/2246	0.62	0/3040
1	3-C	0.38	0/2282	0.61	0/3089
1	3-D	0.39	0/2246	0.62	0/3040
1	4-A	0.38	0/2282	0.59	0/3089
1	4-B	0.41	0/2246	0.63	1/3040 (0.0%)
1	4-C	0.38	0/2282	0.62	0/3089
1	4-D	0.38	0/2246	0.61	0/3040
1	5-A	0.39	0/2282	0.63	0/3089
1	5-B	0.43	0/2246	0.65	1/3040 (0.0%)
1	5-C	0.40	0/2282	0.64	0/3089
1	5-D	0.41	0/2246	0.65	0/3040
1	6-A	0.40	0/2282	0.63	0/3089
1	6-B	0.41	0/2246	0.63	0/3040
1	6-C	0.39	0/2282	0.64	0/3089
1	6-D	0.40	0/2246	0.65	0/3040
1	7-A	0.38	0/2282	0.63	0/3089
1	7-B	0.40	0/2246	0.62	0/3040
1	7-C	0.41	0/2282	0.64	0/3089
1	7-D	0.41	0/2246	0.64	0/3040
1	8-A	0.39	0/2282	0.63	0/3089
1	8-B	0.41	0/2246	0.63	0/3040
1	8-C	0.41	0/2282	0.66	0/3089
1	8-D	0.41	0/2246	0.64	0/3040
All	All	0.39	0/72448	0.63	2/98064 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-B	109	MSE	CA-CB-CG	-6.46	102.32	113.30
1	5-B	109	MSE	CB-CA-C	5.31	121.01	110.40

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	2234	0	2199	160	0
1	1-B	2198	0	2168	122	0
1	1-C	2234	0	2199	148	0
1	1-D	2198	0	2168	142	0
1	2-A	2234	0	2199	181	0
1	2-B	2198	0	2168	140	0
1	2-C	2234	0	2199	167	0
1	2-D	2198	0	2168	128	0
1	3-A	2234	0	2199	152	0
1	3-B	2198	0	2168	180	0
1	3-C	2234	0	2199	213	0
1	3-D	2198	0	2168	126	0
1	4-A	2234	0	2199	204	0
1	4-B	2198	0	2168	154	0
1	4-C	2234	0	2199	172	0
1	4-D	2198	0	2168	155	0
1	5-A	2234	0	2199	188	0
1	5-B	2198	0	2168	115	0
1	5-C	2234	0	2199	150	0
1	5-D	2198	0	2168	149	0
1	6-A	2234	0	2199	209	0
1	6-B	2198	0	2168	148	0
1	6-C	2234	0	2199	200	0
1	6-D	2198	0	2168	140	0
1	7-A	2234	0	2199	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7-B	2198	0	2168	136	0
1	7-C	2234	0	2199	161	0
1	7-D	2198	0	2168	156	0
1	8-A	2234	0	2199	162	0
1	8-B	2198	0	2168	169	0
1	8-C	2234	0	2199	146	0
1	8-D	2198	0	2168	167	0
2	1-A	130	0	0	4	0
2	1-B	177	0	0	10	0
2	1-C	135	0	0	9	0
2	1-D	134	0	0	6	0
2	2-A	137	0	0	5	0
2	2-B	179	0	0	13	0
2	2-C	129	0	0	9	0
2	2-D	131	0	0	8	0
2	3-A	135	0	0	6	0
2	3-B	175	0	0	10	0
2	3-C	132	0	0	16	0
2	3-D	134	0	0	4	0
2	4-A	134	0	0	10	0
2	4-B	173	0	0	11	0
2	4-C	135	0	0	15	0
2	4-D	134	0	0	6	0
2	5-A	134	0	0	7	0
2	5-B	171	0	0	14	0
2	5-C	138	0	0	7	0
2	5-D	133	0	0	16	0
2	6-A	135	0	0	7	0
2	6-B	176	0	0	12	0
2	6-C	132	0	0	7	0
2	6-D	133	0	0	9	0
2	7-A	128	0	0	13	0
2	7-B	177	0	0	12	0
2	7-C	133	0	0	9	0
2	7-D	138	0	0	13	0
2	8-A	135	0	0	7	0
2	8-B	173	0	0	16	0
2	8-C	133	0	0	7	0
2	8-D	135	0	0	14	0
All	All	75520	0	69872	4966	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (4966) 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:C:124:VAL:HG22	1:C:197:ALA:HB3	1.25	1.18
1:A:135:LEU:HD22	1:A:149:MSE:HE2	1.28	1.14
1:A:241:HIS:HB3	2:A:427:HOH:O	1.45	1.13
1:A:238:LEU:HA	1:A:242:MSE:HE3	1.37	1.06
1:C:198:VAL:HB	1:C:231:VAL:HG22	1.34	1.04
1:A:234:GLN:HE22	1:A:275:ILE:HD11	1.22	1.04
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.19	1.02
1:B:51:MSE:HE1	1:C:44:ILE:HD12	1.39	1.02
1:C:249:VAL:HA	1:C:278:MSE:HE2	1.36	1.02
1:B:73:SER:HB3	1:B:155:MSE:SE	2.09	1.02
1:C:140:ARG:HH12	1:C:301:SER:HB2	1.22	1.01
1:B:260:VAL:HG13	1:B:278:MSE:HE1	1.40	1.01
1:A:80:VAL:HG21	1:A:159:VAL:HG11	1.40	1.00
1:A:259:SER:H	1:A:281:SER:HB3	1.22	1.00
1:A:253:ARG:HH22	1:A:330:GLU:HB3	1.25	1.00
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.26	0.99
1:B:187:LEU:HD21	1:B:221:VAL:HG22	1.44	0.98
1:A:241:HIS:HB3	2:A:428:HOH:O	1.60	0.98
1:D:249:VAL:HA	1:D:278:MSE:HE1	1.40	0.98
1:C:54:MSE:HE2	1:C:204:ASP:HB3	1.46	0.98
1:A:127:ILE:HB	1:A:200:VAL:HG22	1.46	0.97
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.27	0.97
1:B:230:VAL:HG11	1:B:287:VAL:HG11	1.46	0.97
1:B:187:LEU:HD21	1:B:221:VAL:HG22	1.48	0.96
1:A:105:ALA:O	1:A:109:MSE:HG2	1.64	0.96
1:C:242:MSE:HE2	1:C:242:MSE:HA	1.45	0.96
1:A:151:GLU:HG3	1:A:152:ILE:H	1.31	0.95
1:C:198:VAL:HB	1:C:231:VAL:HG22	1.48	0.95
1:A:44:ILE:HD12	1:D:51:MSE:HE1	1.48	0.95
1:A:127:ILE:HD12	1:A:200:VAL:HG22	1.48	0.95
1:C:89:VAL:HG22	1:C:99:THR:HG23	1.46	0.95
1:A:127:ILE:HD12	1:A:200:VAL:HG22	1.43	0.94
1:B:227:PRO:HG2	2:B:469:HOH:O	1.66	0.94
1:B:227:PRO:HG2	2:B:469:HOH:O	1.66	0.94
1:A:135:LEU:HD22	1:A:149:MSE:HE2	1.47	0.93
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.32	0.93
1:C:253:ARG:HH22	1:C:330:GLU:HB2	1.32	0.93
1:A:206:ILE:HG23	1:A:207:GLY:H	1.33	0.92
1:A:241:HIS:HB3	2:A:428:HOH:O	1.68	0.92
1:C:200:VAL:HB	1:C:233:THR:HG22	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:MSE:HE2	1:A:242:MSE:HA	1.50	0.92
1:A:72:LYS:HB3	1:C:51:MSE:HB2	1.51	0.91
1:D:249:VAL:HG21	1:D:329:ILE:HG23	1.51	0.91
1:A:222:ALA:HA	1:A:225:LEU:HD12	1.53	0.91
1:B:311:ASN:HD22	1:B:314:ILE:HG12	1.34	0.91
1:A:245:ILE:HA	1:A:248:ILE:HD12	1.52	0.91
1:B:79:ILE:HB	1:B:91:VAL:HB	1.51	0.90
1:B:51:MSE:HE1	1:C:44:ILE:HD12	1.54	0.90
1:A:152:ILE:HD12	1:A:182:ASP:HA	1.50	0.90
1:D:257:LYS:HB2	1:D:283:GLU:HB2	1.54	0.90
1:B:320:CYS:O	1:B:321:LEU:HD23	1.72	0.90
1:A:222:ALA:HA	1:A:225:LEU:HD12	1.54	0.89
1:A:242:MSE:HE2	1:A:242:MSE:HA	1.54	0.89
1:C:127:ILE:HD13	1:C:200:VAL:HG22	1.53	0.89
1:B:196:ASP:OD1	1:B:226:ARG:HD3	1.73	0.89
1:A:242:MSE:HA	1:A:242:MSE:HE2	1.52	0.89
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.38	0.88
1:B:112:HIS:O	1:B:116:CYS:HB2	1.74	0.88
1:D:43:VAL:HG23	1:D:44:ILE:HG13	1.56	0.88
1:B:49:SER:HB2	1:B:51:MSE:HE2	1.56	0.88
1:A:125:LEU:HB3	1:A:198:VAL:HG22	1.56	0.88
1:A:99:THR:HG22	1:A:101:ARG:H	1.39	0.88
1:A:43:VAL:HG13	1:D:43:VAL:HA	1.54	0.88
1:A:238:LEU:HA	1:A:242:MSE:HE3	1.54	0.88
1:C:225:LEU:HD11	1:C:231:VAL:HG23	1.54	0.88
1:C:225:LEU:HD11	1:C:231:VAL:HG13	1.55	0.87
1:A:234:GLN:HE22	1:A:275:ILE:HD11	1.38	0.87
1:A:257:LYS:HB2	1:A:283:GLU:HB2	1.56	0.87
1:A:51:MSE:HG2	2:A:395:HOH:O	1.75	0.86
1:A:68:LEU:HD12	1:A:80:VAL:HG12	1.55	0.86
1:D:200:VAL:HB	1:D:233:THR:HG23	1.56	0.86
1:B:109:MSE:HE1	1:B:310:TYR:HD2	1.40	0.86
1:D:238:LEU:HD22	1:D:325:ALA:HB1	1.56	0.86
1:D:257:LYS:HB2	1:D:283:GLU:HB2	1.56	0.86
1:B:225:LEU:HD22	1:B:229:GLY:HA3	1.56	0.86
1:D:248:ILE:HG22	1:D:278:MSE:HE2	1.57	0.86
1:D:205:PRO:HB2	1:D:210:LYS:HA	1.57	0.86
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.39	0.86
1:B:227:PRO:HG2	2:B:470:HOH:O	1.75	0.86
1:C:242:MSE:HA	1:C:245:ILE:HD12	1.57	0.85
1:A:154:LYS:HB2	1:A:180:ILE:HD13	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:HIS:HB2	1:A:244:ILE:HD12	1.57	0.85
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.11	0.85
1:A:44:ILE:HB	1:D:43:VAL:HG12	1.58	0.85
1:D:198:VAL:HB	1:D:231:VAL:HG22	1.58	0.85
1:C:200:VAL:HB	1:C:233:THR:HG22	1.58	0.85
1:A:55:TRP:HD1	1:A:58:GLU:HG3	1.41	0.85
1:B:122:LYS:HD2	1:B:145:GLU:HG3	1.59	0.85
1:D:161:LYS:HA	1:D:168:ALA:HB2	1.56	0.85
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.40	0.85
1:A:238:LEU:HD11	1:A:321:LEU:HD22	1.56	0.85
1:C:242:MSE:HA	1:C:242:MSE:HE2	1.56	0.85
1:A:292:PRO:HD3	1:A:315:HIS:CD2	2.12	0.85
1:A:122:LYS:HE3	2:A:388:HOH:O	1.77	0.85
1:D:225:LEU:HD11	1:D:231:VAL:HG23	1.59	0.85
1:B:113:LEU:HD23	1:B:279:LEU:HD21	1.59	0.85
1:D:82:GLN:HE22	1:D:87:GLY:HA2	1.40	0.84
1:A:154:LYS:HB2	1:A:180:ILE:HD13	1.59	0.84
1:A:77:ASP:HB2	1:A:93:ASP:HA	1.56	0.84
1:C:292:PRO:HB2	1:C:295:PRO:HB3	1.59	0.84
1:A:299:SER:HA	1:A:302:LYS:HG3	1.60	0.84
1:A:196:ASP:HA	1:A:226:ARG:NH2	1.93	0.84
1:D:130:GLY:HA3	1:D:151:GLU:OE1	1.78	0.84
1:B:136:ARG:HE	1:B:167:VAL:HG12	1.41	0.84
1:A:252:CYS:HB3	1:A:280:CYS:SG	2.18	0.84
1:D:43:VAL:HG23	1:D:44:ILE:HG13	1.57	0.84
1:C:73:SER:HB3	1:C:155:MSE:HG3	1.60	0.84
1:C:148:ASP:HA	1:C:177:ASN:HB3	1.57	0.83
1:A:242:MSE:HB2	2:A:362:HOH:O	1.78	0.83
1:D:267:VAL:HG21	1:D:275:ILE:HB	1.58	0.83
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.14	0.83
1:D:146:GLN:NE2	1:D:177:ASN:HB2	1.93	0.83
1:B:257:LYS:HB2	1:B:283:GLU:HB2	1.59	0.83
1:A:232:CYS:HA	1:A:278:MSE:O	1.78	0.83
1:A:154:LYS:HB2	1:A:180:ILE:HD13	1.61	0.82
1:C:257:LYS:HB3	1:C:283:GLU:HB3	1.59	0.82
1:D:311:ASN:O	1:D:314:ILE:HG22	1.79	0.82
1:D:234:GLN:NE2	1:D:236:GLU:H	1.75	0.82
1:C:278:MSE:HE1	1:C:280:CYS:HB2	1.59	0.82
1:D:311:ASN:HD21	1:D:313:GLU:HB2	1.42	0.82
1:C:109:MSE:HE1	1:C:314:ILE:HG23	1.62	0.82
1:B:257:LYS:HB2	1:B:283:GLU:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD21	1:A:199:ILE:HD11	1.60	0.82
1:D:106:TYR:O	1:D:109:MSE:HB2	1.80	0.82
1:D:69:PHE:HE2	1:D:78:VAL:HB	1.43	0.82
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.14	0.82
1:C:65:GLU:HB3	1:C:82:GLN:HB3	1.60	0.82
1:D:146:GLN:HE21	1:D:177:ASN:HB2	1.43	0.82
1:A:55:TRP:HB2	1:A:58:GLU:OE1	1.80	0.82
1:B:242:MSE:HA	1:B:242:MSE:HE3	1.61	0.82
1:B:208:PRO:HD3	2:B:460:HOH:O	1.79	0.81
1:D:319:PHE:O	1:D:321:LEU:HG	1.79	0.81
1:D:249:VAL:HG22	1:D:278:MSE:SE	2.31	0.81
1:D:238:LEU:HD22	1:D:325:ALA:HB1	1.62	0.81
1:D:109:MSE:HE3	1:D:265:THR:HB	1.62	0.81
1:A:70:GLN:HE22	1:C:70:GLN:HE22	1.25	0.81
1:A:53:PRO:O	1:A:56:PRO:HD3	1.81	0.81
1:C:219:GLN:HE22	1:C:255:ILE:HD12	1.45	0.81
1:C:66:LYS:HB3	1:C:82:GLN:HB3	1.61	0.81
1:C:238:LEU:HD23	1:C:245:ILE:HD13	1.62	0.81
1:C:232:CYS:HA	1:C:278:MSE:O	1.80	0.81
1:A:67:VAL:HG21	1:C:64:VAL:HG11	1.63	0.81
1:C:140:ARG:NH1	1:C:301:SER:HB2	1.96	0.81
1:D:249:VAL:HA	1:D:278:MSE:HE1	1.60	0.81
1:B:196:ASP:OD1	1:B:226:ARG:HD3	1.80	0.81
1:B:135:LEU:HD11	1:B:149:MSE:HG3	1.61	0.80
1:C:311:ASN:ND2	1:C:314:ILE:H	1.77	0.80
1:D:125:LEU:HB3	1:D:198:VAL:HG22	1.63	0.80
1:D:82:GLN:NE2	1:D:87:GLY:HA2	1.95	0.80
1:C:86:TYR:HB3	1:C:99:THR:HG21	1.63	0.80
1:B:198:VAL:HG23	1:B:225:LEU:HD21	1.61	0.80
1:C:151:GLU:OE2	1:C:157:VAL:HG22	1.82	0.80
1:C:131:ASP:O	1:C:167:VAL:HG12	1.80	0.80
1:C:249:VAL:HA	1:C:278:MSE:HE1	1.64	0.80
1:D:152:ILE:HD12	1:D:182:ASP:HA	1.64	0.80
1:C:198:VAL:HB	1:C:231:VAL:HG12	1.63	0.80
1:C:158:ASP:OD2	1:D:45:PRO:HB3	1.80	0.80
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.47	0.80
1:A:72:LYS:HZ1	1:C:53:PRO:HD3	1.47	0.80
1:B:149:MSE:SE	1:B:178:LEU:HD13	2.32	0.80
1:D:263:ALA:HB1	1:D:318:ALA:HB1	1.64	0.79
1:C:324:PHE:HA	1:C:327:LYS:HE3	1.65	0.79
1:A:94:GLY:O	1:A:95:VAL:HG23	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:LYS:HB2	1:D:283:GLU:HB2	1.65	0.79
1:A:69:PHE:HZ	1:A:155:MSE:HE1	1.48	0.79
1:D:234:GLN:HE21	1:D:236:GLU:H	1.26	0.79
1:A:135:LEU:HD13	1:A:149:MSE:SE	2.33	0.79
1:D:146:GLN:NE2	1:D:177:ASN:HB2	1.97	0.79
1:A:252:CYS:O	1:A:260:VAL:HG11	1.82	0.79
1:A:179:VAL:HG12	1:A:179:VAL:O	1.82	0.79
1:C:257:LYS:HB3	1:C:283:GLU:HB3	1.64	0.79
1:A:135:LEU:HD22	1:A:149:MSE:HE2	1.64	0.79
1:A:297:ASP:O	1:A:298:GLU:HB2	1.83	0.78
1:B:134:VAL:HG12	1:B:138:VAL:HG23	1.64	0.78
1:C:148:ASP:OD1	1:C:177:ASN:HB3	1.83	0.78
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.19	0.78
1:D:109:MSE:HE3	1:D:265:THR:CB	2.14	0.78
1:C:193:GLY:H	1:C:224:ALA:HA	1.49	0.78
1:B:238:LEU:HD22	1:B:242:MSE:HE1	1.64	0.78
1:D:136:ARG:HE	1:D:167:VAL:HB	1.48	0.78
1:A:234:GLN:HE22	1:A:275:ILE:HD11	1.48	0.78
1:C:215:LYS:H	1:C:216:PRO:CD	1.97	0.78
1:C:182:ASP:OD1	1:C:184:VAL:HG22	1.83	0.78
1:A:292:PRO:HB2	1:A:295:PRO:HD3	1.66	0.78
1:D:115:LEU:HD21	1:D:138:VAL:HG13	1.64	0.78
1:B:109:MSE:HG3	1:B:265:THR:HG21	1.66	0.78
1:C:236:GLU:HB3	1:C:241:HIS:HD2	1.49	0.78
1:C:249:VAL:HA	1:C:278:MSE:HE2	1.66	0.78
1:D:111:THR:O	1:D:115:LEU:HB2	1.83	0.78
1:C:73:SER:HB3	1:C:155:MSE:SE	2.34	0.78
1:D:87:GLY:HA3	1:D:100:GLU:HB2	1.65	0.78
1:D:198:VAL:HB	1:D:231:VAL:HG22	1.65	0.78
1:D:230:VAL:HG12	1:D:281:SER:OG	1.83	0.77
1:B:183:GLY:HA3	2:B:476:HOH:O	1.84	0.77
1:B:242:MSE:O	1:B:246:GLU:HG3	1.84	0.77
1:A:70:GLN:HG3	1:A:79:ILE:HG12	1.66	0.77
1:D:126:VAL:HB	1:D:149:MSE:SE	2.35	0.77
1:B:73:SER:HB2	1:B:155:MSE:HG3	1.66	0.77
1:D:109:MSE:HE2	1:D:310:TYR:HA	1.65	0.77
1:A:111:THR:O	1:A:115:LEU:HD23	1.82	0.77
1:D:151:GLU:HG2	1:D:157:VAL:HG22	1.66	0.77
1:A:107:GLN:NE2	1:A:133:GLY:HA3	2.00	0.77
1:A:236:GLU:HB3	1:A:241:HIS:NE2	2.00	0.77
1:A:238:LEU:HA	1:A:242:MSE:CE	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HD12	1:B:172:GLU:HG3	1.67	0.77
1:A:107:GLN:NE2	1:A:133:GLY:HA3	2.00	0.77
1:D:196:ASP:OD1	1:D:226:ARG:HD2	1.84	0.77
1:D:225:LEU:HD11	1:D:231:VAL:HG23	1.65	0.77
1:D:249:VAL:HA	1:D:278:MSE:HE2	1.67	0.77
1:A:238:LEU:HA	1:A:242:MSE:HE3	1.66	0.77
1:D:146:GLN:HE21	1:D:177:ASN:HB2	1.50	0.77
1:A:178:LEU:HD12	1:A:179:VAL:H	1.47	0.77
1:A:132:GLY:HA2	1:A:149:MSE:HE1	1.65	0.76
1:A:105:ALA:O	1:A:109:MSE:HB2	1.86	0.76
1:B:192:GLU:HA	1:B:223:ARG:HH12	1.50	0.76
1:D:109:MSE:C	1:D:111:THR:H	1.88	0.76
1:A:223:ARG:HD2	2:A:360:HOH:O	1.85	0.76
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.21	0.76
1:A:115:LEU:HD21	1:A:199:ILE:HD11	1.66	0.76
1:D:109:MSE:CE	1:D:310:TYR:HA	2.15	0.76
1:D:128:GLY:HA2	2:D:551:HOH:O	1.83	0.76
1:C:86:TYR:HB3	1:C:99:THR:HG21	1.68	0.76
1:C:80:VAL:HG21	1:C:159:VAL:HG11	1.67	0.76
1:B:206:ILE:HG22	2:B:360:HOH:O	1.86	0.76
1:A:314:ILE:HD12	1:D:320:CYS:SG	2.25	0.76
1:D:238:LEU:HD22	1:D:242:MSE:HE1	1.67	0.76
1:C:129:GLY:HA2	1:C:149:MSE:SE	2.36	0.76
1:A:241:HIS:CB	1:A:244:ILE:HD12	2.16	0.76
1:C:324:PHE:HA	1:C:327:LYS:HE3	1.67	0.76
1:A:260:VAL:HB	1:A:280:CYS:SG	2.26	0.75
1:A:98:LEU:HD13	1:A:103:GLU:OE1	1.86	0.75
1:D:99:THR:HG21	1:D:269:THR:HG21	1.66	0.75
1:B:243:ASP:HB2	2:B:433:HOH:O	1.85	0.75
1:D:111:THR:O	1:D:115:LEU:HB2	1.86	0.75
1:C:127:ILE:HD12	1:C:127:ILE:H	1.51	0.75
1:C:131:ASP:O	1:C:167:VAL:HG12	1.86	0.75
1:C:242:MSE:HE1	1:C:329:ILE:HD11	1.67	0.75
1:D:43:VAL:HG23	1:D:44:ILE:HG13	1.68	0.75
1:A:111:THR:O	1:A:115:LEU:HD23	1.87	0.75
1:A:51:MSE:HE3	1:C:71:GLY:HA3	1.68	0.75
1:A:86:TYR:HD2	1:A:99:THR:HG21	1.50	0.75
1:B:135:LEU:HD11	1:B:149:MSE:HG3	1.69	0.75
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.20	0.75
1:C:86:TYR:HD2	1:C:99:THR:HG21	1.52	0.75
1:C:99:THR:HB	1:C:102:ASP:OD1	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:H	1:C:162:GLN:HE22	1.35	0.75
1:B:51:MSE:HE1	1:C:44:ILE:HD12	1.67	0.75
1:A:63:LYS:HB3	1:A:84:ALA:HB2	1.68	0.75
1:D:238:LEU:HD22	1:D:325:ALA:HB1	1.67	0.75
1:D:43:VAL:HG23	1:D:44:ILE:HG13	1.68	0.75
1:A:88:LYS:HB3	1:A:164:PHE:CE1	2.22	0.75
1:D:130:GLY:HA3	1:D:156:VAL:HG11	1.69	0.75
1:D:77:ASP:N	1:D:93:ASP:OD1	2.18	0.75
1:C:327:LYS:HB2	2:C:491:HOH:O	1.87	0.74
1:D:238:LEU:HD23	1:D:245:ILE:HD13	1.67	0.74
1:D:198:VAL:O	1:D:231:VAL:HA	1.86	0.74
1:A:296:ILE:HD12	1:A:296:ILE:H	1.50	0.74
1:A:249:VAL:HA	1:A:278:MSE:HE1	1.69	0.74
1:A:260:VAL:HB	1:A:278:MSE:HE1	1.69	0.74
1:B:131:ASP:O	1:B:167:VAL:HB	1.87	0.74
1:A:321:LEU:HD13	1:A:329:ILE:HD12	1.68	0.74
1:D:275:ILE:HG13	1:D:276:GLY:H	1.51	0.74
1:A:104:CYS:HB3	1:A:308:LYS:HE2	1.68	0.74
1:A:178:LEU:HG	1:A:180:ILE:HG13	1.68	0.74
1:B:104:CYS:O	1:B:108:GLU:HB2	1.87	0.74
1:B:241:HIS:HB3	2:B:374:HOH:O	1.87	0.74
1:A:178:LEU:HD12	1:A:179:VAL:H	1.51	0.74
1:C:223:ARG:HA	2:C:477:HOH:O	1.86	0.74
1:C:242:MSE:CE	1:C:242:MSE:HA	2.17	0.74
1:C:296:ILE:HG23	1:C:300:SER:HB2	1.70	0.74
1:C:242:MSE:HA	1:C:242:MSE:CE	2.18	0.74
1:B:129:GLY:HA2	1:B:201:ASP:OD1	1.85	0.74
1:C:105:ALA:O	1:C:109:MSE:HB2	1.87	0.74
1:A:44:ILE:HD12	1:D:51:MSE:HE1	1.68	0.74
1:A:178:LEU:HD12	1:A:179:VAL:H	1.51	0.74
1:A:223:ARG:HD2	2:A:360:HOH:O	1.87	0.74
1:D:99:THR:HG23	1:D:269:THR:HG21	1.69	0.74
1:C:135:LEU:HD13	1:C:149:MSE:HE2	1.69	0.74
1:A:228:GLY:HA2	1:A:282:THR:O	1.87	0.74
1:D:125:LEU:HB3	1:D:198:VAL:HG22	1.69	0.74
1:A:152:ILE:HD12	1:A:182:ASP:HA	1.67	0.74
1:C:129:GLY:HA3	1:C:151:GLU:HB2	1.68	0.74
1:B:230:VAL:CG1	1:B:287:VAL:HG11	2.18	0.74
1:B:109:MSE:HA	1:B:109:MSE:HE3	1.70	0.74
1:A:296:ILE:HG23	1:A:300:SER:HB2	1.69	0.74
1:A:223:ARG:HD2	2:A:360:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:O	1:B:126:VAL:HG12	1.86	0.73
1:B:173:ASP:CG	1:B:175:ARG:HH21	1.90	0.73
1:B:111:THR:O	1:B:115:LEU:HB2	1.89	0.73
1:C:79:ILE:HB	1:C:91:VAL:HB	1.70	0.73
1:B:223:ARG:HD2	2:B:481:HOH:O	1.87	0.73
1:B:173:ASP:HB3	1:B:176:VAL:HG23	1.68	0.73
1:A:161:LYS:HA	1:A:168:ALA:HB2	1.70	0.73
1:A:41:SER:OG	1:D:42:THR:HG21	1.88	0.73
1:D:197:ALA:HA	1:D:230:VAL:O	1.89	0.73
1:D:198:VAL:HG23	1:D:225:LEU:HD21	1.70	0.73
1:D:99:THR:CG2	1:D:269:THR:HG21	2.18	0.73
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.23	0.73
1:B:92:LEU:HB2	1:B:97:GLN:NE2	2.04	0.73
1:A:263:ALA:HB2	1:A:319:PHE:CE1	2.24	0.73
1:D:42:THR:HA	1:D:49:SER:HB2	1.70	0.73
1:A:214:GLU:HB3	1:A:216:PRO:HD2	1.69	0.73
1:A:230:VAL:HA	1:A:280:CYS:O	1.87	0.73
1:A:154:LYS:HB2	1:A:180:ILE:HD13	1.68	0.73
1:D:264:TRP:HA	1:D:276:GLY:HA2	1.70	0.73
1:B:109:MSE:HE3	1:B:113:LEU:HD11	1.71	0.73
1:D:73:SER:HB3	1:D:155:MSE:SE	2.39	0.73
1:C:99:THR:HB	1:C:102:ASP:OD1	1.88	0.73
1:C:324:PHE:HA	1:C:327:LYS:HE3	1.71	0.73
1:B:196:ASP:HA	1:B:226:ARG:HH11	1.54	0.73
1:C:99:THR:HG22	1:C:101:ARG:H	1.52	0.73
1:A:132:GLY:HA2	1:A:149:MSE:HE1	1.69	0.73
1:B:192:GLU:HG3	1:B:223:ARG:HH11	1.52	0.73
1:B:42:THR:HG21	1:C:42:THR:H	1.52	0.73
1:A:51:MSE:HE2	1:C:72:LYS:H	1.54	0.73
1:D:128:GLY:HA2	2:D:551:HOH:O	1.87	0.73
1:C:92:LEU:HB2	1:C:97:GLN:HG3	1.69	0.72
1:A:249:VAL:HG13	1:A:278:MSE:HE1	1.71	0.72
1:C:131:ASP:O	1:C:167:VAL:HG12	1.90	0.72
1:B:109:MSE:HG3	1:B:265:THR:HG21	1.71	0.72
1:B:290:LYS:HD2	2:B:485:HOH:O	1.89	0.72
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.71	0.72
1:C:73:SER:HB2	2:C:339:HOH:O	1.89	0.72
1:A:104:CYS:HB3	1:A:308:LYS:HE2	1.69	0.72
1:A:249:VAL:HG22	1:A:278:MSE:SE	2.39	0.72
1:C:129:GLY:HA2	1:C:151:GLU:HG2	1.71	0.72
1:C:53:PRO:O	1:C:56:PRO:HD3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:HIS:ND1	2:C:525:HOH:O	2.22	0.72
1:D:226:ARG:HD3	1:D:226:ARG:H	1.53	0.72
1:B:44:ILE:HD13	1:C:51:MSE:HE3	1.72	0.72
1:B:326:LYS:O	1:B:330:GLU:HG2	1.89	0.72
1:B:79:ILE:HB	1:B:91:VAL:HB	1.70	0.72
1:D:51:MSE:SE	1:D:51:MSE:N	2.72	0.72
1:C:241:HIS:ND1	2:C:525:HOH:O	2.23	0.72
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.72	0.72
1:B:51:MSE:HE1	1:C:47:TRP:CZ2	2.25	0.72
1:D:149:MSE:HE3	1:D:150:CYS:H	1.54	0.72
1:A:245:ILE:O	1:A:249:VAL:HG23	1.88	0.72
1:C:135:LEU:HD22	1:C:149:MSE:HE1	1.72	0.72
1:B:210:LYS:O	1:B:210:LYS:HD3	1.89	0.72
1:A:308:LYS:O	1:D:324:PHE:HB3	1.88	0.71
1:C:66:LYS:O	1:C:81:PHE:HB2	1.89	0.71
1:D:99:THR:HG21	1:D:269:THR:HG21	1.70	0.71
1:A:242:MSE:HE2	1:A:245:ILE:HD12	1.71	0.71
1:A:238:LEU:HA	1:A:242:MSE:CE	2.20	0.71
1:A:261:ASN:HD22	1:A:289:PHE:HD2	1.36	0.71
1:D:270:TYR:HD2	1:D:275:ILE:HB	1.55	0.71
1:A:108:GLU:HB2	1:A:109:MSE:HE3	1.70	0.71
1:D:83:SER:HB3	1:D:87:GLY:O	1.89	0.71
1:C:86:TYR:HD2	1:C:99:THR:HG21	1.55	0.71
1:D:242:MSE:HE1	2:D:513:HOH:O	1.89	0.71
1:B:272:SER:HA	1:C:268:PRO:HB3	1.72	0.71
1:B:44:ILE:HD13	1:C:51:MSE:HE3	1.72	0.71
1:B:42:THR:HA	1:B:49:SER:HB2	1.72	0.71
1:C:262:TYR:OH	1:C:276:GLY:HA3	1.90	0.71
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.25	0.71
1:C:266:SER:HA	1:C:273:GLY:O	1.90	0.71
1:D:127:ILE:HG23	1:D:150:CYS:HB2	1.71	0.71
1:B:57:GLY:HA2	1:C:63:LYS:HB3	1.70	0.71
1:B:43:VAL:HA	1:C:43:VAL:HG13	1.71	0.71
1:B:188:LYS:HE2	2:B:432:HOH:O	1.91	0.71
1:C:214:GLU:HB3	1:C:216:PRO:HD2	1.71	0.71
1:C:260:VAL:HG22	1:C:280:CYS:SG	2.31	0.71
1:B:210:LYS:O	1:B:210:LYS:HD3	1.91	0.71
1:A:151:GLU:CG	1:A:152:ILE:H	2.03	0.71
1:D:146:GLN:HE21	1:D:177:ASN:HB2	1.55	0.71
1:D:149:MSE:HB3	1:D:178:LEU:HA	1.73	0.71
1:C:169:ILE:HG13	1:C:172:GLU:OE2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:VAL:HG11	1:C:178:LEU:HD21	1.73	0.71
1:C:296:ILE:HG21	1:C:307:LEU:HD21	1.71	0.71
1:D:146:GLN:NE2	1:D:177:ASN:HB2	2.05	0.71
1:B:157:VAL:O	1:B:161:LYS:HB2	1.91	0.71
1:D:184:VAL:HG22	1:D:217:PHE:HD1	1.56	0.71
1:A:125:LEU:HD23	1:A:198:VAL:HG22	1.71	0.71
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.73	0.71
1:A:135:LEU:HD22	1:A:149:MSE:HE2	1.72	0.70
1:B:43:VAL:HA	1:C:43:VAL:HG13	1.72	0.70
1:A:296:ILE:HG23	1:A:300:SER:HB2	1.73	0.70
1:A:252:CYS:SG	1:A:278:MSE:SE	2.99	0.70
1:B:234:GLN:HA	1:B:277:PHE:HD1	1.54	0.70
1:B:238:LEU:HD22	1:B:242:MSE:HE1	1.73	0.70
1:A:238:LEU:HB2	1:A:242:MSE:HE3	1.73	0.70
1:A:51:MSE:HB2	1:C:72:LYS:HB3	1.71	0.70
1:B:135:LEU:HD11	1:B:149:MSE:HG3	1.73	0.70
1:A:308:LYS:O	1:D:324:PHE:HB3	1.90	0.70
1:D:140:ARG:HB3	1:D:296:ILE:HD11	1.71	0.70
1:C:248:ILE:HA	1:C:251:ASN:HD22	1.56	0.70
1:B:322:PRO:HG2	1:B:325:ALA:HB3	1.72	0.70
1:D:43:VAL:HG23	1:D:44:ILE:HG13	1.73	0.70
1:A:106:TYR:O	1:A:110:ILE:HG22	1.90	0.70
1:A:204:ASP:HB3	1:A:205:PRO:HD2	1.71	0.70
1:A:187:LEU:HD21	1:A:221:VAL:HA	1.73	0.70
1:C:154:LYS:HB2	1:C:180:ILE:HD13	1.71	0.70
1:C:249:VAL:HA	1:C:278:MSE:CE	2.16	0.70
1:C:67:VAL:HG13	1:C:70:GLN:HE21	1.54	0.70
1:D:266:SER:O	1:D:268:PRO:HD3	1.92	0.70
1:B:54:MSE:SE	2:B:366:HOH:O	2.58	0.70
1:D:198:VAL:HB	1:D:231:VAL:CG2	2.21	0.70
1:B:109:MSE:HE3	1:B:310:TYR:CD2	2.27	0.70
1:C:232:CYS:HA	1:C:278:MSE:O	1.92	0.70
1:D:202:SER:HB2	1:D:234:GLN:HB3	1.73	0.70
1:A:135:LEU:HB2	1:A:149:MSE:HE1	1.71	0.70
1:D:136:ARG:HG2	2:D:357:HOH:O	1.92	0.70
1:A:262:TYR:CZ	1:A:276:GLY:HA3	2.27	0.70
1:C:83:SER:HB3	1:C:87:GLY:O	1.92	0.70
1:B:198:VAL:HG23	1:B:225:LEU:HD21	1.73	0.70
1:C:109:MSE:HE1	1:C:310:TYR:CD2	2.27	0.70
1:C:321:LEU:HD12	1:C:321:LEU:H	1.57	0.70
1:B:73:SER:CB	1:B:155:MSE:HG3	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD13	1:C:149:MSE:HE2	1.73	0.70
1:A:69:PHE:CZ	1:A:155:MSE:HE1	2.27	0.70
1:C:92:LEU:HD11	1:C:130:GLY:HA2	1.74	0.70
1:B:130:GLY:O	1:B:131:ASP:HB2	1.90	0.70
1:B:243:ASP:HB2	2:B:433:HOH:O	1.92	0.70
1:D:214:GLU:HG3	2:D:409:HOH:O	1.90	0.70
1:D:99:THR:CG2	1:D:269:THR:HG21	2.21	0.70
1:D:308:LYS:NZ	1:D:308:LYS:HB3	2.07	0.69
1:C:152:ILE:HG23	1:C:153:ASP:H	1.57	0.69
1:C:86:TYR:HB3	1:C:99:THR:CG2	2.21	0.69
1:C:86:TYR:HB3	1:C:99:THR:OG1	1.92	0.69
1:C:88:LYS:O	1:C:99:THR:HA	1.92	0.69
1:A:238:LEU:HA	1:A:242:MSE:CE	2.22	0.69
1:C:72:LYS:HE2	1:C:77:ASP:OD1	1.91	0.69
1:A:79:ILE:HG13	2:A:453:HOH:O	1.91	0.69
1:B:135:LEU:HD11	1:B:149:MSE:HG3	1.72	0.69
1:A:262:TYR:HA	1:A:277:PHE:O	1.92	0.69
1:A:66:LYS:HG2	1:A:82:GLN:HB3	1.71	0.69
1:B:42:THR:HA	1:B:49:SER:HB2	1.73	0.69
1:C:253:ARG:HA	1:C:260:VAL:HG21	1.75	0.69
1:D:80:VAL:HG21	1:D:159:VAL:HG11	1.75	0.69
1:C:236:GLU:HB3	1:C:241:HIS:HD2	1.55	0.69
1:C:307:LEU:N	1:C:307:LEU:HD12	2.06	0.69
1:D:249:VAL:HA	1:D:278:MSE:CE	2.22	0.69
1:C:239:TRP:O	1:C:240:LEU:HD23	1.91	0.69
1:D:109:MSE:SE	1:D:113:LEU:HD11	2.42	0.69
1:A:301:SER:HB3	1:A:304:ASN:OD1	1.92	0.69
1:C:86:TYR:HD2	1:C:99:THR:HG21	1.58	0.69
1:C:200:VAL:HB	1:C:233:THR:HG22	1.75	0.69
1:B:307:LEU:HD13	1:B:310:TYR:HD1	1.56	0.69
1:A:86:TYR:HB3	1:A:99:THR:HG21	1.73	0.69
1:B:134:VAL:O	1:B:138:VAL:HG23	1.92	0.69
1:C:107:GLN:NE2	1:C:133:GLY:HA3	2.08	0.69
1:B:241:HIS:HD2	2:B:375:HOH:O	1.74	0.69
1:B:311:ASN:HD21	1:B:313:GLU:HB2	1.55	0.69
1:A:232:CYS:HA	1:A:278:MSE:O	1.92	0.69
1:B:129:GLY:O	1:B:131:ASP:N	2.25	0.69
1:C:70:GLN:HG3	1:C:79:ILE:HG12	1.74	0.69
1:A:178:LEU:HD12	1:A:179:VAL:N	2.07	0.69
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.27	0.69
1:C:200:VAL:HB	1:C:233:THR:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:HD13	1:C:51:MSE:HE3	1.75	0.69
1:C:311:ASN:O	1:C:314:ILE:HG22	1.93	0.69
1:B:157:VAL:HG12	1:B:161:LYS:HE3	1.75	0.69
1:C:311:ASN:ND2	1:C:314:ILE:HD13	2.07	0.69
1:A:296:ILE:HD13	1:A:297:ASP:H	1.57	0.69
1:A:135:LEU:HD21	1:A:176:VAL:HG21	1.74	0.69
1:A:125:LEU:HD21	1:A:187:LEU:HD11	1.73	0.69
1:C:249:VAL:HG22	1:C:278:MSE:HE1	1.75	0.69
1:A:86:TYR:HB3	1:A:99:THR:CG2	2.23	0.68
1:A:51:MSE:HE3	1:C:72:LYS:H	1.58	0.68
1:B:109:MSE:HE3	1:B:113:LEU:HD11	1.73	0.68
1:C:215:LYS:HB2	1:C:216:PRO:HD3	1.75	0.68
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.74	0.68
1:A:220:SER:O	1:A:223:ARG:HG2	1.93	0.68
1:A:327:LYS:HG3	1:A:328:VAL:H	1.58	0.68
1:B:67:VAL:HG22	1:B:81:PHE:HB3	1.76	0.68
1:D:327:LYS:O	1:D:330:GLU:HG3	1.93	0.68
1:A:127:ILE:HD12	1:A:127:ILE:O	1.92	0.68
1:C:87:GLY:HA3	1:C:100:GLU:HB2	1.73	0.68
1:D:104:CYS:O	1:D:108:GLU:HG3	1.93	0.68
1:C:235:ALA:O	1:C:236:GLU:HB2	1.91	0.68
1:C:296:ILE:HB	1:C:307:LEU:HD21	1.74	0.68
1:C:249:VAL:HA	1:C:278:MSE:CE	2.24	0.68
1:A:149:MSE:HG3	1:A:178:LEU:HD13	1.75	0.68
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.28	0.68
1:D:130:GLY:HA2	2:D:553:HOH:O	1.94	0.68
1:C:297:ASP:HB3	2:C:350:HOH:O	1.93	0.68
1:B:110:ILE:HG12	1:B:199:ILE:HG23	1.75	0.68
1:D:99:THR:CG2	1:D:269:THR:HG21	2.24	0.68
1:C:296:ILE:HG23	1:C:300:SER:HB2	1.75	0.68
1:C:68:LEU:HB2	1:C:80:VAL:HG12	1.76	0.68
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.29	0.68
1:D:192:GLU:HG2	1:D:223:ARG:HH11	1.59	0.68
1:B:198:VAL:HG23	1:B:225:LEU:HD21	1.75	0.68
1:B:238:LEU:HD11	1:B:321:LEU:HD13	1.73	0.68
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.27	0.68
1:D:107:GLN:O	1:D:111:THR:HG23	1.93	0.68
1:A:66:LYS:HG2	1:A:82:GLN:HB3	1.74	0.68
1:C:232:CYS:HA	1:C:278:MSE:O	1.94	0.68
1:C:219:GLN:NE2	1:C:255:ILE:HD12	2.09	0.68
1:D:238:LEU:HD12	1:D:264:TRP:CE3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:VAL:HG11	1:D:70:GLN:HG3	1.76	0.68
1:A:178:LEU:HD12	1:A:179:VAL:H	1.58	0.68
1:A:242:MSE:CE	1:A:242:MSE:HA	2.24	0.68
1:C:131:ASP:O	1:C:167:VAL:HG12	1.94	0.68
1:D:200:VAL:HB	1:D:233:THR:OG1	1.93	0.68
1:A:200:VAL:HB	1:A:233:THR:HG22	1.75	0.68
1:B:109:MSE:HE3	1:B:310:TYR:HD2	1.56	0.68
1:D:128:GLY:HA3	1:D:201:ASP:HB3	1.75	0.68
1:B:198:VAL:HG23	1:B:225:LEU:HD21	1.76	0.68
1:B:295:PRO:HA	2:B:444:HOH:O	1.94	0.68
1:A:237:SER:H	1:A:241:HIS:HD2	1.42	0.68
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.28	0.68
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.75	0.68
1:A:43:VAL:H	1:C:162:GLN:NE2	1.92	0.68
1:A:43:VAL:N	1:C:162:GLN:HE22	1.92	0.67
1:B:207:GLY:HA3	2:B:460:HOH:O	1.92	0.67
1:D:153:ASP:OD2	1:D:155:MSE:HB2	1.92	0.67
1:B:127:ILE:HD11	1:B:187:LEU:CD2	2.24	0.67
1:A:162:GLN:O	1:A:162:GLN:HG2	1.94	0.67
1:C:99:THR:O	1:C:103:GLU:HB3	1.94	0.67
1:B:80:VAL:HG21	1:B:159:VAL:HG11	1.75	0.67
1:B:92:LEU:HD12	1:B:97:GLN:HG2	1.75	0.67
1:C:99:THR:HB	1:C:102:ASP:OD1	1.95	0.67
1:C:296:ILE:HG22	1:C:307:LEU:HD11	1.75	0.67
1:A:52:SER:HB3	1:A:55:TRP:CE2	2.29	0.67
1:A:238:LEU:HA	1:A:242:MSE:HE3	1.75	0.67
1:D:198:VAL:HG23	1:D:225:LEU:HD21	1.76	0.67
1:A:234:GLN:NE2	1:A:275:ILE:HD11	2.04	0.67
1:B:166:ASP:O	1:B:167:VAL:HG13	1.94	0.67
1:C:118:ILE:HD11	1:C:121:PRO:HB3	1.76	0.67
1:D:187:LEU:HD21	1:D:221:VAL:HG22	1.75	0.67
1:A:70:GLN:HB3	1:C:48:PHE:HD1	1.59	0.67
1:D:76:GLN:HB2	1:D:93:ASP:OD2	1.94	0.67
1:A:76:GLN:NE2	1:A:156:VAL:HG21	2.08	0.67
1:C:313:GLU:HB2	2:C:404:HOH:O	1.94	0.67
1:D:68:LEU:HD12	1:D:68:LEU:N	2.10	0.67
1:A:51:MSE:N	1:A:51:MSE:SE	2.78	0.67
1:C:161:LYS:HA	1:C:168:ALA:HB1	1.74	0.67
1:B:241:HIS:HD2	2:B:378:HOH:O	1.78	0.67
1:B:263:ALA:HB2	1:B:319:PHE:CD1	2.30	0.67
1:D:261:ASN:HD22	1:D:289:PHE:HD2	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:MSE:HE1	1:A:310:TYR:HB2	1.76	0.67
1:C:109:MSE:HE1	1:C:310:TYR:HD2	1.60	0.67
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.77	0.67
1:B:162:GLN:HG3	2:B:411:HOH:O	1.93	0.67
1:D:236:GLU:HB3	1:D:241:HIS:HB2	1.76	0.67
1:A:245:ILE:HA	1:A:248:ILE:HD12	1.75	0.67
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.29	0.67
1:B:279:LEU:H	1:B:279:LEU:HD22	1.60	0.67
1:D:51:MSE:HA	1:D:55:TRP:HE1	1.60	0.67
1:A:220:SER:O	1:A:223:ARG:HG2	1.95	0.66
1:B:166:ASP:O	1:B:167:VAL:HG13	1.95	0.66
1:B:210:LYS:HD3	1:B:210:LYS:O	1.94	0.66
1:B:104:CYS:O	1:B:108:GLU:HB2	1.94	0.66
1:B:223:ARG:HH21	1:B:224:ALA:HA	1.59	0.66
1:D:130:GLY:HA2	2:D:553:HOH:O	1.95	0.66
1:D:261:ASN:HD22	1:D:289:PHE:HD2	1.43	0.66
1:D:90:LEU:HB3	1:D:98:LEU:HG	1.76	0.66
1:A:72:LYS:H	1:C:51:MSE:HE2	1.60	0.66
1:D:111:THR:CG2	1:D:134:VAL:HG13	2.26	0.66
1:B:278:MSE:HE3	1:B:280:CYS:SG	2.36	0.66
1:D:120:ASN:HD21	1:D:122:LYS:HE3	1.60	0.66
1:A:299:SER:C	1:A:301:SER:H	1.97	0.66
1:C:311:ASN:OD1	1:C:312:ALA:N	2.29	0.66
1:D:198:VAL:HB	1:D:231:VAL:CG2	2.23	0.66
1:A:130:GLY:HA2	1:A:171:TYR:OH	1.96	0.66
1:B:51:MSE:HG2	1:B:59:ALA:HB2	1.76	0.66
1:C:136:ARG:NH1	1:C:167:VAL:HG22	2.10	0.66
1:B:109:MSE:HE1	1:B:310:TYR:CD2	2.26	0.66
1:C:154:LYS:HD3	1:C:154:LYS:O	1.95	0.66
1:B:139:ALA:HB1	1:B:175:ARG:NH2	2.09	0.66
1:C:152:ILE:HA	1:C:181:GLY:N	2.11	0.66
1:B:223:ARG:HD2	2:B:477:HOH:O	1.95	0.66
1:A:51:MSE:HE2	1:C:72:LYS:O	1.95	0.66
1:A:161:LYS:HA	1:A:168:ALA:CB	2.25	0.66
1:D:195:TYR:HB2	1:D:225:LEU:HD23	1.78	0.66
1:C:152:ILE:HD12	1:C:182:ASP:HA	1.78	0.66
1:B:40:PHE:CD1	1:C:42:THR:HG21	2.31	0.66
1:D:92:LEU:HD12	1:D:97:GLN:HG2	1.76	0.66
1:B:98:LEU:HD13	1:B:103:GLU:OE2	1.95	0.66
1:D:238:LEU:HD22	1:D:325:ALA:HB1	1.78	0.66
1:A:178:LEU:HD12	1:A:179:VAL:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ILE:HA	1:C:181:GLY:H	1.60	0.66
1:B:173:ASP:HB3	1:B:176:VAL:HG23	1.77	0.66
1:B:163:PHE:C	1:B:165:PRO:HD3	2.15	0.66
1:A:317:ALA:O	1:A:319:PHE:N	2.29	0.66
1:A:165:PRO:HG2	1:A:166:ASP:H	1.60	0.66
1:A:63:LYS:HB3	1:A:84:ALA:CB	2.26	0.66
1:C:257:LYS:HB2	1:C:283:GLU:OE2	1.96	0.66
1:D:228:GLY:HA3	1:D:285:PRO:HD2	1.78	0.66
1:A:66:LYS:HG2	1:A:82:GLN:HB3	1.77	0.66
1:A:239:TRP:HD1	1:A:274:VAL:HG21	1.61	0.66
1:C:292:PRO:HB3	1:C:315:HIS:ND1	2.10	0.66
1:D:231:VAL:HG21	1:D:256:PHE:CZ	2.31	0.66
1:A:196:ASP:HA	1:A:226:ARG:HH21	1.59	0.65
1:A:52:SER:HB3	1:A:55:TRP:CE2	2.31	0.65
1:C:242:MSE:HG2	2:C:397:HOH:O	1.94	0.65
1:A:178:LEU:HD12	1:A:179:VAL:H	1.61	0.65
1:D:184:VAL:HG22	1:D:217:PHE:CD1	2.31	0.65
1:C:76:GLN:NE2	1:C:92:LEU:HB3	2.11	0.65
1:A:241:HIS:ND1	2:A:425:HOH:O	2.29	0.65
1:D:190:ALA:HA	2:D:401:HOH:O	1.96	0.65
1:A:329:ILE:HG22	1:A:329:ILE:O	1.96	0.65
1:D:270:TYR:CD2	1:D:275:ILE:HB	2.31	0.65
1:C:105:ALA:HB1	1:C:267:VAL:HG22	1.78	0.65
1:C:296:ILE:HG23	1:C:300:SER:HB2	1.79	0.65
1:B:290:LYS:HG2	1:B:291:HIS:CE1	2.31	0.65
1:B:68:LEU:HB3	1:B:163:PHE:CE1	2.31	0.65
1:D:162:GLN:HG2	1:D:162:GLN:O	1.95	0.65
1:C:86:TYR:HB3	1:C:99:THR:CG2	2.26	0.65
1:B:242:MSE:CE	1:B:242:MSE:HA	2.26	0.65
1:C:142:ALA:O	1:C:144:ILE:N	2.29	0.65
1:B:150:CYS:O	1:B:151:GLU:HB2	1.97	0.65
1:A:261:ASN:HD22	1:A:289:PHE:HD2	1.42	0.65
1:C:129:GLY:HA3	1:C:151:GLU:HB2	1.79	0.65
1:C:161:LYS:HG3	1:C:168:ALA:HB1	1.77	0.65
1:C:232:CYS:HA	1:C:278:MSE:O	1.97	0.65
1:A:169:ILE:HD12	1:A:172:GLU:OE2	1.97	0.65
1:B:231:VAL:HG22	1:B:232:CYS:N	2.10	0.65
1:D:123:LYS:HE3	1:D:146:GLN:OE1	1.97	0.65
1:B:152:ILE:HA	1:B:180:ILE:HG23	1.78	0.65
1:A:136:ARG:HH11	1:A:137:GLU:HG2	1.61	0.65
1:A:109:MSE:HE2	1:A:265:THR:OG1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:MSE:SE	1:B:206:ILE:HB	2.47	0.65
1:D:104:CYS:O	1:D:108:GLU:HB2	1.96	0.65
1:A:104:CYS:O	1:A:108:GLU:HG3	1.96	0.65
1:D:193:GLY:O	1:D:226:ARG:HB3	1.96	0.65
1:B:234:GLN:HA	1:B:277:PHE:CD1	2.31	0.65
1:C:141:HIS:ND1	2:C:341:HOH:O	2.29	0.65
1:A:161:LYS:HA	1:A:168:ALA:HB2	1.79	0.65
1:D:162:GLN:O	1:D:162:GLN:HG2	1.96	0.65
1:C:210:LYS:O	1:C:214:GLU:HG2	1.97	0.65
1:D:202:SER:OG	1:D:234:GLN:HB3	1.96	0.65
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.32	0.65
1:C:228:GLY:HA3	1:C:285:PRO:HD2	1.78	0.65
1:A:53:PRO:O	1:A:56:PRO:HD3	1.97	0.65
1:B:168:ALA:HA	1:B:171:TYR:HD2	1.62	0.65
1:B:98:LEU:HD12	1:B:98:LEU:C	2.17	0.65
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.31	0.65
1:A:238:LEU:HD11	1:A:321:LEU:HD22	1.79	0.65
1:D:162:GLN:HG2	1:D:162:GLN:O	1.95	0.65
1:D:48:PHE:O	1:D:61:SER:HA	1.97	0.65
1:A:109:MSE:HE1	1:A:310:TYR:HB2	1.79	0.65
1:A:297:ASP:O	1:A:298:GLU:HB2	1.97	0.65
1:A:109:MSE:HE2	1:A:265:THR:CB	2.27	0.65
1:B:326:LYS:O	1:B:330:GLU:HG2	1.97	0.65
1:B:234:GLN:OE1	1:B:236:GLU:N	2.23	0.65
1:D:69:PHE:HB2	1:D:163:PHE:CZ	2.31	0.65
1:B:42:THR:HA	1:B:49:SER:HB2	1.77	0.65
1:B:92:LEU:HD12	1:B:97:GLN:HE21	1.60	0.65
1:D:128:GLY:HA2	2:D:551:HOH:O	1.96	0.65
1:A:329:ILE:O	1:A:330:GLU:HB2	1.96	0.65
1:D:152:ILE:HA	1:D:181:GLY:H	1.61	0.65
1:B:243:ASP:HA	1:B:246:GLU:CD	2.17	0.65
1:D:109:MSE:HE1	1:D:310:TYR:N	2.11	0.65
1:A:51:MSE:CE	1:C:72:LYS:H	2.09	0.65
1:B:114:PRO:HB3	1:B:232:CYS:HB2	1.78	0.65
1:D:198:VAL:HG23	1:D:225:LEU:HD21	1.79	0.64
1:B:126:VAL:O	1:B:149:MSE:HG2	1.96	0.64
1:D:99:THR:CG2	1:D:269:THR:HG21	2.27	0.64
1:B:265:THR:HG22	1:B:277:PHE:HE2	1.62	0.64
1:C:221:VAL:CG1	1:C:231:VAL:HG21	2.27	0.64
1:A:215:LYS:HD3	1:A:255:ILE:HD11	1.79	0.64
1:D:106:TYR:OH	1:D:234:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD12	1:A:179:VAL:N	2.10	0.64
1:B:210:LYS:O	1:B:210:LYS:HD3	1.97	0.64
1:B:271:PRO:HB3	2:B:447:HOH:O	1.97	0.64
1:B:112:HIS:O	1:B:116:CYS:HB2	1.98	0.64
1:A:223:ARG:HD2	2:A:360:HOH:O	1.97	0.64
1:A:107:GLN:HE22	1:A:133:GLY:HA3	1.60	0.64
1:A:179:VAL:HG11	1:A:186:PHE:HD2	1.62	0.64
1:B:39:CYS:SG	1:C:41:SER:HB3	2.38	0.64
1:A:99:THR:O	1:A:103:GLU:HB3	1.98	0.64
1:A:42:THR:HA	1:C:162:GLN:OE1	1.97	0.64
1:B:263:ALA:HB2	1:B:319:PHE:CD1	2.31	0.64
1:A:78:VAL:O	1:A:79:ILE:HG13	1.97	0.64
1:C:162:GLN:HG3	2:C:467:HOH:O	1.97	0.64
1:C:249:VAL:HG22	1:C:278:MSE:SE	2.46	0.64
1:D:118:ILE:HD11	1:D:121:PRO:HB3	1.79	0.64
1:D:218:PHE:O	1:D:255:ILE:HG21	1.96	0.64
1:A:187:LEU:HD11	1:A:224:ALA:CB	2.27	0.64
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.32	0.64
1:D:265:THR:OG1	2:D:563:HOH:O	2.14	0.64
1:D:243:ASP:OD1	1:D:244:ILE:HG13	1.98	0.64
1:A:238:LEU:HA	1:A:245:ILE:HD12	1.79	0.64
1:D:122:LYS:HE2	1:D:122:LYS:HA	1.78	0.64
1:B:234:GLN:OE1	1:B:236:GLU:N	2.28	0.64
1:A:136:ARG:HD3	1:A:166:ASP:O	1.98	0.64
1:B:149:MSE:HB3	1:B:178:LEU:HD12	1.80	0.64
1:C:265:THR:OG1	1:C:267:VAL:HG23	1.98	0.64
1:A:68:LEU:HB2	1:A:80:VAL:O	1.98	0.64
1:C:227:PRO:HB3	1:C:284:GLY:HA3	1.79	0.64
1:D:109:MSE:HA	1:D:109:MSE:HE3	1.80	0.64
1:B:61:SER:O	1:C:58:GLU:HB2	1.98	0.64
1:A:265:THR:HG22	1:A:275:ILE:HG22	1.80	0.64
1:A:136:ARG:HD3	1:A:166:ASP:O	1.98	0.64
1:A:260:VAL:HG12	1:A:280:CYS:SG	2.38	0.64
1:C:296:ILE:CG2	1:C:307:LEU:HD11	2.27	0.64
1:A:226:ARG:HB2	1:A:227:PRO:HD2	1.79	0.64
1:C:152:ILE:HD12	1:C:182:ASP:HA	1.78	0.64
1:A:311:ASN:ND2	1:A:314:ILE:HD13	2.13	0.64
1:A:314:ILE:HD11	1:D:321:LEU:O	1.97	0.64
1:C:235:ALA:O	1:C:236:GLU:HB2	1.96	0.64
1:B:249:VAL:HA	1:B:278:MSE:HE2	1.80	0.64
1:B:327:LYS:HA	1:B:330:GLU:OE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:HB3	1:A:194:SER:HB3	1.80	0.64
1:C:99:THR:OG1	1:C:269:THR:HG21	1.98	0.64
1:C:136:ARG:NH1	1:C:166:ASP:HB3	2.13	0.64
1:C:109:MSE:HE3	1:C:109:MSE:HA	1.78	0.64
1:A:308:LYS:O	1:D:324:PHE:HB3	1.98	0.64
1:A:182:ASP:OD2	1:A:184:VAL:HG22	1.98	0.64
1:C:97:GLN:HA	1:C:97:GLN:NE2	2.13	0.64
1:C:97:GLN:HA	1:C:97:GLN:HE21	1.63	0.64
1:A:116:CYS:SG	1:A:295:PRO:HA	2.38	0.64
1:A:72:LYS:HB3	1:C:51:MSE:HB2	1.80	0.64
1:D:135:LEU:HD11	1:D:149:MSE:SE	2.49	0.63
1:A:135:LEU:CD2	1:A:149:MSE:HE2	2.28	0.63
1:C:223:ARG:HA	2:C:477:HOH:O	1.98	0.63
1:C:87:GLY:O	1:C:89:VAL:HG23	1.99	0.63
1:C:123:LYS:HA	1:C:146:GLN:O	1.98	0.63
1:A:54:MSE:HE1	1:A:244:ILE:CD1	2.28	0.63
1:C:161:LYS:HA	1:C:168:ALA:CB	2.28	0.63
1:A:242:MSE:HE2	1:A:325:ALA:HA	1.80	0.63
1:A:73:SER:HA	1:A:155:MSE:CE	2.27	0.63
1:C:252:CYS:SG	1:C:278:MSE:HE2	2.38	0.63
1:A:72:LYS:HB3	1:C:51:MSE:HB2	1.79	0.63
1:C:73:SER:HB2	2:C:339:HOH:O	1.98	0.63
1:D:265:THR:O	1:D:274:VAL:HA	1.97	0.63
1:B:152:ILE:HG13	1:B:182:ASP:HA	1.80	0.63
1:B:68:LEU:HB3	1:B:163:PHE:CE1	2.33	0.63
1:C:215:LYS:H	1:C:216:PRO:HD3	1.64	0.63
1:C:232:CYS:HB2	1:C:279:LEU:HD13	1.80	0.63
1:A:231:VAL:HG12	1:A:280:CYS:HB2	1.80	0.63
1:C:134:VAL:O	1:C:138:VAL:HG23	1.97	0.63
1:B:98:LEU:HD13	1:B:103:GLU:OE2	1.98	0.63
1:B:113:LEU:HA	1:B:315:HIS:CE1	2.33	0.63
1:D:132:GLY:HA3	1:D:167:VAL:O	1.99	0.63
1:C:50:GLU:HG2	1:C:50:GLU:O	1.99	0.63
1:B:123:LYS:HB3	1:B:195:TYR:HA	1.80	0.63
1:A:162:GLN:HE22	1:C:43:VAL:N	1.97	0.63
1:C:68:LEU:HB2	1:C:80:VAL:O	1.98	0.63
1:A:297:ASP:O	1:A:298:GLU:HB2	1.99	0.63
1:D:134:VAL:O	1:D:138:VAL:HG23	1.98	0.63
1:D:163:PHE:C	1:D:165:PRO:HD3	2.19	0.63
1:D:192:GLU:HB2	1:D:223:ARG:HH11	1.63	0.63
1:A:182:ASP:OD1	1:A:184:VAL:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:HD3	2:A:360:HOH:O	1.97	0.63
1:B:215:LYS:HB2	1:B:216:PRO:HD3	1.79	0.63
1:B:43:VAL:HG12	1:C:44:ILE:HB	1.80	0.63
1:A:214:GLU:HA	1:A:251:ASN:ND2	2.14	0.63
1:A:193:GLY:HA2	1:A:225:LEU:O	1.98	0.63
1:B:126:VAL:HG22	1:B:199:ILE:HD12	1.80	0.63
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.33	0.63
1:C:301:SER:HB3	1:C:304:ASN:HB2	1.79	0.63
1:D:122:LYS:HA	1:D:144:ILE:HA	1.81	0.63
1:C:107:GLN:HE21	1:C:133:GLY:HA3	1.63	0.63
1:C:329:ILE:O	1:C:330:GLU:HB2	1.98	0.63
1:C:96:ILE:HG21	1:C:269:THR:HG21	1.80	0.63
1:A:152:ILE:O	1:A:152:ILE:HG23	1.98	0.63
1:A:223:ARG:HD2	2:A:360:HOH:O	1.99	0.63
1:C:73:SER:CB	1:C:155:MSE:HG3	2.29	0.63
1:A:153:ASP:OD1	1:A:155:MSE:HB2	1.99	0.63
1:A:223:ARG:HD3	2:A:360:HOH:O	1.98	0.63
1:B:149:MSE:O	1:B:150:CYS:HB2	1.98	0.63
1:C:61:SER:O	1:C:62:LEU:HD23	1.99	0.63
1:A:127:ILE:HD11	1:A:187:LEU:HD11	1.81	0.63
1:A:311:ASN:O	1:A:315:HIS:HB2	1.99	0.63
1:B:169:ILE:HD12	1:B:172:GLU:CG	2.29	0.63
1:B:83:SER:HB3	1:B:87:GLY:O	1.99	0.63
1:C:147:ILE:O	1:C:176:VAL:HA	1.99	0.63
1:C:249:VAL:HA	1:C:278:MSE:CE	2.29	0.63
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.64	0.63
1:D:111:THR:O	1:D:115:LEU:HB2	1.99	0.63
1:B:262:TYR:OH	1:B:276:GLY:HA3	1.98	0.63
1:C:292:PRO:CB	1:C:295:PRO:HB3	2.27	0.63
1:C:88:LYS:H	1:C:100:GLU:HG3	1.64	0.63
1:C:112:HIS:O	1:C:116:CYS:HB2	1.98	0.63
1:A:178:LEU:HD12	1:A:179:VAL:N	2.12	0.63
1:B:109:MSE:O	1:B:113:LEU:HG	1.98	0.63
1:B:54:MSE:SE	1:B:204:ASP:HB3	2.49	0.63
1:A:51:MSE:HE3	1:D:44:ILE:HD13	1.81	0.63
1:A:46:GLY:HA3	1:A:63:LYS:NZ	2.14	0.63
1:B:182:ASP:OD2	1:B:184:VAL:HG12	1.98	0.63
1:D:151:GLU:HG2	1:D:157:VAL:HG22	1.80	0.62
1:D:87:GLY:HA3	1:D:100:GLU:HB2	1.80	0.62
1:D:125:LEU:HG	1:D:127:ILE:HG13	1.80	0.62
1:B:123:LYS:NZ	1:B:146:GLN:NE2	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:HB	1:A:233:THR:HG22	1.81	0.62
1:B:292:PRO:HB3	1:B:315:HIS:CE1	2.33	0.62
1:D:198:VAL:HG23	1:D:225:LEU:HD21	1.80	0.62
1:A:260:VAL:CB	1:A:278:MSE:HE1	2.29	0.62
1:C:311:ASN:O	1:C:314:ILE:HG22	1.99	0.62
1:C:297:ASP:OD1	1:C:298:GLU:N	2.32	0.62
1:D:68:LEU:HB2	1:D:80:VAL:O	1.99	0.62
1:C:129:GLY:CA	1:C:151:GLU:HB2	2.29	0.62
1:A:121:PRO:HA	2:A:386:HOH:O	2.00	0.62
1:D:278:MSE:HA	1:D:278:MSE:HE2	1.78	0.62
1:C:180:ILE:N	1:C:180:ILE:HD12	2.15	0.62
1:A:259:SER:N	1:A:281:SER:HB3	2.04	0.62
1:A:295:PRO:HB2	1:A:310:TYR:HE1	1.64	0.62
1:A:86:TYR:HB3	1:A:99:THR:CG2	2.30	0.62
1:B:173:ASP:HB3	1:B:176:VAL:HG23	1.80	0.62
1:C:238:LEU:HA	1:C:242:MSE:HE3	1.81	0.62
1:B:107:GLN:NE2	1:B:133:GLY:HA3	2.14	0.62
1:B:166:ASP:O	1:B:167:VAL:HG13	2.00	0.62
1:D:245:ILE:C	1:D:247:ASP:H	2.01	0.62
1:B:130:GLY:HA2	1:B:171:TYR:OH	1.99	0.62
1:B:108:GLU:OE1	1:B:307:LEU:HB3	1.99	0.62
1:A:43:VAL:HG13	1:D:43:VAL:HA	1.81	0.62
1:C:152:ILE:HD12	1:C:182:ASP:HA	1.81	0.62
1:C:200:VAL:HB	1:C:233:THR:HG22	1.80	0.62
1:A:51:MSE:CE	1:C:71:GLY:HA3	2.30	0.62
1:A:226:ARG:NH1	2:A:414:HOH:O	2.32	0.62
1:C:180:ILE:HD12	1:C:180:ILE:H	1.64	0.62
1:D:163:PHE:C	1:D:165:PRO:HD3	2.20	0.62
1:D:99:THR:CG2	1:D:269:THR:HG21	2.29	0.62
1:A:99:THR:HG22	1:A:101:ARG:H	1.62	0.62
1:A:154:LYS:HB2	1:A:180:ILE:HD13	1.81	0.62
1:A:179:VAL:HG21	1:A:186:PHE:CE2	2.34	0.62
1:A:219:GLN:OE1	1:A:255:ILE:HD12	1.99	0.62
1:C:86:TYR:CB	1:C:99:THR:HG21	2.30	0.62
1:D:253:ARG:NH1	1:D:330:GLU:HB2	2.15	0.62
1:D:130:GLY:HA2	2:D:553:HOH:O	1.98	0.62
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.31	0.62
1:D:146:GLN:HE21	1:D:177:ASN:CB	2.12	0.62
1:B:320:CYS:SG	1:C:314:ILE:HD12	2.40	0.62
1:C:261:ASN:HD22	1:C:289:PHE:HD2	1.47	0.62
1:B:130:GLY:HA3	1:B:156:VAL:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:ASN:ND2	1:D:313:GLU:HB2	2.14	0.62
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.34	0.62
1:B:42:THR:HA	1:B:49:SER:HB2	1.80	0.62
1:D:271:PRO:O	1:D:272:SER:HB3	1.99	0.62
1:D:124:VAL:HG22	1:D:197:ALA:HB3	1.80	0.62
1:A:135:LEU:HD22	1:A:149:MSE:CE	2.28	0.62
1:C:99:THR:O	1:C:103:GLU:HB3	1.99	0.62
1:B:48:PHE:CZ	1:B:91:VAL:HG11	2.35	0.62
1:B:127:ILE:CD1	1:B:187:LEU:HD22	2.30	0.62
1:C:272:SER:O	1:C:274:VAL:N	2.32	0.62
1:B:236:GLU:HB3	1:B:241:HIS:CE1	2.33	0.62
1:C:203:SER:O	1:C:204:ASP:HB2	2.00	0.62
1:C:297:ASP:OD1	1:C:298:GLU:N	2.33	0.62
1:A:44:ILE:HD12	1:D:51:MSE:CE	2.25	0.62
1:A:108:GLU:HB3	1:A:310:TYR:HB3	1.80	0.62
1:B:109:MSE:CE	1:B:310:TYR:HD2	2.12	0.62
1:A:260:VAL:HB	1:A:278:MSE:CE	2.29	0.62
1:C:226:ARG:HB2	1:C:227:PRO:CD	2.30	0.62
1:B:43:VAL:HG23	1:B:44:ILE:HG13	1.81	0.62
1:D:151:GLU:HG2	1:D:157:VAL:HG23	1.81	0.62
1:C:73:SER:HB2	2:C:339:HOH:O	2.00	0.62
1:A:214:GLU:HA	1:A:251:ASN:HD22	1.65	0.62
1:D:69:PHE:CE2	1:D:78:VAL:HB	2.31	0.62
1:A:80:VAL:HG21	1:A:159:VAL:HB	1.82	0.62
1:C:85:THR:O	1:C:101:ARG:HD2	1.99	0.62
1:D:242:MSE:HE3	1:D:325:ALA:HA	1.81	0.62
1:A:55:TRP:HH2	1:A:95:VAL:HG22	1.65	0.62
1:D:70:GLN:HE22	1:D:79:ILE:HD11	1.64	0.62
1:A:72:LYS:HB3	1:C:51:MSE:HB2	1.82	0.62
1:B:275:ILE:HD13	2:B:347:HOH:O	2.00	0.62
1:C:104:CYS:O	1:C:108:GLU:HB2	2.00	0.62
1:C:109:MSE:HE1	1:C:314:ILE:CG2	2.30	0.62
1:D:118:ILE:HD11	1:D:121:PRO:HB3	1.82	0.62
1:D:55:TRP:HB3	1:D:240:LEU:HD13	1.81	0.62
1:A:86:TYR:HB3	1:A:99:THR:CG2	2.29	0.62
1:A:86:TYR:HB3	1:A:99:THR:HG21	1.81	0.62
1:A:238:LEU:HD23	1:A:245:ILE:HD13	1.82	0.62
1:B:68:LEU:HB3	1:B:163:PHE:CE1	2.35	0.62
1:C:110:ILE:O	1:C:110:ILE:HG23	1.99	0.62
1:D:120:ASN:HD21	1:D:122:LYS:HE3	1.65	0.62
1:A:80:VAL:HG21	1:A:159:VAL:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:HD12	1:A:182:ASP:HA	1.81	0.62
1:B:125:LEU:HG	1:B:127:ILE:HG13	1.81	0.62
1:B:137:GLU:O	1:B:140:ARG:HB3	2.00	0.62
1:C:83:SER:HB2	1:C:89:VAL:HG23	1.82	0.62
1:C:112:HIS:HB3	1:C:116:CYS:SG	2.39	0.62
1:C:152:ILE:HG23	1:C:153:ASP:N	2.14	0.62
1:A:87:GLY:N	2:A:453:HOH:O	2.33	0.62
1:B:98:LEU:HD13	1:B:103:GLU:OE2	2.00	0.62
1:B:127:ILE:HD11	1:B:187:LEU:CD2	2.30	0.62
1:A:261:ASN:HD22	1:A:289:PHE:HD2	1.48	0.61
1:C:236:GLU:HB3	1:C:241:HIS:HD2	1.66	0.61
1:B:169:ILE:HD12	1:B:172:GLU:CG	2.29	0.61
1:C:95:VAL:HB	1:C:97:GLN:NE2	2.15	0.61
1:A:228:GLY:HA2	1:A:282:THR:O	1.99	0.61
1:C:249:VAL:HA	1:C:278:MSE:CE	2.30	0.61
1:D:99:THR:HG23	1:D:269:THR:HG21	1.82	0.61
1:A:126:VAL:HB	1:A:149:MSE:CG	2.30	0.61
1:D:99:THR:HG23	1:D:269:THR:HG21	1.82	0.61
1:B:152:ILE:HD12	1:B:181:GLY:O	2.00	0.61
1:C:154:LYS:HB2	1:C:180:ILE:HD13	1.81	0.61
1:A:86:TYR:CD2	1:A:99:THR:HG21	2.33	0.61
1:B:248:ILE:CG2	1:B:278:MSE:HG3	2.29	0.61
1:B:193:GLY:HA2	1:B:225:LEU:O	2.00	0.61
1:B:231:VAL:HG22	1:B:232:CYS:N	2.15	0.61
1:A:44:ILE:HD12	1:D:51:MSE:HE1	1.83	0.61
1:A:55:TRP:CD1	1:A:58:GLU:HG3	2.30	0.61
1:A:215:LYS:HG2	1:A:255:ILE:HG12	1.82	0.61
1:A:135:LEU:HB2	1:A:149:MSE:CE	2.29	0.61
1:D:271:PRO:O	1:D:272:SER:HB2	2.00	0.61
1:A:121:PRO:HA	1:A:196:ASP:OD1	2.00	0.61
1:B:241:HIS:HD2	2:B:375:HOH:O	1.82	0.61
1:A:123:LYS:HD3	1:A:194:SER:O	2.01	0.61
1:B:242:MSE:HG3	1:B:328:VAL:HG11	1.82	0.61
1:D:151:GLU:HG2	1:D:157:VAL:HG23	1.80	0.61
1:A:79:ILE:HB	1:A:91:VAL:HB	1.81	0.61
1:B:242:MSE:O	1:B:246:GLU:HG3	2.00	0.61
1:D:55:TRP:HB3	1:D:240:LEU:HD13	1.81	0.61
1:B:242:MSE:HB2	2:B:479:HOH:O	1.99	0.61
1:C:296:ILE:HG22	1:C:307:LEU:HD11	1.80	0.61
1:C:271:PRO:O	1:C:272:SER:HB3	1.99	0.61
1:C:161:LYS:HA	1:C:168:ALA:CB	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:O	1:A:56:PRO:HD3	2.00	0.61
1:C:154:LYS:HB2	1:C:180:ILE:HG12	1.82	0.61
1:D:83:SER:HB3	1:D:89:VAL:HG21	1.83	0.61
1:A:279:LEU:HB3	1:A:289:PHE:CD2	2.35	0.61
1:D:226:ARG:HD3	1:D:226:ARG:N	2.15	0.61
1:C:127:ILE:HD11	1:C:187:LEU:HD13	1.81	0.61
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.34	0.61
1:A:227:PRO:HB2	1:A:285:PRO:HD3	1.81	0.61
1:C:295:PRO:HG3	1:C:312:ALA:HB2	1.83	0.61
1:A:212:LEU:HA	1:A:217:PHE:CD2	2.35	0.61
1:A:46:GLY:HA3	1:A:63:LYS:NZ	2.14	0.61
1:B:249:VAL:HG11	1:B:329:ILE:HG23	1.83	0.61
1:C:73:SER:HB2	2:C:339:HOH:O	2.01	0.61
1:D:131:ASP:O	1:D:167:VAL:HB	2.00	0.61
1:B:134:VAL:O	1:B:138:VAL:HG23	2.00	0.61
1:B:206:ILE:HG22	2:B:359:HOH:O	2.00	0.61
1:B:271:PRO:O	1:B:272:SER:HB3	2.01	0.61
1:C:129:GLY:H	1:C:151:GLU:HB2	1.66	0.61
1:D:228:GLY:HA3	1:D:285:PRO:HD2	1.82	0.61
1:D:327:LYS:HD3	2:D:340:HOH:O	2.00	0.61
1:B:248:ILE:HG21	1:B:278:MSE:HG3	1.82	0.61
1:C:236:GLU:HB2	1:C:245:ILE:HG13	1.81	0.61
1:D:92:LEU:HB2	1:D:97:GLN:HE21	1.65	0.61
1:A:123:LYS:HD3	1:A:194:SER:O	2.01	0.61
1:B:98:LEU:C	1:B:98:LEU:HD12	2.20	0.61
1:C:131:ASP:HA	1:C:160:SER:HB3	1.82	0.61
1:D:198:VAL:HG23	1:D:225:LEU:HD21	1.82	0.61
1:A:310:TYR:HA	1:A:314:ILE:HG21	1.83	0.61
1:C:242:MSE:CE	1:C:329:ILE:HD11	2.31	0.61
1:D:261:ASN:HD22	1:D:289:PHE:HD2	1.49	0.61
1:A:52:SER:HB3	1:A:55:TRP:CE2	2.36	0.61
1:A:78:VAL:HB	1:A:155:MSE:SE	2.51	0.61
1:A:67:VAL:HG21	1:C:64:VAL:HG11	1.82	0.61
1:C:105:ALA:CB	1:C:267:VAL:HG22	2.30	0.61
1:B:48:PHE:HE2	1:B:96:ILE:HD11	1.65	0.61
1:C:123:LYS:HE3	1:C:195:TYR:CE1	2.35	0.61
1:A:104:CYS:CB	1:A:308:LYS:HE2	2.30	0.61
1:A:124:VAL:HG13	1:A:197:ALA:HB3	1.82	0.61
1:C:321:LEU:HD13	1:C:329:ILE:HD12	1.83	0.61
1:D:179:VAL:HG12	1:D:181:GLY:H	1.65	0.61
1:B:248:ILE:CG2	1:B:278:MSE:HG3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:VAL:HB	1:C:233:THR:HG22	1.83	0.61
1:A:51:MSE:SE	1:C:72:LYS:H	2.33	0.61
1:C:79:ILE:HB	1:C:91:VAL:HB	1.82	0.61
1:D:109:MSE:HE3	1:D:309:PHE:CD2	2.36	0.61
1:D:54:MSE:SE	1:D:204:ASP:HB3	2.50	0.61
1:D:310:TYR:CZ	1:D:315:HIS:HB2	2.36	0.61
1:B:248:ILE:HG22	1:B:278:MSE:HG3	1.83	0.61
1:B:263:ALA:HB2	1:B:319:PHE:CE1	2.36	0.61
1:C:296:ILE:CG2	1:C:307:LEU:HD21	2.31	0.60
1:D:231:VAL:HG21	1:D:256:PHE:CZ	2.36	0.60
1:C:230:VAL:HA	1:C:280:CYS:O	2.01	0.60
1:A:242:MSE:HE2	1:A:245:ILE:HD12	1.82	0.60
1:A:135:LEU:HD12	1:A:135:LEU:H	1.65	0.60
1:C:327:LYS:HG3	1:C:328:VAL:N	2.15	0.60
1:B:151:GLU:O	1:B:180:ILE:HA	2.01	0.60
1:A:129:GLY:HA2	1:A:201:ASP:OD2	2.01	0.60
1:D:128:GLY:HA3	2:D:553:HOH:O	2.00	0.60
1:A:98:LEU:HB2	1:A:103:GLU:CB	2.29	0.60
1:C:86:TYR:HB3	1:C:99:THR:HG23	1.82	0.60
1:C:99:THR:HG22	1:C:101:ARG:H	1.65	0.60
1:C:311:ASN:HD22	1:C:314:ILE:HB	1.64	0.60
1:A:44:ILE:N	1:A:44:ILE:HD12	2.16	0.60
1:A:58:GLU:HA	1:D:61:SER:O	2.01	0.60
1:D:109:MSE:HE1	1:D:310:TYR:HB2	1.80	0.60
1:A:52:SER:HB3	1:A:55:TRP:CE2	2.36	0.60
1:A:187:LEU:HB3	1:A:220:SER:OG	2.00	0.60
1:B:123:LYS:HE3	1:B:146:GLN:NE2	2.15	0.60
1:B:259:SER:O	1:B:280:CYS:HA	2.00	0.60
1:B:260:VAL:HG13	1:B:280:CYS:SG	2.41	0.60
1:D:261:ASN:HD22	1:D:289:PHE:HD2	1.49	0.60
1:A:220:SER:O	1:A:223:ARG:HG2	2.01	0.60
1:D:238:LEU:HD12	1:D:264:TRP:CE3	2.35	0.60
1:A:242:MSE:O	1:A:246:GLU:HG3	2.02	0.60
1:B:135:LEU:HD11	1:B:149:MSE:SE	2.51	0.60
1:D:107:GLN:O	1:D:111:THR:HG23	2.01	0.60
1:D:151:GLU:HG2	1:D:157:VAL:HG23	1.82	0.60
1:D:233:THR:HB	1:D:278:MSE:HB2	1.82	0.60
1:D:89:VAL:HG22	1:D:99:THR:HG22	1.81	0.60
1:B:127:ILE:HD11	1:B:187:LEU:CD2	2.30	0.60
1:B:187:LEU:HB3	1:B:220:SER:OG	2.01	0.60
1:A:50:GLU:OE2	1:A:96:ILE:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:MSE:HE2	1:B:278:MSE:HA	1.83	0.60
1:C:257:LYS:HE2	2:C:368:HOH:O	2.01	0.60
1:C:297:ASP:OD1	1:C:298:GLU:N	2.32	0.60
1:B:238:LEU:CD2	1:B:242:MSE:HE1	2.30	0.60
1:C:112:HIS:HB3	1:C:116:CYS:SG	2.40	0.60
1:A:242:MSE:CE	1:A:245:ILE:HD12	2.31	0.60
1:A:200:VAL:HB	1:A:233:THR:CG2	2.30	0.60
1:D:261:ASN:HD22	1:D:289:PHE:HD2	1.49	0.60
1:C:76:GLN:OE1	1:C:92:LEU:HB3	2.01	0.60
1:B:329:ILE:HG22	1:B:329:ILE:O	2.00	0.60
1:A:249:VAL:HA	1:A:278:MSE:HE1	1.83	0.60
1:A:161:LYS:HA	1:A:168:ALA:HB2	1.84	0.60
1:D:115:LEU:HD21	1:D:138:VAL:HG13	1.83	0.60
1:B:205:PRO:HD3	1:B:213:PHE:CZ	2.35	0.60
1:A:263:ALA:HB2	1:A:319:PHE:CE1	2.37	0.60
1:C:131:ASP:O	1:C:167:VAL:HG12	2.01	0.60
1:A:245:ILE:HA	1:A:248:ILE:HD12	1.82	0.60
1:B:48:PHE:CE1	1:B:91:VAL:HG21	2.37	0.60
1:D:111:THR:HG22	1:D:134:VAL:HG13	1.84	0.60
1:B:98:LEU:HD13	1:B:103:GLU:CD	2.22	0.60
1:C:265:THR:O	1:C:274:VAL:HA	2.01	0.60
1:D:235:ALA:HB2	1:D:278:MSE:HG2	1.82	0.60
1:B:124:VAL:HG22	1:B:197:ALA:HB3	1.83	0.60
1:D:200:VAL:HG12	1:D:202:SER:HB3	1.81	0.60
1:D:226:ARG:HG2	1:D:226:ARG:HH21	1.67	0.60
1:B:48:PHE:HZ	1:B:91:VAL:HG11	1.65	0.60
1:D:157:VAL:HG13	1:D:171:TYR:CZ	2.36	0.60
1:C:221:VAL:CG1	1:C:231:VAL:HG11	2.32	0.60
1:C:271:PRO:O	1:C:272:SER:HB2	2.02	0.60
1:D:115:LEU:HD23	1:D:141:HIS:CD2	2.37	0.60
1:C:153:ASP:OD2	1:C:156:VAL:HG23	2.00	0.60
1:D:52:SER:C	1:D:54:MSE:H	2.04	0.60
1:A:178:LEU:HD12	1:A:179:VAL:N	2.15	0.60
1:A:319:PHE:O	1:A:321:LEU:HG	2.02	0.60
1:A:131:ASP:O	1:A:167:VAL:HG12	2.01	0.60
1:B:132:GLY:HA3	1:B:167:VAL:O	2.02	0.60
1:C:237:SER:H	1:C:241:HIS:HD2	1.50	0.60
1:D:149:MSE:HB3	1:D:178:LEU:HA	1.84	0.60
1:A:237:SER:H	1:A:241:HIS:CD2	2.20	0.60
1:B:130:GLY:O	1:B:131:ASP:HB2	2.00	0.60
1:B:223:ARG:HD2	2:B:477:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:C	1:B:98:LEU:HD12	2.21	0.60
1:A:238:LEU:HD23	1:A:242:MSE:HE1	1.84	0.60
1:B:118:ILE:HB	1:B:119:PRO:HD2	1.83	0.60
1:D:259:SER:O	1:D:280:CYS:HA	2.02	0.60
1:A:54:MSE:SE	1:A:204:ASP:HB3	2.52	0.60
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.36	0.60
1:D:257:LYS:NZ	2:D:510:HOH:O	2.35	0.60
1:A:68:LEU:HG	1:A:81:PHE:HA	1.83	0.60
1:B:215:LYS:HB2	1:B:216:PRO:HD3	1.84	0.60
1:D:135:LEU:HD22	1:D:147:ILE:HG21	1.83	0.60
1:A:182:ASP:O	1:A:184:VAL:N	2.35	0.60
1:A:79:ILE:O	1:A:90:LEU:HD12	2.02	0.60
1:A:99:THR:O	1:A:103:GLU:HB3	2.01	0.60
1:B:157:VAL:O	1:B:161:LYS:HG3	2.02	0.59
1:C:66:LYS:HG2	1:C:82:GLN:HB3	1.82	0.59
1:D:313:GLU:CD	1:D:313:GLU:H	2.04	0.59
1:C:283:GLU:OE1	1:C:283:GLU:N	2.34	0.59
1:B:206:ILE:HG23	1:B:207:GLY:N	2.17	0.59
1:C:301:SER:HB3	1:C:304:ASN:ND2	2.13	0.59
1:D:225:LEU:HD11	1:D:231:VAL:CG2	2.32	0.59
1:A:327:LYS:HG3	1:A:328:VAL:N	2.16	0.59
1:A:159:VAL:HG13	1:A:163:PHE:HD2	1.67	0.59
1:A:72:LYS:NZ	1:C:53:PRO:HD3	2.15	0.59
1:C:187:LEU:CD2	1:C:221:VAL:HG22	2.32	0.59
1:A:111:THR:OG1	1:A:134:VAL:HG13	2.01	0.59
1:A:321:LEU:HD13	1:A:329:ILE:HD12	1.83	0.59
1:C:123:LYS:HG3	1:C:146:GLN:HB3	1.83	0.59
1:B:111:THR:OG1	1:B:134:VAL:HG13	2.02	0.59
1:C:296:ILE:HG23	1:C:300:SER:HB2	1.84	0.59
1:B:111:THR:O	1:B:115:LEU:HB2	2.02	0.59
1:B:149:MSE:O	1:B:179:VAL:HG22	2.01	0.59
1:A:122:LYS:N	1:A:196:ASP:OD1	2.30	0.59
1:B:192:GLU:HG3	1:B:223:ARG:HG2	1.83	0.59
1:D:241:HIS:CG	2:D:413:HOH:O	2.55	0.59
1:C:69:PHE:HE2	1:D:45:PRO:HD3	1.67	0.59
1:A:206:ILE:HG23	1:A:207:GLY:N	2.17	0.59
1:A:219:GLN:OE1	1:A:255:ILE:HD12	2.02	0.59
1:D:109:MSE:HE3	1:D:309:PHE:HD2	1.66	0.59
1:A:67:VAL:HG21	1:C:64:VAL:HG11	1.83	0.59
1:D:145:GLU:O	1:D:175:ARG:HB3	2.01	0.59
1:B:157:VAL:CG1	1:B:161:LYS:HE3	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.38	0.59
1:A:51:MSE:HE1	1:D:44:ILE:HG21	1.83	0.59
1:C:59:ALA:HA	2:C:373:HOH:O	2.01	0.59
1:C:135:LEU:HD22	1:C:149:MSE:SE	2.51	0.59
1:D:215:LYS:HZ3	1:D:251:ASN:ND2	1.99	0.59
1:D:99:THR:HG21	1:D:269:THR:HG21	1.85	0.59
1:D:69:PHE:HB2	1:D:163:PHE:CE2	2.37	0.59
1:B:164:PHE:O	1:B:167:VAL:HG22	2.01	0.59
1:A:252:CYS:HB3	1:A:280:CYS:SG	2.42	0.59
1:C:206:ILE:HG23	1:C:207:GLY:N	2.17	0.59
1:D:123:LYS:HE3	1:D:146:GLN:OE1	2.02	0.59
1:A:211:GLU:OE1	1:A:212:LEU:HG	2.03	0.59
1:D:109:MSE:HE1	1:D:113:LEU:HD11	1.83	0.59
1:D:80:VAL:HG21	1:D:159:VAL:CG1	2.33	0.59
1:D:89:VAL:HG22	1:D:99:THR:HG22	1.84	0.59
1:A:42:THR:HA	1:C:162:GLN:HE22	1.67	0.59
1:B:231:VAL:O	1:B:231:VAL:HG13	2.03	0.59
1:C:220:SER:HA	1:C:223:ARG:HG2	1.83	0.59
1:C:264:TRP:HA	1:C:275:ILE:O	2.03	0.59
1:D:217:PHE:O	1:D:221:VAL:HG23	2.02	0.59
1:D:109:MSE:HB3	1:D:277:PHE:CE2	2.38	0.59
1:C:97:GLN:HE21	1:C:97:GLN:CA	2.16	0.59
1:A:308:LYS:O	1:D:324:PHE:HB3	2.02	0.59
1:B:108:GLU:CD	1:B:307:LEU:HB3	2.23	0.59
1:C:327:LYS:HG3	1:C:328:VAL:N	2.18	0.59
1:A:109:MSE:HE2	1:A:265:THR:HB	1.84	0.59
1:A:253:ARG:HG2	1:A:260:VAL:HG21	1.83	0.59
1:A:82:GLN:HE21	1:A:87:GLY:HA2	1.68	0.59
1:A:87:GLY:N	2:A:459:HOH:O	2.35	0.59
1:B:227:PRO:HG2	2:B:473:HOH:O	2.01	0.59
1:B:114:PRO:HG2	1:B:115:LEU:H	1.68	0.59
1:B:259:SER:O	1:B:280:CYS:HA	2.02	0.59
1:C:54:MSE:HE1	1:C:236:GLU:HG3	1.84	0.59
1:D:113:LEU:HD23	1:D:315:HIS:ND1	2.18	0.59
1:D:149:MSE:HE1	2:D:552:HOH:O	2.03	0.59
1:D:233:THR:HG22	1:D:234:GLN:H	1.67	0.59
1:C:54:MSE:HE2	1:C:205:PRO:HD2	1.85	0.59
1:D:152:ILE:HG13	2:D:346:HOH:O	2.03	0.59
1:A:135:LEU:HB2	1:A:149:MSE:HE2	1.85	0.59
1:D:263:ALA:HA	1:D:318:ALA:O	2.03	0.59
1:C:198:VAL:HB	1:C:231:VAL:CG1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.38	0.59
1:A:44:ILE:N	1:A:44:ILE:HD12	2.18	0.59
1:B:322:PRO:HG2	1:B:325:ALA:CB	2.33	0.59
1:B:196:ASP:OD1	1:B:226:ARG:HD3	2.02	0.59
1:C:135:LEU:HD13	1:C:149:MSE:HE2	1.85	0.59
1:C:263:ALA:HB2	1:C:319:PHE:CE1	2.38	0.59
1:C:227:PRO:HA	1:C:282:THR:OG1	2.02	0.59
1:D:107:GLN:NE2	1:D:133:GLY:HA3	2.17	0.59
1:A:324:PHE:CD1	1:A:325:ALA:N	2.71	0.59
1:B:122:LYS:HD3	1:B:145:GLU:OE2	2.03	0.58
1:D:68:LEU:HD12	1:D:68:LEU:H	1.65	0.58
1:A:132:GLY:HA2	1:A:149:MSE:HE1	1.84	0.58
1:C:129:GLY:HA2	1:C:149:MSE:SE	2.53	0.58
1:C:53:PRO:O	1:C:56:PRO:HD3	2.03	0.58
1:A:51:MSE:HB3	2:C:363:HOH:O	2.02	0.58
1:B:109:MSE:HE2	1:B:113:LEU:HG	1.85	0.58
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.39	0.58
1:C:327:LYS:HG3	1:C:328:VAL:H	1.68	0.58
1:B:240:LEU:HD11	1:B:272:SER:HB2	1.84	0.58
1:D:164:PHE:O	1:D:167:VAL:HG22	2.04	0.58
1:D:75:TYR:HB2	1:D:153:ASP:OD2	2.02	0.58
1:B:123:LYS:HD3	1:B:194:SER:O	2.03	0.58
1:C:161:LYS:HA	1:C:168:ALA:CB	2.34	0.58
1:A:299:SER:HA	1:A:302:LYS:CG	2.31	0.58
1:D:248:ILE:HG22	1:D:278:MSE:CE	2.33	0.58
1:D:108:GLU:HB3	1:D:109:MSE:HE2	1.86	0.58
1:B:233:THR:HG22	1:B:278:MSE:HB2	1.85	0.58
1:D:105:ALA:O	1:D:109:MSE:HG2	2.04	0.58
1:D:111:THR:O	1:D:115:LEU:HB2	2.02	0.58
1:C:293:LEU:HD12	1:C:293:LEU:N	2.18	0.58
1:C:161:LYS:HA	1:C:168:ALA:HB1	1.84	0.58
1:D:93:ASP:N	2:D:353:HOH:O	2.36	0.58
1:B:54:MSE:SE	2:B:369:HOH:O	2.71	0.58
1:C:48:PHE:O	1:C:61:SER:HA	2.03	0.58
1:C:140:ARG:HB3	1:C:140:ARG:HH11	1.68	0.58
1:A:108:GLU:CD	1:A:307:LEU:HD22	2.24	0.58
1:A:55:TRP:HB3	1:A:240:LEU:HD13	1.85	0.58
1:B:51:MSE:SE	2:B:351:HOH:O	2.70	0.58
1:C:107:GLN:NE2	1:C:133:GLY:HA3	2.18	0.58
1:D:149:MSE:HE2	1:D:151:GLU:CG	2.33	0.58
1:D:40:PHE:O	1:D:42:THR:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HD12	1:B:172:GLU:HG3	1.86	0.58
1:A:262:TYR:HA	1:A:277:PHE:O	2.04	0.58
1:C:248:ILE:HG21	1:C:278:MSE:HG3	1.86	0.58
1:B:109:MSE:HE3	1:B:309:PHE:HD2	1.68	0.58
1:C:68:LEU:HD12	1:C:80:VAL:HG12	1.85	0.58
1:B:123:LYS:HB3	1:B:195:TYR:HA	1.86	0.58
1:C:249:VAL:HA	1:C:278:MSE:HE2	1.85	0.58
1:B:45:PRO:HA	1:C:41:SER:HB3	1.85	0.58
1:A:86:TYR:HD2	1:A:99:THR:HG21	1.69	0.58
1:A:238:LEU:HD23	1:A:242:MSE:HE1	1.86	0.58
1:B:43:VAL:HA	1:C:43:VAL:HG13	1.86	0.58
1:A:107:GLN:HG2	1:A:133:GLY:C	2.24	0.58
1:B:236:GLU:HB3	1:B:241:HIS:ND1	2.19	0.58
1:A:98:LEU:HD13	1:A:103:GLU:OE1	2.03	0.58
1:C:311:ASN:ND2	1:C:314:ILE:N	2.50	0.58
1:B:184:VAL:HG11	1:B:211:GLU:OE1	2.03	0.58
1:A:135:LEU:HD11	1:A:176:VAL:HG22	1.85	0.58
1:B:70:GLN:HG3	1:B:79:ILE:HG12	1.86	0.58
1:C:109:MSE:CE	1:C:310:TYR:HD2	2.16	0.58
1:A:99:THR:HG22	1:A:101:ARG:N	2.15	0.58
1:C:264:TRP:HA	1:C:275:ILE:O	2.04	0.58
1:D:109:MSE:HG2	1:D:265:THR:HG21	1.84	0.58
1:D:112:HIS:O	1:D:116:CYS:HB2	2.03	0.58
1:A:248:ILE:HG22	1:A:278:MSE:HG3	1.84	0.58
1:A:307:LEU:HD13	1:A:310:TYR:HB3	1.84	0.58
1:B:39:CYS:HB2	1:B:70:GLN:HE22	1.69	0.58
1:C:322:PRO:HG2	1:C:325:ALA:HB3	1.85	0.58
1:C:238:LEU:HD23	1:C:242:MSE:HE3	1.85	0.58
1:C:50:GLU:HG2	1:C:55:TRP:HZ2	1.68	0.58
1:D:217:PHE:O	1:D:221:VAL:HG23	2.04	0.58
1:A:311:ASN:CG	1:A:314:ILE:HG22	2.23	0.58
1:D:242:MSE:HE1	1:D:329:ILE:HD11	1.85	0.58
1:D:257:LYS:NZ	2:D:510:HOH:O	2.37	0.58
1:C:50:GLU:OE1	1:C:96:ILE:HD12	2.03	0.58
1:C:244:ILE:HG22	1:C:248:ILE:HG13	1.86	0.58
1:D:52:SER:OG	1:D:54:MSE:HG2	2.04	0.58
1:B:235:ALA:HB2	1:B:278:MSE:HG2	1.85	0.58
1:A:91:VAL:CG1	1:A:95:VAL:H	2.16	0.58
1:B:130:GLY:HA3	1:B:156:VAL:HG11	1.86	0.58
1:B:130:GLY:HA2	1:B:171:TYR:OH	2.04	0.58
1:B:238:LEU:HD11	1:B:321:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:PRO:O	1:C:56:PRO:HD3	2.04	0.58
1:B:196:ASP:OD1	1:B:226:ARG:HD3	2.03	0.58
1:C:98:LEU:HD21	1:C:131:ASP:HB3	1.85	0.58
1:D:94:GLY:O	1:D:95:VAL:HG23	2.02	0.58
1:D:164:PHE:HB2	1:D:167:VAL:HG22	1.85	0.58
1:B:104:CYS:O	1:B:108:GLU:HB2	2.04	0.58
1:B:227:PRO:O	1:B:284:GLY:HA3	2.04	0.58
1:B:129:GLY:O	1:B:131:ASP:N	2.37	0.58
1:C:76:GLN:OE1	1:C:92:LEU:HB3	2.04	0.58
1:B:198:VAL:O	1:B:231:VAL:HA	2.03	0.58
1:D:164:PHE:HB2	1:D:167:VAL:HG22	1.85	0.58
1:A:68:LEU:HD11	1:A:88:LYS:HD2	1.86	0.58
1:C:259:SER:O	1:C:280:CYS:HA	2.04	0.58
1:D:69:PHE:CG	1:D:70:GLN:N	2.70	0.58
1:A:236:GLU:HB3	1:A:241:HIS:HD2	1.65	0.58
1:B:42:THR:HA	1:B:49:SER:CB	2.33	0.58
1:C:184:VAL:HG12	1:C:212:LEU:HD21	1.86	0.58
1:C:75:TYR:O	1:C:76:GLN:HB3	2.04	0.58
1:A:243:ASP:OD2	1:A:244:ILE:HG13	2.03	0.58
1:B:51:MSE:HE3	2:C:530:HOH:O	2.04	0.58
1:B:188:LYS:HE2	2:B:432:HOH:O	2.04	0.58
1:B:278:MSE:O	1:B:279:LEU:C	2.42	0.58
1:D:126:VAL:CG1	1:D:149:MSE:SE	3.02	0.58
1:D:161:LYS:HA	1:D:168:ALA:HB2	1.86	0.57
1:A:162:GLN:HE22	1:C:43:VAL:H	1.51	0.57
1:C:52:SER:OG	1:C:54:MSE:HB2	2.04	0.57
1:B:168:ALA:C	1:B:170:GLY:H	2.07	0.57
1:C:98:LEU:HD11	1:C:164:PHE:CE2	2.39	0.57
1:D:51:MSE:HA	1:D:55:TRP:NE1	2.18	0.57
1:C:70:GLN:NE2	2:C:365:HOH:O	2.37	0.57
1:A:151:GLU:HG3	1:A:152:ILE:N	2.10	0.57
1:A:92:LEU:O	1:A:94:GLY:N	2.37	0.57
1:A:236:GLU:HB3	1:A:241:HIS:HD2	1.68	0.57
1:D:163:PHE:C	1:D:165:PRO:HD3	2.24	0.57
1:D:110:ILE:HG13	1:D:232:CYS:SG	2.44	0.57
1:A:80:VAL:HG21	1:A:159:VAL:HG12	1.85	0.57
1:A:220:SER:O	1:A:223:ARG:HG2	2.04	0.57
1:A:329:ILE:O	1:A:329:ILE:HG22	2.03	0.57
1:A:59:ALA:HB3	1:D:61:SER:HB2	1.86	0.57
1:C:123:LYS:HG3	1:C:146:GLN:CB	2.34	0.57
1:D:173:ASP:HB3	1:D:176:VAL:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:O	1:A:248:ILE:HG13	2.04	0.57
1:B:231:VAL:CG1	1:B:280:CYS:HB2	2.34	0.57
1:A:70:GLN:HE22	1:C:70:GLN:HE22	1.51	0.57
1:B:98:LEU:O	1:B:98:LEU:HD12	2.04	0.57
1:A:51:MSE:HB2	1:C:72:LYS:HB3	1.86	0.57
1:C:135:LEU:HD23	1:C:170:GLY:O	2.04	0.57
1:D:43:VAL:C	1:D:44:ILE:HG13	2.25	0.57
1:A:63:LYS:HB3	1:A:84:ALA:CB	2.35	0.57
1:A:63:LYS:HB3	1:A:84:ALA:HB2	1.87	0.57
1:A:86:TYR:HD2	1:A:99:THR:HG21	1.69	0.57
1:C:297:ASP:HA	2:C:488:HOH:O	2.04	0.57
1:D:110:ILE:HG23	1:D:111:THR:HG23	1.86	0.57
1:A:108:GLU:HG2	1:A:307:LEU:HD22	1.85	0.57
1:C:127:ILE:HD12	1:C:127:ILE:N	2.19	0.57
1:C:261:ASN:HD22	1:C:289:PHE:HD2	1.52	0.57
1:B:130:GLY:O	1:B:131:ASP:HB2	2.04	0.57
1:C:70:GLN:NE2	2:C:363:HOH:O	2.34	0.57
1:D:128:GLY:HA2	2:D:551:HOH:O	2.04	0.57
1:B:242:MSE:HE3	1:B:245:ILE:HB	1.86	0.57
1:D:205:PRO:CB	1:D:210:LYS:HA	2.33	0.57
1:C:126:VAL:O	1:C:149:MSE:HA	2.04	0.57
1:C:99:THR:HG22	1:C:101:ARG:N	2.20	0.57
1:B:130:GLY:O	1:B:131:ASP:CB	2.52	0.57
1:D:114:PRO:HG2	1:D:115:LEU:CD1	2.35	0.57
1:C:292:PRO:O	1:C:295:PRO:HD3	2.03	0.57
1:D:252:CYS:SG	1:D:278:MSE:HE2	2.45	0.57
1:B:54:MSE:HE2	1:B:204:ASP:HB3	1.87	0.57
1:C:219:GLN:HB2	1:C:255:ILE:HD12	1.87	0.57
1:D:111:THR:HG22	1:D:134:VAL:HG13	1.86	0.57
1:A:241:HIS:HB3	1:A:244:ILE:HD12	1.85	0.57
1:A:127:ILE:HB	1:A:200:VAL:CG2	2.29	0.57
1:B:121:PRO:C	1:B:122:LYS:HD2	2.25	0.57
1:A:130:GLY:HA2	1:A:151:GLU:OE2	2.05	0.57
1:B:153:ASP:OD2	1:B:156:VAL:HG23	2.04	0.57
1:D:109:MSE:C	1:D:111:THR:N	2.57	0.57
1:D:227:PRO:HB3	1:D:284:GLY:HA3	1.85	0.57
1:B:326:LYS:HE2	1:B:330:GLU:OE1	2.04	0.57
1:A:43:VAL:HG13	1:D:43:VAL:HA	1.86	0.57
1:D:98:LEU:C	1:D:98:LEU:HD12	2.24	0.57
1:A:149:MSE:HG3	1:A:178:LEU:HD13	1.87	0.57
1:B:98:LEU:HD12	1:B:98:LEU:C	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:TRP:CH2	1:A:95:VAL:HG22	2.39	0.57
1:B:243:ASP:O	1:B:244:ILE:HG13	2.05	0.57
1:C:112:HIS:O	1:C:116:CYS:HB2	2.04	0.57
1:B:326:LYS:HE2	2:B:367:HOH:O	2.04	0.57
1:B:44:ILE:CD1	1:C:51:MSE:HE3	2.35	0.57
1:D:111:THR:HG21	1:D:134:VAL:HG13	1.87	0.57
1:A:271:PRO:O	1:A:272:SER:HB3	2.04	0.57
1:B:163:PHE:C	1:B:165:PRO:HD3	2.24	0.57
1:B:116:CYS:HB3	1:B:294:ASN:O	2.05	0.57
1:D:290:LYS:HD2	1:D:291:HIS:CE1	2.40	0.57
1:D:98:LEU:C	1:D:98:LEU:HD12	2.25	0.57
1:B:98:LEU:HD12	1:B:98:LEU:C	2.25	0.57
1:D:198:VAL:HG23	1:D:225:LEU:HD21	1.85	0.57
1:D:51:MSE:O	1:D:52:SER:HB2	2.05	0.57
1:B:184:VAL:HG11	1:B:211:GLU:CD	2.25	0.57
1:B:103:GLU:HB3	1:B:107:GLN:NE2	2.18	0.57
1:C:88:LYS:H	1:C:100:GLU:HG3	1.69	0.57
1:D:134:VAL:O	1:D:138:VAL:HG23	2.04	0.57
1:A:240:LEU:HD11	1:A:271:PRO:HB2	1.86	0.57
1:A:82:GLN:OE1	1:A:88:LYS:HG3	2.04	0.57
1:B:127:ILE:HD11	1:B:187:LEU:CD2	2.35	0.57
1:B:326:LYS:HE2	2:C:351:HOH:O	2.05	0.57
1:A:238:LEU:CA	1:A:242:MSE:HE3	2.32	0.57
1:C:99:THR:O	1:C:103:GLU:HB3	2.04	0.57
1:B:123:LYS:NZ	1:B:146:GLN:HE22	2.03	0.57
1:D:293:LEU:HD23	1:D:293:LEU:N	2.20	0.57
1:A:194:SER:O	1:A:195:TYR:CG	2.58	0.57
1:A:325:ALA:O	1:A:329:ILE:HB	2.05	0.57
1:B:109:MSE:O	1:B:113:LEU:HB2	2.05	0.57
1:A:329:ILE:HG22	1:A:329:ILE:O	2.05	0.57
1:B:97:GLN:O	1:B:98:LEU:HB3	2.05	0.57
1:A:129:GLY:C	1:A:131:ASP:H	2.07	0.57
1:B:187:LEU:HB3	1:B:220:SER:OG	2.05	0.57
1:D:164:PHE:HB2	1:D:167:VAL:HG22	1.85	0.57
1:B:269:THR:HB	2:B:462:HOH:O	2.04	0.57
1:A:86:TYR:HD2	1:A:99:THR:HG21	1.70	0.57
1:A:260:VAL:HB	1:A:278:MSE:CE	2.35	0.57
1:D:279:LEU:HD12	1:D:289:PHE:CD1	2.40	0.57
1:B:172:GLU:O	1:B:173:ASP:C	2.43	0.57
1:A:215:LYS:HG3	1:A:251:ASN:ND2	2.20	0.57
1:C:135:LEU:HB2	1:C:149:MSE:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:PRO:HG2	1:D:115:LEU:H	1.70	0.57
1:C:108:GLU:OE1	1:C:310:TYR:HB3	2.05	0.57
1:A:179:VAL:HG11	1:A:186:PHE:CD2	2.40	0.57
1:A:104:CYS:CB	1:A:308:LYS:HE2	2.33	0.57
1:C:182:ASP:OD2	1:C:185:ALA:HB2	2.04	0.57
1:D:146:GLN:HG2	1:D:148:ASP:OD1	2.05	0.57
1:A:151:GLU:O	1:A:180:ILE:HA	2.05	0.57
1:A:183:GLY:O	1:A:186:PHE:HB3	2.05	0.57
1:A:59:ALA:HB3	1:D:61:SER:HB2	1.86	0.57
1:D:146:GLN:HE21	1:D:177:ASN:CB	2.16	0.57
1:A:128:GLY:HA2	1:A:151:GLU:OE1	2.04	0.56
1:A:90:LEU:HB3	1:A:98:LEU:HG	1.86	0.56
1:A:105:ALA:O	1:A:109:MSE:CG	2.48	0.56
1:B:192:GLU:HA	1:B:223:ARG:NH1	2.20	0.56
1:B:113:LEU:HA	1:B:315:HIS:CE1	2.40	0.56
1:D:136:ARG:HH21	1:D:167:VAL:HG12	1.70	0.56
1:D:223:ARG:NH1	2:D:402:HOH:O	2.38	0.56
1:C:264:TRP:CZ2	1:C:322:PRO:HD3	2.40	0.56
1:D:184:VAL:HG22	1:D:217:PHE:CD1	2.40	0.56
1:D:91:VAL:HA	1:D:95:VAL:O	2.05	0.56
1:C:166:ASP:HB3	2:C:452:HOH:O	2.05	0.56
1:D:259:SER:O	1:D:280:CYS:HA	2.05	0.56
1:A:297:ASP:O	1:A:298:GLU:HB2	2.04	0.56
1:C:242:MSE:HE2	1:C:242:MSE:HA	1.87	0.56
1:A:212:LEU:HA	1:A:217:PHE:CD2	2.40	0.56
1:C:69:PHE:CE1	1:C:159:VAL:HG21	2.40	0.56
1:B:66:LYS:HD3	1:B:66:LYS:C	2.26	0.56
1:D:261:ASN:HD22	1:D:289:PHE:HD2	1.52	0.56
1:A:206:ILE:HG23	1:A:207:GLY:N	2.21	0.56
1:B:130:GLY:O	1:B:131:ASP:HB2	2.04	0.56
1:D:206:ILE:O	1:D:206:ILE:HG13	2.04	0.56
1:A:103:GLU:HA	2:A:368:HOH:O	2.05	0.56
1:D:109:MSE:HG2	1:D:277:PHE:CE2	2.40	0.56
1:D:260:VAL:HA	1:D:280:CYS:SG	2.45	0.56
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.39	0.56
1:B:161:LYS:HA	1:B:168:ALA:HB1	1.87	0.56
1:B:188:LYS:HE2	2:B:432:HOH:O	2.05	0.56
1:B:123:LYS:HZ1	1:B:146:GLN:NE2	2.04	0.56
1:A:253:ARG:HH22	1:A:330:GLU:CB	2.18	0.56
1:C:98:LEU:HG	1:C:99:THR:N	2.20	0.56
1:D:262:TYR:OH	1:D:276:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLU:HG3	1:B:153:ASP:H	1.71	0.56
1:A:129:GLY:C	1:A:131:ASP:H	2.08	0.56
1:D:163:PHE:C	1:D:165:PRO:HD3	2.25	0.56
1:A:144:ILE:HB	1:A:175:ARG:NH1	2.19	0.56
1:B:236:GLU:HB3	1:B:241:HIS:ND1	2.20	0.56
1:C:119:PRO:HD2	1:C:226:ARG:HH22	1.70	0.56
1:A:215:LYS:HD3	1:A:254:GLU:OE1	2.05	0.56
1:B:103:GLU:O	1:B:107:GLN:HG3	2.05	0.56
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.39	0.56
1:D:120:ASN:ND2	1:D:122:LYS:HE3	2.20	0.56
1:A:179:VAL:HG21	1:A:186:PHE:HE2	1.70	0.56
1:B:130:GLY:HA3	1:B:156:VAL:CG1	2.35	0.56
1:A:206:ILE:HG23	1:A:207:GLY:N	2.12	0.56
1:C:86:TYR:HD2	1:C:99:THR:HG21	1.70	0.56
1:A:109:MSE:CE	1:A:310:TYR:HB2	2.35	0.56
1:A:254:GLU:O	1:A:255:ILE:HD13	2.05	0.56
1:D:69:PHE:HB2	1:D:163:PHE:CZ	2.40	0.56
1:B:218:PHE:O	1:B:255:ILE:HG21	2.06	0.56
1:C:253:ARG:HH12	1:C:330:GLU:HB2	1.71	0.56
1:C:86:TYR:CD2	1:C:99:THR:HG21	2.40	0.56
1:D:243:ASP:OD1	1:D:244:ILE:N	2.39	0.56
1:D:98:LEU:C	1:D:98:LEU:HD12	2.25	0.56
1:A:107:GLN:HG2	1:A:133:GLY:C	2.25	0.56
1:A:145:GLU:O	1:A:175:ARG:HG2	2.06	0.56
1:B:98:LEU:HD12	1:B:98:LEU:C	2.26	0.56
1:C:99:THR:HB	1:C:102:ASP:OD1	2.05	0.56
1:C:324:PHE:O	1:C:328:VAL:HG23	2.06	0.56
1:C:100:GLU:HA	1:C:103:GLU:OE2	2.05	0.56
1:B:54:MSE:HE1	1:B:206:ILE:HB	1.87	0.56
1:B:129:GLY:O	1:B:130:GLY:C	2.43	0.56
1:A:296:ILE:HD13	1:A:297:ASP:N	2.19	0.56
1:C:327:LYS:HG3	1:C:328:VAL:H	1.71	0.56
1:A:241:HIS:O	1:A:245:ILE:HG13	2.05	0.56
1:A:259:SER:O	1:A:280:CYS:HA	2.06	0.56
1:A:90:LEU:HB3	1:A:98:LEU:HG	1.88	0.56
1:C:125:LEU:HB2	1:C:195:TYR:CZ	2.40	0.56
1:D:161:LYS:HA	1:D:168:ALA:HB2	1.88	0.56
1:A:50:GLU:O	1:A:50:GLU:HG2	2.06	0.56
1:C:237:SER:H	1:C:241:HIS:HD2	1.54	0.56
1:A:258:GLY:HA3	1:A:281:SER:OG	2.04	0.56
1:C:155:MSE:O	1:C:159:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:VAL:O	1:D:138:VAL:HG23	2.05	0.56
1:A:47:TRP:CE2	1:A:63:LYS:HD3	2.40	0.56
1:B:242:MSE:HG3	1:B:246:GLU:OE1	2.06	0.56
1:B:234:GLN:HE22	1:B:236:GLU:HA	1.69	0.56
1:D:96:ILE:HG21	1:D:269:THR:CG2	2.36	0.56
1:A:43:VAL:HG12	1:A:44:ILE:N	2.21	0.56
1:A:123:LYS:HD3	1:A:194:SER:O	2.05	0.56
1:A:211:GLU:HA	1:A:214:GLU:HG2	1.86	0.56
1:A:229:GLY:O	1:A:281:SER:HA	2.06	0.56
1:A:254:GLU:O	1:A:255:ILE:HD13	2.05	0.56
1:A:212:LEU:HA	1:A:217:PHE:CD2	2.40	0.56
1:A:237:SER:H	1:A:241:HIS:CD2	2.23	0.56
1:A:99:THR:HG22	1:A:101:ARG:N	2.20	0.56
1:A:265:THR:HG22	1:A:275:ILE:HG22	1.88	0.56
1:C:141:HIS:O	1:C:144:ILE:HG12	2.05	0.56
1:C:86:TYR:CD2	1:C:101:ARG:HD3	2.41	0.56
1:A:145:GLU:O	1:A:175:ARG:HG2	2.06	0.56
1:A:253:ARG:NH2	1:A:330:GLU:HB3	2.08	0.56
1:B:124:VAL:HG13	1:B:197:ALA:O	2.06	0.56
1:B:99:THR:HG23	1:B:269:THR:HG21	1.88	0.56
1:A:292:PRO:HB3	1:A:315:HIS:CE1	2.41	0.56
1:D:323:SER:O	1:D:325:ALA:N	2.39	0.56
1:D:98:LEU:C	1:D:98:LEU:HD12	2.26	0.56
1:B:149:MSE:CE	1:B:171:TYR:HE1	2.19	0.56
1:D:151:GLU:OE2	1:D:157:VAL:HG22	2.06	0.56
1:A:229:GLY:O	1:A:281:SER:HA	2.06	0.56
1:B:237:SER:HA	2:B:355:HOH:O	2.06	0.56
1:A:72:LYS:HZ2	1:C:52:SER:HA	1.71	0.56
1:A:182:ASP:OD2	1:A:184:VAL:HG22	2.06	0.56
1:B:240:LEU:HG	1:B:272:SER:HB2	1.88	0.56
1:C:86:TYR:HD2	1:C:99:THR:HG21	1.70	0.56
1:B:263:ALA:HA	1:B:318:ALA:O	2.06	0.56
1:A:79:ILE:HB	1:A:91:VAL:HB	1.87	0.56
1:D:225:LEU:HD22	1:D:229:GLY:HA3	1.86	0.56
1:B:288:ASP:HB3	2:B:395:HOH:O	2.05	0.56
1:C:307:LEU:HD23	1:C:310:TYR:HB3	1.88	0.56
1:C:155:MSE:O	1:C:159:VAL:HG23	2.06	0.56
1:D:98:LEU:HD12	1:D:98:LEU:C	2.25	0.56
1:C:187:LEU:HD21	1:C:221:VAL:HG22	1.88	0.56
1:C:329:ILE:O	1:C:330:GLU:HB2	2.06	0.56
1:D:131:ASP:O	1:D:167:VAL:HB	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLU:HA	1:C:103:GLU:OE2	2.06	0.56
1:C:68:LEU:HD11	1:C:88:LYS:HG2	1.88	0.56
1:C:129:GLY:N	1:C:151:GLU:HB2	2.21	0.56
1:D:73:SER:HB3	1:D:76:GLN:O	2.06	0.56
1:A:229:GLY:O	1:A:281:SER:HA	2.06	0.56
1:C:187:LEU:HD21	1:C:221:VAL:HG22	1.87	0.56
1:D:184:VAL:HG13	2:D:408:HOH:O	2.06	0.56
1:A:126:VAL:HB	1:A:149:MSE:HG3	1.88	0.56
1:C:96:ILE:HG21	1:C:269:THR:CG2	2.36	0.56
1:D:118:ILE:HD11	1:D:121:PRO:HB3	1.88	0.56
1:A:232:CYS:SG	1:A:277:PHE:CD1	2.99	0.56
1:B:210:LYS:NZ	2:B:475:HOH:O	2.39	0.56
1:D:184:VAL:HA	2:D:410:HOH:O	2.05	0.56
1:C:182:ASP:OD2	1:C:185:ALA:HB2	2.06	0.56
1:D:196:ASP:OD1	1:D:226:ARG:NH2	2.39	0.56
1:D:205:PRO:HG3	1:D:244:ILE:HG21	1.87	0.56
1:B:80:VAL:HG21	1:B:159:VAL:CG1	2.36	0.55
1:C:131:ASP:HB2	1:C:167:VAL:HG11	1.88	0.55
1:B:153:ASP:OD1	1:B:155:MSE:HB3	2.06	0.55
1:B:205:PRO:HA	1:B:210:LYS:HA	1.89	0.55
1:C:311:ASN:ND2	1:C:314:ILE:HB	2.21	0.55
1:D:107:GLN:NE2	1:D:133:GLY:HA3	2.21	0.55
1:B:153:ASP:OD2	1:B:155:MSE:HB3	2.06	0.55
1:B:51:MSE:HG3	1:B:59:ALA:CB	2.36	0.55
1:D:252:CYS:HB2	1:D:278:MSE:HE3	1.86	0.55
1:B:45:PRO:HA	1:C:41:SER:OG	2.06	0.55
1:A:242:MSE:CE	1:A:242:MSE:HA	2.32	0.55
1:A:257:LYS:HB2	1:A:283:GLU:HB2	1.88	0.55
1:C:217:PHE:O	1:C:221:VAL:HG23	2.06	0.55
1:B:311:ASN:OD1	1:B:312:ALA:N	2.39	0.55
1:C:68:LEU:HG	1:C:81:PHE:HA	1.87	0.55
1:A:169:ILE:HD12	1:A:172:GLU:OE2	2.06	0.55
1:B:44:ILE:HD13	1:C:51:MSE:CE	2.37	0.55
1:A:72:LYS:HB3	1:C:51:MSE:CB	2.32	0.55
1:D:262:TYR:HA	1:D:277:PHE:O	2.06	0.55
1:C:200:VAL:O	1:C:233:THR:HA	2.06	0.55
1:D:151:GLU:HG2	1:D:157:VAL:CG2	2.36	0.55
1:D:247:ASP:O	1:D:251:ASN:HB2	2.06	0.55
1:D:328:VAL:O	1:D:330:GLU:N	2.38	0.55
1:A:233:THR:O	1:A:277:PHE:HA	2.06	0.55
1:A:296:ILE:HG22	1:A:297:ASP:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:PHE:CZ	1:D:71:GLY:HA3	2.42	0.55
1:B:40:PHE:HD1	1:C:42:THR:HG21	1.72	0.55
1:A:46:GLY:HA3	1:A:63:LYS:NZ	2.21	0.55
1:B:317:ALA:O	1:B:320:CYS:HB3	2.05	0.55
1:C:124:VAL:HG22	1:C:197:ALA:HB3	1.88	0.55
1:C:193:GLY:H	1:C:224:ALA:CA	2.19	0.55
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.41	0.55
1:C:73:SER:HB2	2:C:340:HOH:O	2.06	0.55
1:D:98:LEU:C	1:D:98:LEU:HD12	2.26	0.55
1:B:105:ALA:O	1:B:109:MSE:HB2	2.05	0.55
1:D:64:VAL:HG22	1:D:81:PHE:CE1	2.41	0.55
1:C:129:GLY:HA2	1:C:149:MSE:SE	2.56	0.55
1:A:51:MSE:HE3	1:C:71:GLY:CA	2.36	0.55
1:C:296:ILE:HD12	1:C:307:LEU:HD11	1.87	0.55
1:A:83:SER:O	1:A:85:THR:N	2.39	0.55
1:A:51:MSE:HE1	2:C:408:HOH:O	2.06	0.55
1:B:69:PHE:O	1:B:79:ILE:HA	2.07	0.55
1:D:40:PHE:O	1:D:42:THR:N	2.39	0.55
1:B:154:LYS:HE3	1:B:158:ASP:OD2	2.06	0.55
1:D:123:LYS:HE3	1:D:146:GLN:NE2	2.22	0.55
1:A:238:LEU:HD23	1:A:245:ILE:HD13	1.87	0.55
1:B:292:PRO:HD3	1:B:315:HIS:NE2	2.21	0.55
1:B:188:LYS:HE2	2:B:432:HOH:O	2.07	0.55
1:C:299:SER:HB2	2:C:422:HOH:O	2.06	0.55
1:C:86:TYR:CD2	1:C:99:THR:HG21	2.40	0.55
1:A:210:LYS:O	1:A:214:GLU:HG2	2.07	0.55
1:A:193:GLY:HA2	1:A:225:LEU:O	2.07	0.55
1:B:145:GLU:O	1:B:175:ARG:HG2	2.06	0.55
1:C:238:LEU:HD23	1:C:245:ILE:HD13	1.87	0.55
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.41	0.55
1:D:260:VAL:HG13	1:D:280:CYS:SG	2.46	0.55
1:D:109:MSE:CE	1:D:309:PHE:HD2	2.19	0.55
1:A:121:PRO:O	1:A:144:ILE:HD13	2.06	0.55
1:A:321:LEU:HD13	1:A:329:ILE:HD12	1.88	0.55
1:B:231:VAL:HG22	1:B:232:CYS:N	2.21	0.55
2:B:486:HOH:O	1:C:313:GLU:HB3	2.06	0.55
1:A:53:PRO:O	1:A:56:PRO:HD3	2.06	0.55
1:B:292:PRO:HB3	1:B:315:HIS:CE1	2.41	0.55
1:C:205:PRO:HG3	1:C:244:ILE:HD13	1.88	0.55
1:C:86:TYR:HB3	1:C:99:THR:HG23	1.89	0.55
1:A:104:CYS:O	1:A:108:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:NH2	1:C:240:LEU:HD23	2.22	0.55
1:C:329:ILE:O	1:C:330:GLU:HB2	2.06	0.55
1:D:153:ASP:OD2	1:D:155:MSE:HB3	2.06	0.55
1:A:61:SER:O	1:D:58:GLU:HA	2.06	0.55
1:B:215:LYS:HG2	1:B:251:ASN:HB3	1.88	0.55
1:A:170:GLY:C	1:A:172:GLU:H	2.10	0.55
1:A:283:GLU:O	1:A:283:GLU:HG2	2.07	0.55
1:C:257:LYS:HE2	2:C:368:HOH:O	2.06	0.55
1:D:111:THR:HG22	1:D:134:VAL:HG13	1.89	0.55
1:D:330:GLU:N	1:D:330:GLU:OE1	2.39	0.55
1:A:98:LEU:HB2	1:A:103:GLU:HB2	1.88	0.55
1:C:311:ASN:HD21	1:C:314:ILE:HD13	1.72	0.55
1:D:115:LEU:HD23	1:D:141:HIS:CD2	2.41	0.55
1:B:323:SER:C	1:B:325:ALA:H	2.10	0.55
1:B:92:LEU:HD12	1:B:97:GLN:HG2	1.88	0.55
1:A:90:LEU:HD23	1:A:91:VAL:N	2.21	0.55
1:C:313:GLU:HB2	2:C:407:HOH:O	2.05	0.55
1:A:172:GLU:HG2	2:A:349:HOH:O	2.07	0.55
1:A:110:ILE:HB	1:A:277:PHE:CZ	2.41	0.55
1:B:293:LEU:HD23	1:B:294:ASN:N	2.21	0.55
1:D:238:LEU:HD22	1:D:325:ALA:CB	2.36	0.55
1:A:136:ARG:HH21	1:A:167:VAL:HG13	1.70	0.55
1:C:154:LYS:O	1:C:158:ASP:HB2	2.07	0.55
1:D:203:SER:O	1:D:204:ASP:C	2.45	0.55
1:D:96:ILE:HG21	1:D:269:THR:CG2	2.37	0.55
1:A:164:PHE:HB3	1:A:167:VAL:HB	1.88	0.55
1:A:219:GLN:OE1	1:A:255:ILE:HD12	2.06	0.55
1:C:124:VAL:HG23	1:C:197:ALA:HB3	1.88	0.55
1:D:131:ASP:O	1:D:167:VAL:HG23	2.07	0.55
1:B:152:ILE:HG12	1:B:152:ILE:O	2.05	0.55
1:C:136:ARG:NH2	1:C:167:VAL:HG13	2.21	0.55
1:D:312:ALA:O	1:D:315:HIS:HB3	2.06	0.55
1:D:288:ASP:OD2	1:D:291:HIS:HB2	2.07	0.55
1:D:87:GLY:O	1:D:89:VAL:HG23	2.07	0.55
1:A:171:TYR:CD1	1:A:178:LEU:HD22	2.42	0.55
1:A:242:MSE:C	1:A:244:ILE:H	2.10	0.55
1:A:76:GLN:CD	1:A:92:LEU:HD22	2.27	0.55
1:B:69:PHE:HB3	1:B:80:VAL:HB	1.89	0.55
1:C:135:LEU:HB3	1:C:170:GLY:HA3	1.88	0.55
1:D:241:HIS:CG	1:D:244:ILE:HD12	2.42	0.55
1:D:96:ILE:HG21	1:D:269:THR:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ASP:OD2	1:C:185:ALA:HB2	2.06	0.55
1:D:125:LEU:HD21	1:D:127:ILE:HD11	1.89	0.55
1:A:132:GLY:HA2	1:A:149:MSE:CE	2.36	0.55
1:D:96:ILE:HG21	1:D:269:THR:CG2	2.37	0.55
1:B:106:TYR:CZ	1:B:110:ILE:HD12	2.42	0.55
1:D:101:ARG:HG2	1:D:101:ARG:O	2.07	0.55
1:B:329:ILE:CG2	1:B:329:ILE:O	2.55	0.55
1:C:149:MSE:HG2	1:C:178:LEU:HD13	1.89	0.55
1:C:73:SER:HB2	2:C:340:HOH:O	2.07	0.55
1:C:90:LEU:HB3	1:C:98:LEU:HG	1.88	0.55
1:D:164:PHE:HB2	1:D:167:VAL:HG22	1.88	0.55
1:A:311:ASN:HD21	1:A:314:ILE:HD13	1.70	0.55
1:B:68:LEU:HB3	1:B:163:PHE:CE1	2.42	0.55
1:B:98:LEU:O	1:B:98:LEU:HD12	2.07	0.55
1:A:45:PRO:HA	1:C:68:LEU:O	2.07	0.55
1:D:88:LYS:HG3	1:D:100:GLU:OE1	2.07	0.55
1:D:151:GLU:OE2	1:D:156:VAL:HB	2.07	0.55
1:B:96:ILE:HG21	1:B:269:THR:CG2	2.37	0.55
1:C:187:LEU:HA	1:C:190:ALA:HB2	1.88	0.55
1:B:78:VAL:HG11	1:B:159:VAL:HG21	1.89	0.55
1:D:129:GLY:HA3	1:D:156:VAL:HG11	1.88	0.55
1:A:122:LYS:N	1:A:196:ASP:OD2	2.40	0.55
1:A:123:LYS:HD3	1:A:194:SER:O	2.07	0.55
1:B:42:THR:HA	1:B:49:SER:CB	2.36	0.55
1:A:53:PRO:O	1:A:56:PRO:HD3	2.07	0.55
1:B:234:GLN:NE2	1:B:236:GLU:H	2.05	0.55
1:D:136:ARG:HH11	1:D:136:ARG:HG2	1.72	0.55
1:C:311:ASN:O	1:C:314:ILE:HG22	2.07	0.55
1:C:87:GLY:O	1:C:89:VAL:HG23	2.06	0.54
1:D:120:ASN:HD21	1:D:122:LYS:HE3	1.72	0.54
1:D:96:ILE:HG21	1:D:269:THR:CG2	2.37	0.54
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.41	0.54
1:A:215:LYS:HG2	1:A:255:ILE:HG12	1.89	0.54
1:C:159:VAL:HG22	1:D:45:PRO:HG2	1.88	0.54
1:C:204:ASP:OD1	1:C:205:PRO:HD2	2.06	0.54
1:C:54:MSE:HE2	1:C:204:ASP:OD2	2.07	0.54
1:A:122:LYS:HE2	1:A:145:GLU:OE1	2.08	0.54
1:A:234:GLN:HE22	1:A:275:ILE:CD1	2.18	0.54
1:A:296:ILE:HD12	1:A:296:ILE:H	1.71	0.54
1:B:150:CYS:HA	1:B:179:VAL:O	2.07	0.54
1:B:239:TRP:O	1:C:101:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASP:OD1	1:A:177:ASN:HB3	2.07	0.54
1:D:107:GLN:NE2	1:D:133:GLY:HA3	2.22	0.54
1:C:86:TYR:HB3	1:C:99:THR:CG2	2.37	0.54
1:A:109:MSE:CE	1:A:310:TYR:HB2	2.37	0.54
1:B:326:LYS:HG2	1:B:330:GLU:CD	2.27	0.54
1:B:129:GLY:HA3	1:B:149:MSE:SE	2.58	0.54
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.43	0.54
1:D:197:ALA:HA	1:D:230:VAL:O	2.06	0.54
1:C:66:LYS:HD3	1:C:68:LEU:HD23	1.89	0.54
1:C:237:SER:H	1:C:241:HIS:HD2	1.54	0.54
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.42	0.54
1:D:118:ILE:CD1	1:D:121:PRO:HB3	2.37	0.54
1:B:327:LYS:O	1:B:327:LYS:HD3	2.06	0.54
1:C:123:LYS:HD3	1:C:194:SER:O	2.08	0.54
1:A:134:VAL:O	1:A:138:VAL:HG23	2.06	0.54
1:A:98:LEU:HD11	1:A:164:PHE:CE1	2.41	0.54
1:A:123:LYS:HG3	1:A:195:TYR:CD1	2.42	0.54
1:A:182:ASP:OD2	1:A:184:VAL:HG22	2.07	0.54
1:A:72:LYS:O	1:C:51:MSE:HG2	2.06	0.54
1:C:257:LYS:HE2	2:C:370:HOH:O	2.07	0.54
1:A:55:TRP:HB3	1:A:240:LEU:HD13	1.89	0.54
1:B:130:GLY:O	1:B:131:ASP:CB	2.56	0.54
1:B:148:ASP:OD1	1:B:177:ASN:HB3	2.07	0.54
1:D:257:LYS:CB	1:D:283:GLU:HB2	2.33	0.54
1:D:125:LEU:HD12	1:D:126:VAL:H	1.70	0.54
1:D:227:PRO:C	1:D:285:PRO:HD2	2.27	0.54
1:B:90:LEU:HB3	1:B:98:LEU:HG	1.89	0.54
1:A:109:MSE:CE	1:A:265:THR:HB	2.38	0.54
1:B:164:PHE:N	1:B:165:PRO:HD3	2.22	0.54
1:B:200:VAL:HG12	1:B:202:SER:H	1.71	0.54
1:B:232:CYS:HA	1:B:278:MSE:O	2.07	0.54
1:C:72:LYS:O	1:C:155:MSE:HE1	2.07	0.54
1:C:329:ILE:HG22	1:C:329:ILE:O	2.07	0.54
1:D:321:LEU:O	1:D:326:LYS:HE3	2.07	0.54
1:A:152:ILE:HD12	1:A:182:ASP:HA	1.89	0.54
1:A:41:SER:HA	1:D:40:PHE:HD1	1.72	0.54
1:C:165:PRO:C	1:C:167:VAL:H	2.11	0.54
1:D:112:HIS:NE2	1:D:137:GLU:HB3	2.23	0.54
1:B:192:GLU:HB2	1:B:223:ARG:NH1	2.22	0.54
1:D:131:ASP:O	1:D:167:VAL:HB	2.08	0.54
1:B:67:VAL:HA	1:B:81:PHE:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:LYS:HA	1:D:157:VAL:HG23	1.90	0.54
1:A:272:SER:HA	1:D:268:PRO:HB3	1.89	0.54
1:C:77:ASP:HB3	1:C:93:ASP:HA	1.90	0.54
1:A:236:GLU:HB3	1:A:241:HIS:HD2	1.73	0.54
1:D:65:GLU:HA	1:D:65:GLU:OE1	2.07	0.54
1:A:184:VAL:O	1:A:188:LYS:HG3	2.08	0.54
1:A:92:LEU:O	1:A:94:GLY:N	2.40	0.54
1:D:69:PHE:HB2	1:D:163:PHE:CE2	2.43	0.54
1:A:169:ILE:HD12	1:A:172:GLU:OE2	2.08	0.54
1:A:329:ILE:HG22	1:A:329:ILE:O	2.07	0.54
1:B:128:GLY:O	1:B:130:GLY:N	2.40	0.54
1:B:307:LEU:HD13	1:B:310:TYR:HD1	1.72	0.54
1:C:329:ILE:O	1:C:330:GLU:HB2	2.07	0.54
1:A:152:ILE:HD12	1:A:182:ASP:HA	1.89	0.54
1:A:104:CYS:HB3	1:A:308:LYS:CE	2.37	0.54
1:A:115:LEU:HB3	1:A:141:HIS:CE1	2.43	0.54
1:C:278:MSE:HE1	1:C:280:CYS:CB	2.36	0.54
1:A:260:VAL:HB	1:A:278:MSE:SE	2.57	0.54
1:B:173:ASP:HB3	1:B:176:VAL:HG23	1.90	0.54
1:C:99:THR:O	1:C:103:GLU:HB3	2.07	0.54
1:D:196:ASP:OD1	1:D:226:ARG:CD	2.55	0.54
1:A:79:ILE:HB	1:A:91:VAL:HB	1.89	0.54
1:C:297:ASP:O	1:C:298:GLU:HB2	2.07	0.54
1:A:121:PRO:O	1:A:144:ILE:HD13	2.07	0.54
1:A:219:GLN:OE1	1:A:255:ILE:HD12	2.07	0.54
1:C:259:SER:N	1:C:281:SER:OG	2.41	0.54
1:D:328:VAL:O	1:D:330:GLU:HG3	2.08	0.54
1:A:145:GLU:O	1:A:175:ARG:HG2	2.07	0.54
1:B:262:TYR:OH	1:B:276:GLY:HA3	2.06	0.54
1:D:250:SER:O	1:D:254:GLU:HG3	2.08	0.54
1:A:108:GLU:OE1	1:A:309:PHE:HB3	2.08	0.54
1:D:64:VAL:HG22	1:D:81:PHE:CD1	2.42	0.54
1:B:86:TYR:CD2	1:B:101:ARG:HB3	2.42	0.54
1:C:134:VAL:O	1:C:138:VAL:HG23	2.07	0.54
1:C:54:MSE:HE2	1:C:204:ASP:HB3	1.90	0.54
1:D:263:ALA:HB2	1:D:319:PHE:CE1	2.42	0.54
1:D:96:ILE:HG21	1:D:269:THR:HG22	1.90	0.54
1:C:329:ILE:HG22	1:C:329:ILE:O	2.07	0.54
1:D:200:VAL:HG12	1:D:202:SER:HB3	1.89	0.54
1:B:263:ALA:HA	1:B:318:ALA:O	2.07	0.54
1:B:72:LYS:O	1:B:155:MSE:HE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD13	1:C:149:MSE:CE	2.37	0.54
1:D:198:VAL:CB	1:D:231:VAL:HG22	2.36	0.54
1:A:297:ASP:OD1	1:A:300:SER:HB2	2.08	0.54
1:C:169:ILE:HG13	1:C:172:GLU:OE1	2.08	0.54
1:B:98:LEU:HD21	1:B:131:ASP:CG	2.28	0.54
1:C:179:VAL:HG12	1:C:180:ILE:N	2.22	0.54
1:D:127:ILE:HD13	1:D:183:GLY:HA3	1.90	0.54
1:D:130:GLY:HA3	1:D:156:VAL:CG1	2.37	0.54
1:A:187:LEU:HD21	1:A:221:VAL:HA	1.89	0.54
1:B:262:TYR:OH	1:B:276:GLY:HA3	2.08	0.54
1:D:107:GLN:NE2	1:D:133:GLY:HA3	2.23	0.54
1:C:150:CYS:SG	1:C:183:GLY:HA2	2.48	0.54
1:B:127:ILE:CD1	1:B:187:LEU:HD22	2.38	0.54
1:D:109:MSE:HE1	1:D:310:TYR:CA	2.38	0.54
1:A:219:GLN:OE1	1:A:255:ILE:HD12	2.08	0.54
1:D:108:GLU:OE1	1:D:310:TYR:N	2.40	0.54
1:D:251:ASN:O	1:D:255:ILE:HG12	2.08	0.54
1:D:271:PRO:O	1:D:272:SER:OG	2.21	0.54
1:D:57:GLY:O	1:D:58:GLU:HB3	2.08	0.54
1:B:148:ASP:CG	1:B:177:ASN:HD22	2.11	0.54
1:C:146:GLN:HA	1:C:175:ARG:HB3	1.90	0.54
1:D:123:LYS:HE3	1:D:146:GLN:HE22	1.72	0.54
1:A:136:ARG:NH1	1:A:137:GLU:HG2	2.23	0.54
1:A:193:GLY:HA2	1:A:225:LEU:C	2.29	0.54
1:A:227:PRO:HB2	1:A:285:PRO:CD	2.38	0.54
1:A:135:LEU:HD21	1:A:176:VAL:HG21	1.90	0.54
1:B:114:PRO:HG2	1:B:115:LEU:H	1.73	0.54
1:D:311:ASN:O	1:D:314:ILE:N	2.40	0.54
1:A:80:VAL:HA	1:A:89:VAL:O	2.08	0.54
1:B:198:VAL:O	1:B:231:VAL:HA	2.08	0.54
1:B:69:PHE:O	1:B:79:ILE:HA	2.08	0.54
1:C:184:VAL:O	1:C:188:LYS:HB2	2.07	0.54
1:A:127:ILE:CB	1:A:200:VAL:HG22	2.31	0.54
1:A:83:SER:HB2	1:A:89:VAL:HG21	1.88	0.54
1:B:279:LEU:HG	1:B:319:PHE:HZ	1.73	0.54
1:A:104:CYS:HB3	1:A:308:LYS:CE	2.37	0.54
1:A:308:LYS:O	1:D:324:PHE:HB3	2.07	0.54
1:B:125:LEU:HB2	1:B:195:TYR:CE1	2.43	0.54
1:B:110:ILE:HD12	1:B:277:PHE:CE1	2.42	0.54
1:B:63:LYS:HB3	1:B:84:ALA:HB3	1.90	0.54
1:A:191:ALA:O	1:A:192:GLU:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HG23	1:B:206:ILE:O	2.07	0.54
1:A:260:VAL:HB	1:A:278:MSE:CE	2.36	0.54
1:B:326:LYS:HB3	1:B:326:LYS:NZ	2.22	0.54
1:B:125:LEU:HD12	1:B:126:VAL:H	1.73	0.54
1:B:50:GLU:OE1	1:B:271:PRO:HD3	2.08	0.54
1:B:66:LYS:O	1:B:82:GLN:N	2.39	0.54
1:D:125:LEU:CD2	1:D:187:LEU:HD13	2.38	0.54
1:B:134:VAL:O	1:B:138:VAL:HG23	2.08	0.54
1:A:85:THR:OG1	1:D:57:GLY:HA3	2.08	0.54
1:D:108:GLU:HB3	1:D:310:TYR:HB2	1.89	0.54
1:B:142:ALA:HB3	2:B:401:HOH:O	2.08	0.54
1:D:110:ILE:HG13	1:D:232:CYS:SG	2.48	0.54
1:A:215:LYS:N	1:A:216:PRO:CD	2.71	0.54
1:C:86:TYR:HB3	1:C:99:THR:CG2	2.35	0.54
1:B:322:PRO:O	1:B:326:LYS:HG3	2.07	0.54
1:C:214:GLU:HB3	1:C:216:PRO:HD2	1.89	0.54
1:B:125:LEU:HD12	1:B:126:VAL:N	2.23	0.54
1:B:83:SER:HB3	1:B:87:GLY:O	2.08	0.54
1:C:233:THR:OG1	1:C:278:MSE:HB2	2.08	0.54
1:B:210:LYS:NZ	2:B:474:HOH:O	2.36	0.53
1:D:161:LYS:HA	1:D:168:ALA:CB	2.38	0.53
1:C:50:GLU:OE2	1:C:96:ILE:HB	2.08	0.53
1:D:311:ASN:OD1	1:D:314:ILE:HB	2.08	0.53
1:B:242:MSE:CE	1:B:325:ALA:HA	2.39	0.53
1:B:92:LEU:HB2	1:B:97:GLN:HE22	1.71	0.53
1:C:154:LYS:HD2	1:C:180:ILE:HG21	1.91	0.53
1:A:178:LEU:HD12	1:A:179:VAL:N	2.23	0.53
1:B:110:ILE:O	1:B:114:PRO:CD	2.57	0.53
1:B:215:LYS:HG2	1:B:251:ASN:HB3	1.90	0.53
1:C:62:LEU:HD12	1:C:62:LEU:N	2.23	0.53
1:D:108:GLU:OE2	1:D:307:LEU:HA	2.08	0.53
1:A:164:PHE:CB	1:A:167:VAL:HB	2.38	0.53
1:C:99:THR:O	1:C:103:GLU:HB3	2.08	0.53
1:D:98:LEU:C	1:D:98:LEU:HD12	2.29	0.53
1:B:152:ILE:HG22	2:B:409:HOH:O	2.09	0.53
1:B:48:PHE:CE2	1:B:96:ILE:HD11	2.42	0.53
1:C:125:LEU:HD12	1:C:126:VAL:H	1.72	0.53
1:D:253:ARG:HH12	1:D:330:GLU:HB2	1.72	0.53
1:A:236:GLU:HB3	1:A:241:HIS:HD2	1.70	0.53
1:C:261:ASN:HD22	1:C:289:PHE:HD2	1.57	0.53
1:A:238:LEU:HD13	1:A:322:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LYS:HD3	1:D:194:SER:O	2.08	0.53
1:D:178:LEU:HD12	1:D:179:VAL:H	1.72	0.53
1:A:52:SER:HB3	1:A:55:TRP:NE1	2.23	0.53
1:A:231:VAL:HG12	1:A:280:CYS:HB2	1.90	0.53
1:B:69:PHE:HB2	1:B:163:PHE:CE2	2.44	0.53
1:B:154:LYS:HG2	1:B:158:ASP:OD2	2.09	0.53
1:B:130:GLY:O	1:B:131:ASP:CB	2.56	0.53
1:C:256:PHE:HB3	1:C:281:SER:O	2.08	0.53
1:A:104:CYS:O	1:A:108:GLU:HG3	2.08	0.53
1:A:211:GLU:HA	1:A:214:GLU:HG2	1.91	0.53
1:B:104:CYS:O	1:B:108:GLU:HB2	2.08	0.53
1:B:44:ILE:HB	1:B:47:TRP:HB2	1.91	0.53
1:D:233:THR:HG22	1:D:234:GLN:N	2.24	0.53
1:A:153:ASP:CG	1:A:156:VAL:HG23	2.29	0.53
1:B:38:ALA:N	1:B:70:GLN:HE22	2.07	0.53
1:C:200:VAL:CG2	1:C:233:THR:HG22	2.38	0.53
1:D:80:VAL:HG21	1:D:159:VAL:HG13	1.90	0.53
1:D:240:LEU:HD11	1:D:271:PRO:HB2	1.91	0.53
1:A:51:MSE:SE	1:C:72:LYS:O	2.77	0.53
1:C:236:GLU:HB3	1:C:241:HIS:HD2	1.74	0.53
1:D:262:TYR:HB2	1:D:278:MSE:SE	2.59	0.53
1:B:50:GLU:N	1:B:51:MSE:HE2	2.24	0.53
1:B:54:MSE:HB2	1:B:55:TRP:CE3	2.43	0.53
1:C:132:GLY:CA	1:C:149:MSE:HE1	2.38	0.53
1:C:65:GLU:OE1	1:C:65:GLU:HA	2.08	0.53
1:A:243:ASP:OD2	1:A:244:ILE:HG13	2.09	0.53
1:B:243:ASP:HB2	2:B:433:HOH:O	2.08	0.53
1:B:48:PHE:O	1:B:61:SER:HA	2.09	0.53
1:B:66:LYS:HD2	1:B:68:LEU:HD23	1.90	0.53
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.43	0.53
1:A:68:LEU:O	1:A:69:PHE:HB2	2.08	0.53
1:B:135:LEU:HD21	1:B:149:MSE:HG2	1.91	0.53
1:B:242:MSE:HG2	1:B:328:VAL:HG21	1.89	0.53
1:D:135:LEU:HB2	1:D:170:GLY:HA3	1.90	0.53
1:A:326:LYS:C	1:A:328:VAL:H	2.10	0.53
1:A:55:TRP:CZ3	1:A:271:PRO:HG3	2.44	0.53
1:D:131:ASP:HA	1:D:160:SER:HB3	1.91	0.53
1:A:67:VAL:O	1:C:46:GLY:HA2	2.07	0.53
1:C:99:THR:O	1:C:103:GLU:HB3	2.08	0.53
1:A:267:VAL:HG11	1:A:270:TYR:CE2	2.43	0.53
1:D:109:MSE:O	1:D:111:THR:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:CG	1:A:180:ILE:HG13	2.37	0.53
1:A:43:VAL:HG12	1:A:44:ILE:N	2.23	0.53
1:B:236:GLU:HB3	1:B:241:HIS:ND1	2.23	0.53
1:A:223:ARG:HD3	2:A:360:HOH:O	2.08	0.53
1:C:55:TRP:CZ3	1:C:271:PRO:HG3	2.44	0.53
1:A:55:TRP:CD2	1:A:271:PRO:HG3	2.43	0.53
1:A:53:PRO:O	1:A:56:PRO:HD3	2.09	0.53
1:C:297:ASP:HA	2:C:488:HOH:O	2.09	0.53
1:C:98:LEU:HD21	1:C:131:ASP:HB3	1.91	0.53
1:B:87:GLY:HA3	1:B:100:GLU:HB2	1.90	0.53
1:B:77:ASP:O	1:B:92:LEU:HA	2.09	0.53
1:C:256:PHE:HB2	1:C:260:VAL:HG21	1.89	0.53
1:C:55:TRP:HH2	1:C:95:VAL:HG22	1.73	0.53
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.89	0.53
1:A:212:LEU:HA	1:A:217:PHE:CD2	2.43	0.53
1:C:131:ASP:HA	1:C:160:SER:CB	2.38	0.53
1:C:297:ASP:HB3	2:C:352:HOH:O	2.07	0.53
1:C:66:LYS:HD3	2:C:447:HOH:O	2.08	0.53
1:D:118:ILE:HD13	1:D:230:VAL:HG22	1.91	0.53
1:C:99:THR:O	1:C:103:GLU:HB3	2.08	0.53
1:A:108:GLU:OE1	1:A:307:LEU:HB3	2.08	0.53
1:C:225:LEU:HD11	1:C:231:VAL:HG23	1.90	0.53
1:C:236:GLU:HB2	1:C:245:ILE:CG1	2.38	0.53
1:D:42:THR:HA	1:D:49:SER:CB	2.39	0.53
1:A:66:LYS:O	1:A:82:GLN:N	2.37	0.53
1:C:151:GLU:HG2	1:C:157:VAL:HG23	1.91	0.53
1:C:66:LYS:HD3	2:C:447:HOH:O	2.08	0.53
1:A:125:LEU:HD23	1:A:198:VAL:HG22	1.91	0.53
1:C:114:PRO:O	1:C:117:SER:HB2	2.09	0.53
1:D:232:CYS:HA	1:D:278:MSE:O	2.08	0.53
1:B:168:ALA:HA	1:B:171:TYR:CD2	2.44	0.53
1:C:82:GLN:HE22	1:C:88:LYS:H	1.57	0.53
1:D:105:ALA:O	1:D:109:MSE:HG2	2.09	0.53
1:D:69:PHE:HB2	1:D:163:PHE:CZ	2.43	0.53
1:B:139:ALA:HB1	1:B:175:ARG:NH2	2.23	0.53
1:C:135:LEU:O	1:C:170:GLY:HA3	2.08	0.53
1:C:241:HIS:HB3	2:C:525:HOH:O	2.09	0.53
1:A:68:LEU:HD22	1:A:88:LYS:HZ3	1.74	0.53
1:D:99:THR:HG23	1:D:269:THR:HG21	1.90	0.53
1:D:96:ILE:HG21	1:D:269:THR:HG22	1.91	0.53
1:A:239:TRP:CD1	1:A:274:VAL:HG21	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLY:HA2	1:B:225:LEU:O	2.09	0.53
1:A:231:VAL:HG22	1:A:232:CYS:N	2.24	0.53
1:B:129:GLY:HA3	1:B:149:MSE:SE	2.58	0.53
1:B:187:LEU:HD21	1:B:221:VAL:CG2	2.30	0.53
1:B:114:PRO:HB3	1:B:279:LEU:CD1	2.39	0.53
1:D:200:VAL:HG12	1:D:202:SER:HB3	1.89	0.53
1:A:128:GLY:O	1:A:130:GLY:N	2.42	0.53
1:C:135:LEU:HD13	1:C:149:MSE:CE	2.38	0.53
1:D:111:THR:O	1:D:115:LEU:HD13	2.08	0.53
1:C:297:ASP:HB3	2:C:351:HOH:O	2.09	0.53
1:B:58:GLU:HA	1:C:61:SER:O	2.09	0.53
1:A:261:ASN:ND2	1:A:261:ASN:N	2.56	0.53
1:A:263:ALA:HB2	1:A:319:PHE:CE1	2.44	0.53
1:A:78:VAL:HG12	1:A:80:VAL:CG2	2.39	0.53
1:B:184:VAL:O	1:B:188:LYS:HG3	2.09	0.53
1:C:228:GLY:CA	1:C:285:PRO:HD2	2.39	0.53
1:C:160:SER:O	1:C:168:ALA:HB2	2.09	0.53
1:C:215:LYS:HE2	1:C:251:ASN:HA	1.90	0.53
1:D:140:ARG:CB	1:D:296:ILE:HD11	2.38	0.53
1:A:137:GLU:OE1	1:A:140:ARG:HD2	2.09	0.53
1:A:157:VAL:HG12	1:A:161:LYS:HE3	1.91	0.53
1:C:218:PHE:HE1	1:C:233:THR:HG21	1.73	0.53
1:D:196:ASP:OD1	1:D:226:ARG:CZ	2.57	0.53
1:B:244:ILE:HG13	2:B:433:HOH:O	2.08	0.53
1:C:185:ALA:O	1:C:188:LYS:HB2	2.09	0.53
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.44	0.53
1:B:172:GLU:O	1:B:173:ASP:C	2.47	0.53
1:C:297:ASP:OD1	1:C:298:GLU:N	2.38	0.53
1:D:200:VAL:O	1:D:233:THR:HG23	2.08	0.53
1:D:264:TRP:CH2	1:D:322:PRO:HD3	2.44	0.53
1:A:121:PRO:O	1:A:144:ILE:HD13	2.09	0.53
1:B:123:LYS:O	1:B:124:VAL:HG23	2.09	0.53
1:B:142:ALA:CB	2:B:401:HOH:O	2.56	0.53
1:D:125:LEU:CD2	1:D:187:LEU:HD13	2.39	0.53
1:D:159:VAL:HG13	1:D:163:PHE:CD2	2.44	0.53
1:C:155:MSE:O	1:C:159:VAL:HG23	2.09	0.53
1:D:252:CYS:HB2	1:D:278:MSE:CE	2.39	0.53
1:A:41:SER:HA	1:D:39:CYS:O	2.08	0.53
1:A:88:LYS:HD2	1:A:163:PHE:O	2.09	0.53
1:B:242:MSE:HE3	1:B:325:ALA:HA	1.91	0.53
1:D:259:SER:O	1:D:280:CYS:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:PRO:HB3	1:D:309:PHE:CD1	2.44	0.53
1:C:257:LYS:HE2	2:C:364:HOH:O	2.08	0.53
1:A:66:LYS:HG2	1:A:82:GLN:HB3	1.90	0.53
1:B:127:ILE:O	1:B:200:VAL:HA	2.09	0.53
1:C:311:ASN:HD21	1:C:314:ILE:N	2.06	0.53
1:B:149:MSE:HB2	1:B:178:LEU:HA	1.91	0.53
1:B:238:LEU:O	1:B:242:MSE:HE2	2.09	0.53
1:A:121:PRO:O	1:A:144:ILE:HD13	2.08	0.53
1:B:242:MSE:HA	1:B:242:MSE:HE3	1.90	0.53
1:B:49:SER:CB	1:B:51:MSE:HE2	2.33	0.53
1:C:68:LEU:HG	1:C:81:PHE:HA	1.91	0.53
1:D:51:MSE:O	1:D:52:SER:HB2	2.09	0.53
1:A:70:GLN:HG3	1:A:79:ILE:HG12	1.91	0.52
1:A:43:VAL:H	1:C:162:GLN:NE2	2.04	0.52
1:C:206:ILE:HG23	1:C:207:GLY:N	2.24	0.52
1:B:127:ILE:HD12	1:B:127:ILE:N	2.24	0.52
1:B:228:GLY:CA	1:B:285:PRO:HD2	2.39	0.52
1:B:48:PHE:HD2	1:B:48:PHE:C	2.12	0.52
1:C:297:ASP:HB3	2:C:349:HOH:O	2.08	0.52
1:B:231:VAL:CG2	1:B:232:CYS:N	2.72	0.52
1:A:134:VAL:O	1:A:138:VAL:HG23	2.09	0.52
1:B:227:PRO:HG2	2:B:467:HOH:O	2.09	0.52
1:C:307:LEU:H	1:C:307:LEU:HD12	1.73	0.52
1:A:242:MSE:HE2	1:A:242:MSE:HA	1.91	0.52
1:A:86:TYR:HB3	1:A:99:THR:HG23	1.91	0.52
1:D:126:VAL:CB	1:D:149:MSE:SE	3.04	0.52
1:A:238:LEU:HD11	1:A:321:LEU:HD22	1.90	0.52
1:C:238:LEU:HD11	1:C:321:LEU:HD22	1.91	0.52
1:B:192:GLU:HG3	1:B:223:ARG:NH1	2.23	0.52
1:B:51:MSE:HG2	1:B:59:ALA:HB2	1.91	0.52
1:A:90:LEU:HD23	1:A:90:LEU:C	2.29	0.52
1:C:253:ARG:HA	1:C:260:VAL:HG21	1.90	0.52
1:C:270:TYR:CD2	1:C:275:ILE:HB	2.44	0.52
1:A:111:THR:OG1	1:A:138:VAL:HG23	2.10	0.52
1:A:260:VAL:CG2	1:A:278:MSE:HE1	2.40	0.52
1:A:105:ALA:O	1:A:109:MSE:HG2	2.09	0.52
1:A:164:PHE:HB3	1:A:167:VAL:HB	1.91	0.52
1:B:309:PHE:CE1	1:C:322:PRO:HB3	2.44	0.52
1:C:63:LYS:HB3	1:C:84:ALA:HB3	1.91	0.52
1:A:131:ASP:HB2	1:A:167:VAL:HG11	1.91	0.52
1:D:313:GLU:N	1:D:313:GLU:CD	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLU:CG	1:A:152:ILE:N	2.71	0.52
1:B:228:GLY:HA3	1:B:285:PRO:HD2	1.90	0.52
1:D:217:PHE:O	1:D:221:VAL:HG23	2.10	0.52
1:D:231:VAL:HG21	1:D:256:PHE:CZ	2.44	0.52
1:A:219:GLN:OE1	1:A:255:ILE:HD12	2.09	0.52
1:C:206:ILE:HG23	1:C:207:GLY:H	1.74	0.52
1:D:109:MSE:CE	1:D:310:TYR:HB2	2.38	0.52
1:D:262:TYR:OH	1:D:276:GLY:HA3	2.10	0.52
1:D:98:LEU:C	1:D:98:LEU:HD12	2.30	0.52
1:B:85:THR:OG1	1:C:57:GLY:HA3	2.10	0.52
1:A:271:PRO:HG2	2:A:378:HOH:O	2.09	0.52
1:B:42:THR:HA	1:B:49:SER:HB2	1.92	0.52
1:C:261:ASN:HD22	1:C:289:PHE:HD2	1.56	0.52
1:D:88:LYS:HB2	1:D:100:GLU:HG3	1.92	0.52
1:A:164:PHE:HB3	1:A:167:VAL:CG2	2.40	0.52
1:B:73:SER:CB	1:B:155:MSE:SE	2.98	0.52
1:B:271:PRO:O	1:B:272:SER:HB3	2.08	0.52
1:C:65:GLU:HB3	1:C:82:GLN:O	2.10	0.52
1:B:126:VAL:CG1	1:B:126:VAL:O	2.57	0.52
1:C:272:SER:C	1:C:274:VAL:H	2.13	0.52
1:D:293:LEU:H	1:D:293:LEU:HD23	1.75	0.52
1:A:313:GLU:HB2	1:D:326:LYS:NZ	2.25	0.52
1:A:104:CYS:O	1:A:108:GLU:HB2	2.10	0.52
1:A:328:VAL:O	1:A:328:VAL:HG12	2.10	0.52
1:A:86:TYR:O	1:A:99:THR:HG23	2.09	0.52
1:C:109:MSE:HE1	1:C:314:ILE:HG23	1.92	0.52
1:D:54:MSE:HE2	1:D:204:ASP:OD1	2.10	0.52
1:B:113:LEU:HB3	1:B:114:PRO:CD	2.38	0.52
1:B:173:ASP:HB3	1:B:176:VAL:HG23	1.91	0.52
1:D:109:MSE:CE	1:D:113:LEU:HD11	2.38	0.52
1:D:245:ILE:C	1:D:247:ASP:N	2.62	0.52
1:D:264:TRP:N	1:D:318:ALA:O	2.40	0.52
1:C:297:ASP:HB3	2:C:352:HOH:O	2.10	0.52
1:A:149:MSE:CG	1:A:178:LEU:HD13	2.38	0.52
1:A:329:ILE:O	1:A:330:GLU:HB2	2.08	0.52
1:B:42:THR:O	1:C:43:VAL:HG13	2.09	0.52
1:D:329:ILE:O	1:D:329:ILE:HG22	2.09	0.52
1:C:206:ILE:HG23	1:C:207:GLY:N	2.24	0.52
1:A:108:GLU:HB3	1:A:112:HIS:HD2	1.74	0.52
1:C:58:GLU:O	1:C:59:ALA:HB2	2.10	0.52
1:A:72:LYS:HB2	1:A:72:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLY:CA	1:B:285:PRO:HD2	2.40	0.52
1:D:68:LEU:HD21	1:D:88:LYS:NZ	2.23	0.52
1:B:51:MSE:HG3	2:B:377:HOH:O	2.08	0.52
1:C:219:GLN:OE1	1:C:255:ILE:HD12	2.08	0.52
1:D:109:MSE:HE3	1:D:265:THR:OG1	2.09	0.52
1:B:227:PRO:HG2	2:B:471:HOH:O	2.08	0.52
1:D:132:GLY:HA3	1:D:167:VAL:O	2.10	0.52
1:D:123:LYS:HD3	1:D:194:SER:O	2.09	0.52
1:A:242:MSE:CE	1:A:245:ILE:HD12	2.40	0.52
1:B:166:ASP:O	1:B:167:VAL:HG13	2.10	0.52
1:A:140:ARG:HA	1:A:304:ASN:OD1	2.09	0.52
1:B:122:LYS:HD3	1:B:145:GLU:OE2	2.08	0.52
1:B:125:LEU:HB2	1:B:195:TYR:CE1	2.44	0.52
1:B:130:GLY:O	1:B:131:ASP:CB	2.57	0.52
1:C:48:PHE:O	1:C:61:SER:HA	2.10	0.52
1:C:86:TYR:HB3	1:C:99:THR:CG2	2.40	0.52
1:D:243:ASP:HA	1:D:246:GLU:OE1	2.09	0.52
1:D:40:PHE:O	1:D:42:THR:N	2.42	0.52
1:A:237:SER:HA	2:A:430:HOH:O	2.08	0.52
1:A:298:GLU:HG2	1:A:305:GLY:O	2.10	0.52
1:A:126:VAL:HB	1:A:149:MSE:HG2	1.92	0.52
1:C:66:LYS:HD3	1:C:68:LEU:CD2	2.39	0.52
1:A:111:THR:C	1:A:114:PRO:HD2	2.29	0.52
1:B:123:LYS:O	1:B:124:VAL:HG23	2.09	0.52
1:B:231:VAL:HG11	1:B:256:PHE:CZ	2.45	0.52
1:A:197:ALA:HA	1:A:230:VAL:O	2.09	0.52
1:B:44:ILE:HD13	1:C:51:MSE:CE	2.39	0.52
1:D:96:ILE:HG21	1:D:269:THR:HG22	1.92	0.52
1:B:54:MSE:SE	1:B:54:MSE:H	2.43	0.52
1:A:215:LYS:N	1:A:251:ASN:HD22	2.08	0.52
1:C:200:VAL:CG2	1:C:233:THR:HG22	2.39	0.52
1:D:263:ALA:HB2	1:D:319:PHE:CE1	2.44	0.52
1:A:288:ASP:O	1:A:290:LYS:N	2.43	0.52
1:B:263:ALA:HB2	1:B:319:PHE:CE1	2.45	0.52
1:C:116:CYS:SG	1:C:294:ASN:O	2.64	0.52
1:A:215:LYS:H	1:A:216:PRO:HD3	1.75	0.52
1:B:98:LEU:HD11	1:B:131:ASP:OD2	2.09	0.52
1:B:234:GLN:HE22	1:B:236:GLU:N	2.08	0.52
1:B:98:LEU:HD12	1:B:98:LEU:C	2.30	0.52
1:C:232:CYS:HA	1:C:278:MSE:O	2.10	0.52
1:C:72:LYS:HE2	1:C:77:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PHE:HZ	1:A:155:MSE:HE2	1.74	0.52
1:B:228:GLY:HA3	1:B:285:PRO:HD2	1.92	0.52
1:D:200:VAL:HB	1:D:233:THR:HG23	1.91	0.52
1:A:104:CYS:O	1:A:108:GLU:HG3	2.10	0.52
1:B:121:PRO:O	1:B:122:LYS:HD2	2.09	0.52
1:C:195:TYR:O	1:C:226:ARG:HG2	2.10	0.52
1:C:155:MSE:O	1:C:159:VAL:HG23	2.10	0.52
1:A:166:ASP:O	1:A:169:ILE:HG22	2.10	0.52
1:A:68:LEU:CD1	1:A:80:VAL:HG12	2.36	0.52
1:B:234:GLN:HE22	1:B:236:GLU:H	1.58	0.52
1:D:76:GLN:CD	1:D:92:LEU:HD22	2.29	0.52
1:A:257:LYS:HB2	2:A:574:HOH:O	2.09	0.52
1:C:187:LEU:HD21	1:C:221:VAL:HA	1.92	0.52
1:C:65:GLU:HA	1:C:65:GLU:OE1	2.10	0.52
1:D:91:VAL:HA	1:D:95:VAL:O	2.09	0.52
1:B:103:GLU:HB3	1:B:107:GLN:NE2	2.25	0.52
1:A:99:THR:HB	1:A:102:ASP:OD1	2.10	0.52
1:B:308:LYS:O	1:C:323:SER:HB2	2.10	0.52
1:A:70:GLN:HE21	1:A:71:GLY:N	2.07	0.52
1:C:100:GLU:HA	1:C:103:GLU:OE2	2.10	0.52
1:C:152:ILE:O	1:C:152:ILE:HG12	2.09	0.52
1:B:123:LYS:O	1:B:195:TYR:HD1	1.92	0.52
1:C:123:LYS:HD3	1:C:194:SER:O	2.10	0.52
1:C:165:PRO:C	1:C:167:VAL:H	2.12	0.52
1:C:182:ASP:OD2	1:C:185:ALA:HB2	2.09	0.52
1:D:263:ALA:HB2	1:D:319:PHE:CE1	2.45	0.52
1:B:234:GLN:NE2	1:B:236:GLU:N	2.57	0.52
1:C:256:PHE:HD1	1:C:282:THR:HG22	1.74	0.52
1:C:307:LEU:N	1:C:307:LEU:CD1	2.73	0.52
1:B:116:CYS:HB3	1:B:294:ASN:O	2.10	0.52
1:C:223:ARG:HA	2:C:477:HOH:O	2.10	0.52
1:C:68:LEU:O	1:C:69:PHE:HB2	2.10	0.52
1:D:161:LYS:HA	1:D:168:ALA:CB	2.39	0.52
1:D:262:TYR:HA	1:D:277:PHE:O	2.10	0.52
1:B:112:HIS:NE2	1:B:307:LEU:HD11	2.25	0.52
1:C:169:ILE:O	1:C:172:GLU:HB2	2.10	0.52
1:D:147:ILE:HB	1:D:176:VAL:HA	1.92	0.52
1:B:263:ALA:HB2	1:B:319:PHE:CE1	2.45	0.52
1:A:151:GLU:O	1:A:180:ILE:HA	2.09	0.52
1:C:99:THR:HB	1:C:102:ASP:OD1	2.10	0.52
1:D:136:ARG:HH11	1:D:136:ARG:HG2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:CD2	1:C:187:LEU:HD13	2.40	0.52
1:C:235:ALA:O	1:C:236:GLU:HB2	2.10	0.52
1:D:109:MSE:HB3	1:D:277:PHE:CZ	2.45	0.52
1:A:261:ASN:OD1	1:A:290:LYS:HE3	2.09	0.52
1:A:324:PHE:O	1:A:327:LYS:HG2	2.10	0.52
1:B:178:LEU:HD12	1:B:179:VAL:H	1.74	0.52
1:D:198:VAL:H	1:D:231:VAL:HG22	1.75	0.52
1:D:126:VAL:HG12	1:D:149:MSE:SE	2.59	0.52
1:C:295:PRO:HG3	1:C:312:ALA:HB2	1.92	0.51
1:B:166:ASP:HB2	2:B:372:HOH:O	2.10	0.51
1:B:223:ARG:NH1	2:B:483:HOH:O	2.42	0.51
1:D:64:VAL:HG22	1:D:81:PHE:CD1	2.45	0.51
1:B:202:SER:OG	1:B:234:GLN:HB3	2.10	0.51
1:C:167:VAL:HG23	2:C:452:HOH:O	2.09	0.51
1:C:170:GLY:HA2	2:C:460:HOH:O	2.09	0.51
1:D:310:TYR:CD1	1:D:311:ASN:N	2.79	0.51
1:B:226:ARG:HG2	1:B:227:PRO:O	2.10	0.51
1:C:80:VAL:HG21	1:C:159:VAL:HG11	1.92	0.51
1:C:166:ASP:O	1:C:169:ILE:HG22	2.10	0.51
1:D:238:LEU:HD12	1:D:264:TRP:CE3	2.44	0.51
1:A:249:VAL:HA	1:A:278:MSE:CE	2.39	0.51
1:B:43:VAL:HG23	1:B:44:ILE:HG13	1.91	0.51
1:D:60:HIS:CE1	1:D:272:SER:H	2.28	0.51
1:B:122:LYS:HA	1:B:144:ILE:HA	1.92	0.51
1:B:122:LYS:HD2	1:B:145:GLU:CG	2.37	0.51
1:C:205:PRO:HB3	1:C:213:PHE:CD1	2.45	0.51
1:A:68:LEU:HB3	1:A:163:PHE:CE1	2.44	0.51
1:B:312:ALA:O	1:B:315:HIS:HB3	2.09	0.51
1:D:312:ALA:O	1:D:315:HIS:HB3	2.10	0.51
1:D:40:PHE:O	1:D:42:THR:N	2.42	0.51
1:A:128:GLY:O	1:A:130:GLY:N	2.44	0.51
1:C:122:LYS:HB3	1:C:145:GLU:HG3	1.92	0.51
1:B:200:VAL:HG11	1:B:212:LEU:HD13	1.91	0.51
1:C:87:GLY:O	1:C:88:LYS:C	2.49	0.51
1:D:96:ILE:HG21	1:D:269:THR:HG22	1.93	0.51
1:A:215:LYS:HD3	1:A:254:GLU:OE1	2.10	0.51
1:B:249:VAL:HG22	1:B:278:MSE:SE	2.59	0.51
1:A:297:ASP:CG	1:A:298:GLU:H	2.13	0.51
1:B:249:VAL:HA	1:B:278:MSE:CE	2.40	0.51
1:B:87:GLY:HA3	1:B:100:GLU:HB2	1.92	0.51
1:C:157:VAL:O	1:C:161:LYS:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:GLU:C	1:D:213:PHE:H	2.13	0.51
1:A:206:ILE:HD11	2:A:448:HOH:O	2.11	0.51
1:D:226:ARG:NH2	1:D:227:PRO:O	2.44	0.51
1:D:99:THR:HG21	1:D:269:THR:HG21	1.90	0.51
1:D:327:LYS:HD3	2:D:342:HOH:O	2.11	0.51
1:B:48:PHE:C	1:B:48:PHE:CD2	2.83	0.51
1:C:53:PRO:O	1:C:56:PRO:HD3	2.10	0.51
1:A:129:GLY:O	1:A:131:ASP:N	2.43	0.51
1:A:310:TYR:CD1	1:A:311:ASN:N	2.78	0.51
1:C:154:LYS:HB2	1:C:180:ILE:CG2	2.39	0.51
1:C:180:ILE:HD12	1:C:180:ILE:H	1.74	0.51
1:A:260:VAL:HA	1:A:280:CYS:HA	1.92	0.51
1:C:141:HIS:O	1:C:142:ALA:C	2.49	0.51
1:C:292:PRO:HB2	1:C:295:PRO:CB	2.38	0.51
1:A:54:MSE:HE2	1:A:54:MSE:HA	1.91	0.51
1:C:232:CYS:HB2	1:C:279:LEU:CD1	2.40	0.51
1:A:260:VAL:HB	1:A:278:MSE:HE2	1.90	0.51
1:A:259:SER:O	1:A:280:CYS:HA	2.10	0.51
1:B:264:TRP:HA	1:B:276:GLY:HA2	1.92	0.51
1:D:257:LYS:CB	1:D:283:GLU:HB2	2.39	0.51
1:A:51:MSE:HE3	1:D:44:ILE:HD13	1.91	0.51
1:B:140:ARG:HE	1:B:307:LEU:HD21	1.76	0.51
1:B:249:VAL:HG11	1:B:329:ILE:CG2	2.40	0.51
1:B:42:THR:HG23	1:C:43:VAL:HG22	1.92	0.51
1:B:51:MSE:CE	1:C:44:ILE:HD12	2.39	0.51
1:C:70:GLN:HG2	1:C:79:ILE:HG23	1.92	0.51
1:B:131:ASP:OD1	1:B:167:VAL:HG21	2.09	0.51
1:B:223:ARG:HG2	1:B:223:ARG:NH1	2.19	0.51
1:B:239:TRP:HB2	1:B:272:SER:OG	2.10	0.51
1:B:187:LEU:HD21	1:B:221:VAL:CG2	2.30	0.51
1:B:71:GLY:O	1:B:72:LYS:HB2	2.09	0.51
1:C:192:GLU:HA	1:C:224:ALA:HA	1.91	0.51
1:D:113:LEU:N	1:D:114:PRO:HD2	2.26	0.51
1:D:42:THR:HA	1:D:49:SER:HB2	1.92	0.51
1:A:130:GLY:O	1:A:131:ASP:HB3	2.10	0.51
1:A:240:LEU:HD11	1:A:271:PRO:HB2	1.91	0.51
1:D:115:LEU:HD23	1:D:141:HIS:CD2	2.45	0.51
1:A:324:PHE:CG	1:A:325:ALA:N	2.78	0.51
1:C:149:MSE:HE2	1:C:171:TYR:HE1	1.75	0.51
1:C:210:LYS:O	1:C:210:LYS:HD3	2.11	0.51
1:A:320:CYS:SG	1:D:317:ALA:HB2	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:NH1	1:C:166:ASP:HB3	2.26	0.51
1:D:73:SER:HB3	1:D:155:MSE:SE	2.61	0.51
1:A:161:LYS:HA	1:A:168:ALA:HB2	1.91	0.51
1:C:79:ILE:HB	1:C:91:VAL:HB	1.91	0.51
1:B:241:HIS:HB3	2:B:376:HOH:O	2.09	0.51
1:C:272:SER:O	1:C:274:VAL:HG22	2.11	0.51
1:A:72:LYS:H	1:C:51:MSE:SE	2.44	0.51
1:C:264:TRP:CZ2	1:C:322:PRO:HD3	2.45	0.51
1:D:108:GLU:CB	1:D:109:MSE:HE2	2.41	0.51
1:C:99:THR:CG2	1:C:102:ASP:H	2.23	0.51
1:A:311:ASN:OD1	1:A:314:ILE:HG22	2.11	0.51
1:B:43:VAL:HG23	1:B:44:ILE:HG13	1.92	0.51
1:D:73:SER:HA	1:D:155:MSE:CE	2.40	0.51
1:A:54:MSE:SE	1:A:205:PRO:HG3	2.60	0.51
1:C:103:GLU:O	1:C:107:GLN:HG3	2.09	0.51
1:C:262:TYR:OH	1:C:276:GLY:HA3	2.11	0.51
1:A:242:MSE:CE	1:A:245:ILE:HD12	2.41	0.51
1:A:297:ASP:O	1:A:298:GLU:HB2	2.11	0.51
1:C:129:GLY:HA3	1:C:151:GLU:HB2	1.93	0.51
1:C:256:PHE:HD1	1:C:282:THR:HA	1.75	0.51
1:A:320:CYS:SG	1:D:317:ALA:HB2	2.51	0.51
1:B:153:ASP:CG	1:B:155:MSE:HB2	2.30	0.51
1:B:252:CYS:SG	1:B:278:MSE:HE2	2.50	0.51
1:C:70:GLN:NE2	2:C:360:HOH:O	2.43	0.51
1:A:125:LEU:HD23	1:A:198:VAL:HG13	1.92	0.51
1:A:238:LEU:HA	1:A:245:ILE:CD1	2.39	0.51
1:B:257:LYS:HE3	1:B:283:GLU:HB2	1.91	0.51
1:C:136:ARG:NH2	1:C:167:VAL:HG13	2.26	0.51
1:C:72:LYS:HE2	1:C:77:ASP:OD1	2.10	0.51
1:A:244:ILE:O	1:A:248:ILE:HG13	2.10	0.51
1:A:261:ASN:HD21	1:A:289:PHE:HD2	1.57	0.51
1:B:51:MSE:CE	1:B:51:MSE:N	2.74	0.51
1:C:134:VAL:HG12	1:C:138:VAL:HG23	1.91	0.51
1:C:171:TYR:CE1	1:C:178:LEU:HD22	2.46	0.51
1:C:198:VAL:HG21	1:C:221:VAL:HG13	1.93	0.51
1:B:127:ILE:HD11	1:B:187:LEU:HD21	1.91	0.51
1:B:126:VAL:HG22	1:B:199:ILE:HD12	1.92	0.51
1:B:324:PHE:HD2	1:C:308:LYS:O	1.94	0.51
1:C:129:GLY:CA	1:C:151:GLU:HB2	2.40	0.51
1:D:228:GLY:N	1:D:285:PRO:HD2	2.25	0.51
1:C:121:PRO:O	1:C:144:ILE:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ASP:OD1	1:C:184:VAL:HG22	2.11	0.51
1:D:185:ALA:O	1:D:186:PHE:C	2.49	0.51
1:A:154:LYS:HB2	1:A:180:ILE:CD1	2.36	0.51
1:D:109:MSE:HE3	1:D:310:TYR:HA	1.93	0.51
1:B:113:LEU:HD23	1:B:315:HIS:CE1	2.46	0.51
1:B:228:GLY:N	1:B:282:THR:OG1	2.44	0.51
1:B:43:VAL:HG23	1:B:44:ILE:HG13	1.92	0.51
1:B:48:PHE:O	1:B:61:SER:HA	2.11	0.51
1:C:329:ILE:O	1:C:329:ILE:HG22	2.11	0.51
1:A:129:GLY:N	1:A:149:MSE:SE	2.94	0.51
1:A:209:ALA:HB1	1:A:212:LEU:HD11	1.92	0.51
1:A:246:GLU:OE1	1:A:328:VAL:HG13	2.11	0.51
1:C:238:LEU:HD11	1:C:321:LEU:CD2	2.41	0.51
1:C:121:PRO:O	1:C:144:ILE:HD13	2.11	0.51
1:A:154:LYS:HB2	1:A:180:ILE:CD1	2.36	0.51
1:B:98:LEU:C	1:B:98:LEU:HD12	2.31	0.51
1:C:131:ASP:HB2	1:C:167:VAL:HG11	1.93	0.51
1:C:329:ILE:HG22	1:C:329:ILE:O	2.09	0.51
1:D:259:SER:O	1:D:280:CYS:HA	2.11	0.51
1:B:79:ILE:H	1:B:79:ILE:HD12	1.76	0.51
1:C:129:GLY:N	1:C:149:MSE:SE	2.94	0.51
1:D:109:MSE:HG2	1:D:265:THR:CB	2.41	0.51
1:B:130:GLY:O	1:B:131:ASP:HB2	2.11	0.51
1:D:227:PRO:O	1:D:285:PRO:HD2	2.11	0.51
1:B:129:GLY:O	1:B:130:GLY:C	2.48	0.51
1:B:205:PRO:HB3	1:B:213:PHE:CE1	2.45	0.51
1:A:127:ILE:HD13	1:A:217:PHE:HZ	1.75	0.51
1:B:296:ILE:HD12	1:B:307:LEU:HD11	1.92	0.51
1:C:169:ILE:HA	1:C:172:GLU:OE1	2.11	0.51
1:C:89:VAL:HA	1:C:98:LEU:O	2.11	0.51
1:D:76:GLN:OE1	1:D:92:LEU:HD22	2.11	0.51
1:B:187:LEU:HG	1:B:221:VAL:HG23	1.93	0.51
1:A:231:VAL:CG1	1:A:280:CYS:HB2	2.41	0.51
1:B:105:ALA:O	1:B:109:MSE:HG2	2.11	0.51
1:B:153:ASP:OD1	1:B:155:MSE:HB3	2.10	0.51
1:A:264:TRP:HD1	1:A:318:ALA:O	1.94	0.51
2:B:490:HOH:O	1:C:51:MSE:HE1	2.11	0.51
1:D:151:GLU:OE1	1:D:152:ILE:N	2.44	0.51
1:D:256:PHE:HD1	1:D:282:THR:HG22	1.76	0.51
1:B:206:ILE:HG23	1:B:207:GLY:H	1.75	0.51
1:B:43:VAL:HG22	1:B:49:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:MSE:HE2	1:D:310:TYR:CA	2.40	0.51
1:A:155:MSE:O	1:A:158:ASP:HB2	2.11	0.51
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.92	0.51
1:B:187:LEU:HD23	1:B:217:PHE:CE1	2.45	0.51
1:A:69:PHE:HZ	1:A:155:MSE:SE	2.44	0.51
1:A:191:ALA:HB3	1:A:194:SER:HB3	1.93	0.51
1:B:96:ILE:HG21	1:B:269:THR:CG2	2.41	0.51
1:D:111:THR:HG22	1:D:134:VAL:HG13	1.93	0.51
1:A:76:GLN:OE1	1:A:92:LEU:HD22	2.11	0.51
1:C:137:GLU:OE1	1:C:140:ARG:HD2	2.11	0.51
1:D:52:SER:C	1:D:54:MSE:N	2.64	0.51
1:A:46:GLY:HA3	1:A:63:LYS:NZ	2.25	0.51
1:C:158:ASP:OD1	1:D:45:PRO:HB3	2.10	0.51
1:C:242:MSE:O	1:C:246:GLU:HB2	2.11	0.51
1:D:92:LEU:HD12	1:D:97:GLN:HG2	1.93	0.51
1:C:66:LYS:HG2	1:C:82:GLN:HB2	1.93	0.51
1:D:257:LYS:HD3	2:D:417:HOH:O	2.11	0.51
1:C:179:VAL:HG12	1:C:180:ILE:H	1.76	0.51
1:D:246:GLU:CD	1:D:328:VAL:HG11	2.30	0.51
1:D:51:MSE:O	1:D:52:SER:CB	2.58	0.51
1:A:164:PHE:HB3	1:A:167:VAL:HB	1.93	0.50
1:A:252:CYS:HB3	1:A:280:CYS:SG	2.51	0.50
1:A:263:ALA:HB2	1:A:319:PHE:CZ	2.45	0.50
1:C:123:LYS:HG2	1:C:195:TYR:HD1	1.75	0.50
1:A:257:LYS:NZ	2:A:566:HOH:O	2.43	0.50
1:A:327:LYS:HG3	1:A:328:VAL:HG23	1.92	0.50
1:A:91:VAL:HG13	1:A:95:VAL:H	1.76	0.50
1:C:329:ILE:O	1:C:329:ILE:HG22	2.11	0.50
1:D:149:MSE:HE2	1:D:151:GLU:HG2	1.92	0.50
1:D:55:TRP:HH2	1:D:204:ASP:OD1	1.94	0.50
1:B:312:ALA:O	1:B:315:HIS:HB3	2.11	0.50
1:C:227:PRO:CB	1:C:284:GLY:HA3	2.40	0.50
1:A:46:GLY:HA3	1:A:63:LYS:NZ	2.26	0.50
1:C:323:SER:O	1:C:327:LYS:HG2	2.12	0.50
1:A:103:GLU:O	1:A:107:GLN:HG3	2.11	0.50
1:B:197:ALA:HA	1:B:230:VAL:O	2.11	0.50
1:B:229:GLY:O	1:B:281:SER:HA	2.11	0.50
1:C:240:LEU:HD11	1:C:272:SER:HB3	1.93	0.50
1:D:105:ALA:O	1:D:109:MSE:HB2	2.11	0.50
1:D:265:THR:CG2	1:D:275:ILE:HG22	2.40	0.50
1:A:80:VAL:HG21	1:A:159:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:HG	1:D:163:PHE:CE1	2.46	0.50
1:A:159:VAL:HG13	1:A:163:PHE:CD2	2.46	0.50
1:A:265:THR:HG22	1:A:275:ILE:HG22	1.92	0.50
1:B:105:ALA:HA	1:B:309:PHE:CG	2.46	0.50
1:A:165:PRO:HG2	1:A:166:ASP:H	1.76	0.50
1:A:44:ILE:N	1:A:44:ILE:CD1	2.74	0.50
1:B:240:LEU:CG	1:B:272:SER:HB2	2.41	0.50
1:C:217:PHE:O	1:C:220:SER:HB3	2.11	0.50
1:B:61:SER:O	1:C:58:GLU:HA	2.11	0.50
1:A:270:TYR:HB3	1:A:271:PRO:HD2	1.93	0.50
1:D:109:MSE:HG2	1:D:265:THR:CG2	2.41	0.50
1:A:54:MSE:O	1:A:56:PRO:HD3	2.12	0.50
1:D:125:LEU:HD12	1:D:126:VAL:H	1.77	0.50
1:A:310:TYR:CD1	1:A:311:ASN:N	2.79	0.50
1:A:323:SER:O	1:A:327:LYS:HG2	2.12	0.50
1:C:118:ILE:HB	1:C:119:PRO:HD2	1.94	0.50
1:C:210:LYS:O	1:C:214:GLU:HG2	2.11	0.50
1:B:236:GLU:HB3	1:B:241:HIS:HB2	1.92	0.50
1:A:136:ARG:HH21	1:A:167:VAL:CG1	2.24	0.50
1:D:151:GLU:HG2	1:D:157:VAL:CG2	2.41	0.50
1:A:328:VAL:C	1:A:330:GLU:H	2.15	0.50
1:C:253:ARG:HA	1:C:260:VAL:HG21	1.93	0.50
1:D:111:THR:CG2	1:D:134:VAL:HG13	2.41	0.50
1:A:99:THR:HB	1:A:102:ASP:OD1	2.12	0.50
1:A:212:LEU:HA	1:A:217:PHE:CD2	2.47	0.50
1:A:242:MSE:O	1:A:245:ILE:HB	2.11	0.50
1:D:275:ILE:HG13	1:D:276:GLY:N	2.25	0.50
1:A:109:MSE:SE	1:A:309:PHE:CD1	3.13	0.50
1:B:144:ILE:HG21	1:B:147:ILE:HG12	1.94	0.50
1:B:65:GLU:HG2	1:B:84:ALA:HA	1.92	0.50
1:A:135:LEU:HD11	1:A:149:MSE:SE	2.62	0.50
1:C:287:VAL:HG11	1:C:289:PHE:CZ	2.46	0.50
1:D:75:TYR:CD2	1:D:153:ASP:HB2	2.47	0.50
1:D:97:GLN:O	1:D:98:LEU:HB3	2.12	0.50
1:B:239:TRP:HD1	1:B:274:VAL:HG21	1.75	0.50
1:D:149:MSE:HE2	1:D:151:GLU:HG3	1.92	0.50
1:D:261:ASN:HB3	2:D:518:HOH:O	2.11	0.50
1:B:51:MSE:HE3	1:B:51:MSE:H	1.76	0.50
1:C:215:LYS:N	1:C:216:PRO:CD	2.74	0.50
1:B:121:PRO:O	1:B:144:ILE:HD13	2.12	0.50
1:B:130:GLY:O	1:B:131:ASP:CB	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:O	1:C:242:MSE:HE3	2.11	0.50
1:B:169:ILE:CG2	1:B:170:GLY:N	2.74	0.50
1:D:88:LYS:H	1:D:100:GLU:CG	2.25	0.50
1:D:328:VAL:C	1:D:330:GLU:H	2.14	0.50
1:B:269:THR:HB	2:B:466:HOH:O	2.11	0.50
1:C:109:MSE:CE	1:C:314:ILE:CG2	2.90	0.50
1:C:165:PRO:HG2	1:C:166:ASP:H	1.77	0.50
1:C:51:MSE:HG2	2:C:405:HOH:O	2.11	0.50
1:C:99:THR:HG22	1:C:101:ARG:N	2.27	0.50
1:B:214:GLU:HB2	2:B:429:HOH:O	2.12	0.50
1:C:126:VAL:O	1:C:149:MSE:HA	2.12	0.50
1:A:279:LEU:HB3	1:A:289:PHE:CD2	2.45	0.50
1:B:278:MSE:C	1:B:278:MSE:SE	3.00	0.50
1:C:123:LYS:HE3	1:C:195:TYR:HE1	1.75	0.50
1:A:186:PHE:O	1:A:190:ALA:HB2	2.12	0.50
1:D:80:VAL:CG2	1:D:159:VAL:HG11	2.40	0.50
1:D:322:PRO:O	1:D:324:PHE:N	2.44	0.50
1:A:267:VAL:HG11	1:A:270:TYR:CE2	2.47	0.50
1:A:310:TYR:CD1	1:A:311:ASN:N	2.79	0.50
1:B:233:THR:HG22	1:B:278:MSE:HB2	1.93	0.50
1:A:109:MSE:HE1	1:A:310:TYR:CB	2.40	0.50
1:A:76:GLN:OE1	1:A:92:LEU:HB3	2.10	0.50
1:B:179:VAL:HG23	1:B:179:VAL:O	2.12	0.50
1:D:114:PRO:HB3	1:D:232:CYS:HB2	1.93	0.50
1:C:220:SER:HA	1:C:223:ARG:HG2	1.93	0.50
1:C:54:MSE:HE2	1:C:205:PRO:HD2	1.92	0.50
1:D:139:ALA:HB1	1:D:175:ARG:NH2	2.26	0.50
1:D:43:VAL:O	1:D:44:ILE:HG13	2.11	0.50
1:A:182:ASP:CG	1:A:183:GLY:H	2.15	0.50
1:A:252:CYS:SG	1:A:278:MSE:HG2	2.52	0.50
1:C:165:PRO:C	1:C:167:VAL:H	2.14	0.50
1:C:328:VAL:HG12	1:C:328:VAL:O	2.12	0.50
1:D:263:ALA:HB2	1:D:319:PHE:CE1	2.46	0.50
1:D:75:TYR:CD2	1:D:153:ASP:HB2	2.47	0.50
1:B:241:HIS:HB3	2:B:433:HOH:O	2.12	0.50
1:D:154:LYS:HG2	1:D:158:ASP:OD2	2.11	0.50
1:D:242:MSE:HE1	1:D:325:ALA:HB2	1.93	0.50
1:C:294:ASN:ND2	2:C:347:HOH:O	2.45	0.50
1:D:60:HIS:CE1	1:D:271:PRO:HA	2.46	0.50
1:B:51:MSE:CE	1:B:51:MSE:H	2.24	0.50
1:C:173:ASP:OD1	1:C:175:ARG:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:PRO:HG3	1:C:312:ALA:HB2	1.93	0.50
1:D:263:ALA:HB2	1:D:319:PHE:CE1	2.46	0.50
1:B:98:LEU:HD12	1:B:98:LEU:O	2.12	0.50
1:D:123:LYS:HE3	1:D:146:GLN:OE1	2.10	0.50
1:A:144:ILE:HB	1:A:175:ARG:NH1	2.26	0.50
1:A:219:GLN:OE1	1:A:255:ILE:HD12	2.11	0.50
1:C:118:ILE:C	1:C:118:ILE:HD12	2.32	0.50
1:C:226:ARG:CB	1:C:227:PRO:CD	2.90	0.50
1:C:235:ALA:HB2	1:C:278:MSE:HG2	1.94	0.50
1:C:310:TYR:HA	1:C:314:ILE:HG21	1.94	0.50
1:A:212:LEU:HA	1:A:217:PHE:CD2	2.47	0.50
1:C:225:LEU:HD11	1:C:231:VAL:HG22	1.94	0.50
1:D:54:MSE:HE1	1:D:204:ASP:CB	2.41	0.50
1:A:145:GLU:O	1:A:175:ARG:HG2	2.11	0.50
1:A:187:LEU:HG	1:A:220:SER:O	2.12	0.50
1:A:219:GLN:OE1	1:A:255:ILE:HG23	2.11	0.50
1:A:301:SER:C	1:A:303:SER:H	2.14	0.50
1:A:56:PRO:HG2	1:D:85:THR:HG21	1.94	0.50
1:B:164:PHE:HB3	1:B:167:VAL:CG2	2.42	0.50
1:A:113:LEU:HD23	1:A:315:HIS:ND1	2.26	0.50
1:B:154:LYS:HG2	1:B:158:ASP:OD2	2.12	0.50
1:B:243:ASP:HB2	2:B:433:HOH:O	2.11	0.50
1:C:227:PRO:HB3	1:C:284:GLY:CA	2.42	0.50
1:C:104:CYS:SG	1:C:309:PHE:HB2	2.51	0.50
1:C:292:PRO:HB3	1:C:315:HIS:NE2	2.26	0.50
1:D:93:ASP:N	2:D:354:HOH:O	2.45	0.50
1:A:86:TYR:HB3	1:A:99:THR:HG21	1.92	0.50
1:C:114:PRO:O	1:C:117:SER:HB2	2.12	0.50
1:A:229:GLY:O	1:A:281:SER:HA	2.11	0.50
1:A:68:LEU:HB2	1:A:80:VAL:HG12	1.94	0.50
1:B:124:VAL:HG13	1:B:197:ALA:HB3	1.94	0.50
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.47	0.50
1:C:321:LEU:HD22	1:C:329:ILE:HD12	1.93	0.50
1:D:131:ASP:CG	2:D:552:HOH:O	2.50	0.50
1:D:136:ARG:HG2	1:D:136:ARG:HH11	1.76	0.50
1:D:257:LYS:NZ	2:D:510:HOH:O	2.45	0.50
1:D:118:ILE:CD1	1:D:121:PRO:HB3	2.42	0.50
1:D:128:GLY:O	1:D:129:GLY:C	2.50	0.50
1:C:233:THR:O	1:C:277:PHE:HA	2.11	0.50
1:D:206:ILE:HG13	1:D:206:ILE:O	2.12	0.50
1:A:311:ASN:O	1:A:314:ILE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:HG2	1:B:227:PRO:N	2.24	0.50
1:C:165:PRO:C	1:C:167:VAL:N	2.65	0.50
1:C:292:PRO:HB3	1:C:315:HIS:CE1	2.47	0.50
1:A:209:ALA:HB1	1:A:212:LEU:CD1	2.42	0.50
1:D:110:ILE:HD13	1:D:201:ASP:HA	1.93	0.50
1:A:261:ASN:HA	2:A:386:HOH:O	2.12	0.50
1:B:106:TYR:CD1	1:B:275:ILE:HG21	2.47	0.50
1:C:49:SER:HB2	1:C:51:MSE:HE1	1.93	0.50
1:D:310:TYR:CD1	1:D:310:TYR:C	2.85	0.50
1:B:205:PRO:HB3	1:B:213:PHE:CE1	2.47	0.50
1:B:48:PHE:O	1:B:61:SER:HA	2.12	0.50
1:D:104:CYS:O	1:D:108:GLU:HG3	2.12	0.50
1:D:111:THR:HG22	1:D:134:VAL:HG13	1.92	0.50
1:A:179:VAL:HG11	1:A:186:PHE:HE2	1.76	0.50
1:A:68:LEU:HB2	1:A:80:VAL:HG12	1.94	0.50
1:D:151:GLU:OE1	1:D:152:ILE:N	2.44	0.50
1:D:113:LEU:N	1:D:114:PRO:CD	2.75	0.50
1:D:141:HIS:NE2	1:D:296:ILE:HD11	2.27	0.50
1:A:283:GLU:HG3	2:A:574:HOH:O	2.10	0.50
1:D:159:VAL:HG13	1:D:163:PHE:HD2	1.76	0.50
1:A:171:TYR:CE1	1:A:178:LEU:HD22	2.47	0.50
1:C:221:VAL:HG13	1:C:231:VAL:HG21	1.93	0.50
1:C:262:TYR:HD2	1:C:321:LEU:HD11	1.77	0.50
1:A:80:VAL:HG21	1:A:159:VAL:HG12	1.94	0.50
1:B:125:LEU:HB2	1:B:195:TYR:CE1	2.47	0.50
1:C:257:LYS:HB3	1:C:283:GLU:HB3	1.93	0.50
1:A:46:GLY:HA3	1:A:63:LYS:HZ1	1.76	0.50
1:C:293:LEU:HD23	1:C:293:LEU:O	2.12	0.50
1:D:113:LEU:N	1:D:114:PRO:HD2	2.27	0.50
1:B:164:PHE:HB3	1:B:167:VAL:CG2	2.42	0.49
1:B:196:ASP:HA	1:B:226:ARG:NH1	2.24	0.49
1:D:76:GLN:HB2	1:D:93:ASP:OD1	2.12	0.49
1:A:232:CYS:HA	1:A:278:MSE:O	2.11	0.49
1:B:265:THR:HG22	1:B:277:PHE:HE2	1.77	0.49
1:B:238:LEU:O	1:B:242:MSE:HE2	2.12	0.49
1:B:271:PRO:HB3	2:B:448:HOH:O	2.12	0.49
1:C:303:SER:C	1:C:305:GLY:H	2.15	0.49
1:D:109:MSE:HE1	1:D:310:TYR:CB	2.42	0.49
1:A:86:TYR:CE2	1:A:101:ARG:HD3	2.47	0.49
1:A:51:MSE:O	1:A:52:SER:HB2	2.11	0.49
1:B:149:MSE:HG3	1:B:149:MSE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:PHE:O	1:D:255:ILE:HG21	2.12	0.49
1:B:275:ILE:O	1:B:275:ILE:CG2	2.60	0.49
1:C:155:MSE:O	1:C:159:VAL:HG23	2.12	0.49
1:C:324:PHE:O	1:C:327:LYS:HG2	2.12	0.49
1:C:73:SER:HB2	2:C:340:HOH:O	2.11	0.49
1:D:90:LEU:HD21	1:D:92:LEU:HD21	1.93	0.49
1:A:146:GLN:HG3	1:A:175:ARG:O	2.12	0.49
1:C:161:LYS:HG3	1:C:168:ALA:CB	2.39	0.49
1:C:327:LYS:HG3	1:C:328:VAL:H	1.77	0.49
1:D:182:ASP:O	1:D:185:ALA:HB3	2.12	0.49
1:D:200:VAL:HB	1:D:233:THR:HG23	1.92	0.49
1:A:98:LEU:HB2	1:A:103:GLU:HB3	1.94	0.49
1:A:267:VAL:HG11	1:A:270:TYR:CE2	2.47	0.49
1:A:66:LYS:O	1:A:81:PHE:HB2	2.12	0.49
1:B:111:THR:CG2	1:B:134:VAL:HG13	2.42	0.49
1:B:123:LYS:HZ3	1:B:146:GLN:HE22	1.60	0.49
1:B:127:ILE:HD11	1:B:187:LEU:HD22	1.94	0.49
1:C:106:TYR:CE1	1:C:275:ILE:HG21	2.47	0.49
1:C:267:VAL:HB	1:C:270:TYR:HD2	1.76	0.49
1:B:89:VAL:HG13	1:B:99:THR:HG22	1.93	0.49
1:A:145:GLU:O	1:A:175:ARG:HG2	2.12	0.49
1:C:230:VAL:HA	1:C:280:CYS:O	2.12	0.49
1:D:238:LEU:HD21	1:D:329:ILE:HD11	1.95	0.49
1:A:307:LEU:N	1:A:307:LEU:HD12	2.26	0.49
1:A:123:LYS:HG2	1:A:146:GLN:HB3	1.93	0.49
1:A:129:GLY:HA2	1:A:201:ASP:OD2	2.12	0.49
1:C:107:GLN:HE22	1:C:136:ARG:HH21	1.61	0.49
1:C:242:MSE:O	1:C:246:GLU:HG3	2.12	0.49
1:C:173:ASP:HB3	1:C:176:VAL:HG23	1.94	0.49
1:C:239:TRP:C	1:C:240:LEU:HD23	2.33	0.49
1:A:182:ASP:CG	1:A:183:GLY:N	2.65	0.49
1:A:244:ILE:O	1:A:248:ILE:HG13	2.12	0.49
1:B:126:VAL:O	1:B:127:ILE:C	2.50	0.49
1:C:103:GLU:HB2	1:C:107:GLN:NE2	2.28	0.49
1:A:125:LEU:HD23	1:A:198:VAL:CG1	2.42	0.49
1:A:80:VAL:HG21	1:A:159:VAL:CB	2.42	0.49
1:B:123:LYS:HE3	1:B:146:GLN:NE2	2.27	0.49
1:B:184:VAL:HA	1:B:217:PHE:CE1	2.46	0.49
1:C:54:MSE:HE1	1:C:244:ILE:HD11	1.94	0.49
1:C:278:MSE:SE	1:C:278:MSE:C	3.01	0.49
1:D:73:SER:HA	1:D:155:MSE:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:THR:HG22	1:D:269:THR:O	2.12	0.49
1:C:257:LYS:HE2	2:C:367:HOH:O	2.11	0.49
1:D:195:TYR:O	1:D:225:LEU:HA	2.12	0.49
1:C:121:PRO:O	1:C:144:ILE:HD13	2.12	0.49
1:A:159:VAL:HG13	1:A:163:PHE:CE2	2.47	0.49
1:B:259:SER:O	1:B:280:CYS:HA	2.12	0.49
1:C:66:LYS:HD3	2:C:447:HOH:O	2.12	0.49
1:D:70:GLN:HE21	1:D:79:ILE:HD11	1.77	0.49
1:A:65:GLU:HB3	1:A:82:GLN:O	2.12	0.49
1:B:187:LEU:HB3	1:B:220:SER:OG	2.13	0.49
1:B:52:SER:C	1:B:54:MSE:H	2.16	0.49
1:C:182:ASP:OD1	1:C:184:VAL:HG22	2.13	0.49
1:B:324:PHE:HD2	1:C:308:LYS:O	1.95	0.49
1:C:85:THR:O	1:C:101:ARG:HD2	2.11	0.49
1:A:132:GLY:CA	1:A:135:LEU:HD13	2.43	0.49
1:A:108:GLU:CG	1:A:307:LEU:HD22	2.42	0.49
1:C:328:VAL:C	1:C:330:GLU:H	2.16	0.49
1:B:134:VAL:O	1:B:138:VAL:HG23	2.11	0.49
1:C:164:PHE:HB3	1:C:167:VAL:HB	1.93	0.49
1:B:214:GLU:HB2	2:B:429:HOH:O	2.12	0.49
1:C:125:LEU:HB2	1:C:195:TYR:CE1	2.47	0.49
1:B:109:MSE:HG2	1:B:265:THR:HB	1.94	0.49
1:C:76:GLN:HG3	1:C:92:LEU:HD22	1.95	0.49
1:D:211:GLU:HG2	1:D:211:GLU:O	2.12	0.49
1:D:77:ASP:O	1:D:92:LEU:HA	2.12	0.49
1:A:151:GLU:O	1:A:180:ILE:HA	2.12	0.49
1:B:97:GLN:O	1:B:98:LEU:HB3	2.11	0.49
1:C:151:GLU:O	1:C:180:ILE:HA	2.13	0.49
1:D:238:LEU:HD21	1:D:262:TYR:CE1	2.47	0.49
1:A:241:HIS:HB3	1:A:244:ILE:HB	1.94	0.49
1:C:109:MSE:HE1	1:C:314:ILE:HG22	1.94	0.49
1:A:267:VAL:HG11	1:A:270:TYR:CE2	2.48	0.49
1:C:223:ARG:HG3	1:C:224:ALA:N	2.28	0.49
1:D:257:LYS:HG3	2:D:414:HOH:O	2.12	0.49
1:A:242:MSE:SE	1:A:245:ILE:HB	2.63	0.49
1:D:50:GLU:OE2	1:D:96:ILE:HB	2.12	0.49
1:B:123:LYS:HE3	1:B:146:GLN:NE2	2.28	0.49
1:A:141:HIS:O	1:A:143:SER:N	2.41	0.49
1:C:296:ILE:HB	1:C:307:LEU:HD11	1.95	0.49
1:D:167:VAL:C	1:D:169:ILE:H	2.15	0.49
1:A:264:TRP:HA	1:A:275:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LYS:C	1:B:210:LYS:HD3	2.33	0.49
1:D:164:PHE:O	1:D:167:VAL:HG22	2.13	0.49
1:A:242:MSE:HA	1:A:242:MSE:CE	2.31	0.49
1:C:237:SER:H	1:C:241:HIS:HD2	1.60	0.49
1:B:113:LEU:HA	1:B:315:HIS:HE1	1.78	0.49
1:D:149:MSE:HE3	1:D:150:CYS:N	2.27	0.49
1:C:301:SER:CB	1:C:304:ASN:HD22	2.21	0.49
1:D:164:PHE:N	1:D:165:PRO:HD3	2.28	0.49
1:A:44:ILE:CD1	1:A:44:ILE:N	2.76	0.49
1:B:134:VAL:HG12	1:B:138:VAL:CG2	2.39	0.49
1:B:144:ILE:HG22	1:B:175:ARG:HD2	1.95	0.49
1:D:114:PRO:HG2	1:D:115:LEU:HD12	1.94	0.49
1:B:326:LYS:C	1:B:328:VAL:H	2.16	0.49
1:C:104:CYS:SG	1:C:105:ALA:N	2.86	0.49
1:C:222:ALA:HA	1:C:225:LEU:HB2	1.95	0.49
1:D:250:SER:O	1:D:254:GLU:HG3	2.12	0.49
1:A:79:ILE:HB	1:A:91:VAL:HB	1.94	0.49
1:B:77:ASP:O	1:B:92:LEU:HA	2.12	0.49
1:C:193:GLY:HA2	1:C:225:LEU:O	2.13	0.49
1:B:108:GLU:HG2	1:B:307:LEU:HD13	1.94	0.49
1:B:44:ILE:O	1:B:47:TRP:HB2	2.13	0.49
1:D:192:GLU:HB2	1:D:223:ARG:NH1	2.28	0.49
1:D:269:THR:O	1:D:269:THR:HG22	2.12	0.49
1:D:311:ASN:O	1:D:313:GLU:N	2.46	0.49
1:D:41:SER:O	1:D:42:THR:HB	2.13	0.49
1:A:129:GLY:HA2	1:A:201:ASP:OD2	2.13	0.49
1:D:257:LYS:HG3	2:D:414:HOH:O	2.12	0.49
1:C:296:ILE:HG22	2:C:344:HOH:O	2.11	0.49
1:B:269:THR:HB	2:B:460:HOH:O	2.12	0.49
1:C:180:ILE:HD12	1:C:180:ILE:N	2.27	0.49
1:C:152:ILE:HD12	1:C:182:ASP:HB2	1.94	0.49
1:C:187:LEU:HA	1:C:190:ALA:HB2	1.93	0.49
1:A:91:VAL:O	1:A:92:LEU:HD23	2.13	0.49
1:B:113:LEU:HB3	1:B:114:PRO:HD3	1.94	0.49
1:C:98:LEU:HD22	1:C:131:ASP:OD2	2.11	0.49
1:C:51:MSE:SE	1:C:51:MSE:N	2.94	0.49
1:B:283:GLU:HB3	2:B:441:HOH:O	2.12	0.49
1:C:97:GLN:O	1:C:98:LEU:HB3	2.13	0.49
1:D:215:LYS:HD2	1:D:255:ILE:HD11	1.94	0.49
1:C:131:ASP:HB2	1:C:167:VAL:HG11	1.94	0.49
1:C:293:LEU:HD23	1:C:293:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:SER:HB2	1:B:53:PRO:CD	2.42	0.49
1:C:197:ALA:HA	1:C:230:VAL:O	2.13	0.49
1:D:327:LYS:O	1:D:330:GLU:HG3	2.12	0.49
1:A:131:ASP:O	1:A:167:VAL:HG12	2.12	0.49
1:A:301:SER:O	1:A:303:SER:N	2.46	0.49
1:A:307:LEU:N	1:A:307:LEU:HD12	2.27	0.49
1:B:111:THR:HG23	1:B:138:VAL:HG22	1.94	0.49
1:C:129:GLY:N	1:C:151:GLU:HB2	2.27	0.49
1:C:151:GLU:O	1:C:180:ILE:HA	2.12	0.49
1:C:327:LYS:HG3	1:C:328:VAL:N	2.27	0.49
1:C:54:MSE:HE2	1:C:204:ASP:CB	2.33	0.49
1:A:159:VAL:O	1:A:163:PHE:HD2	1.96	0.49
1:A:127:ILE:HD12	1:A:200:VAL:CG2	2.43	0.49
1:B:128:GLY:O	1:B:130:GLY:N	2.46	0.49
1:B:153:ASP:OD2	1:B:155:MSE:HB2	2.11	0.49
1:B:98:LEU:HD21	1:B:131:ASP:OD1	2.13	0.49
1:B:160:SER:HA	1:B:164:PHE:HD2	1.76	0.49
1:A:86:TYR:CD2	1:A:101:ARG:HD3	2.47	0.49
1:A:187:LEU:HD21	1:A:221:VAL:HG22	1.94	0.49
1:B:293:LEU:HD23	1:B:294:ASN:N	2.28	0.49
1:A:310:TYR:CD1	1:A:310:TYR:C	2.86	0.49
1:C:104:CYS:HB3	2:C:380:HOH:O	2.13	0.49
1:C:210:LYS:O	1:C:214:GLU:HG2	2.12	0.49
1:D:185:ALA:O	1:D:186:PHE:C	2.50	0.49
1:A:218:PHE:HB2	1:A:255:ILE:HG21	1.95	0.49
1:B:317:ALA:HB2	1:C:320:CYS:SG	2.53	0.49
1:D:129:GLY:O	1:D:156:VAL:HG11	2.12	0.49
1:A:293:LEU:O	1:A:293:LEU:HD23	2.13	0.49
1:C:68:LEU:HD12	1:C:80:VAL:HG12	1.95	0.49
1:C:76:GLN:HG3	1:C:92:LEU:HD22	1.94	0.49
1:A:182:ASP:OD2	1:A:184:VAL:HG22	2.13	0.49
1:A:238:LEU:CD2	1:A:242:MSE:HE1	2.42	0.49
1:B:152:ILE:O	1:B:152:ILE:HG12	2.13	0.49
1:A:50:GLU:O	1:A:55:TRP:NE1	2.40	0.49
1:A:292:PRO:HB3	1:A:315:HIS:CE1	2.47	0.49
1:C:147:ILE:HD12	1:C:175:ARG:HB2	1.95	0.49
1:D:97:GLN:NE2	1:D:97:GLN:HA	2.28	0.49
1:B:151:GLU:HG3	1:B:152:ILE:N	2.27	0.49
1:B:164:PHE:HB3	1:B:167:VAL:CG2	2.43	0.49
1:B:54:MSE:HB2	1:B:55:TRP:CE3	2.48	0.49
1:A:43:VAL:HG13	1:D:43:VAL:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLU:HB3	1:B:216:PRO:HD2	1.95	0.49
1:B:215:LYS:HE2	1:B:251:ASN:OD1	2.13	0.49
1:C:256:PHE:CD1	1:C:282:THR:HG22	2.48	0.49
1:C:263:ALA:HB2	1:C:319:PHE:CE1	2.48	0.49
1:C:297:ASP:OD1	1:C:298:GLU:N	2.33	0.49
1:A:92:LEU:O	1:A:95:VAL:N	2.43	0.49
1:B:210:LYS:C	1:B:210:LYS:HD3	2.32	0.49
1:C:107:GLN:HE22	1:C:136:ARG:NH2	2.11	0.49
1:B:109:MSE:HE3	1:B:309:PHE:CD2	2.46	0.49
1:C:296:ILE:HG22	1:C:297:ASP:N	2.28	0.49
1:B:271:PRO:HG2	2:B:348:HOH:O	2.12	0.49
1:C:88:LYS:HD3	1:C:163:PHE:O	2.13	0.49
1:D:279:LEU:HD12	1:D:289:PHE:CE1	2.48	0.49
1:A:184:VAL:HG12	1:A:217:PHE:CD1	2.48	0.49
1:B:326:LYS:HG2	1:B:330:GLU:OE1	2.13	0.49
1:A:90:LEU:HB2	1:A:164:PHE:CZ	2.47	0.49
1:B:127:ILE:HD11	1:B:187:LEU:HD22	1.94	0.49
1:C:230:VAL:HA	1:C:280:CYS:O	2.12	0.49
1:B:66:LYS:HE3	1:B:68:LEU:HD23	1.95	0.49
1:D:106:TYR:O	1:D:109:MSE:CB	2.58	0.49
1:D:138:VAL:C	1:D:140:ARG:H	2.15	0.49
1:D:200:VAL:CB	1:D:233:THR:HG23	2.34	0.49
1:A:287:VAL:HA	2:A:379:HOH:O	2.12	0.49
1:B:225:LEU:HD22	1:B:229:GLY:CA	2.34	0.49
1:D:124:VAL:HG12	1:D:125:LEU:N	2.27	0.49
1:A:244:ILE:O	1:A:248:ILE:HG13	2.13	0.48
1:C:128:GLY:C	1:C:149:MSE:SE	3.01	0.48
1:D:184:VAL:HG21	1:D:211:GLU:OE1	2.13	0.48
1:B:217:PHE:O	1:B:220:SER:HB3	2.13	0.48
1:D:313:GLU:CD	1:D:313:GLU:H	2.16	0.48
1:A:129:GLY:C	1:A:131:ASP:H	2.17	0.48
1:A:125:LEU:HD13	1:A:195:TYR:CZ	2.47	0.48
1:A:225:LEU:HD11	1:A:231:VAL:HB	1.94	0.48
1:A:129:GLY:HA3	1:A:149:MSE:HE1	1.94	0.48
1:A:212:LEU:HA	1:A:217:PHE:CD2	2.48	0.48
1:B:113:LEU:HD11	1:B:319:PHE:CZ	2.48	0.48
1:C:198:VAL:HG21	1:C:221:VAL:HG13	1.94	0.48
1:A:211:GLU:HA	1:A:214:GLU:CG	2.43	0.48
1:A:46:GLY:O	1:A:63:LYS:HD2	2.13	0.48
1:A:124:VAL:HG23	1:A:144:ILE:HD12	1.95	0.48
1:C:322:PRO:O	1:C:323:SER:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:VAL:O	1:D:231:VAL:HG23	2.12	0.48
1:B:162:GLN:NE2	2:B:453:HOH:O	2.45	0.48
1:B:49:SER:HB2	1:B:51:MSE:HE2	1.94	0.48
1:B:66:LYS:HD3	1:B:67:VAL:N	2.28	0.48
1:C:135:LEU:HD13	1:C:149:MSE:HE2	1.94	0.48
1:D:269:THR:O	1:D:269:THR:HG22	2.13	0.48
1:D:54:MSE:HB2	1:D:55:TRP:CE3	2.48	0.48
1:A:232:CYS:HA	1:A:278:MSE:O	2.13	0.48
1:B:242:MSE:HE3	1:B:324:PHE:HE1	1.78	0.48
1:C:155:MSE:O	1:C:159:VAL:HG23	2.13	0.48
1:D:54:MSE:HE1	1:D:204:ASP:HB3	1.95	0.48
1:B:248:ILE:HG22	1:B:249:VAL:N	2.28	0.48
1:A:199:ILE:HA	1:A:232:CYS:O	2.14	0.48
1:C:296:ILE:CG2	2:C:344:HOH:O	2.61	0.48
1:A:127:ILE:HG22	1:A:150:CYS:HB3	1.94	0.48
1:B:109:MSE:HE2	1:B:113:LEU:HG	1.95	0.48
1:C:112:HIS:O	1:C:116:CYS:HB2	2.12	0.48
1:C:159:VAL:HG22	1:D:45:PRO:CG	2.43	0.48
1:A:89:VAL:HG13	1:A:96:ILE:HG23	1.95	0.48
1:B:246:GLU:HB2	1:B:328:VAL:CG1	2.43	0.48
1:C:98:LEU:HD12	1:C:103:GLU:HB2	1.95	0.48
1:A:131:ASP:HA	1:A:160:SER:HB3	1.95	0.48
1:B:179:VAL:HG21	1:B:186:PHE:CE2	2.48	0.48
1:C:301:SER:HB3	1:C:304:ASN:ND2	2.05	0.48
1:D:111:THR:O	1:D:115:LEU:HB2	2.11	0.48
1:A:271:PRO:O	1:A:272:SER:CB	2.60	0.48
1:A:276:GLY:O	1:A:277:PHE:CG	2.66	0.48
1:B:232:CYS:HA	1:B:278:MSE:O	2.13	0.48
1:B:97:GLN:O	1:B:98:LEU:HB3	2.13	0.48
1:D:99:THR:OG1	1:D:102:ASP:OD1	2.28	0.48
1:B:267:VAL:HG11	1:B:270:TYR:CE2	2.48	0.48
1:D:290:LYS:HD2	1:D:291:HIS:HE1	1.76	0.48
1:A:76:GLN:OE1	1:A:92:LEU:HB3	2.13	0.48
1:D:259:SER:HB3	1:D:281:SER:OG	2.13	0.48
1:A:324:PHE:O	1:A:327:LYS:HG2	2.12	0.48
1:C:65:GLU:O	1:C:66:LYS:HE2	2.13	0.48
1:D:233:THR:HG22	1:D:234:GLN:N	2.28	0.48
1:D:252:CYS:SG	1:D:278:MSE:SE	3.21	0.48
1:D:64:VAL:HG22	1:D:81:PHE:CE1	2.48	0.48
1:A:238:LEU:HD11	1:A:264:TRP:CD2	2.48	0.48
1:B:225:LEU:HB3	1:B:229:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:TYR:CD2	1:C:101:ARG:HD3	2.48	0.48
1:D:242:MSE:HE1	1:D:329:ILE:HD11	1.94	0.48
1:A:245:ILE:O	1:A:249:VAL:HG23	2.12	0.48
1:B:228:GLY:HA3	1:B:285:PRO:HD2	1.95	0.48
1:B:44:ILE:HD13	1:C:51:MSE:HE3	1.95	0.48
1:A:124:VAL:HG23	1:A:144:ILE:HD12	1.95	0.48
1:A:147:ILE:HB	1:A:176:VAL:HA	1.94	0.48
1:B:271:PRO:HG2	2:B:348:HOH:O	2.13	0.48
1:B:90:LEU:HB3	1:B:98:LEU:HG	1.94	0.48
1:B:97:GLN:O	1:B:98:LEU:HB3	2.13	0.48
1:D:111:THR:HG22	1:D:134:VAL:HG13	1.95	0.48
1:A:170:GLY:O	1:A:172:GLU:N	2.46	0.48
1:A:220:SER:O	1:A:223:ARG:HG2	2.13	0.48
1:C:107:GLN:NE2	1:C:136:ARG:HH21	2.10	0.48
1:B:55:TRP:CE3	1:B:271:PRO:HG3	2.48	0.48
1:C:230:VAL:HA	1:C:280:CYS:O	2.13	0.48
1:A:258:GLY:HA3	1:A:281:SER:OG	2.13	0.48
1:A:214:GLU:HB3	1:A:216:PRO:HD2	1.95	0.48
1:C:286:ASP:HA	2:C:399:HOH:O	2.12	0.48
1:C:296:ILE:O	1:C:297:ASP:C	2.51	0.48
1:C:86:TYR:CD2	1:C:99:THR:HG21	2.42	0.48
1:A:125:LEU:HD13	1:A:186:PHE:CE1	2.48	0.48
1:C:147:ILE:O	1:C:177:ASN:N	2.45	0.48
1:A:164:PHE:HB3	1:A:167:VAL:HB	1.95	0.48
1:A:249:VAL:O	1:A:253:ARG:HG2	2.14	0.48
1:A:90:LEU:HB3	1:A:98:LEU:HG	1.95	0.48
1:D:217:PHE:O	1:D:220:SER:HB3	2.13	0.48
1:B:86:TYR:CD2	1:B:101:ARG:HB3	2.48	0.48
1:A:198:VAL:O	1:A:231:VAL:HA	2.14	0.48
1:B:260:VAL:HA	1:B:280:CYS:SG	2.53	0.48
1:C:129:GLY:HA2	1:C:149:MSE:HE3	1.95	0.48
1:C:248:ILE:CG2	1:C:278:MSE:HG3	2.43	0.48
1:B:198:VAL:HG23	1:B:225:LEU:HD21	1.94	0.48
1:C:165:PRO:C	1:C:167:VAL:H	2.16	0.48
1:C:293:LEU:O	1:C:293:LEU:HD23	2.14	0.48
1:A:159:VAL:HG13	1:A:163:PHE:HE2	1.79	0.48
1:C:137:GLU:O	1:C:140:ARG:HB3	2.13	0.48
1:A:253:ARG:HH22	1:A:330:GLU:HB2	1.77	0.48
1:A:88:LYS:HB2	1:A:100:GLU:HG3	1.95	0.48
1:C:293:LEU:O	1:C:293:LEU:HD23	2.13	0.48
1:D:245:ILE:O	1:D:249:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:HIS:ND1	1:B:141:HIS:HE1	2.11	0.48
1:A:131:ASP:O	1:A:167:VAL:HG12	2.13	0.48
1:A:66:LYS:HG2	1:A:82:GLN:CB	2.43	0.48
1:C:193:GLY:HA2	1:C:225:LEU:O	2.13	0.48
1:C:235:ALA:HB3	1:C:277:PHE:N	2.28	0.48
1:A:301:SER:O	1:A:303:SER:N	2.46	0.48
1:B:150:CYS:O	1:B:151:GLU:CB	2.61	0.48
1:D:204:ASP:HB3	1:D:205:PRO:HD2	1.96	0.48
1:A:54:MSE:HA	1:A:54:MSE:HE2	1.94	0.48
1:C:86:TYR:CE2	1:C:101:ARG:HD3	2.48	0.48
1:D:112:HIS:NE2	1:D:137:GLU:OE1	2.47	0.48
1:D:141:HIS:CE1	1:D:296:ILE:HD12	2.49	0.48
1:D:183:GLY:O	1:D:187:LEU:HD23	2.14	0.48
1:D:92:LEU:HB2	1:D:97:GLN:NE2	2.28	0.48
1:D:139:ALA:C	1:D:141:HIS:H	2.15	0.48
1:D:60:HIS:CG	2:D:364:HOH:O	2.66	0.48
1:D:68:LEU:HD23	1:D:163:PHE:CD1	2.49	0.48
1:A:263:ALA:HB2	1:A:319:PHE:CE1	2.49	0.48
1:B:164:PHE:O	1:B:167:VAL:HG23	2.14	0.48
1:C:238:LEU:HD11	1:C:321:LEU:HD22	1.95	0.48
1:D:226:ARG:HG2	1:D:227:PRO:N	2.23	0.48
1:A:149:MSE:HG3	1:A:178:LEU:HD13	1.95	0.48
1:A:196:ASP:HA	1:A:226:ARG:HH21	1.79	0.48
1:B:163:PHE:C	1:B:165:PRO:HD3	2.34	0.48
1:A:243:ASP:HA	1:A:246:GLU:OE1	2.13	0.48
1:D:225:LEU:HD11	1:D:231:VAL:HG22	1.94	0.48
1:A:197:ALA:HA	1:A:230:VAL:O	2.13	0.48
1:A:241:HIS:HB3	2:A:429:HOH:O	2.13	0.48
1:B:115:LEU:HB3	1:B:141:HIS:NE2	2.28	0.48
1:C:196:ASP:OD1	1:C:226:ARG:HD3	2.13	0.48
1:A:121:PRO:HA	2:A:385:HOH:O	2.13	0.48
1:B:228:GLY:HA3	1:B:285:PRO:HD2	1.95	0.48
1:D:310:TYR:CE2	1:D:315:HIS:HB2	2.48	0.48
1:A:214:GLU:HB3	1:A:216:PRO:HD2	1.95	0.48
1:B:241:HIS:HB3	1:B:244:ILE:HD12	1.94	0.48
1:D:60:HIS:CD2	2:D:362:HOH:O	2.66	0.48
1:A:242:MSE:O	1:A:245:ILE:HB	2.13	0.48
1:A:72:LYS:H	1:C:51:MSE:SE	2.46	0.48
1:C:53:PRO:O	1:C:56:PRO:HD3	2.14	0.48
1:C:65:GLU:HA	1:C:65:GLU:OE1	2.12	0.48
1:D:157:VAL:O	1:D:161:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PRO:HB3	1:B:279:LEU:HD12	1.96	0.48
1:B:45:PRO:HB2	2:B:344:HOH:O	2.14	0.48
1:C:165:PRO:C	1:C:167:VAL:H	2.17	0.48
1:C:225:LEU:HD11	1:C:231:VAL:CG2	2.37	0.48
1:C:99:THR:HG22	1:C:101:ARG:N	2.27	0.48
1:D:114:PRO:HG2	1:D:115:LEU:H	1.79	0.48
1:D:128:GLY:N	1:D:149:MSE:HE1	2.29	0.48
1:A:90:LEU:HB3	1:A:98:LEU:HG	1.96	0.48
1:D:171:TYR:C	1:D:173:ASP:H	2.16	0.48
1:C:161:LYS:HA	1:C:168:ALA:HB1	1.95	0.48
1:D:99:THR:HG23	1:D:269:THR:HG21	1.95	0.48
1:B:150:CYS:SG	1:B:183:GLY:HA2	2.53	0.48
1:B:236:GLU:HB3	1:B:241:HIS:ND1	2.28	0.48
1:B:45:PRO:HG3	1:C:43:VAL:HG21	1.95	0.48
1:A:111:THR:OG1	1:A:134:VAL:HG13	2.14	0.48
1:B:278:MSE:SE	1:B:280:CYS:SG	3.22	0.48
1:D:198:VAL:O	1:D:231:VAL:HG22	2.13	0.48
1:D:54:MSE:HB3	1:D:54:MSE:HE3	1.82	0.48
1:A:311:ASN:O	1:A:314:ILE:N	2.47	0.48
1:B:109:MSE:HE1	1:B:318:ALA:HB2	1.96	0.48
1:C:110:ILE:HG12	1:C:199:ILE:HG23	1.96	0.48
1:C:47:TRP:CZ2	1:C:63:LYS:HB2	2.49	0.48
1:C:51:MSE:O	1:C:52:SER:HB2	2.13	0.48
1:B:193:GLY:HA2	1:B:226:ARG:HA	1.95	0.48
1:C:154:LYS:HB2	1:C:180:ILE:HD13	1.94	0.48
1:C:236:GLU:HB2	1:C:245:ILE:HD11	1.96	0.48
1:C:225:LEU:HD13	1:C:282:THR:HG23	1.96	0.48
1:A:79:ILE:HD12	2:A:449:HOH:O	2.13	0.48
1:A:41:SER:HG	1:D:42:THR:HG21	1.76	0.48
1:A:244:ILE:O	1:A:248:ILE:HG13	2.13	0.48
1:B:213:PHE:O	1:B:251:ASN:ND2	2.47	0.48
1:B:134:VAL:O	1:B:138:VAL:HG23	2.13	0.48
1:B:236:GLU:HB3	1:B:241:HIS:ND1	2.29	0.48
1:D:98:LEU:O	1:D:98:LEU:HD12	2.13	0.48
1:B:195:TYR:HB2	1:B:224:ALA:O	2.14	0.48
1:B:45:PRO:HB2	2:B:344:HOH:O	2.13	0.48
1:A:108:GLU:HB2	1:A:109:MSE:CE	2.39	0.48
1:C:173:ASP:OD1	1:C:175:ARG:HB2	2.14	0.48
1:C:109:MSE:CE	1:C:314:ILE:HG23	2.40	0.48
1:D:112:HIS:O	1:D:113:LEU:C	2.51	0.48
1:B:163:PHE:O	1:B:165:PRO:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG12	1:A:161:LYS:HE3	1.96	0.48
1:A:240:LEU:HG	1:A:272:SER:HB3	1.95	0.48
1:C:287:VAL:HG11	1:C:289:PHE:CE1	2.49	0.48
1:D:149:MSE:HG2	1:D:178:LEU:HD13	1.94	0.48
1:D:252:CYS:CB	1:D:278:MSE:HE3	2.44	0.48
1:D:231:VAL:HG21	1:D:256:PHE:CZ	2.48	0.48
1:D:257:LYS:HG2	1:D:283:GLU:OE1	2.12	0.48
1:B:205:PRO:HB3	1:B:213:PHE:CD1	2.49	0.48
1:C:182:ASP:OD2	1:C:184:VAL:HG22	2.13	0.48
1:A:104:CYS:O	1:A:108:GLU:HG3	2.13	0.48
1:A:270:TYR:HB3	2:A:380:HOH:O	2.12	0.48
1:A:50:GLU:CD	1:A:96:ILE:HG13	2.34	0.48
1:B:205:PRO:HB2	1:B:210:LYS:HG2	1.95	0.48
1:C:321:LEU:N	1:C:321:LEU:HD12	2.26	0.48
1:A:76:GLN:HG3	1:A:78:VAL:HG22	1.95	0.48
1:B:196:ASP:OD1	1:B:226:ARG:HD3	2.14	0.48
1:B:78:VAL:HA	1:B:92:LEU:HD23	1.95	0.48
1:D:142:ALA:HB2	2:D:376:HOH:O	2.12	0.48
1:B:257:LYS:CB	1:B:283:GLU:HB2	2.37	0.48
1:D:108:GLU:OE1	1:D:310:TYR:N	2.47	0.48
1:D:167:VAL:C	1:D:169:ILE:H	2.16	0.48
1:A:239:TRP:CD2	1:D:268:PRO:HG2	2.49	0.48
1:B:127:ILE:HB	1:B:200:VAL:HG22	1.96	0.48
1:C:308:LYS:NZ	2:C:372:HOH:O	2.47	0.48
1:A:132:GLY:O	1:A:135:LEU:HD13	2.14	0.48
1:B:192:GLU:HB2	1:B:223:ARG:NH1	2.28	0.48
1:C:234:GLN:OE1	1:C:236:GLU:N	2.44	0.48
1:B:80:VAL:HG21	1:B:159:VAL:CG1	2.44	0.48
1:C:236:GLU:HB2	1:C:245:ILE:CD1	2.44	0.48
1:C:238:LEU:HD11	1:C:321:LEU:HD22	1.94	0.48
1:A:159:VAL:HG13	1:A:163:PHE:CE2	2.48	0.48
1:A:226:ARG:HD2	1:A:227:PRO:O	2.13	0.48
1:A:231:VAL:CG1	1:A:280:CYS:HB2	2.43	0.48
1:A:98:LEU:HD12	1:A:98:LEU:C	2.34	0.48
1:D:279:LEU:O	1:D:289:PHE:CE2	2.67	0.48
1:A:228:GLY:HA3	1:A:285:PRO:HD2	1.96	0.48
1:B:162:GLN:OE1	2:B:453:HOH:O	2.20	0.48
1:B:163:PHE:O	1:B:165:PRO:HD3	2.13	0.48
1:B:234:GLN:NE2	1:B:234:GLN:O	2.45	0.48
1:C:98:LEU:HD23	1:C:131:ASP:OD2	2.14	0.48
1:D:279:LEU:HD12	1:D:289:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:GLY:HA3	1:D:285:PRO:HD2	1.96	0.48
1:A:76:GLN:OE1	1:A:92:LEU:HD13	2.13	0.48
1:B:217:PHE:O	1:B:220:SER:HB3	2.14	0.48
1:C:50:GLU:OE1	1:C:96:ILE:HD12	2.14	0.48
1:D:88:LYS:H	1:D:100:GLU:HG3	1.79	0.48
1:C:165:PRO:HA	1:C:168:ALA:HB3	1.96	0.48
1:C:311:ASN:HD21	1:C:314:ILE:H	1.53	0.48
1:C:159:VAL:CG2	1:D:45:PRO:HG2	2.44	0.48
1:D:66:LYS:O	1:D:81:PHE:HB2	2.14	0.48
1:B:110:ILE:CG2	1:B:111:THR:N	2.77	0.48
1:D:308:LYS:HZ3	1:D:308:LYS:HB3	1.78	0.48
1:B:249:VAL:HG22	1:B:278:MSE:SE	2.64	0.48
1:B:263:ALA:HB2	1:B:319:PHE:CE1	2.48	0.48
1:A:122:LYS:O	1:A:144:ILE:HG23	2.13	0.48
1:A:152:ILE:HG23	1:A:153:ASP:N	2.29	0.48
1:C:167:VAL:C	1:C:169:ILE:H	2.17	0.48
1:D:119:PRO:HG3	2:D:412:HOH:O	2.14	0.48
1:A:237:SER:H	1:A:241:HIS:CD2	2.32	0.48
1:B:270:TYR:O	1:B:271:PRO:C	2.51	0.48
1:B:97:GLN:O	1:B:98:LEU:HB3	2.14	0.47
1:C:193:GLY:HA2	1:C:225:LEU:O	2.13	0.47
1:D:245:ILE:O	1:D:249:VAL:HG23	2.14	0.47
1:D:151:GLU:HG2	1:D:157:VAL:CG2	2.44	0.47
1:D:269:THR:HG22	1:D:269:THR:O	2.13	0.47
1:B:113:LEU:HA	1:B:315:HIS:CE1	2.49	0.47
1:B:66:LYS:O	1:B:68:LEU:N	2.47	0.47
1:C:184:VAL:HG23	1:C:185:ALA:N	2.29	0.47
1:A:125:LEU:CD2	1:A:187:LEU:HD11	2.44	0.47
1:A:55:TRP:CD1	1:A:55:TRP:O	2.67	0.47
1:B:112:HIS:NE2	1:B:137:GLU:OE1	2.42	0.47
1:D:223:ARG:HH11	1:D:223:ARG:HG3	1.79	0.47
1:B:113:LEU:CD1	1:B:279:LEU:HG	2.44	0.47
1:D:245:ILE:O	1:D:247:ASP:N	2.47	0.47
1:A:108:GLU:OE1	1:A:309:PHE:N	2.45	0.47
1:C:158:ASP:HA	1:C:161:LYS:HE3	1.95	0.47
1:A:162:GLN:NE2	1:C:42:THR:HB	2.29	0.47
1:A:321:LEU:CD1	1:A:326:LYS:HG3	2.44	0.47
1:A:95:VAL:O	1:A:97:GLN:NE2	2.47	0.47
1:B:106:TYR:O	1:B:109:MSE:N	2.47	0.47
1:B:135:LEU:HD11	1:B:149:MSE:HG3	1.96	0.47
1:B:99:THR:HG23	1:B:269:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:SER:OG	1:B:86:TYR:N	2.43	0.47
1:C:154:LYS:HD3	1:C:154:LYS:C	2.34	0.47
1:C:236:GLU:HG3	1:C:241:HIS:CD2	2.49	0.47
1:D:263:ALA:O	1:D:277:PHE:N	2.47	0.47
1:D:329:ILE:O	1:D:330:GLU:HB2	2.13	0.47
1:A:296:ILE:HB	1:A:307:LEU:HD11	1.96	0.47
1:A:165:PRO:HG2	1:A:166:ASP:H	1.78	0.47
1:A:51:MSE:HE3	1:C:72:LYS:N	2.25	0.47
1:B:173:ASP:HB3	1:B:176:VAL:CG2	2.44	0.47
1:B:257:LYS:HE3	1:B:283:GLU:HB2	1.96	0.47
1:B:57:GLY:HA2	1:C:63:LYS:HB3	1.95	0.47
1:A:161:LYS:NZ	2:A:343:HOH:O	2.40	0.47
1:A:238:LEU:C	1:A:238:LEU:HD12	2.35	0.47
1:B:164:PHE:O	1:B:167:VAL:HG23	2.14	0.47
1:A:238:LEU:HD22	1:A:242:MSE:HE1	1.95	0.47
1:D:322:PRO:O	1:D:325:ALA:N	2.46	0.47
1:A:126:VAL:O	1:A:149:MSE:HA	2.14	0.47
1:A:206:ILE:HG23	1:A:207:GLY:N	2.29	0.47
1:A:310:TYR:HE2	1:A:315:HIS:HD1	1.61	0.47
1:B:51:MSE:HG3	1:B:59:ALA:HB2	1.96	0.47
1:C:206:ILE:HG23	1:C:207:GLY:N	2.29	0.47
1:D:99:THR:OG1	1:D:102:ASP:OD1	2.28	0.47
1:A:241:HIS:HB3	1:A:244:ILE:HB	1.96	0.47
1:D:124:VAL:HG13	1:D:197:ALA:O	2.14	0.47
1:A:121:PRO:O	1:A:144:ILE:HD13	2.15	0.47
1:B:109:MSE:CE	1:B:310:TYR:HB2	2.45	0.47
1:C:99:THR:HG22	1:C:101:ARG:H	1.79	0.47
1:D:112:HIS:O	1:D:116:CYS:HB2	2.13	0.47
1:B:140:ARG:NH2	1:B:307:LEU:HD23	2.28	0.47
1:C:194:SER:HB2	2:C:479:HOH:O	2.14	0.47
1:D:259:SER:O	1:D:280:CYS:HA	2.14	0.47
1:A:88:LYS:HB3	1:A:164:PHE:CE1	2.49	0.47
1:A:215:LYS:N	1:A:216:PRO:CD	2.77	0.47
1:A:51:MSE:HE3	2:A:395:HOH:O	2.15	0.47
1:C:313:GLU:HG3	2:C:490:HOH:O	2.13	0.47
1:C:68:LEU:HB3	1:C:163:PHE:CE1	2.49	0.47
1:B:80:VAL:HA	1:B:89:VAL:O	2.15	0.47
1:C:124:VAL:HG22	1:C:197:ALA:CB	2.19	0.47
1:C:92:LEU:HD11	1:C:130:GLY:CA	2.43	0.47
1:C:147:ILE:HB	1:C:176:VAL:HG22	1.97	0.47
1:A:260:VAL:HG23	1:A:278:MSE:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:THR:OG1	1:D:137:GLU:HB3	2.14	0.47
1:A:238:LEU:HD12	1:A:264:TRP:CE3	2.49	0.47
1:A:133:GLY:O	1:A:137:GLU:HG2	2.14	0.47
1:B:210:LYS:HD3	1:B:210:LYS:C	2.34	0.47
1:C:73:SER:HB3	1:C:155:MSE:SE	2.64	0.47
1:D:178:LEU:HD12	1:D:179:VAL:N	2.30	0.47
1:A:263:ALA:HB2	1:A:319:PHE:CE1	2.49	0.47
1:B:112:HIS:O	1:B:116:CYS:HB2	2.15	0.47
1:C:198:VAL:HG23	1:C:225:LEU:HD21	1.95	0.47
1:B:61:SER:O	1:C:58:GLU:HA	2.14	0.47
1:D:157:VAL:O	1:D:161:LYS:HG3	2.15	0.47
1:C:154:LYS:HB2	1:C:180:ILE:CG1	2.43	0.47
1:D:111:THR:HG22	1:D:134:VAL:HG13	1.96	0.47
1:D:52:SER:HB3	1:D:55:TRP:CE2	2.49	0.47
1:B:252:CYS:HB3	1:B:280:CYS:SG	2.53	0.47
1:B:324:PHE:C	1:B:324:PHE:CD1	2.87	0.47
1:A:109:MSE:SE	1:A:318:ALA:HB2	2.64	0.47
1:A:150:CYS:SG	1:A:179:VAL:HB	2.55	0.47
1:C:72:LYS:HE2	1:C:77:ASP:OD1	2.13	0.47
1:A:264:TRP:CZ2	1:A:322:PRO:HD3	2.49	0.47
1:D:198:VAL:CB	1:D:231:VAL:HG22	2.40	0.47
1:B:125:LEU:HB2	1:B:195:TYR:CE1	2.49	0.47
1:D:125:LEU:HB3	1:D:198:VAL:HG22	1.95	0.47
1:A:257:LYS:HG3	1:A:283:GLU:HB2	1.96	0.47
1:D:54:MSE:HB2	1:D:55:TRP:CE3	2.49	0.47
1:A:115:LEU:HD11	1:A:124:VAL:HG21	1.97	0.47
1:C:222:ALA:HA	1:C:282:THR:CG2	2.44	0.47
1:C:311:ASN:CG	1:C:314:ILE:HD13	2.34	0.47
1:D:256:PHE:HD1	1:D:282:THR:CG2	2.26	0.47
1:B:98:LEU:HD12	1:B:98:LEU:O	2.15	0.47
1:C:236:GLU:O	1:C:275:ILE:HD12	2.14	0.47
1:A:165:PRO:HG2	1:A:166:ASP:H	1.79	0.47
1:B:110:ILE:O	1:B:114:PRO:HD2	2.14	0.47
1:B:192:GLU:HG3	1:B:223:ARG:HG2	1.96	0.47
1:B:54:MSE:SE	2:B:567:HOH:O	2.82	0.47
1:C:79:ILE:HB	1:C:91:VAL:HB	1.97	0.47
1:A:79:ILE:HB	1:A:91:VAL:HB	1.96	0.47
1:B:172:GLU:O	1:B:173:ASP:C	2.52	0.47
1:B:42:THR:HA	1:B:49:SER:CB	2.44	0.47
1:B:43:VAL:HG23	1:B:44:ILE:HG13	1.96	0.47
1:A:301:SER:HB3	1:A:304:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:VAL:CG2	1:B:232:CYS:N	2.77	0.47
1:A:299:SER:C	1:A:301:SER:N	2.66	0.47
1:A:78:VAL:HG12	1:A:79:ILE:N	2.30	0.47
1:B:160:SER:HA	1:B:164:PHE:HD2	1.79	0.47
1:C:181:GLY:O	1:C:182:ASP:C	2.52	0.47
1:A:154:LYS:HG2	1:A:158:ASP:OD2	2.14	0.47
1:A:253:ARG:CG	1:A:260:VAL:HG21	2.45	0.47
1:A:310:TYR:C	1:A:310:TYR:CD1	2.87	0.47
1:C:169:ILE:HA	1:C:172:GLU:OE1	2.15	0.47
1:D:136:ARG:HG2	1:D:136:ARG:HH11	1.79	0.47
1:C:206:ILE:HG23	1:C:207:GLY:N	2.29	0.47
1:D:111:THR:CG2	1:D:134:VAL:HG13	2.44	0.47
1:D:99:THR:OG1	1:D:100:GLU:N	2.46	0.47
1:A:162:GLN:OE1	1:C:42:THR:HB	2.13	0.47
1:A:169:ILE:O	1:A:172:GLU:HB2	2.15	0.47
1:A:257:LYS:HB2	1:A:283:GLU:HG3	1.95	0.47
1:A:310:TYR:HE2	1:A:315:HIS:ND1	2.11	0.47
1:A:44:ILE:HD12	1:D:51:MSE:HE1	1.96	0.47
1:B:44:ILE:HD13	1:C:51:MSE:CE	2.45	0.47
1:D:198:VAL:O	1:D:231:VAL:HG13	2.15	0.47
1:D:42:THR:HA	1:D:49:SER:HB2	1.96	0.47
1:A:107:GLN:O	1:A:110:ILE:HG22	2.14	0.47
1:A:206:ILE:HG23	1:A:207:GLY:N	2.29	0.47
1:A:54:MSE:HE2	1:A:54:MSE:HA	1.97	0.47
1:D:108:GLU:HG2	1:D:137:GLU:HG3	1.96	0.47
1:C:135:LEU:HB3	1:C:170:GLY:HA3	1.96	0.47
1:C:169:ILE:HA	1:C:172:GLU:OE2	2.13	0.47
1:C:263:ALA:HB2	1:C:319:PHE:CE1	2.49	0.47
1:D:69:PHE:O	1:D:79:ILE:HA	2.14	0.47
1:B:136:ARG:NE	1:B:167:VAL:HG12	2.20	0.47
1:C:121:PRO:O	1:C:144:ILE:HD13	2.15	0.47
1:D:111:THR:CG2	1:D:134:VAL:HG13	2.44	0.47
1:D:64:VAL:HG12	1:D:65:GLU:N	2.30	0.47
1:B:199:ILE:HA	1:B:232:CYS:O	2.14	0.47
1:C:141:HIS:HB2	1:C:144:ILE:HG12	1.96	0.47
1:C:169:ILE:C	1:C:171:TYR:H	2.17	0.47
1:C:262:TYR:HA	1:C:277:PHE:O	2.14	0.47
1:A:326:LYS:HE3	1:D:313:GLU:OE1	2.15	0.47
1:B:308:LYS:C	1:C:323:SER:HB2	2.35	0.47
1:C:242:MSE:HA	1:C:242:MSE:HE2	1.97	0.47
1:C:104:CYS:HB2	1:C:308:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:THR:OG1	1:D:137:GLU:HB3	2.14	0.47
1:D:136:ARG:HE	1:D:167:VAL:CB	2.20	0.47
1:D:68:LEU:CD1	1:D:81:PHE:HA	2.45	0.47
1:A:127:ILE:HD12	1:A:127:ILE:C	2.35	0.47
1:A:90:LEU:HD22	1:A:97:GLN:CB	2.44	0.47
1:B:327:LYS:HD3	1:B:327:LYS:C	2.35	0.47
1:A:125:LEU:HD21	1:A:187:LEU:HD11	1.97	0.47
1:C:248:ILE:O	1:C:248:ILE:HG22	2.13	0.47
1:C:322:PRO:HG2	1:C:325:ALA:CB	2.45	0.47
1:D:139:ALA:C	1:D:141:HIS:H	2.17	0.47
1:A:122:LYS:O	1:A:144:ILE:HG23	2.15	0.47
1:A:296:ILE:HG21	1:A:301:SER:OG	2.14	0.47
1:D:55:TRP:O	1:D:58:GLU:HG2	2.15	0.47
1:A:64:VAL:HG12	1:A:65:GLU:N	2.29	0.47
1:B:164:PHE:N	1:B:165:PRO:HD3	2.30	0.47
1:D:182:ASP:OD2	1:D:184:VAL:HB	2.15	0.47
1:D:69:PHE:O	1:D:79:ILE:HA	2.14	0.47
1:A:104:CYS:O	1:A:108:GLU:HG3	2.14	0.47
1:A:187:LEU:O	1:A:190:ALA:HB3	2.15	0.47
1:A:295:PRO:CB	1:A:310:TYR:HE1	2.26	0.47
1:C:72:LYS:HE2	1:C:77:ASP:CG	2.35	0.47
1:B:103:GLU:O	1:B:107:GLN:HG3	2.15	0.47
1:B:307:LEU:HD13	1:B:310:TYR:HD1	1.79	0.47
1:B:91:VAL:HA	1:B:95:VAL:O	2.14	0.47
1:C:161:LYS:HA	1:C:168:ALA:HB2	1.96	0.47
1:C:116:CYS:SG	1:C:295:PRO:HA	2.55	0.47
1:D:241:HIS:HB3	1:D:244:ILE:HB	1.96	0.47
1:A:121:PRO:HA	2:A:386:HOH:O	2.15	0.47
1:B:111:THR:O	1:B:115:LEU:HB2	2.14	0.47
1:C:223:ARG:HA	2:C:477:HOH:O	2.15	0.47
1:D:313:GLU:CD	1:D:313:GLU:H	2.17	0.47
1:B:249:VAL:HG21	1:B:329:ILE:HG21	1.97	0.47
1:D:107:GLN:CD	1:D:133:GLY:HA3	2.35	0.47
1:B:242:MSE:HA	1:B:242:MSE:HE3	1.96	0.47
1:B:272:SER:OG	1:B:274:VAL:HG22	2.14	0.47
1:B:274:VAL:HG13	2:C:398:HOH:O	2.15	0.47
1:B:81:PHE:CE2	1:B:89:VAL:HB	2.50	0.47
1:B:321:LEU:O	1:C:314:ILE:HD11	2.14	0.47
1:C:50:GLU:HG2	1:C:55:TRP:HZ2	1.79	0.47
1:D:123:LYS:HB3	1:D:195:TYR:HA	1.96	0.47
1:A:298:GLU:OE1	1:A:302:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:MSE:SE	1:B:54:MSE:N	2.98	0.47
1:C:323:SER:C	1:C:325:ALA:H	2.17	0.47
1:C:68:LEU:O	1:C:69:PHE:HB2	2.14	0.47
1:D:107:GLN:CD	1:D:133:GLY:HA3	2.34	0.47
1:A:149:MSE:CG	1:A:178:LEU:HD13	2.44	0.47
1:B:106:TYR:OH	1:B:234:GLN:HG3	2.15	0.47
1:B:278:MSE:SE	1:B:279:LEU:N	2.98	0.47
1:C:123:LYS:HG2	1:C:195:TYR:CD1	2.50	0.47
1:A:129:GLY:H	1:A:149:MSE:SE	2.48	0.47
1:B:78:VAL:O	1:B:79:ILE:HG13	2.14	0.47
1:C:165:PRO:HG2	1:C:166:ASP:H	1.80	0.47
1:C:169:ILE:HA	1:C:172:GLU:OE2	2.14	0.47
1:D:136:ARG:HG2	2:D:356:HOH:O	2.15	0.47
1:D:326:LYS:NZ	2:D:351:HOH:O	2.48	0.47
1:D:78:VAL:C	1:D:79:ILE:HG13	2.35	0.47
1:A:76:GLN:OE1	1:A:92:LEU:HB3	2.15	0.47
1:C:229:GLY:O	1:C:281:SER:HA	2.15	0.47
1:C:49:SER:HB3	1:C:61:SER:OG	2.15	0.47
1:D:262:TYR:HD2	1:D:278:MSE:HE3	1.80	0.47
1:D:328:VAL:HG13	2:D:415:HOH:O	2.15	0.47
1:B:121:PRO:O	1:B:144:ILE:HD13	2.15	0.47
1:A:111:THR:OG1	1:A:134:VAL:HG13	2.14	0.47
1:A:206:ILE:HG23	1:A:207:GLY:H	1.80	0.47
1:A:293:LEU:O	1:A:293:LEU:HD23	2.15	0.47
1:A:92:LEU:O	1:A:93:ASP:C	2.53	0.47
1:C:261:ASN:HD21	1:C:289:PHE:HB2	1.78	0.47
1:B:192:GLU:HG3	1:B:223:ARG:HG2	1.96	0.47
1:C:152:ILE:HD12	1:C:182:ASP:HB2	1.97	0.47
1:C:58:GLU:N	1:C:58:GLU:CD	2.68	0.47
1:D:250:SER:HA	1:D:253:ARG:HD2	1.97	0.47
1:A:120:ASN:O	1:A:122:LYS:HE2	2.15	0.47
1:C:104:CYS:O	1:C:108:GLU:HB2	2.14	0.47
1:C:245:ILE:O	1:C:249:VAL:HG23	2.15	0.47
1:D:234:GLN:HE21	1:D:236:GLU:N	2.04	0.47
1:D:313:GLU:CD	1:D:313:GLU:N	2.68	0.47
1:A:239:TRP:O	1:D:101:ARG:NH2	2.48	0.47
1:A:94:GLY:O	1:A:95:VAL:CG2	2.60	0.47
1:D:110:ILE:CD1	1:D:201:ASP:HA	2.44	0.47
1:A:109:MSE:HG3	1:A:265:THR:OG1	2.13	0.47
1:A:170:GLY:C	1:A:172:GLU:N	2.69	0.47
1:A:69:PHE:HE1	1:A:78:VAL:HB	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:O	1:D:44:ILE:HG13	2.14	0.47
1:D:92:LEU:HD12	1:D:97:GLN:HG2	1.97	0.47
1:A:191:ALA:HB3	1:A:194:SER:HB3	1.97	0.47
1:A:227:PRO:HB2	1:A:284:GLY:HA3	1.97	0.47
1:A:68:LEU:HB2	1:A:80:VAL:HG12	1.97	0.47
1:A:92:LEU:O	1:A:94:GLY:N	2.48	0.47
1:C:151:GLU:HG2	1:C:157:VAL:CG2	2.44	0.47
1:C:164:PHE:HB3	1:C:167:VAL:HB	1.97	0.47
1:D:296:ILE:HG23	1:D:307:LEU:HD11	1.96	0.47
1:C:198:VAL:O	1:C:231:VAL:HA	2.14	0.47
1:D:60:HIS:CD2	2:D:364:HOH:O	2.68	0.47
1:A:72:LYS:HA	1:A:77:ASP:HA	1.96	0.47
1:D:139:ALA:C	1:D:175:ARG:HH12	2.17	0.47
1:A:92:LEU:O	1:A:95:VAL:N	2.48	0.47
1:B:125:LEU:HA	1:B:148:ASP:O	2.15	0.47
1:A:106:TYR:HE2	1:A:201:ASP:OD2	1.97	0.47
1:C:165:PRO:O	1:C:167:VAL:N	2.48	0.47
1:D:90:LEU:HB3	1:D:98:LEU:CD1	2.45	0.47
1:C:324:PHE:CD1	1:C:325:ALA:N	2.83	0.47
1:B:155:MSE:O	1:B:159:VAL:HG23	2.15	0.47
1:B:63:LYS:NZ	2:B:534:HOH:O	2.37	0.47
1:C:97:GLN:NE2	1:C:97:GLN:CA	2.77	0.47
1:A:139:ALA:O	1:A:141:HIS:N	2.48	0.47
1:B:231:VAL:HG12	1:B:280:CYS:O	2.15	0.47
1:B:327:LYS:HG2	1:B:327:LYS:O	2.15	0.47
1:B:85:THR:HG21	1:C:56:PRO:O	2.14	0.47
1:C:68:LEU:HB2	1:C:80:VAL:HG12	1.98	0.47
1:A:134:VAL:O	1:A:138:VAL:HG23	2.15	0.46
1:A:310:TYR:CD1	1:A:311:ASN:N	2.83	0.46
1:D:164:PHE:O	1:D:167:VAL:HG22	2.15	0.46
1:D:274:VAL:HG23	1:D:274:VAL:O	2.15	0.46
1:D:60:HIS:CD2	2:D:360:HOH:O	2.69	0.46
1:C:125:LEU:HB2	1:C:195:TYR:CE1	2.50	0.46
1:C:66:LYS:HG2	1:C:67:VAL:N	2.30	0.46
1:C:82:GLN:NE2	1:C:88:LYS:N	2.63	0.46
1:D:51:MSE:O	1:D:52:SER:CB	2.63	0.46
1:B:235:ALA:HB2	1:B:278:MSE:HB2	1.96	0.46
1:C:55:TRP:HH2	1:C:95:VAL:HG13	1.80	0.46
1:A:215:LYS:HG2	1:A:255:ILE:CG1	2.44	0.46
1:C:82:GLN:HE22	1:C:88:LYS:HE3	1.78	0.46
1:A:108:GLU:CD	1:A:307:LEU:HB3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LEU:H	1:C:307:LEU:CD1	2.28	0.46
1:C:89:VAL:HG13	1:C:96:ILE:HG23	1.96	0.46
1:A:288:ASP:OD1	1:A:290:LYS:HB2	2.16	0.46
1:A:279:LEU:HB3	1:A:289:PHE:CD2	2.50	0.46
1:A:324:PHE:CE1	1:A:325:ALA:HB2	2.50	0.46
1:B:269:THR:O	1:B:269:THR:HG22	2.14	0.46
1:C:206:ILE:HG23	1:C:207:GLY:N	2.29	0.46
1:C:238:LEU:HD23	1:C:245:ILE:HD13	1.96	0.46
1:A:96:ILE:HD12	1:A:269:THR:HG23	1.97	0.46
1:D:191:ALA:HB3	1:D:194:SER:HB3	1.97	0.46
1:D:241:HIS:ND1	1:D:244:ILE:HD12	2.30	0.46
1:A:80:VAL:HG21	1:A:159:VAL:CG1	2.44	0.46
1:A:173:ASP:HB3	1:A:176:VAL:CG2	2.44	0.46
1:A:124:VAL:HG13	1:A:197:ALA:HB3	1.96	0.46
1:A:97:GLN:NE2	1:A:97:GLN:HA	2.30	0.46
1:D:60:HIS:CD2	2:D:364:HOH:O	2.68	0.46
1:C:245:ILE:HA	1:C:248:ILE:HD12	1.97	0.46
1:C:150:CYS:SG	1:C:181:GLY:O	2.74	0.46
1:D:60:HIS:CD2	2:D:360:HOH:O	2.68	0.46
1:B:146:GLN:HA	1:B:175:ARG:HB3	1.97	0.46
1:C:136:ARG:HH12	1:C:167:VAL:HG22	1.80	0.46
1:C:154:LYS:HB2	1:C:180:ILE:HG21	1.97	0.46
1:D:136:ARG:HH11	1:D:136:ARG:HG2	1.80	0.46
1:D:98:LEU:O	1:D:98:LEU:HD12	2.14	0.46
1:D:114:PRO:HG2	1:D:115:LEU:H	1.79	0.46
1:C:66:LYS:HE2	1:C:68:LEU:HA	1.97	0.46
1:A:52:SER:HB3	1:A:55:TRP:CE2	2.49	0.46
1:D:118:ILE:HD11	1:D:121:PRO:HB3	1.96	0.46
1:B:129:GLY:HA3	2:B:575:HOH:O	2.15	0.46
1:B:240:LEU:HD21	1:B:272:SER:HB2	1.97	0.46
1:D:73:SER:C	1:D:75:TYR:H	2.17	0.46
1:B:157:VAL:HG13	1:B:171:TYR:CZ	2.50	0.46
1:C:165:PRO:HG2	1:C:166:ASP:H	1.81	0.46
1:D:263:ALA:HB2	1:D:319:PHE:CE1	2.50	0.46
1:B:113:LEU:N	1:B:114:PRO:HD2	2.29	0.46
1:B:243:ASP:HA	1:B:246:GLU:OE1	2.15	0.46
1:C:197:ALA:HA	1:C:230:VAL:O	2.14	0.46
1:C:307:LEU:N	1:C:307:LEU:HD12	2.30	0.46
1:D:111:THR:HG21	1:D:134:VAL:HA	1.97	0.46
1:D:205:PRO:HG3	1:D:244:ILE:HD13	1.97	0.46
1:B:108:GLU:OE1	1:B:310:TYR:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:GLU:H	1:D:313:GLU:CD	2.18	0.46
1:B:113:LEU:HD11	1:B:319:PHE:HZ	1.80	0.46
1:D:259:SER:O	1:D:280:CYS:HA	2.16	0.46
1:B:133:GLY:O	1:B:137:GLU:HG2	2.15	0.46
1:C:132:GLY:HA3	1:C:149:MSE:HE1	1.96	0.46
1:C:310:TYR:CD1	1:C:310:TYR:C	2.89	0.46
1:A:79:ILE:CG2	1:A:80:VAL:N	2.78	0.46
1:B:195:TYR:O	1:B:225:LEU:HD23	2.15	0.46
1:B:206:ILE:HG23	1:B:206:ILE:O	2.15	0.46
1:B:68:LEU:H	1:B:81:PHE:HA	1.79	0.46
1:D:310:TYR:CD1	1:D:310:TYR:C	2.89	0.46
1:D:69:PHE:HB2	1:D:163:PHE:CZ	2.50	0.46
1:A:299:SER:O	1:A:301:SER:N	2.49	0.46
1:C:225:LEU:HB3	1:C:229:GLY:HA3	1.96	0.46
1:C:313:GLU:HG3	2:C:490:HOH:O	2.14	0.46
1:D:158:ASP:O	1:D:161:LYS:HB2	2.16	0.46
1:A:92:LEU:O	1:A:95:VAL:N	2.44	0.46
1:C:268:PRO:O	1:C:270:TYR:N	2.49	0.46
1:A:135:LEU:HD12	1:A:135:LEU:N	2.31	0.46
1:A:290:LYS:HD3	2:A:373:HOH:O	2.15	0.46
1:A:51:MSE:CG	2:A:395:HOH:O	2.48	0.46
1:C:127:ILE:HG12	1:C:217:PHE:CZ	2.51	0.46
1:C:173:ASP:HB3	1:C:176:VAL:HG23	1.97	0.46
1:C:252:CYS:HB3	1:C:280:CYS:SG	2.56	0.46
1:D:86:TYR:O	1:D:100:GLU:HB2	2.15	0.46
1:D:90:LEU:HB3	1:D:98:LEU:CG	2.44	0.46
1:D:107:GLN:CD	1:D:133:GLY:HA3	2.36	0.46
1:A:80:VAL:CG2	1:A:159:VAL:HG11	2.30	0.46
1:A:310:TYR:CG	1:A:311:ASN:N	2.83	0.46
1:C:283:GLU:H	1:C:283:GLU:CD	2.19	0.46
1:C:100:GLU:HA	1:C:103:GLU:OE2	2.15	0.46
1:C:262:TYR:HA	1:C:277:PHE:O	2.16	0.46
1:D:169:ILE:HG23	1:D:170:GLY:N	2.30	0.46
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.80	0.46
1:A:86:TYR:O	1:A:99:THR:HG23	2.16	0.46
1:D:111:THR:CG2	1:D:134:VAL:HG13	2.45	0.46
1:D:141:HIS:O	1:D:143:SER:N	2.48	0.46
1:B:86:TYR:CD2	1:B:101:ARG:HB3	2.50	0.46
1:C:222:ALA:HA	1:C:282:THR:HG21	1.96	0.46
1:B:200:VAL:C	1:B:202:SER:H	2.17	0.46
1:C:303:SER:C	1:C:305:GLY:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLY:O	1:A:277:PHE:CG	2.68	0.46
1:C:152:ILE:HG13	1:C:182:ASP:N	2.31	0.46
1:D:242:MSE:CE	1:D:325:ALA:HA	2.43	0.46
1:D:76:GLN:CD	1:D:92:LEU:HD22	2.36	0.46
1:C:109:MSE:HE2	1:C:113:LEU:HG	1.96	0.46
1:A:298:GLU:O	1:A:301:SER:O	2.32	0.46
1:C:151:GLU:O	1:C:180:ILE:HA	2.14	0.46
1:C:154:LYS:HD3	1:C:158:ASP:HB2	1.97	0.46
1:D:187:LEU:HB3	1:D:220:SER:OG	2.14	0.46
1:A:153:ASP:C	1:A:153:ASP:OD1	2.53	0.46
1:B:233:THR:HG23	2:B:471:HOH:O	2.14	0.46
1:B:82:GLN:HE22	1:B:88:LYS:HG3	1.81	0.46
1:A:225:LEU:HB2	1:A:282:THR:HG21	1.98	0.46
1:C:169:ILE:O	1:C:172:GLU:HB2	2.15	0.46
1:D:274:VAL:C	1:D:275:ILE:O	2.53	0.46
1:B:42:THR:HG23	1:C:42:THR:O	2.14	0.46
1:A:243:ASP:OD2	1:A:244:ILE:HG13	2.16	0.46
1:B:149:MSE:HE1	1:B:171:TYR:HE1	1.80	0.46
1:B:257:LYS:CB	1:B:283:GLU:HB2	2.40	0.46
1:A:297:ASP:CG	1:A:298:GLU:N	2.68	0.46
1:C:236:GLU:O	1:C:276:GLY:HA3	2.15	0.46
1:B:170:GLY:C	1:B:172:GLU:H	2.19	0.46
1:C:161:LYS:HA	1:C:168:ALA:CB	2.45	0.46
1:D:112:HIS:ND1	1:D:141:HIS:HE1	2.12	0.46
1:D:114:PRO:HG2	1:D:115:LEU:H	1.80	0.46
1:A:223:ARG:CD	2:A:360:HOH:O	2.61	0.46
1:B:198:VAL:O	1:B:231:VAL:HA	2.15	0.46
1:B:96:ILE:HG21	1:B:269:THR:CG2	2.46	0.46
1:D:262:TYR:OH	1:D:276:GLY:HA3	2.16	0.46
1:A:310:TYR:C	1:A:310:TYR:CD1	2.88	0.46
1:A:292:PRO:HB3	1:A:315:HIS:ND1	2.30	0.46
1:B:109:MSE:O	1:B:113:LEU:HB2	2.16	0.46
1:D:122:LYS:HD3	1:D:145:GLU:OE2	2.15	0.46
1:D:249:VAL:HG21	1:D:329:ILE:HG23	1.98	0.46
1:B:148:ASP:OD1	1:B:177:ASN:HB3	2.16	0.46
1:B:228:GLY:N	1:B:282:THR:OG1	2.49	0.46
1:B:324:PHE:CD1	1:B:325:ALA:N	2.83	0.46
1:D:112:HIS:O	1:D:116:CYS:HB2	2.15	0.46
1:D:128:GLY:HA2	2:D:551:HOH:O	2.16	0.46
1:B:113:LEU:HD23	1:B:315:HIS:ND1	2.31	0.46
1:D:113:LEU:N	1:D:114:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD23	1:A:176:VAL:HG21	1.97	0.46
1:B:136:ARG:HH21	1:B:167:VAL:HG12	1.80	0.46
1:D:54:MSE:SE	1:D:206:ILE:HB	2.65	0.46
1:D:233:THR:O	1:D:277:PHE:HA	2.14	0.46
1:D:68:LEU:HG	1:D:163:PHE:HE1	1.81	0.46
1:D:265:THR:OG1	1:D:266:SER:N	2.49	0.46
1:A:46:GLY:HA3	1:A:63:LYS:HZ1	1.81	0.46
1:C:112:HIS:CE1	1:C:141:HIS:HE2	2.34	0.46
1:B:85:THR:HG1	1:C:57:GLY:HA3	1.80	0.46
1:C:125:LEU:HB2	1:C:195:TYR:CE1	2.51	0.46
1:C:263:ALA:O	1:C:276:GLY:HA2	2.16	0.46
1:A:125:LEU:HD13	1:A:186:PHE:CE1	2.51	0.46
1:A:257:LYS:NZ	2:A:566:HOH:O	2.49	0.46
1:B:113:LEU:HB3	1:B:279:LEU:HD11	1.96	0.46
1:C:198:VAL:HG21	1:C:221:VAL:HG13	1.98	0.46
1:D:115:LEU:HD23	1:D:141:HIS:CD2	2.50	0.46
1:A:236:GLU:HB2	1:A:245:ILE:CG1	2.45	0.46
1:B:249:VAL:HG22	1:B:278:MSE:CE	2.45	0.46
1:B:320:CYS:HB3	1:C:313:GLU:HB3	1.97	0.46
1:D:115:LEU:HB3	1:D:141:HIS:NE2	2.30	0.46
1:D:269:THR:O	1:D:269:THR:HG22	2.15	0.46
1:A:70:GLN:NE2	1:A:71:GLY:N	2.63	0.46
1:A:323:SER:C	1:A:325:ALA:H	2.18	0.46
1:A:99:THR:HG22	1:A:101:ARG:N	2.31	0.46
1:A:228:GLY:N	1:A:282:THR:OG1	2.49	0.46
1:A:58:GLU:HA	1:D:61:SER:O	2.15	0.46
1:C:324:PHE:HA	1:C:327:LYS:CE	2.41	0.46
1:A:206:ILE:HG13	1:A:207:GLY:N	2.31	0.46
1:B:249:VAL:HG22	1:B:278:MSE:SE	2.66	0.46
1:D:187:LEU:HD21	1:D:221:VAL:HG22	1.97	0.46
1:D:97:GLN:HA	1:D:97:GLN:NE2	2.31	0.46
1:A:236:GLU:O	1:A:275:ILE:HD12	2.15	0.46
1:A:43:VAL:HG13	1:D:43:VAL:CA	2.45	0.46
1:C:125:LEU:HD12	1:C:148:ASP:O	2.15	0.46
1:D:279:LEU:HG	1:D:319:PHE:HZ	1.80	0.46
1:C:134:VAL:O	1:C:138:VAL:HG23	2.16	0.46
1:C:129:GLY:CA	1:C:151:GLU:HB2	2.44	0.46
1:D:200:VAL:HB	1:D:233:THR:CG2	2.46	0.46
1:A:135:LEU:HD21	1:A:176:VAL:HG11	1.96	0.46
1:A:226:ARG:HD2	1:A:227:PRO:O	2.16	0.46
1:D:314:ILE:HA	1:D:317:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PRO:HB3	1:C:283:GLU:O	2.15	0.46
1:A:88:LYS:N	1:A:100:GLU:OE1	2.49	0.46
1:B:48:PHE:O	1:B:61:SER:HA	2.15	0.46
1:B:91:VAL:HA	1:B:95:VAL:O	2.16	0.46
1:D:245:ILE:O	1:D:249:VAL:HG23	2.16	0.46
1:A:238:LEU:O	1:A:242:MSE:HE3	2.15	0.46
1:A:314:ILE:HA	1:D:320:CYS:SG	2.56	0.46
1:B:164:PHE:N	1:B:165:PRO:HD3	2.30	0.46
1:B:324:PHE:C	1:B:324:PHE:CD1	2.89	0.46
1:C:185:ALA:O	1:C:188:LYS:HB2	2.14	0.46
1:D:294:ASN:HB2	2:D:425:HOH:O	2.16	0.46
1:A:301:SER:O	1:A:302:LYS:C	2.53	0.46
1:B:141:HIS:CE1	1:B:296:ILE:HD12	2.51	0.46
1:C:154:LYS:HB2	1:C:180:ILE:HD13	1.98	0.46
1:C:45:PRO:O	1:C:47:TRP:HD1	1.99	0.46
1:B:108:GLU:OE1	1:B:310:TYR:N	2.49	0.46
1:B:40:PHE:HA	1:C:42:THR:HG23	1.98	0.46
1:C:100:GLU:HA	1:C:103:GLU:OE2	2.16	0.46
1:A:260:VAL:HB	1:A:278:MSE:HE2	1.97	0.46
1:B:211:GLU:HA	1:B:214:GLU:OE1	2.14	0.46
1:B:72:LYS:HA	1:B:77:ASP:HA	1.97	0.46
1:D:68:LEU:H	1:D:68:LEU:CD1	2.29	0.46
1:A:311:ASN:H	1:A:314:ILE:HG22	1.81	0.46
1:D:90:LEU:HD23	1:D:98:LEU:HG	1.97	0.46
1:B:164:PHE:O	1:B:167:VAL:HG23	2.16	0.46
1:B:167:VAL:C	1:B:169:ILE:N	2.70	0.46
1:C:278:MSE:HE2	1:C:278:MSE:HA	1.98	0.46
1:D:110:ILE:HA	1:D:232:CYS:SG	2.56	0.46
1:D:263:ALA:HB2	1:D:319:PHE:CD1	2.51	0.46
1:B:150:CYS:HG	1:B:181:GLY:C	2.19	0.46
1:C:227:PRO:C	1:C:285:PRO:HD2	2.36	0.46
1:C:202:SER:O	1:C:234:GLN:HB3	2.16	0.46
1:D:113:LEU:N	1:D:114:PRO:HD2	2.31	0.46
1:A:113:LEU:N	1:A:114:PRO:CD	2.77	0.46
1:A:110:ILE:HG21	1:A:134:VAL:HG22	1.98	0.46
1:A:295:PRO:HG3	1:A:312:ALA:HB2	1.98	0.46
1:A:313:GLU:HG3	2:D:351:HOH:O	2.16	0.46
1:B:77:ASP:O	1:B:92:LEU:HA	2.15	0.46
1:A:135:LEU:HD21	1:A:176:VAL:HG11	1.98	0.46
1:A:309:PHE:O	1:A:309:PHE:CD1	2.69	0.46
1:A:50:GLU:OE2	1:A:96:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LYS:HG2	1:B:251:ASN:HB3	1.97	0.45
1:B:329:ILE:O	1:B:330:GLU:C	2.55	0.45
1:C:230:VAL:HA	1:C:280:CYS:O	2.15	0.45
1:C:283:GLU:N	1:C:283:GLU:OE1	2.43	0.45
1:D:141:HIS:C	1:D:143:SER:H	2.20	0.45
1:B:49:SER:HA	1:B:60:HIS:O	2.16	0.45
1:C:98:LEU:HD12	1:C:103:GLU:HB3	1.99	0.45
1:D:120:ASN:ND2	1:D:122:LYS:HE3	2.31	0.45
1:C:47:TRP:CE2	1:C:63:LYS:HD3	2.50	0.45
1:C:65:GLU:OE1	1:C:65:GLU:HA	2.16	0.45
1:D:146:GLN:HE21	1:D:177:ASN:CB	2.26	0.45
1:A:243:ASP:CG	1:A:244:ILE:H	2.19	0.45
1:A:279:LEU:HB3	1:A:289:PHE:CE2	2.52	0.45
1:A:86:TYR:HB3	1:A:99:THR:CG2	2.46	0.45
1:D:54:MSE:HB2	1:D:55:TRP:CE3	2.51	0.45
1:A:210:LYS:C	1:A:212:LEU:H	2.20	0.45
1:C:214:GLU:HB3	1:C:216:PRO:HD2	1.99	0.45
1:A:154:LYS:HG3	1:A:180:ILE:HD13	1.98	0.45
1:A:43:VAL:CG1	1:A:44:ILE:N	2.79	0.45
1:B:136:ARG:HH11	1:B:136:ARG:HG3	1.81	0.45
1:B:223:ARG:C	1:B:223:ARG:HE	2.18	0.45
1:C:274:VAL:HG23	1:C:274:VAL:O	2.17	0.45
1:D:215:LYS:NZ	1:D:251:ASN:ND2	2.64	0.45
1:D:228:GLY:HA3	1:D:285:PRO:HD2	1.97	0.45
1:A:107:GLN:CD	1:A:133:GLY:HA3	2.37	0.45
1:A:126:VAL:HG12	1:A:127:ILE:N	2.31	0.45
1:B:236:GLU:HB3	1:B:241:HIS:ND1	2.31	0.45
1:C:230:VAL:HA	1:C:280:CYS:O	2.15	0.45
1:A:163:PHE:HE1	1:C:45:PRO:HB3	1.82	0.45
1:D:89:VAL:HG22	1:D:99:THR:HG22	1.97	0.45
1:C:229:GLY:O	1:C:281:SER:HA	2.16	0.45
1:C:248:ILE:HG21	1:C:278:MSE:HG3	1.98	0.45
1:D:323:SER:O	1:D:326:LYS:N	2.49	0.45
1:C:324:PHE:CD1	1:C:325:ALA:N	2.84	0.45
1:D:155:MSE:HG3	1:D:159:VAL:HG23	1.98	0.45
1:D:60:HIS:CE1	1:D:271:PRO:HA	2.51	0.45
1:A:125:LEU:HB2	1:A:195:TYR:CE1	2.51	0.45
1:A:123:LYS:HG3	1:A:195:TYR:HD1	1.80	0.45
1:A:313:GLU:HG3	2:D:350:HOH:O	2.15	0.45
1:A:324:PHE:O	1:A:328:VAL:HG23	2.16	0.45
1:C:90:LEU:HB3	1:C:98:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:PHE:N	1:D:165:PRO:HD3	2.31	0.45
1:D:201:ASP:O	1:D:202:SER:O	2.34	0.45
1:A:148:ASP:OD1	1:A:177:ASN:HB3	2.15	0.45
1:A:192:GLU:HG2	2:A:424:HOH:O	2.15	0.45
1:A:307:LEU:N	1:A:307:LEU:HD12	2.31	0.45
1:A:313:GLU:HG3	2:D:351:HOH:O	2.15	0.45
1:B:139:ALA:HB1	1:B:175:ARG:HH21	1.81	0.45
1:C:264:TRP:CZ2	1:C:322:PRO:HD3	2.51	0.45
1:D:51:MSE:CA	1:D:55:TRP:HE1	2.29	0.45
1:A:159:VAL:HG13	1:A:163:PHE:HE2	1.81	0.45
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.80	0.45
1:A:115:LEU:CD2	1:A:199:ILE:HD11	2.43	0.45
1:A:54:MSE:CE	1:A:206:ILE:HD13	2.45	0.45
1:C:328:VAL:C	1:C:330:GLU:H	2.19	0.45
1:A:253:ARG:HH22	1:A:330:GLU:HB3	1.80	0.45
1:C:68:LEU:HB2	1:C:80:VAL:CG1	2.44	0.45
1:D:38:ALA:C	1:D:40:PHE:H	2.20	0.45
1:A:125:LEU:HD13	1:A:195:TYR:OH	2.16	0.45
1:B:111:THR:HG22	1:B:115:LEU:HD22	1.97	0.45
1:C:180:ILE:HD11	2:C:389:HOH:O	2.16	0.45
1:D:249:VAL:HG22	1:D:278:MSE:SE	2.67	0.45
1:A:125:LEU:HD13	1:A:186:PHE:CE1	2.52	0.45
1:A:109:MSE:HE3	1:A:314:ILE:HG13	1.98	0.45
1:D:249:VAL:HG11	1:D:329:ILE:HG23	1.97	0.45
1:A:129:GLY:HA3	1:A:149:MSE:HE1	1.98	0.45
1:B:239:TRP:CD2	1:C:268:PRO:HG2	2.51	0.45
1:C:104:CYS:O	1:C:108:GLU:HG3	2.17	0.45
1:D:52:SER:HB3	1:D:55:TRP:CE2	2.50	0.45
1:A:59:ALA:O	1:D:61:SER:HB2	2.17	0.45
1:A:135:LEU:CD2	1:A:149:MSE:HE2	2.20	0.45
1:B:327:LYS:HG2	1:B:327:LYS:O	2.16	0.45
1:C:128:GLY:O	1:C:129:GLY:C	2.54	0.45
1:A:131:ASP:HB2	1:A:167:VAL:CG1	2.46	0.45
1:B:54:MSE:HB3	1:B:55:TRP:CE3	2.51	0.45
1:C:328:VAL:C	1:C:330:GLU:H	2.20	0.45
1:B:113:LEU:HB2	1:B:114:PRO:CD	2.46	0.45
1:C:103:GLU:HB2	1:C:107:GLN:NE2	2.31	0.45
1:B:55:TRP:HB2	1:B:58:GLU:HG2	1.99	0.45
1:D:125:LEU:HB2	1:D:195:TYR:CE1	2.50	0.45
1:A:301:SER:O	1:A:302:LYS:C	2.54	0.45
1:C:248:ILE:O	1:C:278:MSE:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLN:HE22	1:C:43:VAL:N	2.14	0.45
1:D:151:GLU:HG2	1:D:157:VAL:CG2	2.46	0.45
1:A:253:ARG:HG3	1:A:253:ARG:HH11	1.81	0.45
1:C:151:GLU:O	1:C:180:ILE:HA	2.16	0.45
1:D:239:TRP:O	1:D:240:LEU:HD23	2.16	0.45
1:A:242:MSE:O	1:A:244:ILE:N	2.49	0.45
1:B:291:HIS:HA	1:B:292:PRO:HD2	1.84	0.45
1:C:292:PRO:C	1:C:293:LEU:HD12	2.36	0.45
1:A:133:GLY:C	1:A:135:LEU:N	2.69	0.45
1:C:149:MSE:HE2	1:C:171:TYR:CE1	2.51	0.45
1:C:151:GLU:OE1	1:C:152:ILE:N	2.49	0.45
1:D:321:LEU:HB3	1:D:322:PRO:HD2	1.98	0.45
1:B:163:PHE:C	1:B:165:PRO:HD3	2.37	0.45
1:A:154:LYS:HG2	1:A:158:ASP:OD2	2.16	0.45
1:B:240:LEU:HB2	1:B:241:HIS:CE1	2.52	0.45
1:C:152:ILE:HG12	1:C:152:ILE:O	2.17	0.45
1:C:279:LEU:HB3	1:C:289:PHE:CD1	2.52	0.45
1:A:163:PHE:HE1	1:C:45:PRO:HB3	1.82	0.45
1:B:109:MSE:HG3	1:B:265:THR:HG21	1.98	0.45
1:B:205:PRO:HB3	1:B:213:PHE:CD1	2.52	0.45
1:C:173:ASP:HB3	1:C:176:VAL:HG23	1.99	0.45
1:C:236:GLU:HG3	1:C:241:HIS:CD2	2.52	0.45
1:C:301:SER:CB	1:C:304:ASN:HD22	2.20	0.45
1:C:86:TYR:CD2	1:C:101:ARG:HD3	2.51	0.45
1:A:329:ILE:O	1:A:330:GLU:HB2	2.17	0.45
1:B:200:VAL:HG12	1:B:202:SER:H	1.81	0.45
1:B:223:ARG:NH2	2:B:369:HOH:O	2.50	0.45
1:B:113:LEU:O	1:B:315:HIS:HE1	1.99	0.45
1:A:215:LYS:HG2	1:A:255:ILE:CG1	2.46	0.45
1:B:161:LYS:HE2	2:B:412:HOH:O	2.16	0.45
1:C:215:LYS:N	1:C:216:PRO:CD	2.71	0.45
1:A:211:GLU:O	1:A:217:PHE:HB2	2.16	0.45
1:D:257:LYS:HB2	1:D:283:GLU:CB	2.39	0.45
1:A:129:GLY:HA3	1:A:171:TYR:OH	2.17	0.45
1:A:171:TYR:HE1	1:A:178:LEU:HD13	1.81	0.45
1:B:217:PHE:O	1:B:220:SER:HB3	2.17	0.45
1:D:52:SER:HB3	1:D:55:TRP:CE2	2.51	0.45
1:A:202:SER:O	1:A:234:GLN:NE2	2.49	0.45
1:A:308:LYS:O	1:D:324:PHE:HB3	2.17	0.45
1:C:328:VAL:C	1:C:330:GLU:N	2.70	0.45
1:D:138:VAL:O	1:D:141:HIS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ALA:HB2	1:D:278:MSE:HG2	1.98	0.45
1:B:239:TRP:CD2	1:C:268:PRO:HG2	2.52	0.45
1:D:99:THR:OG1	1:D:102:ASP:OD1	2.28	0.45
1:A:169:ILE:O	1:A:172:GLU:HB2	2.16	0.45
1:B:151:GLU:HG3	1:B:153:ASP:H	1.81	0.45
1:B:108:GLU:HG2	1:B:307:LEU:HD22	1.99	0.45
1:D:49:SER:HB2	1:D:51:MSE:HE2	1.99	0.45
1:B:52:SER:OG	1:B:54:MSE:SE	2.84	0.45
1:C:221:VAL:HG12	1:C:225:LEU:HD12	1.98	0.45
1:D:68:LEU:CD1	1:D:68:LEU:N	2.80	0.45
1:A:198:VAL:O	1:A:231:VAL:HG23	2.16	0.45
1:B:269:THR:HG22	1:B:269:THR:O	2.17	0.45
1:D:83:SER:OG	1:D:86:TYR:HB2	2.17	0.45
1:B:169:ILE:CG2	1:B:170:GLY:N	2.80	0.45
1:C:98:LEU:HD21	1:C:164:PHE:CE2	2.51	0.45
1:A:135:LEU:HD22	1:A:149:MSE:SE	2.67	0.45
1:B:233:THR:O	1:B:277:PHE:HA	2.17	0.45
1:C:222:ALA:HA	1:C:225:LEU:HD12	1.97	0.45
1:A:215:LYS:N	1:A:216:PRO:CD	2.79	0.45
1:B:240:LEU:HD23	1:C:101:ARG:NH2	2.31	0.45
1:D:324:PHE:CD1	1:D:324:PHE:C	2.90	0.45
1:A:236:GLU:HB3	1:A:241:HIS:NE2	2.31	0.45
1:D:65:GLU:HB3	1:D:82:GLN:O	2.16	0.45
1:C:53:PRO:O	1:C:56:PRO:HD3	2.16	0.45
1:D:171:TYR:O	1:D:173:ASP:N	2.48	0.45
1:A:215:LYS:HB2	1:A:251:ASN:ND2	2.32	0.45
1:A:54:MSE:HE1	1:A:206:ILE:HD13	1.98	0.45
1:D:111:THR:OG1	1:D:137:GLU:HB3	2.16	0.45
1:A:200:VAL:HG21	1:A:217:PHE:HZ	1.82	0.45
1:A:296:ILE:HD13	1:A:307:LEU:HD11	1.97	0.45
1:D:149:MSE:HG2	1:D:178:LEU:HD13	1.97	0.45
1:C:110:ILE:HG12	1:C:199:ILE:CG2	2.46	0.45
1:B:257:LYS:HE3	1:B:283:GLU:HB2	1.98	0.45
1:B:259:SER:O	1:B:280:CYS:HA	2.17	0.45
1:A:251:ASN:O	1:A:255:ILE:HG12	2.17	0.45
1:A:42:THR:HA	1:C:162:GLN:NE2	2.31	0.45
1:B:44:ILE:HD11	1:C:49:SER:CB	2.46	0.45
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.52	0.45
1:B:109:MSE:HE2	1:B:310:TYR:HB2	1.98	0.45
1:B:240:LEU:CD2	1:B:272:SER:HB2	2.46	0.45
1:B:51:MSE:HA	1:B:55:TRP:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:TRP:CZ2	1:C:322:PRO:HD3	2.52	0.45
1:D:232:CYS:HA	1:D:278:MSE:O	2.17	0.45
1:A:68:LEU:O	1:A:69:PHE:CB	2.64	0.45
1:A:82:GLN:HE22	1:A:87:GLY:HA2	1.82	0.45
1:B:324:PHE:C	1:B:324:PHE:CD1	2.90	0.45
1:B:225:LEU:HD22	1:B:229:GLY:HA3	1.99	0.45
1:C:54:MSE:HG3	2:C:480:HOH:O	2.15	0.45
1:A:101:ARG:NH2	1:D:239:TRP:O	2.49	0.45
1:A:208:PRO:C	1:A:210:LYS:H	2.20	0.45
1:A:215:LYS:HB2	1:A:251:ASN:ND2	2.32	0.45
1:A:257:LYS:NZ	2:A:566:HOH:O	2.50	0.45
1:A:329:ILE:O	1:A:329:ILE:HG22	2.16	0.45
1:C:55:TRP:HB2	1:C:240:LEU:HD13	1.97	0.45
1:B:47:TRP:HZ3	1:C:58:GLU:HA	1.81	0.45
1:D:256:PHE:HD1	1:D:282:THR:HG22	1.82	0.45
1:D:323:SER:OG	1:D:324:PHE:N	2.50	0.45
1:A:278:MSE:HE2	1:A:278:MSE:HA	1.98	0.45
1:B:136:ARG:HE	1:B:167:VAL:HA	1.82	0.45
1:C:85:THR:HG1	1:C:86:TYR:HD1	1.65	0.45
1:D:116:CYS:SG	1:D:296:ILE:HG13	2.56	0.45
1:D:65:GLU:HB3	1:D:82:GLN:O	2.16	0.45
1:B:252:CYS:HB3	1:B:280:CYS:SG	2.57	0.45
1:B:51:MSE:SE	2:B:377:HOH:O	2.85	0.45
1:A:45:PRO:HA	1:C:68:LEU:O	2.17	0.45
1:C:88:LYS:HB2	1:C:164:PHE:CE2	2.51	0.45
1:A:64:VAL:HG13	1:A:81:PHE:CD1	2.52	0.45
1:C:136:ARG:NH1	1:C:166:ASP:O	2.49	0.45
1:C:63:LYS:HB3	1:C:84:ALA:HB3	1.98	0.45
1:D:164:PHE:O	1:D:167:VAL:HG22	2.16	0.45
1:D:54:MSE:HE2	1:D:204:ASP:OD1	2.17	0.45
1:A:131:ASP:O	1:A:167:VAL:HG12	2.17	0.45
1:B:190:ALA:O	1:B:191:ALA:C	2.55	0.45
1:B:237:SER:HA	2:B:355:HOH:O	2.15	0.45
1:C:221:VAL:CG1	1:C:231:VAL:HG21	2.47	0.45
1:D:226:ARG:HG2	1:D:227:PRO:N	2.32	0.45
1:D:236:GLU:CB	1:D:241:HIS:HB2	2.44	0.45
1:A:267:VAL:HB	1:A:270:TYR:HD2	1.82	0.45
1:A:231:VAL:CG1	1:A:280:CYS:HB2	2.46	0.45
1:A:98:LEU:C	1:A:98:LEU:HD12	2.37	0.45
1:B:89:VAL:HG13	1:B:99:THR:HG22	1.97	0.45
1:D:231:VAL:HG21	1:D:256:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:SER:HB3	1:A:55:TRP:CE2	2.52	0.45
1:C:154:LYS:HG2	1:C:154:LYS:O	2.17	0.45
1:B:44:ILE:HG21	1:C:51:MSE:CE	2.47	0.45
1:A:57:GLY:O	1:D:62:LEU:HA	2.17	0.45
1:C:283:GLU:N	1:C:283:GLU:OE1	2.48	0.45
1:A:123:LYS:HG2	1:A:195:TYR:CD1	2.52	0.45
1:A:70:GLN:HG3	1:A:79:ILE:HG12	1.98	0.45
1:B:324:PHE:C	1:B:324:PHE:CD1	2.91	0.45
1:B:69:PHE:HB3	1:B:80:VAL:HB	1.98	0.45
1:A:73:SER:HA	1:A:155:MSE:SE	2.67	0.45
1:A:68:LEU:CD2	1:A:88:LYS:HZ3	2.29	0.45
1:B:169:ILE:O	1:B:169:ILE:HG13	2.16	0.45
1:B:271:PRO:HG2	2:B:348:HOH:O	2.16	0.45
1:C:225:LEU:HD11	1:C:231:VAL:CG2	2.47	0.45
1:D:313:GLU:H	1:D:313:GLU:CD	2.19	0.45
1:A:298:GLU:C	1:A:300:SER:H	2.20	0.45
1:A:171:TYR:CD1	1:A:178:LEU:HD22	2.52	0.45
1:A:255:ILE:HG22	1:A:256:PHE:N	2.31	0.45
1:B:167:VAL:C	1:B:169:ILE:N	2.70	0.45
1:B:267:VAL:HG11	1:B:270:TYR:CD2	2.50	0.45
1:A:238:LEU:CA	1:A:242:MSE:HE3	2.42	0.45
1:A:54:MSE:HE2	1:A:54:MSE:HA	1.99	0.45
1:C:125:LEU:HB2	1:C:195:TYR:CZ	2.52	0.45
1:B:173:ASP:O	1:B:175:ARG:N	2.50	0.45
1:C:238:LEU:O	1:C:242:MSE:HE3	2.17	0.45
1:A:66:LYS:NZ	1:A:66:LYS:HB2	2.32	0.45
1:B:87:GLY:HA3	1:B:100:GLU:HB2	1.99	0.45
1:A:55:TRP:CB	1:A:240:LEU:HD13	2.47	0.45
1:C:225:LEU:HD11	1:C:231:VAL:HG22	1.99	0.45
1:B:135:LEU:HA	1:B:135:LEU:HD23	1.81	0.45
1:B:49:SER:HA	1:B:61:SER:HA	1.99	0.45
1:B:50:GLU:CA	1:B:51:MSE:HE2	2.46	0.45
1:D:157:VAL:O	1:D:161:LYS:HG3	2.17	0.45
1:B:328:VAL:C	1:B:330:GLU:H	2.21	0.45
1:B:108:GLU:HG2	1:B:137:GLU:CD	2.38	0.45
1:B:204:ASP:O	1:B:206:ILE:N	2.50	0.45
1:B:50:GLU:C	1:B:51:MSE:HG3	2.37	0.45
1:B:79:ILE:HD12	1:B:79:ILE:H	1.81	0.45
1:B:125:LEU:HB2	1:B:195:TYR:CE1	2.52	0.44
1:B:244:ILE:HG13	2:B:433:HOH:O	2.17	0.44
1:B:259:SER:O	1:B:280:CYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:CD2	1:C:187:LEU:HD13	2.47	0.44
1:B:119:PRO:O	1:B:120:ASN:C	2.54	0.44
1:B:157:VAL:HG13	1:B:171:TYR:CZ	2.52	0.44
1:B:309:PHE:CE1	1:C:322:PRO:HB3	2.52	0.44
1:D:99:THR:OG1	1:D:102:ASP:OD1	2.30	0.44
2:A:376:HOH:O	1:D:327:LYS:HD3	2.17	0.44
1:A:132:GLY:C	1:A:135:LEU:HD13	2.36	0.44
1:A:144:ILE:HG22	1:A:175:ARG:HD2	1.98	0.44
1:B:288:ASP:HB3	2:B:395:HOH:O	2.16	0.44
1:C:184:VAL:HG12	1:C:212:LEU:CD2	2.46	0.44
1:C:238:LEU:HD11	1:C:321:LEU:HD22	1.98	0.44
1:B:206:ILE:HG23	1:B:207:GLY:N	2.32	0.44
1:A:197:ALA:HA	1:A:230:VAL:O	2.16	0.44
1:A:51:MSE:HE3	1:D:44:ILE:CD1	2.47	0.44
1:C:107:GLN:HG2	1:C:133:GLY:O	2.17	0.44
1:C:137:GLU:OE1	1:C:140:ARG:NE	2.50	0.44
1:A:79:ILE:HG22	1:A:80:VAL:N	2.31	0.44
1:B:169:ILE:HD12	1:B:172:GLU:HB2	1.99	0.44
1:B:69:PHE:HB2	1:B:163:PHE:CE2	2.52	0.44
1:C:324:PHE:CD1	1:C:325:ALA:N	2.85	0.44
1:D:135:LEU:HD22	1:D:147:ILE:HG21	1.98	0.44
1:B:275:ILE:HD12	1:B:275:ILE:HA	1.74	0.44
1:C:46:GLY:HA3	1:C:63:LYS:NZ	2.33	0.44
1:D:271:PRO:O	1:D:272:SER:OG	2.27	0.44
1:A:293:LEU:C	1:A:293:LEU:HD23	2.38	0.44
1:A:46:GLY:O	1:A:63:LYS:HD2	2.17	0.44
1:C:223:ARG:HA	2:C:477:HOH:O	2.16	0.44
1:B:123:LYS:HZ3	1:B:146:GLN:NE2	2.15	0.44
1:B:132:GLY:O	1:B:135:LEU:HB2	2.18	0.44
1:B:51:MSE:SE	2:C:530:HOH:O	2.85	0.44
1:C:82:GLN:HE22	1:C:88:LYS:N	2.15	0.44
1:D:129:GLY:CA	1:D:156:VAL:HG11	2.48	0.44
1:A:248:ILE:CG2	1:A:278:MSE:HG3	2.48	0.44
1:C:258:GLY:HA3	1:C:281:SER:OG	2.17	0.44
1:D:202:SER:HB2	1:D:213:PHE:CE1	2.51	0.44
1:B:205:PRO:HB2	1:B:210:LYS:HG3	1.98	0.44
1:B:234:GLN:HE22	1:B:236:GLU:CA	2.30	0.44
1:B:310:TYR:CD1	1:B:310:TYR:C	2.90	0.44
1:B:61:SER:O	1:C:59:ALA:N	2.45	0.44
1:C:214:GLU:CB	1:C:216:PRO:HD2	2.42	0.44
1:C:283:GLU:CD	1:C:283:GLU:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ASP:HB3	2:C:350:HOH:O	2.17	0.44
1:D:69:PHE:HZ	1:D:155:MSE:SE	2.50	0.44
1:C:241:HIS:HB3	1:C:244:ILE:HB	1.98	0.44
1:B:233:THR:O	1:B:277:PHE:HA	2.17	0.44
1:D:238:LEU:HD22	1:D:325:ALA:CB	2.39	0.44
1:A:288:ASP:CG	1:A:291:HIS:HD1	2.21	0.44
1:B:173:ASP:HB3	1:B:176:VAL:CG2	2.42	0.44
1:D:141:HIS:O	1:D:144:ILE:HG12	2.18	0.44
1:D:90:LEU:HB3	1:D:98:LEU:HG	1.98	0.44
1:A:98:LEU:HD22	1:A:103:GLU:OE1	2.17	0.44
1:A:324:PHE:CD1	1:A:325:ALA:N	2.86	0.44
1:B:205:PRO:HB3	1:B:213:PHE:CE1	2.52	0.44
1:D:169:ILE:HG23	1:D:170:GLY:N	2.33	0.44
1:A:83:SER:O	1:A:84:ALA:C	2.56	0.44
1:A:99:THR:O	1:A:103:GLU:HB3	2.17	0.44
1:B:191:ALA:O	1:B:223:ARG:NH2	2.50	0.44
1:B:296:ILE:HD12	1:B:307:LEU:HD11	2.00	0.44
1:C:140:ARG:NH2	1:C:304:ASN:HB2	2.32	0.44
1:A:135:LEU:CD1	1:A:135:LEU:H	2.28	0.44
1:B:70:GLN:HA	1:B:79:ILE:HG12	2.00	0.44
1:A:43:VAL:HG12	1:A:44:ILE:N	2.32	0.44
1:C:99:THR:HG22	1:C:102:ASP:OD1	2.17	0.44
1:C:198:VAL:HG23	1:C:225:LEU:HD21	1.98	0.44
1:C:233:THR:OG1	1:C:278:MSE:HB2	2.16	0.44
1:C:50:GLU:C	1:C:51:MSE:SE	3.05	0.44
1:A:329:ILE:O	1:A:330:GLU:HB2	2.17	0.44
1:C:296:ILE:HG22	2:C:344:HOH:O	2.16	0.44
1:C:68:LEU:CD1	1:C:88:LYS:HD3	2.47	0.44
1:A:70:GLN:HE22	1:C:79:ILE:HD13	1.82	0.44
1:A:108:GLU:HB3	1:A:112:HIS:HD2	1.82	0.44
1:A:129:GLY:C	1:A:131:ASP:N	2.71	0.44
1:A:298:GLU:C	1:A:300:SER:N	2.70	0.44
1:C:123:LYS:HD3	1:C:194:SER:O	2.17	0.44
1:C:165:PRO:HG2	2:C:452:HOH:O	2.18	0.44
1:C:328:VAL:O	1:C:330:GLU:N	2.51	0.44
1:C:76:GLN:OE1	1:C:92:LEU:HD13	2.16	0.44
1:D:118:ILE:HG13	1:D:121:PRO:HD3	2.00	0.44
1:C:259:SER:O	1:C:280:CYS:HA	2.17	0.44
1:D:245:ILE:O	1:D:249:VAL:HG23	2.17	0.44
1:A:98:LEU:C	1:A:98:LEU:HD12	2.37	0.44
1:A:243:ASP:OD2	1:A:244:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:VAL:HA	1:C:280:CYS:O	2.17	0.44
1:C:70:GLN:HE21	1:C:70:GLN:HB2	1.65	0.44
1:D:310:TYR:CG	1:D:311:ASN:N	2.86	0.44
1:A:72:LYS:HB3	1:C:51:MSE:HB2	2.00	0.44
1:B:214:GLU:HB2	2:B:429:HOH:O	2.17	0.44
1:C:193:GLY:N	1:C:224:ALA:HA	2.27	0.44
1:D:125:LEU:HD12	1:D:126:VAL:N	2.32	0.44
1:D:91:VAL:HG13	1:D:95:VAL:C	2.38	0.44
1:B:189:ASN:ND2	2:B:347:HOH:O	2.45	0.44
1:C:236:GLU:HG3	1:C:241:HIS:NE2	2.33	0.44
1:D:264:TRP:CZ2	1:D:322:PRO:HD3	2.52	0.44
1:A:241:HIS:HB3	1:A:244:ILE:HD12	1.98	0.44
1:A:119:PRO:HD3	1:A:293:LEU:CD2	2.48	0.44
1:A:73:SER:HA	1:A:155:MSE:HE3	2.00	0.44
1:A:78:VAL:HG12	1:A:80:VAL:HG22	2.00	0.44
1:A:68:LEU:HD22	1:A:88:LYS:NZ	2.32	0.44
1:C:80:VAL:HG21	1:C:159:VAL:CG1	2.47	0.44
1:C:164:PHE:HA	1:C:165:PRO:HD2	1.88	0.44
1:D:151:GLU:OE1	1:D:152:ILE:N	2.41	0.44
1:A:122:LYS:HE2	1:A:145:GLU:HG3	2.00	0.44
1:A:252:CYS:CB	1:A:278:MSE:SE	3.15	0.44
1:A:78:VAL:HG12	1:A:79:ILE:N	2.33	0.44
1:B:238:LEU:HD23	1:B:245:ILE:HD13	1.98	0.44
1:C:200:VAL:CB	1:C:233:THR:HG22	2.39	0.44
1:D:182:ASP:CG	1:D:183:GLY:H	2.21	0.44
1:D:236:GLU:HB3	2:D:413:HOH:O	2.18	0.44
1:C:296:ILE:HG23	1:C:300:SER:CB	2.41	0.44
1:B:149:MSE:O	1:B:179:VAL:HB	2.18	0.44
1:C:63:LYS:HG3	1:C:63:LYS:O	2.16	0.44
1:A:124:VAL:O	1:A:147:ILE:HA	2.17	0.44
1:B:231:VAL:HG22	1:B:232:CYS:H	1.81	0.44
1:B:314:ILE:HG13	1:C:322:PRO:HA	2.00	0.44
1:C:86:TYR:O	1:C:99:THR:HG22	2.17	0.44
1:A:171:TYR:HA	1:A:176:VAL:HG11	2.00	0.44
1:C:75:TYR:O	1:C:76:GLN:HB3	2.16	0.44
1:D:103:GLU:HG2	2:D:345:HOH:O	2.18	0.44
1:D:248:ILE:HG22	1:D:278:MSE:HG3	2.00	0.44
1:A:123:LYS:HD3	1:A:194:SER:O	2.16	0.44
1:A:202:SER:HB2	1:A:213:PHE:CE1	2.53	0.44
1:B:125:LEU:HD12	1:B:126:VAL:H	1.83	0.44
1:A:326:LYS:O	1:A:330:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLN:HG2	1:A:153:ASP:OD2	2.17	0.44
1:A:267:VAL:HG11	1:A:270:TYR:CE2	2.53	0.44
1:A:43:VAL:CG1	1:A:44:ILE:N	2.80	0.44
1:C:164:PHE:HA	1:C:165:PRO:HD2	1.81	0.44
1:D:161:LYS:HE2	2:D:357:HOH:O	2.16	0.44
1:D:228:GLY:CA	1:D:285:PRO:HD2	2.47	0.44
1:D:43:VAL:C	1:D:44:ILE:HG13	2.37	0.44
1:D:69:PHE:CD2	1:D:70:GLN:N	2.86	0.44
1:D:76:GLN:HB2	1:D:93:ASP:OD1	2.17	0.44
1:B:113:LEU:CD2	1:B:279:LEU:HD21	2.39	0.44
1:C:297:ASP:OD1	1:C:298:GLU:N	2.51	0.44
1:A:51:MSE:SE	1:C:72:LYS:H	2.51	0.44
1:D:60:HIS:CE1	1:D:271:PRO:HA	2.52	0.44
1:A:238:LEU:HD23	1:A:242:MSE:HE1	1.99	0.44
1:B:223:ARG:HD2	2:B:483:HOH:O	2.17	0.44
1:C:187:LEU:HD21	1:C:221:VAL:HG22	1.99	0.44
1:C:301:SER:HB3	1:C:304:ASN:HB2	1.98	0.44
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.52	0.44
1:D:44:ILE:HG23	1:D:45:PRO:HD2	1.99	0.44
1:A:157:VAL:CG1	1:A:161:LYS:HE3	2.47	0.44
1:A:90:LEU:HD21	1:A:92:LEU:HG	1.99	0.44
1:B:149:MSE:HE2	1:B:171:TYR:CE1	2.53	0.44
1:B:75:TYR:CE2	1:B:152:ILE:HG13	2.52	0.44
1:B:114:PRO:HB3	1:B:232:CYS:HB2	1.98	0.44
1:C:165:PRO:HD2	2:C:452:HOH:O	2.17	0.44
1:C:249:VAL:HG22	1:C:278:MSE:SE	2.68	0.44
1:A:301:SER:HB3	1:A:304:ASN:CG	2.37	0.44
1:C:257:LYS:HD2	1:C:257:LYS:HA	1.81	0.44
1:C:310:TYR:CD1	1:C:311:ASN:N	2.85	0.44
1:D:98:LEU:HD11	1:D:164:PHE:CE2	2.53	0.44
1:D:60:HIS:CD2	2:D:362:HOH:O	2.71	0.44
1:B:122:LYS:O	1:B:144:ILE:HG23	2.17	0.44
1:B:168:ALA:C	1:B:170:GLY:N	2.69	0.44
1:B:218:PHE:O	1:B:255:ILE:HG21	2.17	0.44
1:D:240:LEU:HD11	1:D:271:PRO:HB2	2.00	0.44
1:A:107:GLN:HG2	1:A:134:VAL:N	2.32	0.44
1:C:112:HIS:CE1	1:C:141:HIS:HE2	2.36	0.44
1:C:234:GLN:OE1	1:C:236:GLU:N	2.49	0.44
1:D:271:PRO:O	1:D:272:SER:CB	2.65	0.44
1:A:154:LYS:HG2	1:A:158:ASP:OD2	2.17	0.44
1:C:165:PRO:HG2	1:C:166:ASP:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ILE:O	1:C:249:VAL:HG23	2.18	0.44
1:C:310:TYR:CD1	1:C:311:ASN:N	2.85	0.44
1:C:86:TYR:CD2	1:C:101:ARG:HD3	2.52	0.44
1:A:104:CYS:O	1:A:108:GLU:HB2	2.17	0.44
1:A:81:PHE:O	1:A:88:LYS:HA	2.17	0.44
1:B:78:VAL:O	1:B:79:ILE:HG13	2.17	0.44
1:C:200:VAL:CB	1:C:233:THR:HG22	2.47	0.44
1:A:64:VAL:HG11	1:C:67:VAL:HG21	1.99	0.44
1:D:164:PHE:HB2	1:D:167:VAL:CG2	2.48	0.44
1:D:116:CYS:SG	1:D:296:ILE:HG13	2.58	0.44
1:D:60:HIS:CG	2:D:360:HOH:O	2.71	0.44
1:A:108:GLU:OE1	1:A:309:PHE:HB3	2.17	0.44
1:B:231:VAL:CG2	1:B:232:CYS:H	2.31	0.44
1:C:136:ARG:CZ	1:C:167:VAL:HG13	2.47	0.44
1:C:238:LEU:HD23	1:C:245:ILE:HD13	1.99	0.44
1:C:60:HIS:HE2	1:C:271:PRO:HA	1.82	0.44
1:C:86:TYR:HB3	1:C:99:THR:HG23	2.00	0.44
1:C:145:GLU:HG2	2:C:463:HOH:O	2.17	0.44
1:D:210:LYS:O	1:D:214:GLU:HG3	2.17	0.44
1:D:109:MSE:CE	1:D:265:THR:OG1	2.66	0.44
1:A:130:GLY:HA3	1:A:151:GLU:HG2	1.98	0.44
1:A:140:ARG:CD	1:A:296:ILE:HG21	2.48	0.44
1:A:238:LEU:CD1	1:A:322:PRO:HD2	2.48	0.44
1:C:193:GLY:HA2	1:C:225:LEU:C	2.38	0.44
1:D:162:GLN:NE2	2:D:389:HOH:O	2.50	0.44
1:A:245:ILE:O	1:A:248:ILE:HB	2.18	0.44
1:B:222:ALA:HB2	1:B:256:PHE:CE1	2.52	0.44
1:B:190:ALA:O	1:B:223:ARG:NH2	2.50	0.44
1:C:104:CYS:O	1:C:108:GLU:HG3	2.18	0.44
1:C:210:LYS:HE2	2:C:396:HOH:O	2.17	0.44
1:D:60:HIS:CE1	1:D:271:PRO:HA	2.52	0.44
1:A:311:ASN:CG	1:A:314:ILE:HD13	2.37	0.44
1:A:324:PHE:CE1	1:A:325:ALA:HB2	2.52	0.44
1:D:109:MSE:HG2	1:D:265:THR:HB	2.00	0.44
1:D:109:MSE:SE	1:D:309:PHE:HD2	2.51	0.44
1:A:125:LEU:HD12	1:A:148:ASP:OD2	2.17	0.44
1:D:200:VAL:HB	1:D:233:THR:CB	2.48	0.44
1:C:141:HIS:HB2	1:C:144:ILE:CG1	2.48	0.44
1:C:230:VAL:HG11	1:C:287:VAL:HG11	1.99	0.44
1:D:187:LEU:HD21	1:D:221:VAL:HG22	1.99	0.44
1:A:234:GLN:HE22	1:A:275:ILE:CD1	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HG13	1:A:277:PHE:CE1	2.53	0.44
1:B:206:ILE:HG23	1:B:207:GLY:N	2.33	0.44
1:C:287:VAL:HG11	1:C:289:PHE:CZ	2.52	0.44
1:D:138:VAL:C	1:D:140:ARG:H	2.21	0.44
1:A:328:VAL:C	1:A:330:GLU:H	2.21	0.44
1:A:73:SER:CA	1:A:155:MSE:SE	3.16	0.44
1:C:130:GLY:HA2	1:C:156:VAL:HG11	1.99	0.44
1:C:222:ALA:O	1:C:225:LEU:HB2	2.18	0.44
1:D:271:PRO:O	1:D:272:SER:CB	2.65	0.44
1:A:142:ALA:HB3	2:A:417:HOH:O	2.18	0.44
1:A:237:SER:H	1:A:241:HIS:HD2	1.66	0.44
1:C:328:VAL:C	1:C:330:GLU:H	2.20	0.44
1:D:245:ILE:O	1:D:249:VAL:HG23	2.18	0.44
1:A:115:LEU:C	1:A:117:SER:H	2.21	0.44
1:B:149:MSE:O	1:B:178:LEU:HA	2.18	0.44
1:B:238:LEU:O	1:B:242:MSE:SE	2.86	0.44
1:D:198:VAL:HG23	1:D:225:LEU:CD2	2.44	0.44
1:A:122:LYS:HE2	1:A:145:GLU:CD	2.39	0.44
1:A:202:SER:O	1:A:234:GLN:NE2	2.51	0.44
1:B:155:MSE:HE1	2:B:454:HOH:O	2.17	0.44
1:B:259:SER:O	1:B:281:SER:N	2.48	0.44
1:D:196:ASP:OD1	1:D:226:ARG:HD2	2.18	0.44
1:D:113:LEU:HA	1:D:315:HIS:CE1	2.52	0.44
1:B:164:PHE:HB2	1:B:167:VAL:HG22	1.99	0.44
1:A:122:LYS:HG2	1:A:145:GLU:CD	2.39	0.44
1:B:184:VAL:O	1:B:188:LYS:HB2	2.17	0.44
1:D:44:ILE:HG23	1:D:45:PRO:HD2	1.99	0.44
1:A:59:ALA:HB3	1:D:61:SER:HB2	2.00	0.44
1:A:50:GLU:C	1:A:51:MSE:SE	3.06	0.44
1:B:130:GLY:HA3	1:B:156:VAL:HG12	1.99	0.44
1:A:238:LEU:O	1:A:242:MSE:HG2	2.18	0.44
1:A:312:ALA:O	1:A:315:HIS:HB3	2.18	0.44
1:B:264:TRP:CZ3	1:B:274:VAL:HG11	2.52	0.44
1:C:275:ILE:HG13	1:C:276:GLY:N	2.32	0.44
1:D:114:PRO:HG2	1:D:115:LEU:H	1.83	0.44
1:D:164:PHE:HB2	1:D:167:VAL:CG2	2.48	0.44
1:A:129:GLY:O	1:A:131:ASP:N	2.51	0.44
1:B:99:THR:O	1:B:103:GLU:HG3	2.18	0.44
1:B:162:GLN:NE2	2:B:364:HOH:O	2.43	0.44
1:C:173:ASP:HB3	1:C:176:VAL:HG23	2.00	0.44
1:C:275:ILE:HA	1:C:275:ILE:HD12	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:HB3	1:D:163:PHE:CE1	2.53	0.44
1:A:186:PHE:O	1:A:190:ALA:HB2	2.18	0.44
1:A:270:TYR:HD2	1:A:275:ILE:HB	1.82	0.44
1:A:293:LEU:HD23	1:A:293:LEU:C	2.38	0.44
1:B:163:PHE:C	1:B:164:PHE:HD2	2.20	0.44
1:B:165:PRO:C	1:B:167:VAL:H	2.21	0.44
1:B:125:LEU:O	1:B:198:VAL:HA	2.18	0.44
1:B:278:MSE:O	1:B:279:LEU:O	2.35	0.44
1:B:307:LEU:HD13	1:B:310:TYR:CD1	2.51	0.44
1:D:125:LEU:HB2	1:D:195:TYR:CE1	2.52	0.44
1:D:248:ILE:CG2	1:D:278:MSE:HG3	2.48	0.44
1:A:97:GLN:O	1:A:98:LEU:HB3	2.18	0.43
1:D:323:SER:O	1:D:324:PHE:C	2.54	0.43
1:A:215:LYS:N	1:A:216:PRO:CD	2.81	0.43
1:A:129:GLY:C	1:A:131:ASP:N	2.72	0.43
1:B:130:GLY:HA3	1:B:151:GLU:CG	2.48	0.43
1:B:152:ILE:CG1	1:B:182:ASP:HA	2.47	0.43
1:B:49:SER:HA	1:B:61:SER:HA	1.98	0.43
1:C:193:GLY:HA2	1:C:226:ARG:N	2.33	0.43
1:C:266:SER:O	1:C:268:PRO:HD3	2.17	0.43
1:C:79:ILE:HG22	1:C:80:VAL:N	2.33	0.43
1:D:69:PHE:HE2	1:D:78:VAL:HB	1.82	0.43
1:A:155:MSE:HG2	2:A:344:HOH:O	2.18	0.43
1:A:264:TRP:CD1	1:A:321:LEU:HD23	2.53	0.43
1:C:149:MSE:O	1:C:178:LEU:HD12	2.18	0.43
1:C:171:TYR:CD1	1:C:178:LEU:HD22	2.52	0.43
1:B:51:MSE:CE	1:C:44:ILE:HD12	2.38	0.43
1:D:93:ASP:N	2:D:352:HOH:O	2.50	0.43
1:B:237:SER:HA	2:B:356:HOH:O	2.17	0.43
1:C:111:THR:O	1:C:115:LEU:HG	2.18	0.43
1:D:108:GLU:HB3	1:D:310:TYR:HB2	1.99	0.43
1:B:51:MSE:HE2	1:B:51:MSE:N	2.33	0.43
1:D:132:GLY:HA3	1:D:167:VAL:O	2.18	0.43
1:A:182:ASP:CG	2:A:354:HOH:O	2.56	0.43
1:C:329:ILE:HG22	1:C:329:ILE:O	2.17	0.43
1:C:86:TYR:CD2	1:C:99:THR:HG21	2.51	0.43
1:D:91:VAL:HG13	1:D:95:VAL:O	2.17	0.43
1:A:91:VAL:HG12	1:A:92:LEU:N	2.33	0.43
1:C:226:ARG:HB2	1:C:227:PRO:HD3	2.00	0.43
1:D:233:THR:HG22	1:D:234:GLN:O	2.18	0.43
1:C:159:VAL:HG13	1:C:163:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:PRO:HB3	1:D:232:CYS:HB2	2.00	0.43
1:D:271:PRO:O	1:D:272:SER:OG	2.29	0.43
1:A:103:GLU:HG3	1:A:104:CYS:N	2.33	0.43
1:A:164:PHE:HB2	1:A:167:VAL:HB	2.00	0.43
1:C:173:ASP:HA	1:C:174:PRO:HD3	1.91	0.43
1:B:200:VAL:HG21	1:B:217:PHE:HZ	1.84	0.43
1:B:223:ARG:CG	1:B:223:ARG:NH1	2.81	0.43
1:C:154:LYS:HD2	1:C:180:ILE:HG12	1.99	0.43
1:C:221:VAL:HG11	1:C:231:VAL:HG11	1.99	0.43
1:A:126:VAL:HG11	1:A:149:MSE:HE1	2.00	0.43
1:C:62:LEU:HD12	1:C:89:VAL:HG21	2.00	0.43
1:D:111:THR:OG1	1:D:112:HIS:N	2.51	0.43
1:D:264:TRP:CZ3	1:D:274:VAL:HG11	2.52	0.43
1:D:321:LEU:HD13	1:D:329:ILE:HD12	2.00	0.43
1:A:134:VAL:O	1:A:138:VAL:HG23	2.18	0.43
1:B:131:ASP:HA	1:B:160:SER:HB3	1.99	0.43
1:B:58:GLU:HA	1:C:61:SER:O	2.17	0.43
1:A:184:VAL:HG23	1:A:185:ALA:N	2.33	0.43
1:A:191:ALA:O	1:A:192:GLU:C	2.56	0.43
1:A:296:ILE:CG2	1:A:297:ASP:N	2.81	0.43
1:B:111:THR:HG23	1:B:138:VAL:HG22	2.00	0.43
1:B:266:SER:O	1:B:268:PRO:HD3	2.18	0.43
1:C:122:LYS:HB3	1:C:145:GLU:HG3	2.00	0.43
1:C:225:LEU:HD22	1:C:229:GLY:HA3	2.00	0.43
2:B:487:HOH:O	1:C:274:VAL:HG13	2.17	0.43
1:B:169:ILE:HG23	1:B:170:GLY:N	2.33	0.43
1:B:48:PHE:HE2	1:B:96:ILE:HD11	1.82	0.43
1:D:279:LEU:HD12	1:D:289:PHE:CE1	2.53	0.43
1:A:239:TRP:HD1	1:A:274:VAL:CG2	2.29	0.43
1:D:139:ALA:HB1	1:D:175:ARG:HH22	1.82	0.43
1:A:168:ALA:HA	1:A:171:TYR:CE2	2.53	0.43
1:A:191:ALA:HB3	1:A:194:SER:HB3	2.00	0.43
1:A:214:GLU:HB3	1:A:216:PRO:HD2	2.00	0.43
1:B:103:GLU:O	1:B:107:GLN:HG3	2.18	0.43
1:B:181:GLY:O	1:B:182:ASP:C	2.56	0.43
1:B:236:GLU:HB3	1:B:241:HIS:CE1	2.53	0.43
1:B:69:PHE:HB3	1:B:80:VAL:HB	2.00	0.43
1:D:271:PRO:O	1:D:272:SER:OG	2.29	0.43
1:A:313:GLU:HB2	1:D:326:LYS:HZ1	1.83	0.43
1:A:226:ARG:HB2	1:A:227:PRO:HD2	1.99	0.43
1:B:111:THR:O	1:B:115:LEU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:HG12	1:C:225:LEU:HD12	2.00	0.43
1:C:274:VAL:HG13	2:C:396:HOH:O	2.18	0.43
1:C:264:TRP:HA	1:C:276:GLY:HA2	2.00	0.43
1:C:289:PHE:HB3	1:C:319:PHE:CZ	2.54	0.43
1:C:68:LEU:HB2	1:C:80:VAL:O	2.17	0.43
1:D:82:GLN:NE2	1:D:83:SER:O	2.47	0.43
1:D:68:LEU:HD21	1:D:88:LYS:HZ3	1.82	0.43
1:A:86:TYR:O	1:A:99:THR:HG23	2.18	0.43
1:C:245:ILE:HA	1:C:248:ILE:HD12	2.00	0.43
1:A:66:LYS:HG2	1:A:67:VAL:N	2.33	0.43
1:D:136:ARG:HH11	1:D:136:ARG:HG2	1.83	0.43
1:A:46:GLY:O	1:A:63:LYS:HD2	2.18	0.43
1:A:91:VAL:O	1:A:92:LEU:HD23	2.17	0.43
1:D:244:ILE:O	1:D:248:ILE:HG13	2.18	0.43
1:C:176:VAL:HG12	1:C:177:ASN:N	2.32	0.43
1:D:149:MSE:HG2	1:D:178:LEU:HD13	1.99	0.43
1:A:178:LEU:HD12	1:A:179:VAL:N	2.30	0.43
1:A:197:ALA:HA	1:A:230:VAL:O	2.18	0.43
1:B:289:PHE:HB3	1:B:319:PHE:CZ	2.54	0.43
1:C:324:PHE:CD1	1:C:324:PHE:O	2.71	0.43
1:A:301:SER:O	1:A:304:ASN:N	2.46	0.43
1:B:212:LEU:HD22	1:B:217:PHE:CZ	2.53	0.43
1:B:99:THR:HG23	1:B:269:THR:HG21	2.01	0.43
1:C:200:VAL:CB	1:C:233:THR:HG22	2.45	0.43
1:C:242:MSE:HE1	1:C:329:ILE:CD1	2.44	0.43
1:D:145:GLU:O	1:D:175:ARG:HG2	2.18	0.43
1:D:248:ILE:CG2	1:D:278:MSE:HG3	2.48	0.43
1:A:323:SER:HB2	1:D:308:LYS:O	2.18	0.43
1:D:59:ALA:C	1:D:61:SER:H	2.20	0.43
1:A:110:ILE:HG23	1:A:111:THR:N	2.33	0.43
1:A:68:LEU:H	1:A:81:PHE:HA	1.83	0.43
1:C:123:LYS:HD2	2:C:479:HOH:O	2.18	0.43
1:C:310:TYR:CD1	1:C:311:ASN:N	2.86	0.43
1:D:191:ALA:HB3	1:D:194:SER:HB3	1.99	0.43
1:B:115:LEU:C	1:B:117:SER:H	2.22	0.43
1:A:258:GLY:HA3	1:A:281:SER:OG	2.17	0.43
1:A:67:VAL:CG2	1:C:64:VAL:HG11	2.39	0.43
1:A:234:GLN:HA	1:A:277:PHE:CD1	2.53	0.43
1:D:311:ASN:O	1:D:312:ALA:C	2.56	0.43
1:A:123:LYS:HG2	1:A:195:TYR:CD1	2.53	0.43
1:A:242:MSE:HE2	1:A:245:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:HG21	1:B:186:PHE:HE2	1.84	0.43
1:B:228:GLY:N	1:B:285:PRO:HD2	2.33	0.43
1:C:135:LEU:HD12	1:C:135:LEU:HA	1.88	0.43
1:C:164:PHE:HA	1:C:165:PRO:HD2	1.84	0.43
1:A:231:VAL:CG1	1:A:280:CYS:HB2	2.48	0.43
1:A:44:ILE:O	1:A:45:PRO:O	2.36	0.43
1:C:123:LYS:NZ	1:C:146:GLN:HG2	2.33	0.43
1:C:173:ASP:O	1:C:176:VAL:HG23	2.18	0.43
1:D:328:VAL:HG13	2:D:411:HOH:O	2.18	0.43
1:A:45:PRO:HA	1:C:68:LEU:O	2.18	0.43
1:D:148:ASP:OD2	1:D:195:TYR:HE1	2.01	0.43
1:A:262:TYR:OH	1:A:276:GLY:HA3	2.19	0.43
1:B:113:LEU:N	1:B:114:PRO:HD2	2.33	0.43
1:C:117:SER:O	1:C:118:ILE:HG23	2.18	0.43
1:D:106:TYR:CD1	1:D:275:ILE:HG21	2.54	0.43
1:D:311:ASN:OD1	1:D:312:ALA:N	2.51	0.43
1:A:113:LEU:N	1:A:114:PRO:CD	2.80	0.43
1:B:118:ILE:HG21	1:B:230:VAL:HG13	2.00	0.43
1:C:131:ASP:HB2	1:C:167:VAL:CG1	2.48	0.43
1:D:233:THR:O	1:D:277:PHE:HA	2.18	0.43
1:D:99:THR:CG2	1:D:269:THR:HG21	2.42	0.43
1:A:211:GLU:C	1:A:213:PHE:H	2.22	0.43
1:A:296:ILE:HG23	1:A:300:SER:HB2	2.00	0.43
1:C:294:ASN:O	1:C:294:ASN:CG	2.55	0.43
1:C:140:ARG:NH1	1:C:301:SER:HB2	2.33	0.43
1:D:278:MSE:HA	1:D:278:MSE:HE2	2.01	0.43
1:B:43:VAL:C	1:B:44:ILE:HG13	2.39	0.43
1:A:98:LEU:O	1:A:98:LEU:HD12	2.17	0.43
1:B:141:HIS:CE1	1:B:296:ILE:HD11	2.53	0.43
1:B:53:PRO:HD3	2:B:379:HOH:O	2.19	0.43
1:B:135:LEU:HD11	1:B:149:MSE:CG	2.42	0.43
1:C:152:ILE:HG23	1:C:153:ASP:N	2.34	0.43
1:A:86:TYR:HD2	1:A:99:THR:HG21	1.83	0.43
1:B:109:MSE:HG2	1:B:310:TYR:HB2	2.01	0.43
1:A:50:GLU:OE1	1:A:95:VAL:HA	2.18	0.43
1:C:103:GLU:O	1:C:107:GLN:HG3	2.18	0.43
1:A:252:CYS:HB3	1:A:280:CYS:HG	1.77	0.43
1:A:299:SER:C	1:A:301:SER:H	2.21	0.43
1:C:266:SER:O	1:C:267:VAL:HG23	2.18	0.43
1:D:324:PHE:C	1:D:324:PHE:CD1	2.92	0.43
1:D:69:PHE:O	1:D:79:ILE:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:SER:CB	1:A:287:VAL:HB	2.49	0.43
1:A:227:PRO:C	1:A:285:PRO:HD2	2.39	0.43
1:D:60:HIS:HE1	1:D:269:THR:C	2.21	0.43
1:B:67:VAL:HA	1:B:81:PHE:HA	2.00	0.43
1:B:48:PHE:CE2	1:B:96:ILE:HD11	2.53	0.43
1:C:253:ARG:NH2	1:C:330:GLU:HB2	2.15	0.43
1:A:125:LEU:HD23	1:A:125:LEU:O	2.19	0.43
1:A:293:LEU:HD23	1:A:293:LEU:C	2.39	0.43
1:C:306:PRO:HB2	2:C:547:HOH:O	2.19	0.43
1:C:311:ASN:OD1	1:C:313:GLU:N	2.33	0.43
1:C:238:LEU:HD11	1:C:321:LEU:HD22	2.00	0.43
1:C:60:HIS:NE2	1:C:271:PRO:HA	2.33	0.43
1:A:206:ILE:O	1:A:206:ILE:HG13	2.17	0.43
1:A:262:TYR:OH	1:A:276:GLY:HA3	2.18	0.43
1:A:270:TYR:HB3	1:A:271:PRO:HD2	2.01	0.43
1:A:98:LEU:C	1:A:98:LEU:HD12	2.39	0.43
1:C:290:LYS:NZ	2:C:349:HOH:O	2.52	0.43
1:D:48:PHE:HB2	1:D:64:VAL:CG2	2.47	0.43
1:D:65:GLU:O	1:D:66:LYS:HB2	2.18	0.43
1:A:106:TYR:HE2	1:A:201:ASP:OD2	2.01	0.43
1:A:244:ILE:HG22	1:A:248:ILE:HD11	2.01	0.43
1:B:113:LEU:HD12	1:B:279:LEU:HG	1.99	0.43
1:B:163:PHE:O	1:B:165:PRO:HD3	2.19	0.43
1:D:246:GLU:HB2	1:D:328:VAL:HG11	2.00	0.43
1:D:60:HIS:HE1	1:D:272:SER:H	1.65	0.43
1:A:161:LYS:HA	1:A:168:ALA:HB1	2.00	0.43
1:B:218:PHE:C	1:B:255:ILE:HG21	2.39	0.43
1:C:295:PRO:HB3	1:C:310:TYR:OH	2.18	0.43
1:D:218:PHE:CE2	1:D:252:CYS:SG	3.12	0.43
1:A:328:VAL:O	1:A:328:VAL:HG12	2.18	0.43
1:A:50:GLU:HG3	1:A:95:VAL:HA	2.01	0.43
1:B:134:VAL:O	1:B:138:VAL:HG23	2.18	0.43
1:D:203:SER:HA	1:D:234:GLN:OE1	2.19	0.43
1:D:310:TYR:C	1:D:310:TYR:CD1	2.91	0.43
1:C:204:ASP:C	1:C:206:ILE:H	2.22	0.43
1:A:184:VAL:O	1:A:188:LYS:HG3	2.18	0.43
1:A:238:LEU:HD11	1:A:321:LEU:HD22	2.00	0.43
1:A:236:GLU:HB3	1:A:241:HIS:HB2	2.01	0.43
1:B:263:ALA:O	1:B:277:PHE:N	2.50	0.43
1:B:136:ARG:HB3	1:B:136:ARG:NH1	2.33	0.43
1:B:150:CYS:SG	1:B:186:PHE:HB2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:THR:HG21	1:B:269:THR:HG21	2.01	0.43
1:C:243:ASP:CG	1:C:244:ILE:H	2.22	0.43
1:B:103:GLU:OE1	1:B:167:VAL:HG11	2.18	0.43
1:C:200:VAL:HB	1:C:233:THR:HG22	2.00	0.43
1:C:231:VAL:HG21	1:C:256:PHE:CZ	2.53	0.43
1:D:114:PRO:HG2	1:D:115:LEU:HD13	1.99	0.43
1:A:288:ASP:OD1	1:A:290:LYS:HB2	2.19	0.43
1:B:205:PRO:HB3	1:B:213:PHE:CD1	2.54	0.43
1:C:49:SER:HB2	1:C:51:MSE:SE	2.68	0.43
1:D:60:HIS:CE1	1:D:271:PRO:HA	2.54	0.43
1:A:140:ARG:HD3	1:A:296:ILE:HG21	1.99	0.43
1:D:128:GLY:C	1:D:130:GLY:N	2.72	0.43
1:B:173:ASP:OD2	1:B:175:ARG:NH2	2.49	0.43
1:A:107:GLN:HB3	1:A:137:GLU:HG3	2.00	0.43
1:A:249:VAL:HA	1:A:278:MSE:CE	2.47	0.43
1:B:113:LEU:N	1:B:114:PRO:HD2	2.34	0.43
1:B:151:GLU:O	1:B:180:ILE:HA	2.19	0.43
1:C:128:GLY:N	1:C:149:MSE:SE	3.02	0.43
1:C:89:VAL:HG12	1:C:90:LEU:N	2.33	0.43
1:D:198:VAL:HG23	1:D:225:LEU:CD2	2.47	0.43
1:A:54:MSE:HB3	1:A:55:TRP:CE3	2.54	0.43
1:A:109:MSE:SE	1:A:309:PHE:CE1	3.22	0.43
1:C:60:HIS:HE2	1:C:270:TYR:C	2.22	0.43
1:D:144:ILE:HG21	1:D:147:ILE:HG12	2.01	0.43
1:A:129:GLY:O	1:A:131:ASP:N	2.52	0.43
1:A:141:HIS:HB2	1:A:144:ILE:HG12	2.00	0.43
1:C:151:GLU:HG3	1:C:153:ASP:H	1.84	0.43
1:C:48:PHE:O	1:C:61:SER:HA	2.18	0.43
1:D:111:THR:HA	1:D:199:ILE:HD13	2.00	0.43
1:D:115:LEU:N	1:D:115:LEU:HD12	2.34	0.43
1:A:226:ARG:NH1	2:A:412:HOH:O	2.52	0.43
1:B:184:VAL:HA	1:B:217:PHE:CD1	2.54	0.43
1:C:242:MSE:SE	1:C:329:ILE:HG13	2.69	0.43
1:C:48:PHE:O	1:C:61:SER:HA	2.19	0.43
1:D:115:LEU:HD23	1:D:141:HIS:CD2	2.54	0.43
1:D:288:ASP:OD2	1:D:291:HIS:ND1	2.52	0.43
1:B:51:MSE:HG3	1:B:59:ALA:HB1	2.01	0.43
1:D:125:LEU:HD21	1:D:127:ILE:HD11	2.01	0.43
1:D:221:VAL:HG11	1:D:231:VAL:HG13	2.01	0.43
1:D:232:CYS:HA	1:D:278:MSE:O	2.18	0.43
1:C:162:GLN:CG	2:C:467:HOH:O	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:GLU:HA	2:D:370:HOH:O	2.19	0.43
1:D:218:PHE:C	1:D:255:ILE:HG21	2.40	0.43
1:B:173:ASP:HB3	1:B:176:VAL:HG23	2.01	0.43
1:B:188:LYS:HD3	2:B:421:HOH:O	2.18	0.43
1:D:154:LYS:HA	1:D:157:VAL:CG2	2.48	0.43
1:B:135:LEU:HD21	1:B:149:MSE:CG	2.49	0.43
1:A:310:TYR:CD1	1:A:311:ASN:N	2.87	0.43
1:B:270:TYR:O	1:B:271:PRO:C	2.57	0.43
1:D:130:GLY:CA	2:D:553:HOH:O	2.60	0.43
1:D:242:MSE:HE1	1:D:324:PHE:O	2.19	0.43
1:D:242:MSE:HE1	1:D:325:ALA:HA	2.00	0.43
1:A:122:LYS:HE2	1:A:145:GLU:OE1	2.18	0.43
1:D:236:GLU:HB3	2:D:409:HOH:O	2.19	0.43
1:D:262:TYR:CZ	1:D:276:GLY:HA3	2.54	0.43
1:B:109:MSE:HE2	1:B:113:LEU:CG	2.49	0.43
1:C:173:ASP:HB3	1:C:176:VAL:CG2	2.49	0.43
1:D:56:PRO:HG2	2:D:347:HOH:O	2.19	0.43
1:A:329:ILE:O	1:A:329:ILE:HG23	2.19	0.43
1:A:54:MSE:HB3	1:A:55:TRP:CE3	2.54	0.43
1:C:259:SER:O	1:C:280:CYS:HA	2.18	0.43
1:C:76:GLN:HB2	1:C:93:ASP:CG	2.39	0.43
1:D:291:HIS:HA	1:D:292:PRO:HD2	1.93	0.43
1:A:324:PHE:CD1	1:A:324:PHE:C	2.92	0.43
1:B:231:VAL:CG2	1:B:232:CYS:N	2.82	0.43
1:B:251:ASN:O	1:B:254:GLU:N	2.46	0.43
1:A:109:MSE:SE	1:A:310:TYR:HD2	2.52	0.43
1:B:122:LYS:HD3	1:B:145:GLU:OE2	2.19	0.43
1:B:179:VAL:HG21	1:B:186:PHE:CE2	2.53	0.43
1:D:88:LYS:HB2	1:D:164:PHE:HE2	1.84	0.43
1:C:112:HIS:HB3	1:C:116:CYS:SG	2.58	0.42
1:C:98:LEU:HD22	1:C:131:ASP:OD1	2.18	0.42
1:C:152:ILE:HD12	1:C:182:ASP:CA	2.49	0.42
1:C:69:PHE:C	1:C:69:PHE:CD1	2.91	0.42
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.84	0.42
1:A:301:SER:C	1:A:303:SER:N	2.72	0.42
1:B:200:VAL:HG12	1:B:202:SER:N	2.34	0.42
1:D:291:HIS:HA	1:D:292:PRO:HD2	1.87	0.42
1:B:323:SER:O	1:B:325:ALA:N	2.52	0.42
1:A:324:PHE:CD1	1:A:325:ALA:N	2.87	0.42
1:A:242:MSE:SE	1:A:325:ALA:HA	2.69	0.42
1:B:263:ALA:HA	1:B:318:ALA:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLU:O	1:B:276:GLY:N	2.52	0.42
1:A:235:ALA:HB2	1:A:278:MSE:HG2	2.00	0.42
1:D:102:ASP:OD2	1:D:269:THR:HG23	2.18	0.42
1:B:257:LYS:HE3	1:B:283:GLU:HB2	2.00	0.42
1:C:173:ASP:HA	1:C:174:PRO:HD3	1.86	0.42
1:C:203:SER:H	1:C:209:ALA:CB	2.32	0.42
1:A:310:TYR:C	1:A:310:TYR:CD1	2.92	0.42
1:C:80:VAL:HG21	1:C:159:VAL:HG12	2.00	0.42
1:B:309:PHE:CZ	1:C:322:PRO:HB3	2.54	0.42
1:B:63:LYS:HB2	1:C:57:GLY:HA2	2.01	0.42
1:C:72:LYS:HA	1:C:77:ASP:HA	2.01	0.42
1:A:43:VAL:HG13	1:D:43:VAL:C	2.38	0.42
1:A:67:VAL:O	1:C:46:GLY:HA2	2.18	0.42
1:B:167:VAL:C	1:B:169:ILE:N	2.72	0.42
1:B:169:ILE:CG2	1:B:170:GLY:N	2.82	0.42
1:A:184:VAL:HG23	1:A:185:ALA:N	2.34	0.42
1:B:267:VAL:HG11	1:B:270:TYR:CE2	2.54	0.42
1:C:234:GLN:C	1:C:234:GLN:NE2	2.72	0.42
1:C:112:HIS:O	1:C:116:CYS:HB2	2.18	0.42
1:C:185:ALA:C	1:C:187:LEU:H	2.22	0.42
1:A:132:GLY:CA	1:A:149:MSE:HE1	2.47	0.42
1:B:210:LYS:NZ	1:B:214:GLU:OE2	2.52	0.42
1:B:310:TYR:CD1	1:B:310:TYR:C	2.91	0.42
1:C:129:GLY:HA3	1:C:151:GLU:HB2	2.00	0.42
1:C:166:ASP:HA	1:C:169:ILE:CG2	2.48	0.42
1:D:182:ASP:OD2	1:D:184:VAL:HB	2.19	0.42
1:D:217:PHE:O	1:D:220:SER:HB3	2.19	0.42
1:D:326:LYS:NZ	2:D:350:HOH:O	2.52	0.42
1:D:48:PHE:HE2	1:D:96:ILE:HG12	1.83	0.42
1:B:184:VAL:HG23	1:B:217:PHE:HD1	1.84	0.42
1:A:249:VAL:O	1:A:252:CYS:HB2	2.18	0.42
1:A:298:GLU:C	1:A:300:SER:N	2.72	0.42
1:B:240:LEU:O	2:B:481:HOH:O	2.21	0.42
1:C:324:PHE:O	1:C:327:LYS:HG2	2.19	0.42
1:C:55:TRP:CE3	1:C:271:PRO:HG3	2.54	0.42
1:D:169:ILE:HG23	1:D:170:GLY:N	2.34	0.42
1:D:124:VAL:HG22	1:D:197:ALA:HB3	2.01	0.42
1:A:211:GLU:HA	1:A:214:GLU:CG	2.49	0.42
1:A:212:LEU:HD12	1:A:212:LEU:H	1.83	0.42
1:A:68:LEU:HD13	1:A:163:PHE:CD1	2.53	0.42
1:A:70:GLN:HE22	1:C:70:GLN:NE2	2.04	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:O	1:A:93:ASP:C	2.58	0.42
1:B:45:PRO:HD3	1:C:43:VAL:HG21	2.01	0.42
1:A:55:TRP:HB3	1:A:240:LEU:HD13	2.01	0.42
1:A:98:LEU:C	1:A:98:LEU:HD12	2.40	0.42
1:C:129:GLY:O	1:C:131:ASP:N	2.44	0.42
1:A:131:ASP:OD2	1:A:132:GLY:N	2.53	0.42
1:B:313:GLU:CD	1:B:313:GLU:H	2.23	0.42
1:C:198:VAL:HG23	1:C:225:LEU:HD21	2.00	0.42
1:D:114:PRO:HG2	1:D:115:LEU:H	1.83	0.42
1:D:162:GLN:NE2	2:D:385:HOH:O	2.52	0.42
1:A:226:ARG:HH21	1:A:226:ARG:HG2	1.84	0.42
1:A:52:SER:OG	1:A:54:MSE:HB2	2.20	0.42
1:B:205:PRO:HB3	1:B:213:PHE:CD1	2.54	0.42
1:D:105:ALA:HA	1:D:309:PHE:CG	2.54	0.42
1:B:134:VAL:O	1:B:138:VAL:N	2.37	0.42
1:B:228:GLY:N	1:B:285:PRO:HD2	2.34	0.42
1:C:240:LEU:HD11	1:C:272:SER:HB3	2.00	0.42
1:D:88:LYS:HG2	1:D:163:PHE:O	2.19	0.42
1:D:269:THR:HG22	1:D:269:THR:O	2.19	0.42
1:A:70:GLN:HE22	1:C:70:GLN:NE2	2.16	0.42
1:C:116:CYS:SG	1:C:295:PRO:HA	2.59	0.42
1:D:111:THR:O	1:D:114:PRO:HG2	2.20	0.42
1:D:125:LEU:HD12	1:D:126:VAL:H	1.85	0.42
1:D:65:GLU:HB3	1:D:82:GLN:O	2.18	0.42
1:A:160:SER:O	1:A:164:PHE:HD2	2.02	0.42
1:A:144:ILE:O	1:A:175:ARG:HD2	2.19	0.42
1:A:208:PRO:CG	2:A:401:HOH:O	2.67	0.42
1:D:279:LEU:HD12	1:D:289:PHE:CE1	2.55	0.42
1:A:48:PHE:O	1:A:61:SER:HA	2.19	0.42
1:C:193:GLY:HA2	1:C:225:LEU:O	2.19	0.42
1:D:42:THR:HB	1:D:47:TRP:O	2.19	0.42
1:D:52:SER:O	1:D:54:MSE:N	2.52	0.42
1:A:125:LEU:HD12	1:A:148:ASP:HB2	2.01	0.42
1:C:169:ILE:HG12	2:C:460:HOH:O	2.19	0.42
1:C:289:PHE:HB3	1:C:319:PHE:CZ	2.55	0.42
1:C:324:PHE:CD1	1:C:325:ALA:N	2.87	0.42
1:D:88:LYS:O	1:D:99:THR:HA	2.18	0.42
1:C:157:VAL:HG13	1:C:171:TYR:CZ	2.54	0.42
1:C:252:CYS:SG	1:C:278:MSE:HE3	2.59	0.42
1:D:265:THR:HG23	1:D:267:VAL:HG23	2.02	0.42
1:A:164:PHE:HB3	1:A:167:VAL:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:HB2	1:A:319:PHE:CE1	2.54	0.42
1:B:238:LEU:HD22	1:B:242:MSE:SE	2.69	0.42
1:B:240:LEU:CD1	1:B:272:SER:HB2	2.47	0.42
1:D:135:LEU:HD12	1:D:171:TYR:CD1	2.55	0.42
1:D:152:ILE:CG2	1:D:153:ASP:N	2.82	0.42
1:D:65:GLU:HB3	1:D:82:GLN:O	2.19	0.42
1:A:99:THR:CG2	1:A:101:ARG:H	2.32	0.42
1:A:157:VAL:HG12	1:A:161:LYS:HE3	2.02	0.42
1:D:111:THR:OG1	1:D:137:GLU:HB3	2.20	0.42
1:D:129:GLY:O	1:D:130:GLY:O	2.37	0.42
1:D:169:ILE:HA	1:D:172:GLU:OE1	2.20	0.42
1:A:288:ASP:C	1:A:290:LYS:N	2.73	0.42
1:C:125:LEU:HB2	1:C:195:TYR:CE1	2.54	0.42
1:C:267:VAL:HG11	1:C:270:TYR:CD2	2.54	0.42
1:D:225:LEU:HD22	1:D:229:GLY:CA	2.50	0.42
1:A:75:TYR:CZ	1:A:152:ILE:HG12	2.54	0.42
1:A:310:TYR:CD1	1:A:311:ASN:N	2.88	0.42
1:C:121:PRO:O	1:C:144:ILE:HD13	2.20	0.42
1:D:162:GLN:NE2	2:D:387:HOH:O	2.52	0.42
1:D:259:SER:O	1:D:280:CYS:HA	2.19	0.42
1:D:48:PHE:HE2	1:D:50:GLU:HB2	1.84	0.42
1:A:55:TRP:HZ3	1:A:204:ASP:OD2	2.02	0.42
1:C:238:LEU:HA	1:C:242:MSE:CE	2.49	0.42
1:D:131:ASP:C	1:D:167:VAL:HB	2.40	0.42
1:D:138:VAL:HG12	1:D:144:ILE:HG13	2.01	0.42
1:A:69:PHE:CE2	1:B:45:PRO:HD3	2.54	0.42
1:B:264:TRP:CZ3	1:B:274:VAL:HG11	2.54	0.42
1:C:129:GLY:N	1:C:151:GLU:HB2	2.34	0.42
1:C:219:GLN:HB2	1:C:255:ILE:HD12	2.01	0.42
1:A:261:ASN:ND2	1:A:289:PHE:HD2	2.15	0.42
1:B:223:ARG:NH1	2:B:480:HOH:O	2.52	0.42
1:B:140:ARG:NE	1:B:307:LEU:HD21	2.35	0.42
1:C:114:PRO:HG2	1:C:115:LEU:H	1.83	0.42
1:C:257:LYS:HE2	2:C:368:HOH:O	2.19	0.42
1:A:223:ARG:HG3	1:A:224:ALA:N	2.35	0.42
1:B:124:VAL:HG23	1:B:144:ILE:HD12	2.00	0.42
1:B:52:SER:C	1:B:54:MSE:N	2.73	0.42
1:C:232:CYS:HA	1:C:278:MSE:O	2.20	0.42
1:B:43:VAL:CA	1:C:43:VAL:HG13	2.46	0.42
1:A:80:VAL:HG21	1:A:159:VAL:HG12	2.01	0.42
1:A:43:VAL:HG12	1:A:44:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLU:OE1	1:C:167:VAL:HG21	2.20	0.42
1:D:131:ASP:HA	1:D:160:SER:CB	2.50	0.42
1:D:45:PRO:O	1:D:47:TRP:HD1	2.02	0.42
1:A:169:ILE:HG23	1:A:170:GLY:N	2.34	0.42
1:B:326:LYS:O	1:B:327:LYS:C	2.57	0.42
1:B:95:VAL:HG21	1:B:204:ASP:OD2	2.19	0.42
1:C:225:LEU:HD22	1:C:229:GLY:HA3	2.01	0.42
1:B:122:LYS:HD3	1:B:145:GLU:OE2	2.19	0.42
1:B:165:PRO:C	1:B:167:VAL:H	2.23	0.42
1:C:43:VAL:CG1	1:C:44:ILE:N	2.82	0.42
1:A:262:TYR:C	1:A:262:TYR:CD1	2.93	0.42
1:B:107:GLN:HG2	1:B:133:GLY:C	2.40	0.42
1:B:326:LYS:O	1:B:330:GLU:HG2	2.20	0.42
1:C:146:GLN:HG2	1:C:147:ILE:N	2.34	0.42
1:C:215:LYS:N	1:C:216:PRO:CD	2.82	0.42
1:C:236:GLU:O	1:C:276:GLY:N	2.53	0.42
1:C:310:TYR:CD1	1:C:311:ASN:N	2.88	0.42
1:C:322:PRO:O	1:C:324:PHE:N	2.52	0.42
1:D:47:TRP:CE2	1:D:63:LYS:HB2	2.54	0.42
1:A:73:SER:C	1:A:75:TYR:H	2.21	0.42
1:C:148:ASP:OD1	1:C:177:ASN:HB3	2.20	0.42
1:C:198:VAL:HG11	1:C:221:VAL:HG13	2.01	0.42
1:C:226:ARG:HG3	1:C:227:PRO:N	2.35	0.42
1:D:109:MSE:SE	1:D:310:TYR:HD2	2.53	0.42
1:D:321:LEU:HD13	1:D:329:ILE:HD12	2.01	0.42
1:B:310:TYR:C	1:B:310:TYR:CD1	2.92	0.42
1:A:310:TYR:HA	1:A:314:ILE:HG21	2.02	0.42
1:B:249:VAL:HG22	1:B:278:MSE:HE3	2.02	0.42
1:D:310:TYR:CD1	1:D:310:TYR:C	2.93	0.42
1:D:96:ILE:HG21	1:D:269:THR:HG22	2.02	0.42
1:A:264:TRP:CD1	1:A:321:LEU:HD23	2.54	0.42
1:A:92:LEU:O	1:A:93:ASP:C	2.57	0.42
1:A:151:GLU:HG2	1:A:157:VAL:CG2	2.50	0.42
1:A:90:LEU:HD22	1:A:97:GLN:HB3	2.01	0.42
1:B:105:ALA:O	1:B:108:GLU:N	2.53	0.42
1:B:131:ASP:N	1:B:171:TYR:OH	2.53	0.42
1:B:167:VAL:C	1:B:169:ILE:N	2.72	0.42
1:C:107:GLN:NE2	1:C:133:GLY:HA3	2.35	0.42
1:A:47:TRP:HZ3	1:D:58:GLU:N	2.18	0.42
1:A:103:GLU:HB2	1:A:107:GLN:NE2	2.35	0.42
1:A:226:ARG:HB2	1:A:227:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLY:O	1:C:136:ARG:HB3	2.19	0.42
1:A:173:ASP:HB3	1:A:176:VAL:CG2	2.47	0.42
1:D:221:VAL:CG1	1:D:231:VAL:HG21	2.50	0.42
1:D:311:ASN:O	1:D:314:ILE:N	2.52	0.42
1:D:97:GLN:HA	1:D:97:GLN:OE1	2.20	0.42
1:A:88:LYS:N	1:A:100:GLU:OE1	2.45	0.42
1:A:122:LYS:HE2	1:A:145:GLU:OE1	2.19	0.42
1:A:232:CYS:HA	1:A:278:MSE:O	2.20	0.42
1:A:77:ASP:HB2	1:A:93:ASP:CA	2.39	0.42
1:C:52:SER:HB3	1:C:55:TRP:CE2	2.55	0.42
1:D:239:TRP:O	1:D:240:LEU:HD23	2.20	0.42
1:A:171:TYR:CD1	1:A:178:LEU:HD22	2.55	0.42
1:C:279:LEU:HB3	1:C:289:PHE:CG	2.54	0.42
1:A:279:LEU:HB3	1:A:289:PHE:CE2	2.55	0.42
1:A:297:ASP:CG	1:A:298:GLU:N	2.72	0.42
1:C:141:HIS:HB2	1:C:144:ILE:HG12	2.01	0.42
1:C:73:SER:CB	1:C:155:MSE:SE	3.12	0.42
1:C:252:CYS:HB2	1:C:278:MSE:HE3	2.01	0.42
1:C:87:GLY:O	1:C:88:LYS:C	2.56	0.42
1:D:288:ASP:OD1	1:D:291:HIS:N	2.52	0.42
1:C:297:ASP:OD1	1:C:298:GLU:N	2.35	0.42
1:A:277:PHE:HB3	1:A:279:LEU:HD22	2.02	0.42
1:A:43:VAL:O	1:A:45:PRO:HD3	2.19	0.42
1:B:118:ILE:HD13	1:B:230:VAL:HG22	2.02	0.42
1:C:129:GLY:CA	1:C:151:GLU:HB2	2.49	0.42
1:D:52:SER:HB3	1:D:55:TRP:CE2	2.55	0.42
1:D:63:LYS:HG2	1:D:84:ALA:HB2	2.02	0.42
1:A:245:ILE:O	1:A:249:VAL:HG23	2.19	0.42
1:A:297:ASP:H	1:A:300:SER:HB3	1.84	0.42
1:A:57:GLY:O	1:A:58:GLU:O	2.37	0.42
1:D:264:TRP:CZ3	1:D:274:VAL:HG21	2.55	0.42
1:A:99:THR:HG22	1:A:101:ARG:N	2.35	0.42
1:B:267:VAL:HG11	1:B:270:TYR:CD2	2.54	0.42
1:C:123:LYS:HG2	1:C:195:TYR:CE1	2.55	0.42
1:D:126:VAL:HG11	1:D:149:MSE:CE	2.50	0.42
1:A:70:GLN:HE21	1:A:79:ILE:HD11	1.85	0.42
1:B:136:ARG:HD3	1:B:167:VAL:HA	2.01	0.42
1:B:236:GLU:HB3	1:B:237:SER:H	1.69	0.42
1:B:307:LEU:CD1	1:B:310:TYR:HD1	2.28	0.42
1:B:74:ASP:N	1:B:74:ASP:OD2	2.52	0.42
1:D:112:HIS:O	1:D:113:LEU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASN:HA	1:D:121:PRO:HD2	1.97	0.42
1:D:158:ASP:O	1:D:161:LYS:HB2	2.20	0.42
1:A:130:GLY:O	1:A:131:ASP:HB3	2.19	0.42
1:B:266:SER:O	1:B:267:VAL:CG2	2.67	0.42
1:B:87:GLY:HA3	1:B:100:GLU:HB2	2.01	0.42
1:C:151:GLU:HG3	1:C:153:ASP:H	1.84	0.42
1:A:323:SER:OG	1:D:311:ASN:HB3	2.20	0.42
1:D:324:PHE:CG	1:D:325:ALA:N	2.87	0.42
1:D:329:ILE:O	1:D:330:GLU:HB2	2.19	0.42
1:D:72:LYS:HG3	1:D:77:ASP:OD1	2.19	0.42
1:A:187:LEU:HD21	1:A:221:VAL:HG22	2.01	0.42
1:A:241:HIS:HB3	1:A:244:ILE:HB	2.02	0.42
1:A:46:GLY:O	1:A:63:LYS:HD2	2.20	0.42
1:D:256:PHE:CD1	1:D:282:THR:HG22	2.53	0.42
1:B:123:LYS:O	1:B:195:TYR:HA	2.19	0.42
1:B:293:LEU:C	1:B:295:PRO:HD3	2.40	0.42
1:C:148:ASP:HA	1:C:177:ASN:CB	2.38	0.42
1:C:289:PHE:O	1:C:315:HIS:HE1	2.02	0.42
1:C:72:LYS:HD2	1:C:77:ASP:OD1	2.19	0.42
1:D:244:ILE:O	1:D:248:ILE:HG13	2.20	0.42
1:D:97:GLN:HE21	1:D:97:GLN:HA	1.82	0.42
1:A:211:GLU:OE1	1:A:211:GLU:N	2.49	0.42
1:A:293:LEU:HD23	1:A:293:LEU:C	2.40	0.42
1:A:43:VAL:C	1:A:44:ILE:HD12	2.40	0.42
1:B:169:ILE:HA	1:B:169:ILE:HD12	1.91	0.42
1:C:137:GLU:CD	1:C:140:ARG:HE	2.23	0.42
1:C:61:SER:O	1:C:62:LEU:HD23	2.19	0.42
1:D:161:LYS:HA	1:D:168:ALA:CB	2.50	0.42
1:D:39:CYS:C	1:D:41:SER:H	2.22	0.42
1:A:257:LYS:HE2	1:A:283:GLU:OE2	2.20	0.42
1:C:229:GLY:O	1:C:281:SER:HA	2.19	0.42
1:C:251:ASN:O	1:C:255:ILE:HG12	2.20	0.42
1:D:113:LEU:N	1:D:114:PRO:HD2	2.33	0.42
1:D:313:GLU:CD	1:D:313:GLU:N	2.73	0.42
1:A:244:ILE:O	1:A:248:ILE:HG13	2.20	0.42
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.55	0.42
1:D:260:VAL:HG13	1:D:280:CYS:SG	2.60	0.42
1:B:101:ARG:HG2	1:B:101:ARG:O	2.18	0.42
1:A:314:ILE:HD13	1:D:321:LEU:O	2.20	0.42
1:D:43:VAL:CG2	1:D:44:ILE:HG13	2.40	0.42
1:A:169:ILE:O	1:A:172:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ILE:HG23	1:D:170:GLY:N	2.34	0.42
1:D:80:VAL:HG12	1:D:80:VAL:O	2.20	0.42
1:A:253:ARG:HH22	1:A:330:GLU:HB2	1.84	0.42
1:B:242:MSE:CG	1:B:328:VAL:HG21	2.50	0.42
1:C:152:ILE:HD12	1:C:182:ASP:HA	2.02	0.42
1:C:262:TYR:OH	1:C:276:GLY:HA3	2.20	0.42
1:C:310:TYR:CD1	1:C:311:ASN:N	2.88	0.42
1:D:131:ASP:HA	1:D:160:SER:HB3	2.01	0.42
1:A:293:LEU:C	1:A:293:LEU:HD23	2.40	0.42
1:B:96:ILE:HG21	1:B:269:THR:HG22	2.01	0.42
1:C:50:GLU:OE2	1:C:95:VAL:HA	2.19	0.42
1:D:149:MSE:HE2	1:D:151:GLU:HB2	2.02	0.42
1:A:169:ILE:HG23	1:A:170:GLY:N	2.34	0.42
1:B:115:LEU:HD23	1:B:141:HIS:CD2	2.54	0.42
1:C:107:GLN:CD	1:C:133:GLY:HA3	2.40	0.42
1:C:182:ASP:OD1	1:C:184:VAL:HG22	2.19	0.42
1:C:125:LEU:HD23	1:C:198:VAL:HG22	2.02	0.42
1:C:215:LYS:HB2	1:C:216:PRO:HD3	2.02	0.42
1:C:200:VAL:CG2	1:C:233:THR:HG22	2.50	0.42
1:C:95:VAL:O	1:C:97:GLN:HG2	2.20	0.42
1:A:257:LYS:NZ	2:A:566:HOH:O	2.52	0.42
1:A:47:TRP:HE3	1:A:61:SER:OG	2.01	0.42
1:D:118:ILE:HD11	1:D:197:ALA:HB2	2.00	0.42
1:A:291:HIS:HA	1:A:292:PRO:HD2	1.86	0.42
1:C:151:GLU:OE1	1:C:152:ILE:N	2.51	0.42
1:D:267:VAL:HB	1:D:270:TYR:HB2	2.01	0.42
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.85	0.42
1:A:51:MSE:O	1:C:72:LYS:HD2	2.19	0.42
1:A:55:TRP:O	1:A:55:TRP:CD1	2.73	0.42
1:A:72:LYS:HE2	2:A:396:HOH:O	2.20	0.42
1:B:229:GLY:O	1:B:281:SER:HA	2.20	0.42
1:D:53:PRO:O	1:D:56:PRO:HD3	2.20	0.42
1:B:238:LEU:HD13	1:B:325:ALA:HB1	2.02	0.42
1:B:67:VAL:HG22	1:B:81:PHE:CB	2.49	0.42
1:B:85:THR:O	1:B:101:ARG:HD2	2.20	0.42
1:D:131:ASP:O	1:D:167:VAL:HB	2.20	0.42
1:A:291:HIS:O	1:A:292:PRO:C	2.57	0.42
1:C:65:GLU:OE1	1:C:65:GLU:HA	2.19	0.42
1:D:113:LEU:N	1:D:114:PRO:HD2	2.35	0.42
1:A:134:VAL:HG12	1:A:138:VAL:HG23	2.02	0.42
1:A:86:TYR:HD2	1:A:99:THR:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:TRP:CZ2	1:C:51:MSE:SE	3.23	0.42
1:A:279:LEU:HB3	1:A:289:PHE:CD1	2.55	0.42
1:A:44:ILE:HG23	1:A:45:PRO:HD2	2.01	0.42
1:C:104:CYS:CB	1:C:308:LYS:HB2	2.49	0.42
1:C:108:GLU:OE1	1:C:307:LEU:HB3	2.19	0.42
1:C:123:LYS:HE3	1:C:195:TYR:CE1	2.55	0.42
1:C:223:ARG:C	1:C:225:LEU:H	2.24	0.42
1:D:126:VAL:HB	1:D:149:MSE:SE	2.70	0.42
1:B:113:LEU:HD23	1:B:315:HIS:ND1	2.34	0.42
1:D:329:ILE:O	1:D:329:ILE:HG22	2.19	0.42
1:A:113:LEU:HD23	1:A:315:HIS:CE1	2.55	0.42
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.85	0.42
1:A:236:GLU:HB3	1:A:241:HIS:NE2	2.34	0.42
1:A:301:SER:O	1:A:302:LYS:C	2.57	0.42
1:B:162:GLN:NE2	2:B:364:HOH:O	2.45	0.42
1:B:243:ASP:N	2:B:433:HOH:O	2.52	0.42
1:C:234:GLN:OE1	1:C:235:ALA:N	2.53	0.42
1:D:241:HIS:ND1	2:D:411:HOH:O	2.37	0.42
1:A:304:ASN:HB3	2:A:374:HOH:O	2.19	0.42
1:B:152:ILE:HA	1:B:180:ILE:CG2	2.47	0.42
1:B:125:LEU:HB2	1:B:195:TYR:CD1	2.55	0.42
1:C:111:THR:HG21	1:C:137:GLU:HB3	2.01	0.42
1:C:275:ILE:HG13	1:C:276:GLY:H	1.84	0.42
1:A:279:LEU:O	1:A:280:CYS:SG	2.75	0.42
1:A:50:GLU:OE2	1:A:95:VAL:HG13	2.19	0.42
1:B:107:GLN:HG2	1:B:134:VAL:N	2.35	0.42
1:D:184:VAL:HG13	2:D:410:HOH:O	2.20	0.42
1:A:96:ILE:CG2	1:A:269:THR:HG21	2.49	0.42
1:C:125:LEU:HB2	1:C:195:TYR:CE1	2.55	0.42
1:C:66:LYS:HG2	1:C:82:GLN:HB3	2.01	0.42
1:D:122:LYS:HG2	1:D:143:SER:O	2.20	0.42
1:D:279:LEU:HB3	1:D:289:PHE:CD2	2.55	0.42
1:A:235:ALA:HB3	1:A:262:TYR:HE2	1.85	0.41
1:A:51:MSE:HB2	1:C:72:LYS:HB3	2.02	0.41
1:B:42:THR:HA	1:B:49:SER:CB	2.50	0.41
1:C:169:ILE:HA	1:C:172:GLU:CD	2.41	0.41
1:D:186:PHE:C	1:D:186:PHE:CD1	2.93	0.41
1:D:83:SER:OG	1:D:86:TYR:N	2.41	0.41
1:C:297:ASP:CG	1:C:300:SER:HG	2.22	0.41
1:D:96:ILE:HG21	1:D:269:THR:HG21	2.01	0.41
1:A:83:SER:HB2	1:A:89:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:GLY:O	1:C:281:SER:HA	2.18	0.41
1:D:250:SER:O	1:D:253:ARG:HB2	2.20	0.41
1:A:55:TRP:HA	1:A:56:PRO:HD2	1.93	0.41
1:B:229:GLY:O	1:B:281:SER:HA	2.20	0.41
1:C:127:ILE:CD1	1:C:127:ILE:H	2.26	0.41
1:A:308:LYS:O	1:D:324:PHE:HD2	2.02	0.41
1:A:264:TRP:HA	1:A:275:ILE:O	2.19	0.41
1:D:103:GLU:O	1:D:107:GLN:HB2	2.20	0.41
1:D:48:PHE:H	1:D:64:VAL:HG23	1.85	0.41
1:C:200:VAL:HG11	1:C:217:PHE:CE2	2.55	0.41
1:D:186:PHE:C	1:D:186:PHE:CD1	2.94	0.41
1:A:279:LEU:HD23	1:A:319:PHE:CE1	2.54	0.41
1:C:272:SER:O	2:C:337:HOH:O	2.22	0.41
1:A:115:LEU:C	1:A:117:SER:N	2.73	0.41
1:A:262:TYR:OH	1:A:276:GLY:HA3	2.19	0.41
1:A:238:LEU:HA	1:A:242:MSE:HE1	1.99	0.41
1:B:104:CYS:O	1:B:108:GLU:HB2	2.20	0.41
1:B:140:ARG:HH21	1:B:307:LEU:HD23	1.85	0.41
1:B:229:GLY:O	1:B:281:SER:HA	2.21	0.41
1:D:130:GLY:O	1:D:160:SER:OG	2.34	0.41
1:D:135:LEU:O	1:D:136:ARG:C	2.58	0.41
1:A:179:VAL:HG11	1:A:186:PHE:CE2	2.54	0.41
1:A:229:GLY:O	1:A:281:SER:HA	2.19	0.41
1:B:149:MSE:SE	1:B:151:GLU:HB2	2.70	0.41
1:C:82:GLN:NE2	1:C:88:LYS:HG3	2.35	0.41
1:A:230:VAL:HA	1:A:280:CYS:O	2.19	0.41
1:A:279:LEU:HB3	1:A:289:PHE:CE1	2.56	0.41
1:B:206:ILE:CG2	1:B:207:GLY:N	2.83	0.41
1:B:47:TRP:CZ2	1:B:63:LYS:HE2	2.55	0.41
1:A:129:GLY:C	1:A:131:ASP:N	2.73	0.41
1:A:311:ASN:O	1:A:313:GLU:N	2.53	0.41
1:D:167:VAL:C	1:D:169:ILE:N	2.74	0.41
1:D:242:MSE:HE1	1:D:325:ALA:CB	2.50	0.41
1:A:121:PRO:HG2	1:A:144:ILE:HD11	2.02	0.41
1:A:170:GLY:C	1:A:172:GLU:N	2.72	0.41
1:C:258:GLY:HA3	1:C:281:SER:OG	2.20	0.41
1:A:176:VAL:HG12	1:A:177:ASN:N	2.35	0.41
1:A:234:GLN:NE2	1:A:275:ILE:HD11	2.21	0.41
1:A:55:TRP:CD1	1:A:55:TRP:O	2.73	0.41
1:B:86:TYR:O	1:B:99:THR:HB	2.20	0.41
1:A:264:TRP:HA	1:A:275:ILE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG13	2:A:376:HOH:O	2.20	0.41
1:B:271:PRO:O	1:B:272:SER:CB	2.66	0.41
1:B:76:GLN:HB2	1:B:93:ASP:CG	2.41	0.41
1:C:209:ALA:O	1:C:212:LEU:HD13	2.20	0.41
1:C:46:GLY:HA3	1:C:63:LYS:HZ1	1.85	0.41
1:D:241:HIS:O	1:D:245:ILE:HG13	2.20	0.41
1:A:135:LEU:HD21	1:A:176:VAL:HG11	2.02	0.41
1:A:146:GLN:HA	1:A:175:ARG:O	2.21	0.41
1:A:149:MSE:HE3	1:A:171:TYR:CE1	2.55	0.41
1:B:53:PRO:O	1:B:56:PRO:HD3	2.20	0.41
1:C:113:LEU:N	1:C:114:PRO:HD2	2.36	0.41
1:D:324:PHE:C	1:D:324:PHE:CD1	2.94	0.41
1:D:69:PHE:HE2	1:D:78:VAL:HB	1.84	0.41
1:A:127:ILE:HD12	1:A:200:VAL:HG22	2.02	0.41
1:A:79:ILE:HG22	1:A:80:VAL:N	2.34	0.41
1:B:51:MSE:SE	1:C:44:ILE:HD12	2.70	0.41
1:B:78:VAL:HG11	1:B:159:VAL:HG21	2.01	0.41
1:C:82:GLN:NE2	1:C:88:LYS:N	2.68	0.41
1:D:206:ILE:HG23	1:D:207:GLY:N	2.35	0.41
1:A:156:VAL:HG12	1:A:157:VAL:N	2.34	0.41
1:A:113:LEU:HA	1:A:113:LEU:HD23	1.94	0.41
1:B:104:CYS:O	1:B:108:GLU:HB2	2.21	0.41
1:B:169:ILE:CG2	1:B:170:GLY:N	2.83	0.41
1:C:215:LYS:N	1:C:216:PRO:HD3	2.32	0.41
1:D:76:GLN:OE1	1:D:92:LEU:HD22	2.20	0.41
1:B:127:ILE:HD11	1:B:187:LEU:HD23	1.98	0.41
1:A:49:SER:HB2	1:A:51:MSE:SE	2.70	0.41
1:C:200:VAL:HB	1:C:233:THR:CG2	2.34	0.41
1:C:202:SER:HB2	1:C:213:PHE:CE1	2.55	0.41
1:B:308:LYS:O	1:C:324:PHE:HB3	2.20	0.41
1:D:128:GLY:C	1:D:130:GLY:N	2.71	0.41
1:A:121:PRO:HA	2:A:382:HOH:O	2.18	0.41
1:C:184:VAL:CG2	1:C:185:ALA:N	2.84	0.41
1:D:164:PHE:HB2	1:D:167:VAL:CG2	2.50	0.41
1:A:192:GLU:HG2	2:A:425:HOH:O	2.20	0.41
1:B:173:ASP:OD1	1:B:175:ARG:NH2	2.50	0.41
1:C:89:VAL:HG12	1:C:90:LEU:N	2.35	0.41
1:D:103:GLU:HA	2:D:372:HOH:O	2.20	0.41
1:D:107:GLN:NE2	2:D:373:HOH:O	2.52	0.41
1:A:161:LYS:HA	1:A:168:ALA:CB	2.46	0.41
1:C:106:TYR:HE2	1:C:201:ASP:OD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:GLN:HG2	1:C:79:ILE:HG12	2.01	0.41
1:A:214:GLU:CB	1:A:216:PRO:HD2	2.50	0.41
1:B:114:PRO:HG2	1:B:115:LEU:H	1.86	0.41
1:B:132:GLY:HA3	1:B:167:VAL:O	2.20	0.41
1:B:150:CYS:SG	1:B:181:GLY:O	2.78	0.41
1:C:112:HIS:HB3	1:C:116:CYS:SG	2.61	0.41
1:C:147:ILE:O	1:C:176:VAL:HA	2.20	0.41
1:C:50:GLU:HG2	1:C:55:TRP:CZ2	2.55	0.41
1:B:106:TYR:CZ	1:B:110:ILE:HD12	2.55	0.41
1:B:134:VAL:O	1:B:138:VAL:HG23	2.20	0.41
1:B:323:SER:C	1:B:325:ALA:N	2.72	0.41
1:C:324:PHE:O	1:C:324:PHE:HD1	2.04	0.41
1:C:82:GLN:HE22	1:C:88:LYS:HG3	1.85	0.41
1:D:72:LYS:HD2	1:D:77:ASP:OD1	2.19	0.41
1:A:72:LYS:HZ3	1:A:72:LYS:HB2	1.85	0.41
1:C:191:ALA:O	1:C:192:GLU:C	2.59	0.41
1:A:98:LEU:HD12	1:A:98:LEU:C	2.40	0.41
1:B:109:MSE:SE	1:B:314:ILE:CG2	3.18	0.41
1:C:50:GLU:CG	1:C:55:TRP:HZ2	2.31	0.41
1:C:79:ILE:HG22	1:C:80:VAL:N	2.35	0.41
1:D:110:ILE:HG12	1:D:199:ILE:HG23	2.03	0.41
1:A:116:CYS:SG	1:A:295:PRO:HA	2.60	0.41
1:A:257:LYS:HE3	1:A:257:LYS:HB3	1.92	0.41
1:A:233:THR:O	1:A:277:PHE:HD1	2.03	0.41
1:A:70:GLN:HG3	1:A:79:ILE:HA	2.02	0.41
1:B:324:PHE:CD1	1:B:324:PHE:C	2.94	0.41
1:C:215:LYS:HE3	1:C:251:ASN:OD1	2.20	0.41
1:A:239:TRP:HB2	1:A:272:SER:OG	2.20	0.41
1:B:130:GLY:HA3	1:B:156:VAL:HG11	2.01	0.41
1:B:199:ILE:HA	1:B:232:CYS:O	2.20	0.41
1:C:106:TYR:HE2	1:C:201:ASP:OD2	2.02	0.41
1:D:184:VAL:HG22	1:D:217:PHE:HD1	1.84	0.41
1:B:248:ILE:HG22	1:B:278:MSE:HG3	2.02	0.41
1:D:128:GLY:HA3	1:D:149:MSE:HE1	2.02	0.41
1:D:54:MSE:O	1:D:241:HIS:NE2	2.53	0.41
1:A:197:ALA:HA	1:A:230:VAL:O	2.20	0.41
1:D:121:PRO:O	1:D:144:ILE:HD13	2.20	0.41
1:D:108:GLU:OE2	1:D:307:LEU:HD23	2.21	0.41
1:D:55:TRP:O	1:D:58:GLU:HG2	2.19	0.41
1:A:86:TYR:CE2	1:A:101:ARG:HD3	2.55	0.41
1:A:288:ASP:OD2	1:A:291:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLU:O	1:B:276:GLY:N	2.52	0.41
1:B:155:MSE:O	1:B:159:VAL:HG23	2.19	0.41
1:B:72:LYS:HB2	1:B:77:ASP:OD1	2.20	0.41
1:D:108:GLU:OE1	1:D:310:TYR:N	2.53	0.41
1:A:267:VAL:CG1	1:A:270:TYR:CD2	2.99	0.41
1:B:123:LYS:HE3	1:B:146:GLN:CD	2.41	0.41
1:B:161:LYS:HA	1:B:168:ALA:HB1	2.02	0.41
1:B:216:PRO:HD2	2:B:429:HOH:O	2.19	0.41
1:B:290:LYS:HE2	2:B:484:HOH:O	2.20	0.41
1:C:173:ASP:OD1	1:C:175:ARG:N	2.46	0.41
1:C:223:ARG:HG3	1:C:224:ALA:N	2.36	0.41
1:C:237:SER:H	1:C:241:HIS:HD2	1.69	0.41
1:A:311:ASN:O	1:A:313:GLU:N	2.53	0.41
1:A:242:MSE:C	1:A:244:ILE:N	2.72	0.41
1:A:264:TRP:HD1	1:A:318:ALA:O	2.03	0.41
1:A:97:GLN:O	1:A:98:LEU:HB3	2.18	0.41
1:B:169:ILE:HA	1:B:172:GLU:HG2	2.03	0.41
1:C:127:ILE:O	1:C:127:ILE:HG22	2.21	0.41
1:C:283:GLU:OE2	1:C:283:GLU:N	2.44	0.41
1:A:218:PHE:HB3	1:A:256:PHE:HE1	1.86	0.41
1:D:317:ALA:O	1:D:319:PHE:N	2.54	0.41
1:C:135:LEU:HD12	1:C:135:LEU:HA	1.89	0.41
1:C:238:LEU:HD22	1:C:242:MSE:HE1	2.02	0.41
1:D:118:ILE:HD11	1:D:121:PRO:HB3	2.03	0.41
1:D:50:GLU:C	1:D:51:MSE:SE	3.09	0.41
1:A:135:LEU:HD23	1:A:170:GLY:C	2.41	0.41
1:B:163:PHE:O	1:B:165:PRO:HD3	2.21	0.41
1:D:109:MSE:SE	1:D:309:PHE:CD2	3.24	0.41
1:D:159:VAL:O	1:D:163:PHE:HB2	2.20	0.41
1:D:223:ARG:NH2	2:D:526:HOH:O	2.53	0.41
1:A:206:ILE:CG2	1:A:207:GLY:N	2.83	0.41
1:B:123:LYS:HE3	1:B:146:GLN:NE2	2.35	0.41
1:B:179:VAL:HG21	1:B:186:PHE:CE2	2.56	0.41
1:B:245:ILE:O	1:B:248:ILE:HB	2.21	0.41
1:B:269:THR:HG22	1:B:269:THR:O	2.20	0.41
1:C:164:PHE:HB3	1:C:167:VAL:CG2	2.50	0.41
1:C:182:ASP:OD2	1:C:184:VAL:HG22	2.21	0.41
1:C:200:VAL:HB	1:C:233:THR:CG2	2.48	0.41
1:C:206:ILE:HG23	1:C:207:GLY:H	1.86	0.41
1:C:310:TYR:CD1	1:C:311:ASN:N	2.89	0.41
1:C:82:GLN:HE22	1:C:88:LYS:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:MSE:H	1:A:109:MSE:HG2	1.66	0.41
1:B:164:PHE:HB2	1:B:167:VAL:CG2	2.51	0.41
1:B:191:ALA:O	1:B:223:ARG:NH1	2.54	0.41
1:B:205:PRO:HD3	1:B:213:PHE:CZ	2.56	0.41
1:B:215:LYS:HE3	1:B:254:GLU:HB2	2.03	0.41
1:C:225:LEU:HD11	1:C:231:VAL:CG1	2.39	0.41
1:A:231:VAL:O	1:A:231:VAL:HG13	2.20	0.41
1:B:239:TRP:CD2	1:C:268:PRO:HG2	2.56	0.41
1:C:204:ASP:CG	1:C:205:PRO:HD2	2.40	0.41
1:C:310:TYR:HA	1:C:314:ILE:HG21	2.01	0.41
1:A:127:ILE:HD13	1:A:217:PHE:CZ	2.55	0.41
1:A:80:VAL:HG21	1:A:159:VAL:CG1	2.49	0.41
1:B:172:GLU:O	1:B:173:ASP:C	2.58	0.41
1:B:264:TRP:HA	1:B:276:GLY:HA2	2.02	0.41
1:D:60:HIS:HE1	1:D:272:SER:N	2.19	0.41
1:A:215:LYS:H	1:A:216:PRO:CD	2.33	0.41
1:C:86:TYR:CD2	1:C:101:ARG:HD3	2.56	0.41
1:D:231:VAL:HG23	1:D:280:CYS:HB2	2.01	0.41
1:D:257:LYS:HD3	2:D:417:HOH:O	2.21	0.41
1:A:329:ILE:O	1:A:329:ILE:CG2	2.66	0.41
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.82	0.41
1:B:275:ILE:O	1:B:275:ILE:HG23	2.19	0.41
1:B:146:GLN:HA	1:B:175:ARG:HB3	2.03	0.41
1:B:66:LYS:HG3	2:B:383:HOH:O	2.20	0.41
1:D:186:PHE:O	1:D:190:ALA:HB2	2.20	0.41
1:D:232:CYS:HA	1:D:278:MSE:O	2.20	0.41
1:D:261:ASN:HB3	1:D:319:PHE:CE1	2.56	0.41
1:D:210:LYS:O	1:D:214:GLU:HG3	2.20	0.41
1:D:60:HIS:CE1	1:D:271:PRO:HA	2.56	0.41
1:A:125:LEU:HD13	1:A:186:PHE:HE1	1.85	0.41
1:A:310:TYR:C	1:A:310:TYR:CD1	2.94	0.41
1:A:98:LEU:HD12	1:A:98:LEU:C	2.41	0.41
1:C:267:VAL:HG11	1:C:270:TYR:CE2	2.56	0.41
1:D:108:GLU:HB3	1:D:310:TYR:CB	2.50	0.41
1:D:123:LYS:HG3	1:D:146:GLN:HB3	2.03	0.41
1:A:154:LYS:HG3	1:A:180:ILE:HD13	2.02	0.41
1:A:151:GLU:O	1:A:180:ILE:HA	2.20	0.41
1:A:214:GLU:HA	1:A:251:ASN:HD22	1.83	0.41
1:B:113:LEU:HG	1:B:279:LEU:HD21	2.03	0.41
1:B:264:TRP:H	1:B:264:TRP:HD1	1.69	0.41
1:B:74:ASP:OD1	1:B:74:ASP:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLU:HG2	1:C:55:TRP:CZ2	2.52	0.41
1:A:154:LYS:C	1:A:156:VAL:N	2.74	0.41
1:A:249:VAL:HA	1:A:278:MSE:HE2	2.02	0.41
1:A:307:LEU:H	1:A:307:LEU:HD12	1.85	0.41
1:B:157:VAL:O	1:B:161:LYS:HG3	2.21	0.41
1:C:178:LEU:HD12	1:C:179:VAL:H	1.85	0.41
1:B:173:ASP:HB2	2:B:361:HOH:O	2.20	0.41
1:B:253:ARG:HG3	2:B:371:HOH:O	2.21	0.41
1:A:72:LYS:NZ	1:C:52:SER:HA	2.35	0.41
1:D:151:GLU:OE1	1:D:152:ILE:N	2.54	0.41
1:D:225:LEU:HD11	1:D:231:VAL:CG2	2.38	0.41
1:B:114:PRO:HB3	1:B:279:LEU:CD1	2.50	0.41
1:B:49:SER:CB	1:B:51:MSE:HE2	2.50	0.41
1:C:66:LYS:HD3	2:C:447:HOH:O	2.20	0.41
1:A:124:VAL:O	1:A:147:ILE:HA	2.21	0.41
1:C:132:GLY:O	1:C:135:LEU:HB3	2.21	0.41
1:D:76:GLN:HB2	1:D:93:ASP:CG	2.41	0.41
1:A:99:THR:HG22	1:A:101:ARG:H	1.86	0.41
1:A:108:GLU:HB3	1:A:112:HIS:HD2	1.86	0.41
1:A:244:ILE:O	1:A:244:ILE:HG22	2.21	0.41
1:C:192:GLU:HA	1:C:223:ARG:O	2.21	0.41
1:C:73:SER:CA	1:C:155:MSE:SE	3.19	0.41
1:A:121:PRO:O	1:A:144:ILE:HD13	2.20	0.41
1:B:241:HIS:HD2	2:B:376:HOH:O	2.04	0.41
1:C:140:ARG:NH2	1:C:305:GLY:O	2.53	0.41
1:C:310:TYR:C	1:C:310:TYR:CD1	2.94	0.41
1:D:167:VAL:C	1:D:169:ILE:N	2.74	0.41
1:D:182:ASP:OD2	1:D:184:VAL:HB	2.21	0.41
1:A:279:LEU:H	1:A:279:LEU:HD22	1.85	0.41
1:B:103:GLU:CD	1:B:167:VAL:HG11	2.40	0.41
1:B:259:SER:O	1:B:280:CYS:HA	2.21	0.41
1:D:186:PHE:CD1	1:D:186:PHE:C	2.93	0.41
1:A:258:GLY:HA3	1:A:281:SER:OG	2.19	0.41
1:B:230:VAL:HG12	1:B:281:SER:HB3	2.03	0.41
1:B:308:LYS:O	1:C:323:SER:HB2	2.21	0.41
1:B:109:MSE:CE	1:B:318:ALA:HB2	2.51	0.41
1:C:200:VAL:CG2	1:C:233:THR:HG22	2.51	0.41
1:C:63:LYS:O	1:C:63:LYS:HG3	2.21	0.41
1:A:118:ILE:O	1:A:118:ILE:HG13	2.21	0.41
1:C:329:ILE:O	1:C:330:GLU:HB2	2.21	0.41
1:C:80:VAL:HA	1:C:89:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:PHE:O	1:D:165:PRO:HD3	2.21	0.41
1:D:123:LYS:HD3	1:D:194:SER:O	2.21	0.41
1:A:195:TYR:O	1:A:226:ARG:HG3	2.19	0.41
1:B:124:VAL:HG22	1:B:197:ALA:HB3	2.03	0.41
1:A:170:GLY:C	1:A:172:GLU:N	2.73	0.41
1:B:136:ARG:NH1	1:B:137:GLU:OE2	2.53	0.41
1:A:267:VAL:CG1	1:A:270:TYR:CD2	3.04	0.41
1:D:148:ASP:OD1	1:D:177:ASN:ND2	2.44	0.41
1:A:242:MSE:CA	1:A:242:MSE:HE2	2.36	0.41
1:A:301:SER:O	1:A:302:LYS:C	2.58	0.41
1:A:69:PHE:C	1:A:69:PHE:CD1	2.93	0.41
1:D:169:ILE:HA	1:D:172:GLU:OE1	2.21	0.41
1:A:249:VAL:O	1:A:253:ARG:HG3	2.20	0.41
1:A:327:LYS:HB3	1:A:327:LYS:HE2	1.89	0.41
1:D:134:VAL:O	1:D:138:VAL:HG23	2.21	0.41
1:D:149:MSE:HB3	1:D:178:LEU:HA	2.03	0.41
1:D:256:PHE:CD1	1:D:282:THR:CG2	3.04	0.41
1:D:98:LEU:O	1:D:98:LEU:HD12	2.21	0.41
1:A:125:LEU:HA	1:A:148:ASP:O	2.21	0.41
1:A:290:LYS:HD3	2:A:373:HOH:O	2.21	0.41
1:B:288:ASP:OD1	1:B:290:LYS:N	2.51	0.41
1:B:324:PHE:C	1:B:324:PHE:CD1	2.94	0.41
1:B:41:SER:C	1:B:51:MSE:HE3	2.41	0.41
1:C:107:GLN:CD	1:C:133:GLY:HA3	2.41	0.41
1:C:161:LYS:HA	1:C:168:ALA:HB2	2.02	0.41
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.56	0.41
1:D:109:MSE:CG	1:D:277:PHE:CE2	3.03	0.41
1:A:214:GLU:CB	1:A:216:PRO:HD2	2.51	0.41
1:C:147:ILE:HB	1:C:175:ARG:O	2.21	0.41
1:D:110:ILE:HG23	1:D:111:THR:N	2.35	0.41
1:D:217:PHE:O	1:D:220:SER:HB3	2.20	0.41
1:D:310:TYR:CD1	1:D:310:TYR:C	2.94	0.41
1:A:132:GLY:HA2	1:A:135:LEU:HD13	2.02	0.41
1:A:144:ILE:HB	1:A:175:ARG:NH1	2.36	0.41
1:B:109:MSE:HB3	1:B:109:MSE:HE2	2.00	0.41
1:D:206:ILE:HG23	1:D:207:GLY:N	2.35	0.41
1:D:215:LYS:N	1:D:216:PRO:CD	2.84	0.41
1:D:83:SER:HG	1:D:86:TYR:H	1.69	0.41
1:A:278:MSE:O	1:A:279:LEU:C	2.59	0.41
1:A:50:GLU:HG2	1:A:50:GLU:O	2.21	0.41
1:B:155:MSE:O	1:B:159:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:C	1:B:44:ILE:HG13	2.42	0.41
1:C:206:ILE:CG2	1:C:207:GLY:N	2.84	0.41
1:C:60:HIS:CE1	2:C:373:HOH:O	2.73	0.41
1:A:85:THR:HG21	1:D:56:PRO:O	2.21	0.41
1:A:133:GLY:O	1:A:134:VAL:C	2.59	0.41
1:A:192:GLU:HB2	1:A:223:ARG:HH12	1.86	0.41
1:A:308:LYS:N	1:A:308:LYS:HD3	2.36	0.41
1:A:86:TYR:O	1:A:99:THR:HG23	2.21	0.41
1:C:301:SER:CB	1:C:304:ASN:HD22	2.14	0.41
1:D:150:CYS:HA	1:D:179:VAL:O	2.20	0.41
1:A:48:PHE:O	1:A:61:SER:HA	2.20	0.41
1:B:232:CYS:HA	1:B:278:MSE:O	2.21	0.41
1:B:51:MSE:CG	2:B:377:HOH:O	2.68	0.41
1:D:79:ILE:HD12	2:D:495:HOH:O	2.21	0.41
1:A:259:SER:O	1:A:281:SER:N	2.53	0.41
1:A:49:SER:O	1:A:51:MSE:SE	2.89	0.41
1:B:178:LEU:HD12	1:B:179:VAL:N	2.36	0.41
1:B:38:ALA:C	1:B:40:PHE:H	2.24	0.41
1:C:102:ASP:OD2	1:C:268:PRO:HD2	2.21	0.41
1:B:97:GLN:O	1:B:98:LEU:CB	2.69	0.41
1:C:124:VAL:O	1:C:147:ILE:HA	2.20	0.41
1:C:125:LEU:HD22	1:C:195:TYR:CE2	2.55	0.41
1:D:92:LEU:HD21	1:D:156:VAL:CG2	2.50	0.41
1:A:267:VAL:CG1	1:A:270:TYR:CD2	3.01	0.41
1:A:67:VAL:O	1:C:46:GLY:HA2	2.20	0.41
1:C:113:LEU:N	1:C:114:PRO:HD2	2.36	0.41
1:D:193:GLY:HA2	1:D:225:LEU:O	2.21	0.41
1:A:76:GLN:HG3	1:A:78:VAL:HG22	2.03	0.41
1:B:98:LEU:HB2	1:B:103:GLU:HG2	2.02	0.41
1:C:137:GLU:CD	1:C:140:ARG:HE	2.24	0.41
1:C:238:LEU:HD22	1:C:242:MSE:HE1	2.03	0.41
1:A:270:TYR:HA	1:A:271:PRO:HD2	1.89	0.41
1:B:110:ILE:HG13	1:B:232:CYS:SG	2.61	0.41
1:D:76:GLN:OE1	1:D:92:LEU:HB3	2.21	0.41
1:B:323:SER:O	1:B:326:LYS:N	2.51	0.41
1:B:326:LYS:HG2	1:B:330:GLU:HB2	2.03	0.41
1:C:150:CYS:HA	1:C:179:VAL:O	2.20	0.41
1:D:113:LEU:N	1:D:114:PRO:CD	2.83	0.41
1:D:183:GLY:HA2	1:D:186:PHE:HB3	2.02	0.41
1:C:236:GLU:O	1:C:276:GLY:N	2.54	0.41
1:A:154:LYS:CB	1:A:180:ILE:HD13	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:CD1	1:A:322:PRO:HD2	2.51	0.41
1:B:107:GLN:OE1	1:B:133:GLY:HA3	2.21	0.41
1:B:145:GLU:O	1:B:175:ARG:HG2	2.21	0.41
1:B:229:GLY:O	1:B:281:SER:HA	2.21	0.41
1:C:80:VAL:HG21	1:C:159:VAL:HG11	2.03	0.41
1:C:254:GLU:O	1:C:255:ILE:HD13	2.21	0.41
1:D:127:ILE:N	1:D:199:ILE:O	2.54	0.41
1:A:69:PHE:C	1:A:69:PHE:CD1	2.94	0.41
1:C:165:PRO:C	1:C:167:VAL:N	2.73	0.41
1:B:46:GLY:N	1:C:41:SER:OG	2.43	0.41
1:A:122:LYS:NZ	2:A:417:HOH:O	2.51	0.41
1:A:171:TYR:CE1	1:A:178:LEU:HD22	2.56	0.41
1:A:296:ILE:CG2	1:A:300:SER:HB2	2.51	0.41
1:B:217:PHE:O	1:B:220:SER:HB3	2.21	0.41
1:C:220:SER:HA	1:C:223:ARG:HG2	2.03	0.41
1:C:48:PHE:HE2	1:C:96:ILE:HD11	1.85	0.41
1:A:69:PHE:CZ	1:A:155:MSE:SE	3.24	0.41
1:B:213:PHE:HA	1:B:218:PHE:HE2	1.86	0.41
1:C:69:PHE:O	1:C:80:VAL:HG23	2.21	0.41
1:D:130:GLY:HA2	2:D:553:HOH:O	2.21	0.41
1:A:98:LEU:HD21	1:A:131:ASP:HB3	2.03	0.41
1:A:54:MSE:O	1:A:241:HIS:HE1	2.04	0.41
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.56	0.41
1:D:163:PHE:O	1:D:165:PRO:HD3	2.21	0.41
1:D:51:MSE:CB	2:D:352:HOH:O	2.68	0.41
1:D:54:MSE:HB3	1:D:241:HIS:CE1	2.55	0.41
1:B:252:CYS:SG	1:B:278:MSE:HE2	2.62	0.40
1:C:123:LYS:HD3	1:C:194:SER:O	2.21	0.40
1:C:133:GLY:O	1:C:136:ARG:HB3	2.21	0.40
1:A:311:ASN:H	1:A:314:ILE:HG22	1.86	0.40
1:C:164:PHE:HB3	1:C:167:VAL:HB	2.03	0.40
1:C:110:ILE:HG12	1:C:199:ILE:HG23	2.04	0.40
1:C:205:PRO:HB3	1:C:213:PHE:CD1	2.56	0.40
1:C:82:GLN:HA	1:C:82:GLN:HE21	1.86	0.40
1:D:113:LEU:HD23	1:D:315:HIS:ND1	2.36	0.40
1:D:196:ASP:OD1	1:D:226:ARG:HD3	2.21	0.40
1:C:265:THR:OG1	1:C:267:VAL:CG2	2.68	0.40
1:C:87:GLY:N	2:C:565:HOH:O	2.50	0.40
1:A:43:VAL:HG13	1:D:43:VAL:HA	2.03	0.40
1:A:268:PRO:HG2	1:D:239:TRP:CD2	2.56	0.40
1:A:47:TRP:CE3	1:A:61:SER:OG	2.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:HD21	1:C:221:VAL:HA	2.03	0.40
1:A:108:GLU:OE1	1:A:309:PHE:N	2.55	0.40
1:A:154:LYS:CB	1:A:180:ILE:HD13	2.51	0.40
1:C:206:ILE:HG23	1:C:207:GLY:N	2.36	0.40
1:D:157:VAL:HG11	1:D:178:LEU:HD21	2.02	0.40
1:D:215:LYS:HG3	2:D:407:HOH:O	2.20	0.40
1:D:223:ARG:HH11	1:D:223:ARG:HG2	1.86	0.40
1:C:283:GLU:HG2	1:C:283:GLU:O	2.21	0.40
1:D:259:SER:O	1:D:281:SER:N	2.48	0.40
1:A:70:GLN:HE21	1:A:79:ILE:CD1	2.34	0.40
1:B:291:HIS:HA	1:B:292:PRO:HD2	1.79	0.40
1:B:54:MSE:HB2	1:B:55:TRP:CE3	2.56	0.40
1:C:254:GLU:O	1:C:255:ILE:HG12	2.21	0.40
1:C:271:PRO:O	1:C:272:SER:CB	2.66	0.40
1:D:222:ALA:HB2	1:D:256:PHE:CE1	2.56	0.40
1:D:69:PHE:CE2	1:D:159:VAL:HG21	2.56	0.40
1:A:226:ARG:NH1	2:A:413:HOH:O	2.54	0.40
1:A:324:PHE:C	1:A:324:PHE:CD1	2.94	0.40
1:A:328:VAL:C	1:A:330:GLU:N	2.74	0.40
1:B:78:VAL:HG22	1:B:92:LEU:CD2	2.51	0.40
1:B:88:LYS:O	1:B:99:THR:HA	2.22	0.40
1:C:110:ILE:HG23	1:C:111:THR:N	2.35	0.40
1:D:183:GLY:O	1:D:187:LEU:N	2.42	0.40
1:A:206:ILE:CG2	1:A:207:GLY:N	2.83	0.40
1:B:47:TRP:HZ2	2:B:377:HOH:O	2.04	0.40
1:C:269:THR:H	1:C:269:THR:HG1	1.62	0.40
1:C:80:VAL:HG21	1:C:159:VAL:HG12	2.04	0.40
1:D:159:VAL:HG13	1:D:163:PHE:CD2	2.57	0.40
1:A:55:TRP:HB2	1:A:58:GLU:CG	2.51	0.40
1:B:291:HIS:HA	1:B:292:PRO:HD2	1.80	0.40
1:D:328:VAL:HG23	1:D:329:ILE:HG13	2.02	0.40
1:A:121:PRO:HA	2:A:386:HOH:O	2.21	0.40
1:A:153:ASP:OD1	1:A:155:MSE:HB3	2.21	0.40
1:A:61:SER:HB2	1:D:59:ALA:HB3	2.03	0.40
1:B:241:HIS:CD2	2:B:376:HOH:O	2.73	0.40
1:B:44:ILE:HB	1:B:47:TRP:HB2	2.03	0.40
1:C:262:TYR:HD1	1:C:278:MSE:SE	2.54	0.40
1:C:329:ILE:HG22	1:C:329:ILE:O	2.21	0.40
1:D:114:PRO:HG2	1:D:115:LEU:H	1.86	0.40
1:A:112:HIS:HB3	1:A:116:CYS:SG	2.61	0.40
1:A:310:TYR:O	1:A:311:ASN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:MSE:HB2	1:B:55:TRP:CE3	2.56	0.40
1:C:137:GLU:OE1	1:C:140:ARG:NE	2.52	0.40
1:D:152:ILE:HG23	1:D:153:ASP:N	2.36	0.40
1:D:223:ARG:NH2	2:D:526:HOH:O	2.54	0.40
1:D:270:TYR:HD2	1:D:275:ILE:HD13	1.85	0.40
1:A:125:LEU:HD13	1:A:186:PHE:CE1	2.56	0.40
1:B:98:LEU:HD12	1:B:98:LEU:O	2.21	0.40
1:D:180:ILE:O	1:D:180:ILE:HG22	2.21	0.40
1:D:219:GLN:O	1:D:223:ARG:HB2	2.21	0.40
1:A:239:TRP:CD2	1:D:268:PRO:HG2	2.56	0.40
1:A:279:LEU:HB3	1:A:289:PHE:CE2	2.56	0.40
1:D:182:ASP:HA	2:D:502:HOH:O	2.21	0.40
1:D:248:ILE:HG22	1:D:278:MSE:SE	2.72	0.40
1:A:238:LEU:O	1:A:242:MSE:HE3	2.20	0.40
1:C:100:GLU:HA	1:C:103:GLU:OE2	2.21	0.40
1:B:45:PRO:HD3	1:C:43:VAL:HG21	2.02	0.40
1:A:304:ASN:HD22	1:A:304:ASN:C	2.25	0.40
1:C:296:ILE:CG2	1:C:307:LEU:HD11	2.48	0.40
1:C:61:SER:C	1:C:62:LEU:HD12	2.42	0.40
1:A:79:ILE:HG22	1:A:80:VAL:N	2.36	0.40
1:B:120:ASN:O	1:B:122:LYS:HD2	2.22	0.40
1:B:320:CYS:C	1:B:321:LEU:HD23	2.39	0.40
1:C:309:PHE:O	1:C:310:TYR:O	2.39	0.40
1:C:51:MSE:HA	1:C:59:ALA:HB2	2.03	0.40
1:A:249:VAL:HA	1:A:278:MSE:SE	2.72	0.40
1:A:296:ILE:HG23	1:A:300:SER:HB2	2.02	0.40
1:B:105:ALA:O	1:B:106:TYR:C	2.59	0.40
1:B:257:LYS:HE3	1:B:283:GLU:CB	2.51	0.40
1:C:123:LYS:HD2	1:C:146:GLN:OE1	2.21	0.40
1:C:310:TYR:C	1:C:310:TYR:CD1	2.95	0.40
1:C:76:GLN:HB2	1:C:93:ASP:OD1	2.22	0.40
1:D:127:ILE:HG21	1:D:183:GLY:HA3	2.03	0.40
1:D:200:VAL:C	1:D:202:SER:H	2.24	0.40
1:C:247:ASP:O	1:C:251:ASN:ND2	2.54	0.40
1:C:65:GLU:OE2	1:C:82:GLN:HG2	2.22	0.40
1:C:278:MSE:SE	1:C:279:LEU:N	3.05	0.40
1:C:43:VAL:HG12	1:C:44:ILE:O	2.22	0.40
1:D:214:GLU:HG3	2:D:407:HOH:O	2.21	0.40
1:D:245:ILE:HD13	1:D:262:TYR:OH	2.21	0.40
1:A:230:VAL:CA	1:A:280:CYS:O	2.64	0.40
1:A:298:GLU:O	1:A:300:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:O	1:A:326:LYS:HB3	2.20	0.40
1:D:107:GLN:O	1:D:111:THR:HG23	2.21	0.40
1:D:198:VAL:N	1:D:231:VAL:HG22	2.36	0.40
1:D:40:PHE:O	1:D:42:THR:N	2.53	0.40
1:A:72:LYS:HB3	1:C:51:MSE:CB	2.48	0.40
1:B:187:LEU:O	1:B:189:ASN:N	2.54	0.40
1:B:313:GLU:OE1	1:C:326:LYS:HE3	2.21	0.40
1:C:110:ILE:CG2	1:C:111:THR:N	2.84	0.40
1:D:288:ASP:C	1:D:290:LYS:H	2.23	0.40
1:A:173:ASP:HA	1:A:174:PRO:HD3	1.92	0.40
1:B:110:ILE:HG23	1:B:111:THR:N	2.35	0.40
1:C:128:GLY:O	1:C:129:GLY:C	2.60	0.40
1:C:137:GLU:CD	1:C:140:ARG:HE	2.24	0.40
1:C:242:MSE:HE2	1:C:325:ALA:HA	2.02	0.40
1:D:162:GLN:HE21	1:D:163:PHE:N	2.19	0.40
1:C:80:VAL:HG21	1:C:159:VAL:CG1	2.51	0.40
1:C:131:ASP:HB2	1:C:167:VAL:HG11	2.04	0.40
1:C:43:VAL:CG1	1:C:44:ILE:N	2.85	0.40
1:D:110:ILE:HB	1:D:277:PHE:HE1	1.87	0.40
1:A:169:ILE:O	1:A:172:GLU:HB2	2.21	0.40
1:B:319:PHE:O	1:B:321:LEU:HG	2.22	0.40
1:C:169:ILE:O	1:C:171:TYR:N	2.54	0.40
1:C:123:LYS:HD3	1:C:194:SER:O	2.21	0.40
1:A:209:ALA:HA	1:A:211:GLU:OE1	2.22	0.40
1:A:256:PHE:CG	1:A:280:CYS:HB3	2.56	0.40
1:A:264:TRP:HA	1:A:275:ILE:O	2.22	0.40
1:A:288:ASP:OD2	1:A:291:HIS:HB2	2.22	0.40
1:A:327:LYS:HE2	1:A:327:LYS:HB3	1.92	0.40
1:B:242:MSE:O	1:B:246:GLU:N	2.54	0.40
1:C:301:SER:HB3	1:C:304:ASN:ND2	2.16	0.40
1:A:170:GLY:O	1:A:172:GLU:N	2.54	0.40
1:A:289:PHE:O	1:A:315:HIS:NE2	2.51	0.40
1:A:288:ASP:C	1:A:290:LYS:H	2.25	0.40
1:D:260:VAL:HG12	1:D:278:MSE:HE1	2.04	0.40
1:A:311:ASN:HB3	1:D:323:SER:OG	2.22	0.40
1:A:98:LEU:HD12	1:A:98:LEU:C	2.42	0.40
1:C:82:GLN:OE1	1:C:88:LYS:HG2	2.21	0.40
1:B:172:GLU:OE2	2:B:414:HOH:O	2.22	0.40
1:B:178:LEU:HD12	1:B:179:VAL:N	2.35	0.40
1:B:284:GLY:O	1:B:285:PRO:C	2.59	0.40
1:D:257:LYS:NZ	2:D:510:HOH:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD23	1:B:141:HIS:CD2	2.56	0.40
1:B:173:ASP:HA	1:B:174:PRO:HD3	1.97	0.40
1:B:49:SER:HA	1:B:60:HIS:O	2.21	0.40
1:B:98:LEU:HD11	1:B:164:PHE:CE1	2.56	0.40
1:C:129:GLY:H	1:C:151:GLU:HB2	1.85	0.40
1:D:125:LEU:HD12	1:D:126:VAL:N	2.34	0.40
1:D:238:LEU:HD21	1:D:329:ILE:HD11	2.03	0.40
1:A:239:TRP:O	1:A:240:LEU:HD23	2.21	0.40
1:C:105:ALA:O	1:C:109:MSE:HG2	2.20	0.40
1:C:183:GLY:HA2	1:C:186:PHE:HB2	2.04	0.40
1:D:159:VAL:HG13	1:D:163:PHE:HD2	1.86	0.40
1:D:329:ILE:O	1:D:330:GLU:C	2.60	0.40
1:A:246:GLU:OE2	1:A:328:VAL:HG11	2.22	0.40
1:A:72:LYS:O	1:C:51:MSE:HE2	2.22	0.40
1:B:327:LYS:HD3	1:B:327:LYS:C	2.41	0.40
1:C:82:GLN:HA	1:C:82:GLN:NE2	2.37	0.40
1:D:218:PHE:O	1:D:221:VAL:N	2.55	0.40
1:A:88:LYS:O	1:A:99:THR:HA	2.22	0.40
1:B:160:SER:HB3	1:B:167:VAL:HG21	2.04	0.40
1:B:54:MSE:HG3	1:B:55:TRP:CZ3	2.57	0.40
1:A:139:ALA:HA	1:A:175:ARG:NH2	2.35	0.40
1:A:64:VAL:HG12	1:A:65:GLU:N	2.36	0.40
1:A:301:SER:HB3	1:A:304:ASN:OD1	2.21	0.40
1:B:236:GLU:HB3	1:B:237:SER:H	1.73	0.40
1:C:215:LYS:N	1:C:216:PRO:CD	2.84	0.40
1:C:244:ILE:HG22	1:C:248:ILE:HD12	2.02	0.40
1:C:52:SER:HA	1:C:53:PRO:HD3	1.94	0.40
1:A:76:GLN:HB2	1:A:93:ASP:CG	2.42	0.40
1:B:127:ILE:HD11	1:B:187:LEU:CD2	2.52	0.40
1:C:152:ILE:CG2	1:C:153:ASP:N	2.84	0.40
1:C:329:ILE:O	1:C:329:ILE:HG22	2.22	0.40
1:C:52:SER:HB3	1:C:55:TRP:CE2	2.57	0.40
1:D:161:LYS:HA	1:D:168:ALA:HB2	2.03	0.40
1:A:184:VAL:CG2	1:A:185:ALA:N	2.85	0.40
1:B:231:VAL:CG1	1:B:280:CYS:HB2	2.52	0.40
1:D:157:VAL:HG13	1:D:171:TYR:CZ	2.56	0.40
1:D:179:VAL:CG1	1:D:180:ILE:N	2.84	0.40
1:A:157:VAL:CG1	1:A:161:LYS:HE3	2.50	0.40
1:A:170:GLY:O	1:A:172:GLU:N	2.54	0.40
1:A:182:ASP:O	1:A:185:ALA:HB3	2.21	0.40
1:A:243:ASP:CG	1:A:244:ILE:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:O	1:A:276:GLY:HA2	2.22	0.40
1:A:69:PHE:CD1	1:A:69:PHE:C	2.95	0.40
1:B:200:VAL:HG12	1:B:200:VAL:O	2.22	0.40
1:B:292:PRO:HB3	1:B:315:HIS:CE1	2.57	0.40
1:C:311:ASN:H	1:C:314:ILE:HG22	1.87	0.40
1:D:164:PHE:HB2	1:D:167:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	288/334 (86%)	244 (85%)	33 (12%)	11 (4%)	3	7
1	1-B	281/334 (84%)	241 (86%)	33 (12%)	7 (2%)	5	14
1	1-C	288/334 (86%)	249 (86%)	29 (10%)	10 (4%)	3	8
1	1-D	281/334 (84%)	227 (81%)	44 (16%)	10 (4%)	3	7
1	2-A	288/334 (86%)	243 (84%)	32 (11%)	13 (4%)	2	5
1	2-B	281/334 (84%)	245 (87%)	31 (11%)	5 (2%)	8	21
1	2-C	288/334 (86%)	242 (84%)	33 (12%)	13 (4%)	2	5
1	2-D	281/334 (84%)	246 (88%)	28 (10%)	7 (2%)	5	14
1	3-A	288/334 (86%)	243 (84%)	31 (11%)	14 (5%)	2	4
1	3-B	281/334 (84%)	217 (77%)	47 (17%)	17 (6%)	1	2
1	3-C	288/334 (86%)	229 (80%)	46 (16%)	13 (4%)	2	5
1	3-D	281/334 (84%)	244 (87%)	33 (12%)	4 (1%)	11	28
1	4-A	288/334 (86%)	242 (84%)	31 (11%)	15 (5%)	2	3
1	4-B	281/334 (84%)	243 (86%)	28 (10%)	10 (4%)	3	7
1	4-C	288/334 (86%)	243 (84%)	30 (10%)	15 (5%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-D	281/334 (84%)	233 (83%)	40 (14%)	8 (3%)	5	11
1	5-A	288/334 (86%)	232 (81%)	44 (15%)	12 (4%)	3	5
1	5-B	281/334 (84%)	242 (86%)	33 (12%)	6 (2%)	7	18
1	5-C	288/334 (86%)	233 (81%)	42 (15%)	13 (4%)	2	5
1	5-D	281/334 (84%)	225 (80%)	42 (15%)	14 (5%)	2	4
1	6-A	288/334 (86%)	241 (84%)	31 (11%)	16 (6%)	2	3
1	6-B	281/334 (84%)	234 (83%)	35 (12%)	12 (4%)	2	5
1	6-C	288/334 (86%)	238 (83%)	36 (12%)	14 (5%)	2	4
1	6-D	281/334 (84%)	234 (83%)	35 (12%)	12 (4%)	2	5
1	7-A	288/334 (86%)	234 (81%)	39 (14%)	15 (5%)	2	3
1	7-B	281/334 (84%)	247 (88%)	32 (11%)	2 (1%)	22	46
1	7-C	288/334 (86%)	248 (86%)	25 (9%)	15 (5%)	2	3
1	7-D	281/334 (84%)	235 (84%)	36 (13%)	10 (4%)	3	7
1	8-A	288/334 (86%)	249 (86%)	27 (9%)	12 (4%)	3	5
1	8-B	281/334 (84%)	229 (82%)	41 (15%)	11 (4%)	3	6
1	8-C	288/334 (86%)	242 (84%)	37 (13%)	9 (3%)	4	9
1	8-D	281/334 (84%)	240 (85%)	36 (13%)	5 (2%)	8	21
All	All	9104/10688 (85%)	7634 (84%)	1120 (12%)	350 (4%)	3	7

All (350) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	69	PHE
1	1-A	298	GLU
1	1-B	167	VAL
1	1-B	236	GLU
1	1-C	165	PRO
1	1-C	236	GLU
1	1-D	172	GLU
1	1-D	312	ALA
1	2-A	93	ASP
1	2-B	236	GLU
1	2-C	191	ALA
1	2-C	297	ASP
1	2-D	131	ASP
1	2-D	191	ALA

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Mol	Chain	Res	Type
1	3-A	45	PRO
1	3-A	84	ALA
1	3-A	93	ASP
1	3-B	130	GLY
1	3-B	191	ALA
1	3-C	310	TYR
1	4-A	298	GLU
1	4-A	302	LYS
1	4-A	312	ALA
1	4-B	129	GLY
1	4-B	130	GLY
1	4-B	150	CYS
1	4-B	167	VAL
1	4-B	236	GLU
1	4-C	73	SER
1	4-C	192	GLU
1	4-C	206	ILE
1	4-C	214	GLU
1	4-C	215	LYS
1	4-C	236	GLU
1	4-D	202	SER
1	5-A	58	GLU
1	5-A	131	ASP
1	5-B	236	GLU
1	5-B	244	ILE
1	5-C	142	ALA
1	5-C	143	SER
1	5-D	323	SER
1	6-A	165	PRO
1	6-A	202	SER
1	6-B	151	GLU
1	6-B	194	SER
1	6-B	236	GLU
1	6-C	131	ASP
1	6-C	203	SER
1	6-C	236	GLU
1	6-D	131	ASP
1	6-D	329	ILE
1	7-A	93	ASP
1	7-A	183	GLY
1	7-A	318	ALA
1	7-B	131	ASP

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Mol	Chain	Res	Type
1	7-C	165	PRO
1	7-C	236	GLU
1	7-C	323	SER
1	7-D	131	ASP
1	8-A	131	ASP
1	8-A	298	GLU
1	8-A	302	LYS
1	8-B	236	GLU
1	8-C	226	ARG
1	8-D	52	SER
1	8-D	131	ASP
1	1-A	129	GLY
1	1-A	149	MSE
1	1-A	165	PRO
1	1-A	236	GLU
1	1-A	302	LYS
1	1-B	73	SER
1	1-B	131	ASP
1	1-C	298	GLU
1	1-D	142	ALA
1	1-D	323	SER
1	1-D	324	PHE
1	1-D	329	ILE
1	2-A	298	GLU
1	2-A	302	LYS
1	2-A	329	ILE
1	2-B	131	ASP
1	2-B	310	TYR
1	2-C	131	ASP
1	2-C	296	ILE
1	2-C	302	LYS
1	2-D	129	GLY
1	2-D	275	ILE
1	3-A	46	GLY
1	3-A	130	GLY
1	3-A	192	GLU
1	3-A	298	GLU
1	3-B	67	VAL
1	3-B	127	ILE
1	3-B	129	GLY
1	3-B	212	LEU
1	3-C	269	THR

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Mol	Chain	Res	Type
1	3-C	273	GLY
1	3-C	298	GLU
1	4-A	129	GLY
1	4-B	72	LYS
1	4-B	131	ASP
1	4-C	165	PRO
1	4-C	182	ASP
1	4-C	298	GLU
1	4-C	302	LYS
1	4-D	130	GLY
1	5-A	95	VAL
1	5-A	128	GLY
1	5-A	165	PRO
1	5-A	312	ALA
1	5-B	131	ASP
1	5-B	167	VAL
1	5-C	110	ILE
1	5-C	131	ASP
1	5-C	298	GLU
1	5-C	302	LYS
1	5-D	41	SER
1	5-D	110	ILE
1	5-D	130	GLY
1	5-D	202	SER
1	6-A	180	ILE
1	6-A	203	SER
1	6-A	243	ASP
1	6-A	258	GLY
1	6-A	283	GLU
1	6-A	298	GLU
1	6-A	301	SER
1	6-A	302	LYS
1	6-B	41	SER
1	6-B	129	GLY
1	6-B	131	ASP
1	6-B	241	HIS
1	6-C	298	GLU
1	6-D	39	CYS
1	6-D	73	SER
1	6-D	130	GLY
1	6-D	212	LEU
1	7-A	140	ARG

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Mol	Chain	Res	Type
1	7-A	142	ALA
1	7-A	206	ILE
1	7-A	236	GLU
1	7-A	283	GLU
1	7-A	297	ASP
1	7-C	69	PHE
1	7-C	298	GLU
1	7-D	130	GLY
1	7-D	236	GLU
1	7-D	272	SER
1	8-A	165	PRO
1	8-B	131	ASP
1	8-B	255	ILE
1	8-B	279	LEU
1	8-C	131	ASP
1	8-C	298	GLU
1	1-C	166	ASP
1	1-C	182	ASP
1	1-D	236	GLU
1	2-C	93	ASP
1	2-D	41	SER
1	3-A	69	PHE
1	3-A	302	LYS
1	3-B	131	ASP
1	3-B	172	GLU
1	3-B	173	ASP
1	3-B	208	PRO
1	3-B	324	PHE
1	3-C	272	SER
1	3-D	52	SER
1	3-D	236	GLU
1	3-D	292	PRO
1	4-A	131	ASP
1	4-A	236	GLU
1	4-B	328	VAL
1	4-D	114	PRO
1	4-D	131	ASP
1	4-D	236	GLU
1	5-A	236	GLU
1	5-A	289	PHE
1	5-C	111	THR
1	5-D	268	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5-D	329	ILE
1	6-A	114	PRO
1	6-A	171	TYR
1	6-A	214	GLU
1	6-C	101	ARG
1	6-C	302	LYS
1	6-D	139	ALA
1	7-A	114	PRO
1	7-A	202	SER
1	7-C	272	SER
1	7-C	302	LYS
1	7-D	73	SER
1	7-D	312	ALA
1	7-D	318	ALA
1	8-A	69	PHE
1	8-A	271	PRO
1	8-B	166	ASP
1	8-C	129	GLY
1	8-C	302	LYS
1	8-D	41	SER
1	1-A	300	SER
1	1-C	114	PRO
1	1-D	186	PHE
1	2-A	152	ILE
1	2-A	182	ASP
1	2-B	173	ASP
1	2-C	105	ALA
1	2-C	298	GLU
1	3-A	128	GLY
1	3-B	120	ASN
1	3-B	174	PRO
1	3-C	186	PHE
1	4-A	114	PRO
1	4-A	258	GLY
1	4-C	166	ASP
1	4-C	204	ASP
1	4-D	66	LYS
1	4-D	96	ILE
1	5-C	120	ASN
1	5-C	165	PRO
1	5-C	166	ASP
1	5-D	58	GLU

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Mol	Chain	Res	Type
1	5-D	246	GLU
1	6-B	295	PRO
1	6-C	296	ILE
1	6-D	236	GLU
1	7-A	321	LEU
1	7-C	114	PRO
1	7-C	209	ALA
1	7-C	255	ILE
1	8-A	236	GLU
1	8-B	167	VAL
1	8-B	188	LYS
1	8-C	191	ALA
1	8-D	114	PRO
1	1-A	202	SER
1	1-B	292	PRO
1	1-C	131	ASP
1	1-C	160	SER
1	1-D	42	THR
1	2-A	192	GLU
1	2-C	114	PRO
1	2-C	166	ASP
1	2-D	292	PRO
1	3-B	41	SER
1	3-C	59	ALA
1	3-C	243	ASP
1	3-C	296	ILE
1	3-D	290	LYS
1	4-A	180	ILE
1	4-A	272	SER
1	4-A	306	PRO
1	4-A	311	ASN
1	4-B	105	ALA
1	4-C	120	ASN
1	4-D	105	ALA
1	5-A	114	PRO
1	5-B	166	ASP
1	5-C	52	SER
1	5-D	66	LYS
1	5-D	203	SER
1	6-A	192	GLU
1	6-B	327	LYS
1	6-C	114	PRO

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Mol	Chain	Res	Type
1	6-C	297	ASP
1	6-D	272	SER
1	6-D	323	SER
1	7-C	202	SER
1	7-D	120	ASN
1	8-A	255	ILE
1	8-A	268	PRO
1	8-B	268	PRO
1	8-C	202	SER
1	8-D	286	ASP
1	1-A	301	SER
1	1-B	114	PRO
1	1-D	46	GLY
1	2-A	69	PHE
1	2-A	130	GLY
1	2-C	182	ASP
1	3-A	131	ASP
1	3-B	180	ILE
1	3-B	202	SER
1	3-C	255	ILE
1	3-C	268	PRO
1	4-A	318	ALA
1	4-B	292	PRO
1	5-A	306	PRO
1	5-B	114	PRO
1	5-D	45	PRO
1	6-B	98	LEU
1	6-B	142	ALA
1	6-C	102	ASP
1	6-C	312	ALA
1	6-D	327	LYS
1	7-A	289	PHE
1	7-C	207	GLY
1	7-D	204	ASP
1	8-A	212	LEU
1	8-A	258	GLY
1	8-C	69	PHE
1	1-B	258	GLY
1	2-A	114	PRO
1	2-A	258	GLY
1	2-C	165	PRO
1	3-A	296	ILE

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Mol	Chain	Res	Type
1	4-C	205	PRO
1	5-D	167	VAL
1	6-C	268	PRO
1	7-C	205	PRO
1	8-A	152	ILE
1	1-C	129	GLY
1	2-C	244	ILE
1	3-A	114	PRO
1	3-B	152	ILE
1	3-C	114	PRO
1	4-C	114	PRO
1	5-A	96	ILE
1	5-D	292	PRO
1	6-A	179	VAL
1	6-B	144	ILE
1	6-C	244	ILE
1	7-A	120	ASN
1	7-A	130	GLY
1	1-C	205	PRO
1	2-A	296	ILE
1	2-B	268	PRO
1	3-C	170	GLY
1	4-A	130	GLY
1	4-A	296	ILE
1	5-A	258	GLY
1	6-D	206	ILE
1	7-C	329	ILE
1	7-D	206	ILE
1	8-B	129	GLY
1	1-A	258	GLY
1	2-D	274	VAL
1	3-A	258	GLY
1	5-C	114	PRO
1	5-C	292	PRO
1	6-A	296	ILE
1	7-B	329	ILE
1	7-C	167	VAL
1	8-B	52	SER
1	8-B	275	ILE
1	8-C	130	GLY
1	2-A	165	PRO
1	6-C	130	GLY

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	249/276 (90%)	245 (98%)	4 (2%)	62	85
1	1-B	243/276 (88%)	234 (96%)	9 (4%)	34	63
1	1-C	249/276 (90%)	244 (98%)	5 (2%)	55	81
1	1-D	243/276 (88%)	233 (96%)	10 (4%)	30	59
1	2-A	249/276 (90%)	242 (97%)	7 (3%)	43	73
1	2-B	243/276 (88%)	235 (97%)	8 (3%)	38	67
1	2-C	249/276 (90%)	240 (96%)	9 (4%)	35	64
1	2-D	243/276 (88%)	234 (96%)	9 (4%)	34	63
1	3-A	249/276 (90%)	240 (96%)	9 (4%)	35	64
1	3-B	243/276 (88%)	232 (96%)	11 (4%)	27	55
1	3-C	249/276 (90%)	237 (95%)	12 (5%)	25	53
1	3-D	243/276 (88%)	235 (97%)	8 (3%)	38	67
1	4-A	249/276 (90%)	237 (95%)	12 (5%)	25	53
1	4-B	243/276 (88%)	231 (95%)	12 (5%)	25	52
1	4-C	249/276 (90%)	239 (96%)	10 (4%)	31	60
1	4-D	243/276 (88%)	238 (98%)	5 (2%)	53	80
1	5-A	249/276 (90%)	234 (94%)	15 (6%)	19	42
1	5-B	243/276 (88%)	228 (94%)	15 (6%)	18	40
1	5-C	249/276 (90%)	240 (96%)	9 (4%)	35	64
1	5-D	243/276 (88%)	228 (94%)	15 (6%)	18	40
1	6-A	249/276 (90%)	236 (95%)	13 (5%)	23	49
1	6-B	243/276 (88%)	231 (95%)	12 (5%)	25	52
1	6-C	249/276 (90%)	238 (96%)	11 (4%)	28	56
1	6-D	243/276 (88%)	233 (96%)	10 (4%)	30	59
1	7-A	249/276 (90%)	231 (93%)	18 (7%)	14	34
1	7-B	243/276 (88%)	227 (93%)	16 (7%)	16	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-C	249/276 (90%)	244 (98%)	5 (2%)	55	81
1	7-D	243/276 (88%)	236 (97%)	7 (3%)	42	71
1	8-A	249/276 (90%)	241 (97%)	8 (3%)	39	68
1	8-B	243/276 (88%)	227 (93%)	16 (7%)	16	38
1	8-C	249/276 (90%)	241 (97%)	8 (3%)	39	68
1	8-D	243/276 (88%)	231 (95%)	12 (5%)	25	52
All	All	7872/8832 (89%)	7542 (96%)	330 (4%)	30	58

All (330) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	115	LEU
1	1-A	260	VAL
1	1-A	264	TRP
1	1-A	304	ASN
1	1-B	60	HIS
1	1-B	113	LEU
1	1-B	115	LEU
1	1-B	162	GLN
1	1-B	167	VAL
1	1-B	233	THR
1	1-B	241	HIS
1	1-B	264	TRP
1	1-B	286	ASP
1	1-C	77	ASP
1	1-C	204	ASP
1	1-C	234	GLN
1	1-C	236	GLU
1	1-C	264	TRP
1	1-D	97	GLN
1	1-D	99	THR
1	1-D	109	MSE
1	1-D	116	CYS
1	1-D	162	GLN
1	1-D	166	ASP
1	1-D	226	ARG
1	1-D	234	GLN
1	1-D	264	TRP
1	1-D	330	GLU
1	2-A	54	MSE

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Mol	Chain	Res	Type
1	2-A	97	GLN
1	2-A	104	CYS
1	2-A	107	GLN
1	2-A	148	ASP
1	2-A	149	MSE
1	2-A	264	TRP
1	2-B	48	PHE
1	2-B	60	HIS
1	2-B	115	LEU
1	2-B	226	ARG
1	2-B	233	THR
1	2-B	264	TRP
1	2-B	272	SER
1	2-B	311	ASN
1	2-C	74	ASP
1	2-C	98	LEU
1	2-C	234	GLN
1	2-C	261	ASN
1	2-C	264	TRP
1	2-C	278	MSE
1	2-C	283	GLU
1	2-C	293	LEU
1	2-C	327	LYS
1	2-D	97	GLN
1	2-D	131	ASP
1	2-D	155	MSE
1	2-D	166	ASP
1	2-D	234	GLN
1	2-D	264	TRP
1	2-D	278	MSE
1	2-D	286	ASP
1	2-D	330	GLU
1	3-A	54	MSE
1	3-A	97	GLN
1	3-A	107	GLN
1	3-A	115	LEU
1	3-A	204	ASP
1	3-A	226	ARG
1	3-A	238	LEU
1	3-A	241	HIS
1	3-A	330	GLU
1	3-B	54	MSE

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Mol	Chain	Res	Type
1	3-B	60	HIS
1	3-B	74	ASP
1	3-B	76	GLN
1	3-B	97	GLN
1	3-B	115	LEU
1	3-B	166	ASP
1	3-B	234	GLN
1	3-B	241	HIS
1	3-B	264	TRP
1	3-B	316	SER
1	3-C	58	GLU
1	3-C	65	GLU
1	3-C	93	ASP
1	3-C	98	LEU
1	3-C	140	ARG
1	3-C	146	GLN
1	3-C	155	MSE
1	3-C	226	ARG
1	3-C	236	GLU
1	3-C	264	TRP
1	3-C	265	THR
1	3-C	311	ASN
1	3-D	51	MSE
1	3-D	68	LEU
1	3-D	162	GLN
1	3-D	166	ASP
1	3-D	226	ARG
1	3-D	234	GLN
1	3-D	264	TRP
1	3-D	286	ASP
1	4-A	66	LYS
1	4-A	97	GLN
1	4-A	115	LEU
1	4-A	122	LYS
1	4-A	187	LEU
1	4-A	204	ASP
1	4-A	211	GLU
1	4-A	239	TRP
1	4-A	241	HIS
1	4-A	264	TRP
1	4-A	296	ILE
1	4-A	306	PRO

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Mol	Chain	Res	Type
1	4-B	60	HIS
1	4-B	76	GLN
1	4-B	97	GLN
1	4-B	115	LEU
1	4-B	153	ASP
1	4-B	167	VAL
1	4-B	226	ARG
1	4-B	233	THR
1	4-B	241	HIS
1	4-B	264	TRP
1	4-B	278	MSE
1	4-B	324	PHE
1	4-C	48	PHE
1	4-C	60	HIS
1	4-C	220	SER
1	4-C	234	GLN
1	4-C	236	GLU
1	4-C	247	ASP
1	4-C	253	ARG
1	4-C	264	TRP
1	4-C	268	PRO
1	4-C	298	GLU
1	4-D	97	GLN
1	4-D	131	ASP
1	4-D	166	ASP
1	4-D	226	ARG
1	4-D	264	TRP
1	5-A	50	GLU
1	5-A	51	MSE
1	5-A	54	MSE
1	5-A	60	HIS
1	5-A	97	GLN
1	5-A	211	GLU
1	5-A	223	ARG
1	5-A	234	GLN
1	5-A	241	HIS
1	5-A	260	VAL
1	5-A	264	TRP
1	5-A	296	ILE
1	5-A	298	GLU
1	5-A	306	PRO
1	5-A	329	ILE

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Mol	Chain	Res	Type
1	5-B	60	HIS
1	5-B	113	LEU
1	5-B	115	LEU
1	5-B	116	CYS
1	5-B	149	MSE
1	5-B	166	ASP
1	5-B	167	VAL
1	5-B	220	SER
1	5-B	226	ARG
1	5-B	234	GLN
1	5-B	240	LEU
1	5-B	242	MSE
1	5-B	264	TRP
1	5-B	293	LEU
1	5-B	327	LYS
1	5-C	51	MSE
1	5-C	98	LEU
1	5-C	109	MSE
1	5-C	131	ASP
1	5-C	241	HIS
1	5-C	242	MSE
1	5-C	253	ARG
1	5-C	264	TRP
1	5-C	293	LEU
1	5-D	55	TRP
1	5-D	115	LEU
1	5-D	131	ASP
1	5-D	158	ASP
1	5-D	166	ASP
1	5-D	226	ARG
1	5-D	234	GLN
1	5-D	247	ASP
1	5-D	261	ASN
1	5-D	264	TRP
1	5-D	267	VAL
1	5-D	268	PRO
1	5-D	311	ASN
1	5-D	324	PHE
1	5-D	330	GLU
1	6-A	51	MSE
1	6-A	97	GLN
1	6-A	204	ASP

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Mol	Chain	Res	Type
1	6-A	234	GLN
1	6-A	241	HIS
1	6-A	259	SER
1	6-A	260	VAL
1	6-A	261	ASN
1	6-A	264	TRP
1	6-A	296	ILE
1	6-A	298	GLU
1	6-A	310	TYR
1	6-A	330	GLU
1	6-B	51	MSE
1	6-B	73	SER
1	6-B	97	GLN
1	6-B	115	LEU
1	6-B	131	ASP
1	6-B	214	GLU
1	6-B	219	GLN
1	6-B	223	ARG
1	6-B	253	ARG
1	6-B	264	TRP
1	6-B	274	VAL
1	6-B	293	LEU
1	6-C	60	HIS
1	6-C	99	THR
1	6-C	107	GLN
1	6-C	109	MSE
1	6-C	149	MSE
1	6-C	242	MSE
1	6-C	264	TRP
1	6-C	278	MSE
1	6-C	280	CYS
1	6-C	298	GLU
1	6-C	313	GLU
1	6-D	97	GLN
1	6-D	115	LEU
1	6-D	131	ASP
1	6-D	166	ASP
1	6-D	226	ARG
1	6-D	231	VAL
1	6-D	264	TRP
1	6-D	293	LEU
1	6-D	324	PHE

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Mol	Chain	Res	Type
1	6-D	330	GLU
1	7-A	51	MSE
1	7-A	88	LYS
1	7-A	97	GLN
1	7-A	107	GLN
1	7-A	115	LEU
1	7-A	117	SER
1	7-A	125	LEU
1	7-A	136	ARG
1	7-A	192	GLU
1	7-A	204	ASP
1	7-A	233	THR
1	7-A	264	TRP
1	7-A	265	THR
1	7-A	278	MSE
1	7-A	290	LYS
1	7-A	308	LYS
1	7-A	314	ILE
1	7-A	321	LEU
1	7-B	52	SER
1	7-B	60	HIS
1	7-B	74	ASP
1	7-B	97	GLN
1	7-B	107	GLN
1	7-B	109	MSE
1	7-B	115	LEU
1	7-B	149	MSE
1	7-B	166	ASP
1	7-B	187	LEU
1	7-B	221	VAL
1	7-B	226	ARG
1	7-B	234	GLN
1	7-B	264	TRP
1	7-B	265	THR
1	7-B	314	ILE
1	7-C	77	ASP
1	7-C	204	ASP
1	7-C	234	GLN
1	7-C	236	GLU
1	7-C	297	ASP
1	7-D	93	ASP
1	7-D	131	ASP

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Mol	Chain	Res	Type
1	7-D	166	ASP
1	7-D	226	ARG
1	7-D	264	TRP
1	7-D	266	SER
1	7-D	320	CYS
1	8-A	60	HIS
1	8-A	99	THR
1	8-A	115	LEU
1	8-A	226	ARG
1	8-A	234	GLN
1	8-A	241	HIS
1	8-A	264	TRP
1	8-A	265	THR
1	8-B	60	HIS
1	8-B	66	LYS
1	8-B	83	SER
1	8-B	115	LEU
1	8-B	149	MSE
1	8-B	166	ASP
1	8-B	167	VAL
1	8-B	178	LEU
1	8-B	189	ASN
1	8-B	220	SER
1	8-B	226	ARG
1	8-B	234	GLN
1	8-B	241	HIS
1	8-B	264	TRP
1	8-B	274	VAL
1	8-B	278	MSE
1	8-C	51	MSE
1	8-C	109	MSE
1	8-C	236	GLU
1	8-C	261	ASN
1	8-C	264	TRP
1	8-C	298	GLU
1	8-C	308	LYS
1	8-C	321	LEU
1	8-D	51	MSE
1	8-D	68	LEU
1	8-D	77	ASP
1	8-D	111	THR
1	8-D	166	ASP

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Mol	Chain	Res	Type
1	8-D	214	GLU
1	8-D	226	ARG
1	8-D	234	GLN
1	8-D	264	TRP
1	8-D	278	MSE
1	8-D	286	ASP
1	8-D	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	70	GLN
1	1-A	82	GLN
1	1-A	97	GLN
1	1-A	241	HIS
1	1-B	82	GLN
1	1-B	120	ASN
1	1-B	146	GLN
1	1-B	234	GLN
1	1-C	70	GLN
1	1-C	82	GLN
1	1-C	107	GLN
1	1-C	162	GLN
1	1-C	241	HIS
1	1-C	261	ASN
1	1-C	304	ASN
1	1-D	60	HIS
1	1-D	70	GLN
1	1-D	120	ASN
1	1-D	146	GLN
1	1-D	162	GLN
1	1-D	234	GLN
1	1-D	261	ASN
1	2-A	70	GLN
1	2-A	82	GLN
1	2-A	97	GLN
1	2-A	107	GLN
1	2-A	241	HIS
1	2-A	251	ASN
1	2-A	261	ASN
1	2-B	120	ASN
1	2-B	146	GLN

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Mol	Chain	Res	Type
1	2-B	162	GLN
1	2-C	70	GLN
1	2-C	82	GLN
1	2-C	97	GLN
1	2-C	241	HIS
1	2-C	304	ASN
1	2-D	60	HIS
1	2-D	97	GLN
1	2-D	120	ASN
1	2-D	146	GLN
1	2-D	162	GLN
1	2-D	261	ASN
1	3-A	97	GLN
1	3-A	146	GLN
1	3-A	241	HIS
1	3-A	251	ASN
1	3-B	146	GLN
1	3-C	82	GLN
1	3-C	234	GLN
1	3-C	241	HIS
1	3-C	261	ASN
1	3-C	304	ASN
1	3-C	315	HIS
1	3-D	97	GLN
1	3-D	146	GLN
1	3-D	162	GLN
1	3-D	234	GLN
1	3-D	261	ASN
1	3-D	291	HIS
1	4-A	70	GLN
1	4-A	97	GLN
1	4-A	162	GLN
1	4-A	251	ASN
1	4-A	261	ASN
1	4-A	304	ASN
1	4-B	70	GLN
1	4-B	120	ASN
1	4-B	141	HIS
1	4-B	146	GLN
1	4-B	162	GLN
1	4-B	234	GLN
1	4-B	241	HIS

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Mol	Chain	Res	Type
1	4-C	107	GLN
1	4-C	219	GLN
1	4-C	241	HIS
1	4-C	261	ASN
1	4-C	304	ASN
1	4-D	60	HIS
1	4-D	97	GLN
1	4-D	162	GLN
1	4-D	234	GLN
1	4-D	261	ASN
1	5-A	70	GLN
1	5-A	76	GLN
1	5-A	97	GLN
1	5-A	241	HIS
1	5-A	251	ASN
1	5-B	76	GLN
1	5-B	97	GLN
1	5-B	107	GLN
1	5-B	120	ASN
1	5-C	70	GLN
1	5-C	82	GLN
1	5-C	251	ASN
1	5-C	261	ASN
1	5-C	304	ASN
1	5-D	60	HIS
1	5-D	70	GLN
1	5-D	97	GLN
1	5-D	177	ASN
1	5-D	251	ASN
1	5-D	311	ASN
1	6-A	70	GLN
1	6-A	162	GLN
1	6-A	261	ASN
1	6-B	70	GLN
1	6-B	82	GLN
1	6-B	97	GLN
1	6-B	146	GLN
1	6-B	177	ASN
1	6-B	234	GLN
1	6-C	76	GLN
1	6-C	97	GLN
1	6-C	146	GLN

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Mol	Chain	Res	Type
1	6-C	241	HIS
1	6-C	261	ASN
1	6-C	304	ASN
1	6-D	60	HIS
1	6-D	70	GLN
1	6-D	120	ASN
1	6-D	146	GLN
1	6-D	162	GLN
1	6-D	251	ASN
1	6-D	261	ASN
1	7-A	70	GLN
1	7-A	82	GLN
1	7-A	97	GLN
1	7-A	234	GLN
1	7-A	241	HIS
1	7-B	97	GLN
1	7-B	120	ASN
1	7-B	146	GLN
1	7-C	82	GLN
1	7-C	107	GLN
1	7-C	146	GLN
1	7-C	162	GLN
1	7-C	241	HIS
1	7-C	261	ASN
1	7-C	304	ASN
1	7-D	60	HIS
1	7-D	97	GLN
1	7-D	141	HIS
1	7-D	162	GLN
1	8-A	70	GLN
1	8-A	97	GLN
1	8-A	146	GLN
1	8-A	251	ASN
1	8-A	261	ASN
1	8-B	120	ASN
1	8-B	146	GLN
1	8-C	70	GLN
1	8-C	82	GLN
1	8-C	241	HIS
1	8-C	304	ASN
1	8-D	60	HIS
1	8-D	97	GLN

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Mol	Chain	Res	Type
1	8-D	120	ASN
1	8-D	146	GLN
1	8-D	162	GLN
1	8-D	189	ASN
1	8-D	261	ASN
1	8-D	291	HIS

### 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	1-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	1-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	1-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	2-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	2-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	2-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	2-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	3-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	3-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	3-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	3-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	4-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	4-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	4-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	4-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	5-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	5-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	5-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	5-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	6-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	6-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	6-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	6-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	7-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	7-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	7-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	7-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
1	8-A	283/334 (84%)	0.23	23 (8%) 12 10	12, 35, 82, 101	283 (100%)
1	8-B	278/334 (83%)	-0.12	9 (3%) 47 48	10, 30, 62, 100	278 (100%)
1	8-C	283/334 (84%)	0.33	36 (12%) 3 3	15, 35, 80, 112	283 (100%)
1	8-D	278/334 (83%)	0.06	12 (4%) 35 33	11, 31, 70, 104	278 (100%)
All	All	8976/10688 (83%)	0.13	640 (7%) 15 14	10, 33, 75, 112	8976 (100%)

All (640) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-C	207	GLY	10.5
1	2-C	207	GLY	10.5
1	3-C	207	GLY	10.5
1	4-C	207	GLY	10.5
1	5-C	207	GLY	10.5
1	6-C	207	GLY	10.5
1	7-C	207	GLY	10.5
1	8-C	207	GLY	10.5
1	1-A	206	ILE	6.2
1	2-A	206	ILE	6.2
1	3-A	206	ILE	6.2
1	4-A	206	ILE	6.2
1	5-A	206	ILE	6.2
1	6-A	206	ILE	6.2
1	7-A	206	ILE	6.2
1	8-A	206	ILE	6.2
1	1-C	166	ASP	5.8
1	2-C	166	ASP	5.8
1	3-C	166	ASP	5.8
1	4-C	166	ASP	5.8
1	5-C	166	ASP	5.8
1	6-C	166	ASP	5.8
1	7-C	166	ASP	5.8
1	8-C	166	ASP	5.8
1	1-C	301	SER	5.7
1	2-C	301	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	3-C	301	SER	5.7
1	4-C	301	SER	5.7
1	5-C	301	SER	5.7
1	6-C	301	SER	5.7
1	7-C	301	SER	5.7
1	8-C	301	SER	5.7
1	1-A	166	ASP	5.5
1	2-A	166	ASP	5.5
1	3-A	166	ASP	5.5
1	4-A	166	ASP	5.5
1	5-A	166	ASP	5.5
1	6-A	166	ASP	5.5
1	7-A	166	ASP	5.5
1	8-A	166	ASP	5.5
1	1-C	206	ILE	5.4
1	2-C	206	ILE	5.4
1	3-C	206	ILE	5.4
1	4-C	206	ILE	5.4
1	5-C	206	ILE	5.4
1	6-C	206	ILE	5.4
1	7-C	206	ILE	5.4
1	8-C	206	ILE	5.4
1	1-C	205	PRO	5.0
1	2-C	205	PRO	5.0
1	3-C	205	PRO	5.0
1	4-C	205	PRO	5.0
1	5-C	205	PRO	5.0
1	6-C	205	PRO	5.0
1	7-C	205	PRO	5.0
1	8-C	205	PRO	5.0
1	1-C	208	PRO	4.5
1	2-C	208	PRO	4.5
1	3-C	208	PRO	4.5
1	4-C	208	PRO	4.5
1	5-C	208	PRO	4.5
1	6-C	208	PRO	4.5
1	7-C	208	PRO	4.5
1	8-C	208	PRO	4.5
1	1-C	298	GLU	4.2
1	2-C	298	GLU	4.2
1	3-C	298	GLU	4.2
1	4-C	298	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	5-C	298	GLU	4.2
1	6-C	298	GLU	4.2
1	7-C	298	GLU	4.2
1	8-C	298	GLU	4.2
1	1-C	169	ILE	4.2
1	2-C	169	ILE	4.2
1	3-C	169	ILE	4.2
1	4-C	169	ILE	4.2
1	5-C	169	ILE	4.2
1	6-C	169	ILE	4.2
1	7-C	169	ILE	4.2
1	8-C	169	ILE	4.2
1	1-C	227	PRO	4.0
1	2-C	227	PRO	4.0
1	3-C	227	PRO	4.0
1	4-C	227	PRO	4.0
1	5-C	227	PRO	4.0
1	6-C	227	PRO	4.0
1	7-C	227	PRO	4.0
1	8-C	227	PRO	4.0
1	1-D	39	CYS	4.0
1	2-D	39	CYS	4.0
1	3-D	39	CYS	4.0
1	4-D	39	CYS	4.0
1	5-D	39	CYS	4.0
1	6-D	39	CYS	4.0
1	7-D	39	CYS	4.0
1	8-D	39	CYS	4.0
1	1-D	129	GLY	3.9
1	2-D	129	GLY	3.9
1	3-D	129	GLY	3.9
1	4-D	129	GLY	3.9
1	5-D	129	GLY	3.9
1	6-D	129	GLY	3.9
1	7-D	129	GLY	3.9
1	8-D	129	GLY	3.9
1	1-C	129	GLY	3.7
1	2-C	129	GLY	3.7
1	3-C	129	GLY	3.7
1	4-C	129	GLY	3.7
1	5-C	129	GLY	3.7
1	6-C	129	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	7-C	129	GLY	3.7
1	8-C	129	GLY	3.7
1	1-B	243	ASP	3.6
1	2-B	243	ASP	3.6
1	3-B	243	ASP	3.6
1	4-B	243	ASP	3.6
1	5-B	243	ASP	3.6
1	6-B	243	ASP	3.6
1	7-B	243	ASP	3.6
1	8-B	243	ASP	3.6
1	1-B	40	PHE	3.5
1	2-B	40	PHE	3.5
1	3-B	40	PHE	3.5
1	4-B	40	PHE	3.5
1	5-B	40	PHE	3.5
1	6-B	40	PHE	3.5
1	7-B	40	PHE	3.5
1	8-B	40	PHE	3.5
1	1-A	209	ALA	3.4
1	2-A	209	ALA	3.4
1	3-A	209	ALA	3.4
1	4-A	209	ALA	3.4
1	5-A	209	ALA	3.4
1	6-A	209	ALA	3.4
1	7-A	209	ALA	3.4
1	8-A	209	ALA	3.4
1	1-D	166	ASP	3.4
1	2-D	166	ASP	3.4
1	3-D	166	ASP	3.4
1	4-D	166	ASP	3.4
1	5-D	166	ASP	3.4
1	6-D	166	ASP	3.4
1	7-D	166	ASP	3.4
1	8-D	166	ASP	3.4
1	1-D	131	ASP	3.4
1	2-D	131	ASP	3.4
1	3-D	131	ASP	3.4
1	4-D	131	ASP	3.4
1	5-D	131	ASP	3.4
1	6-D	131	ASP	3.4
1	7-D	131	ASP	3.4
1	8-D	131	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	208	PRO	3.3
1	2-A	208	PRO	3.3
1	3-A	208	PRO	3.3
1	4-A	208	PRO	3.3
1	5-A	208	PRO	3.3
1	6-A	208	PRO	3.3
1	7-A	208	PRO	3.3
1	8-A	208	PRO	3.3
1	1-A	169	ILE	3.2
1	2-A	169	ILE	3.2
1	3-A	169	ILE	3.2
1	4-A	169	ILE	3.2
1	5-A	169	ILE	3.2
1	6-A	169	ILE	3.2
1	7-A	169	ILE	3.2
1	8-A	169	ILE	3.2
1	1-C	209	ALA	3.2
1	2-C	209	ALA	3.2
1	3-C	209	ALA	3.2
1	4-C	209	ALA	3.2
1	5-C	209	ALA	3.2
1	6-C	209	ALA	3.2
1	7-C	209	ALA	3.2
1	8-C	209	ALA	3.2
1	1-D	40	PHE	3.2
1	2-D	40	PHE	3.2
1	3-D	40	PHE	3.2
1	4-D	40	PHE	3.2
1	5-D	40	PHE	3.2
1	6-D	40	PHE	3.2
1	7-D	40	PHE	3.2
1	8-D	40	PHE	3.2
1	1-C	286	ASP	3.1
1	2-C	286	ASP	3.1
1	3-C	286	ASP	3.1
1	4-C	286	ASP	3.1
1	5-C	286	ASP	3.1
1	6-C	286	ASP	3.1
1	7-C	286	ASP	3.1
1	8-C	286	ASP	3.1
1	1-A	207	GLY	3.1
1	2-A	207	GLY	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	3-A	207	GLY	3.1
1	4-A	207	GLY	3.1
1	5-A	207	GLY	3.1
1	6-A	207	GLY	3.1
1	7-A	207	GLY	3.1
1	8-A	207	GLY	3.1
1	1-B	206	ILE	3.1
1	2-B	206	ILE	3.1
1	3-B	206	ILE	3.1
1	4-B	206	ILE	3.1
1	5-B	206	ILE	3.1
1	6-B	206	ILE	3.1
1	7-B	206	ILE	3.1
1	8-B	206	ILE	3.1
1	1-C	303	SER	3.0
1	2-C	303	SER	3.0
1	3-C	303	SER	3.0
1	4-C	303	SER	3.0
1	5-C	303	SER	3.0
1	6-C	303	SER	3.0
1	7-C	303	SER	3.0
1	8-C	303	SER	3.0
1	1-C	200	VAL	3.0
1	2-C	200	VAL	3.0
1	3-C	200	VAL	3.0
1	4-C	200	VAL	3.0
1	5-C	200	VAL	3.0
1	6-C	200	VAL	3.0
1	7-C	200	VAL	3.0
1	8-C	200	VAL	3.0
1	1-A	189	ASN	3.0
1	2-A	189	ASN	3.0
1	3-A	189	ASN	3.0
1	4-A	189	ASN	3.0
1	5-A	189	ASN	3.0
1	6-A	189	ASN	3.0
1	7-A	189	ASN	3.0
1	8-A	189	ASN	3.0
1	1-C	216	PRO	3.0
1	2-C	216	PRO	3.0
1	3-C	216	PRO	3.0
1	4-C	216	PRO	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	5-C	216	PRO	3.0
1	6-C	216	PRO	3.0
1	7-C	216	PRO	3.0
1	8-C	216	PRO	3.0
1	1-B	74	ASP	3.0
1	2-B	74	ASP	3.0
1	3-B	74	ASP	3.0
1	4-B	74	ASP	3.0
1	5-B	74	ASP	3.0
1	6-B	74	ASP	3.0
1	7-B	74	ASP	3.0
1	8-B	74	ASP	3.0
1	1-C	327	LYS	3.0
1	2-C	327	LYS	3.0
1	3-C	327	LYS	3.0
1	4-C	327	LYS	3.0
1	5-C	327	LYS	3.0
1	6-C	327	LYS	3.0
1	7-C	327	LYS	3.0
1	8-C	327	LYS	3.0
1	1-D	206	ILE	3.0
1	2-D	206	ILE	3.0
1	3-D	206	ILE	3.0
1	4-D	206	ILE	3.0
1	5-D	206	ILE	3.0
1	6-D	206	ILE	3.0
1	7-D	206	ILE	3.0
1	8-D	206	ILE	3.0
1	1-C	189	ASN	2.9
1	2-C	189	ASN	2.9
1	3-C	189	ASN	2.9
1	4-C	189	ASN	2.9
1	5-C	189	ASN	2.9
1	6-C	189	ASN	2.9
1	7-C	189	ASN	2.9
1	8-C	189	ASN	2.9
1	1-A	283	GLU	2.9
1	2-A	283	GLU	2.9
1	3-A	283	GLU	2.9
1	4-A	283	GLU	2.9
1	5-A	283	GLU	2.9
1	6-A	283	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	7-A	283	GLU	2.9
1	8-A	283	GLU	2.9
1	1-C	167	VAL	2.9
1	2-C	167	VAL	2.9
1	3-C	167	VAL	2.9
1	4-C	167	VAL	2.9
1	5-C	167	VAL	2.9
1	6-C	167	VAL	2.9
1	7-C	167	VAL	2.9
1	8-C	167	VAL	2.9
1	1-C	306	PRO	2.8
1	2-C	306	PRO	2.8
1	3-C	306	PRO	2.8
1	4-C	306	PRO	2.8
1	5-C	306	PRO	2.8
1	6-C	306	PRO	2.8
1	7-C	306	PRO	2.8
1	8-C	306	PRO	2.8
1	1-B	208	PRO	2.8
1	2-B	208	PRO	2.8
1	3-B	208	PRO	2.8
1	4-B	208	PRO	2.8
1	5-B	208	PRO	2.8
1	6-B	208	PRO	2.8
1	7-B	208	PRO	2.8
1	8-B	208	PRO	2.8
1	1-C	130	GLY	2.8
1	2-C	130	GLY	2.8
1	3-C	130	GLY	2.8
1	4-C	130	GLY	2.8
1	5-C	130	GLY	2.8
1	6-C	130	GLY	2.8
1	7-C	130	GLY	2.8
1	8-C	130	GLY	2.8
1	1-A	185	ALA	2.7
1	2-A	185	ALA	2.7
1	3-A	185	ALA	2.7
1	4-A	185	ALA	2.7
1	5-A	185	ALA	2.7
1	6-A	185	ALA	2.7
1	7-A	185	ALA	2.7
1	8-A	185	ALA	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1-C	165	PRO	2.7
1	2-C	165	PRO	2.7
1	3-C	165	PRO	2.7
1	4-C	165	PRO	2.7
1	5-C	165	PRO	2.7
1	6-C	165	PRO	2.7
1	7-C	165	PRO	2.7
1	8-C	165	PRO	2.7
1	1-C	304	ASN	2.7
1	2-C	304	ASN	2.7
1	3-C	304	ASN	2.7
1	4-C	304	ASN	2.7
1	5-C	304	ASN	2.7
1	6-C	304	ASN	2.7
1	7-C	304	ASN	2.7
1	8-C	304	ASN	2.7
1	1-A	172	GLU	2.6
1	2-A	172	GLU	2.6
1	3-A	172	GLU	2.6
1	4-A	172	GLU	2.6
1	5-A	172	GLU	2.6
1	6-A	172	GLU	2.6
1	7-A	172	GLU	2.6
1	8-A	172	GLU	2.6
1	1-A	129	GLY	2.6
1	1-D	130	GLY	2.6
1	2-A	129	GLY	2.6
1	2-D	130	GLY	2.6
1	3-A	129	GLY	2.6
1	3-D	130	GLY	2.6
1	4-A	129	GLY	2.6
1	4-D	130	GLY	2.6
1	5-A	129	GLY	2.6
1	5-D	130	GLY	2.6
1	6-A	129	GLY	2.6
1	6-D	130	GLY	2.6
1	7-A	129	GLY	2.6
1	7-D	130	GLY	2.6
1	8-A	129	GLY	2.6
1	8-D	130	GLY	2.6
1	1-C	210	LYS	2.6
1	2-C	210	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	3-C	210	LYS	2.6
1	4-C	210	LYS	2.6
1	5-C	210	LYS	2.6
1	6-C	210	LYS	2.6
1	7-C	210	LYS	2.6
1	8-C	210	LYS	2.6
1	1-A	174	PRO	2.6
1	2-A	174	PRO	2.6
1	3-A	174	PRO	2.6
1	4-A	174	PRO	2.6
1	5-A	174	PRO	2.6
1	6-A	174	PRO	2.6
1	7-A	174	PRO	2.6
1	8-A	174	PRO	2.6
1	1-C	329	ILE	2.5
1	2-C	329	ILE	2.5
1	3-C	329	ILE	2.5
1	4-C	329	ILE	2.5
1	5-C	329	ILE	2.5
1	6-C	329	ILE	2.5
1	7-C	329	ILE	2.5
1	8-C	329	ILE	2.5
1	1-A	74	ASP	2.5
1	2-A	74	ASP	2.5
1	3-A	74	ASP	2.5
1	4-A	74	ASP	2.5
1	5-A	74	ASP	2.5
1	6-A	74	ASP	2.5
1	7-A	74	ASP	2.5
1	8-A	74	ASP	2.5
1	1-A	303	SER	2.5
1	2-A	303	SER	2.5
1	3-A	303	SER	2.5
1	4-A	303	SER	2.5
1	5-A	303	SER	2.5
1	6-A	303	SER	2.5
1	7-A	303	SER	2.5
1	8-A	303	SER	2.5
1	1-D	305	GLY	2.4
1	2-D	305	GLY	2.4
1	3-D	305	GLY	2.4
1	4-D	305	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	5-D	305	GLY	2.4
1	6-D	305	GLY	2.4
1	7-D	305	GLY	2.4
1	8-D	305	GLY	2.4
1	1-A	250	SER	2.4
1	2-A	250	SER	2.4
1	3-A	250	SER	2.4
1	4-A	250	SER	2.4
1	5-A	250	SER	2.4
1	6-A	250	SER	2.4
1	7-A	250	SER	2.4
1	8-A	250	SER	2.4
1	1-A	41	SER	2.4
1	1-B	77	ASP	2.4
1	2-A	41	SER	2.4
1	2-B	77	ASP	2.4
1	3-A	41	SER	2.4
1	3-B	77	ASP	2.4
1	4-A	41	SER	2.4
1	4-B	77	ASP	2.4
1	5-A	41	SER	2.4
1	5-B	77	ASP	2.4
1	6-A	41	SER	2.4
1	6-B	77	ASP	2.4
1	7-A	41	SER	2.4
1	7-B	77	ASP	2.4
1	8-A	41	SER	2.4
1	8-B	77	ASP	2.4
1	1-A	211	GLU	2.4
1	2-A	211	GLU	2.4
1	3-A	211	GLU	2.4
1	4-A	211	GLU	2.4
1	5-A	211	GLU	2.4
1	6-A	211	GLU	2.4
1	7-A	211	GLU	2.4
1	8-A	211	GLU	2.4
1	1-A	165	PRO	2.3
1	2-A	165	PRO	2.3
1	3-A	165	PRO	2.3
1	4-A	165	PRO	2.3
1	5-A	165	PRO	2.3
1	6-A	165	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	7-A	165	PRO	2.3
1	8-A	165	PRO	2.3
1	1-C	180	ILE	2.3
1	2-C	180	ILE	2.3
1	3-C	180	ILE	2.3
1	4-C	180	ILE	2.3
1	5-C	180	ILE	2.3
1	6-C	180	ILE	2.3
1	7-C	180	ILE	2.3
1	8-C	180	ILE	2.3
1	1-C	179	VAL	2.3
1	2-C	179	VAL	2.3
1	3-C	179	VAL	2.3
1	4-C	179	VAL	2.3
1	5-C	179	VAL	2.3
1	6-C	179	VAL	2.3
1	7-C	179	VAL	2.3
1	8-C	179	VAL	2.3
1	1-C	131	ASP	2.3
1	2-C	131	ASP	2.3
1	3-C	131	ASP	2.3
1	4-C	131	ASP	2.3
1	5-C	131	ASP	2.3
1	6-C	131	ASP	2.3
1	7-C	131	ASP	2.3
1	8-C	131	ASP	2.3
1	1-C	330	GLU	2.3
1	2-C	330	GLU	2.3
1	3-C	330	GLU	2.3
1	4-C	330	GLU	2.3
1	5-C	330	GLU	2.3
1	6-C	330	GLU	2.3
1	7-C	330	GLU	2.3
1	8-C	330	GLU	2.3
1	1-A	301	SER	2.3
1	2-A	301	SER	2.3
1	3-A	301	SER	2.3
1	4-A	301	SER	2.3
1	5-A	301	SER	2.3
1	6-A	301	SER	2.3
1	7-A	301	SER	2.3
1	8-A	301	SER	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1-D	192	GLU	2.3
1	2-D	192	GLU	2.3
1	3-D	192	GLU	2.3
1	4-D	192	GLU	2.3
1	5-D	192	GLU	2.3
1	6-D	192	GLU	2.3
1	7-D	192	GLU	2.3
1	8-D	192	GLU	2.3
1	1-B	207	GLY	2.3
1	2-B	207	GLY	2.3
1	3-B	207	GLY	2.3
1	4-B	207	GLY	2.3
1	5-B	207	GLY	2.3
1	6-B	207	GLY	2.3
1	7-B	207	GLY	2.3
1	8-B	207	GLY	2.3
1	1-D	327	LYS	2.3
1	2-D	327	LYS	2.3
1	3-D	327	LYS	2.3
1	4-D	327	LYS	2.3
1	5-D	327	LYS	2.3
1	6-D	327	LYS	2.3
1	7-D	327	LYS	2.3
1	8-D	327	LYS	2.3
1	1-C	285	PRO	2.2
1	2-C	285	PRO	2.2
1	3-C	285	PRO	2.2
1	4-C	285	PRO	2.2
1	5-C	285	PRO	2.2
1	6-C	285	PRO	2.2
1	7-C	285	PRO	2.2
1	8-C	285	PRO	2.2
1	1-C	299	SER	2.2
1	2-C	299	SER	2.2
1	3-C	299	SER	2.2
1	4-C	299	SER	2.2
1	5-C	299	SER	2.2
1	6-C	299	SER	2.2
1	7-C	299	SER	2.2
1	8-C	299	SER	2.2
1	1-A	328	VAL	2.1
1	2-A	328	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	3-A	328	VAL	2.1
1	4-A	328	VAL	2.1
1	5-A	328	VAL	2.1
1	6-A	328	VAL	2.1
1	7-A	328	VAL	2.1
1	8-A	328	VAL	2.1
1	1-C	194	SER	2.1
1	2-C	194	SER	2.1
1	3-C	194	SER	2.1
1	4-C	194	SER	2.1
1	5-C	194	SER	2.1
1	6-C	194	SER	2.1
1	7-C	194	SER	2.1
1	8-C	194	SER	2.1
1	1-C	75	TYR	2.1
1	2-C	75	TYR	2.1
1	3-C	75	TYR	2.1
1	4-C	75	TYR	2.1
1	5-C	75	TYR	2.1
1	6-C	75	TYR	2.1
1	7-C	75	TYR	2.1
1	8-C	75	TYR	2.1
1	1-B	73	SER	2.1
1	2-B	73	SER	2.1
1	3-B	73	SER	2.1
1	4-B	73	SER	2.1
1	5-B	73	SER	2.1
1	6-B	73	SER	2.1
1	7-B	73	SER	2.1
1	8-B	73	SER	2.1
1	1-A	305	GLY	2.1
1	2-A	305	GLY	2.1
1	3-A	305	GLY	2.1
1	4-A	305	GLY	2.1
1	5-A	305	GLY	2.1
1	6-A	305	GLY	2.1
1	7-A	305	GLY	2.1
1	8-A	305	GLY	2.1
1	1-D	73	SER	2.1
1	2-D	73	SER	2.1
1	3-D	73	SER	2.1
1	4-D	73	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	5-D	73	SER	2.1
1	6-D	73	SER	2.1
1	7-D	73	SER	2.1
1	8-D	73	SER	2.1
1	1-A	180	ILE	2.1
1	2-A	180	ILE	2.1
1	3-A	180	ILE	2.1
1	4-A	180	ILE	2.1
1	5-A	180	ILE	2.1
1	6-A	180	ILE	2.1
1	7-A	180	ILE	2.1
1	8-A	180	ILE	2.1
1	1-B	283	GLU	2.1
1	2-B	283	GLU	2.1
1	3-B	283	GLU	2.1
1	4-B	283	GLU	2.1
1	5-B	283	GLU	2.1
1	6-B	283	GLU	2.1
1	7-B	283	GLU	2.1
1	8-B	283	GLU	2.1
1	1-A	214	GLU	2.1
1	2-A	214	GLU	2.1
1	3-A	214	GLU	2.1
1	4-A	214	GLU	2.1
1	5-A	214	GLU	2.1
1	6-A	214	GLU	2.1
1	7-A	214	GLU	2.1
1	8-A	214	GLU	2.1
1	1-C	232	CYS	2.1
1	2-C	232	CYS	2.1
1	3-C	232	CYS	2.1
1	4-C	232	CYS	2.1
1	5-C	232	CYS	2.1
1	6-C	232	CYS	2.1
1	7-C	232	CYS	2.1
1	8-C	232	CYS	2.1
1	1-C	182	ASP	2.1
1	2-C	182	ASP	2.1
1	3-C	182	ASP	2.1
1	4-C	182	ASP	2.1
1	5-C	182	ASP	2.1
1	6-C	182	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	7-C	182	ASP	2.1
1	8-C	182	ASP	2.1
1	1-D	207	GLY	2.0
1	2-D	207	GLY	2.0
1	3-D	207	GLY	2.0
1	4-D	207	GLY	2.0
1	5-D	207	GLY	2.0
1	6-D	207	GLY	2.0
1	7-D	207	GLY	2.0
1	8-D	207	GLY	2.0
1	1-C	172	GLU	2.0
1	2-C	172	GLU	2.0
1	3-C	172	GLU	2.0
1	4-C	172	GLU	2.0
1	5-C	172	GLU	2.0
1	6-C	172	GLU	2.0
1	7-C	172	GLU	2.0
1	8-C	172	GLU	2.0
1	1-C	56	PRO	2.0
1	2-C	56	PRO	2.0
1	3-C	56	PRO	2.0
1	4-C	56	PRO	2.0
1	5-C	56	PRO	2.0
1	6-C	56	PRO	2.0
1	7-C	56	PRO	2.0
1	8-C	56	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.