



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 08:55 PM GMT

PDB ID : 2Q4C  
Title : Ensemble refinement of the protein crystal structure of annexin from Arabidopsis thaliana gene At1g35720  
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 : 2.51 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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

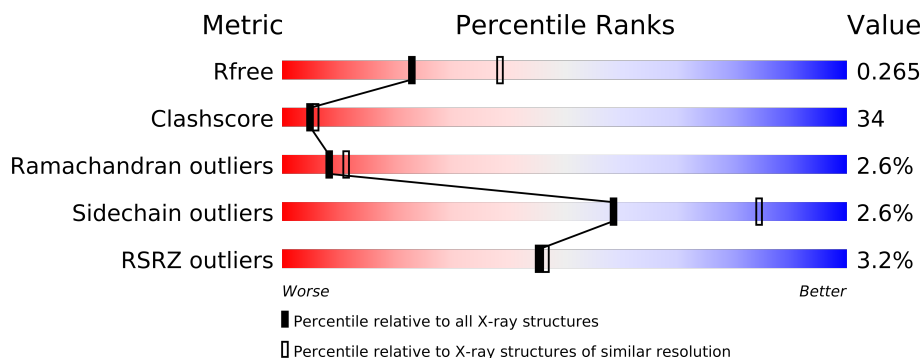
MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683



# 1 Overall quality at a glance

The reported resolution of this entry is 2.51 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)



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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	1-A	317	
1	1-B	317	
1	2-A	317	
1	2-B	317	
1	3-A	317	
1	3-B	317	
1	4-A	317	
1	4-B	317	
1	5-A	317	
1	5-B	317	
1	6-A	317	
1	6-B	317	
1	7-A	317	
1	7-B	317	

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Mol	Chain	Length	Quality of chain
1	8-A	317	
1	8-B	317	



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 42008 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Annexin D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	1-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	2-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	2-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	3-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	3-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	4-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	4-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	5-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	5-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	6-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	6-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	7-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	7-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	8-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	8-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			



There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9SYT0
B	1	SER	-	EXPRESSION TAG	UNP Q9SYT0

- Molecule 2 is water.

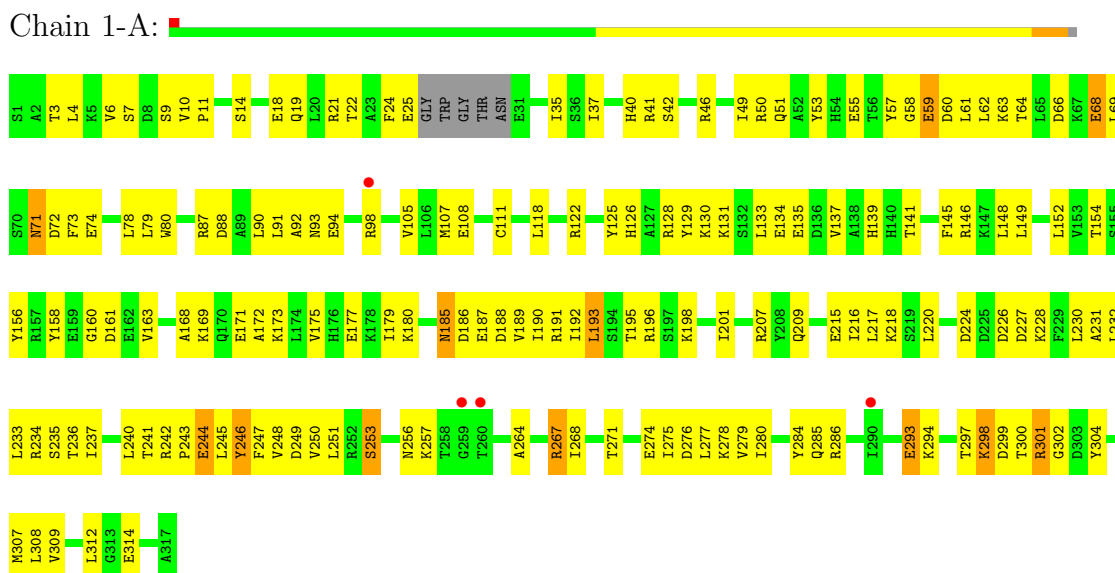
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	170	Total O 170 170	0	0
2	1-B	111	Total O 111 111	0	0
2	2-A	167	Total O 167 167	0	0
2	2-B	114	Total O 114 114	0	0
2	3-A	164	Total O 164 164	0	0
2	3-B	117	Total O 117 117	0	0
2	4-A	167	Total O 167 167	0	0
2	4-B	114	Total O 114 114	0	0
2	5-A	171	Total O 171 171	0	0
2	5-B	110	Total O 110 110	0	0
2	6-A	165	Total O 165 165	0	0
2	6-B	116	Total O 116 116	0	0
2	7-A	165	Total O 165 165	0	0
2	7-B	116	Total O 116 116	0	0
2	8-A	165	Total O 165 165	0	0
2	8-B	116	Total O 116 116	0	0



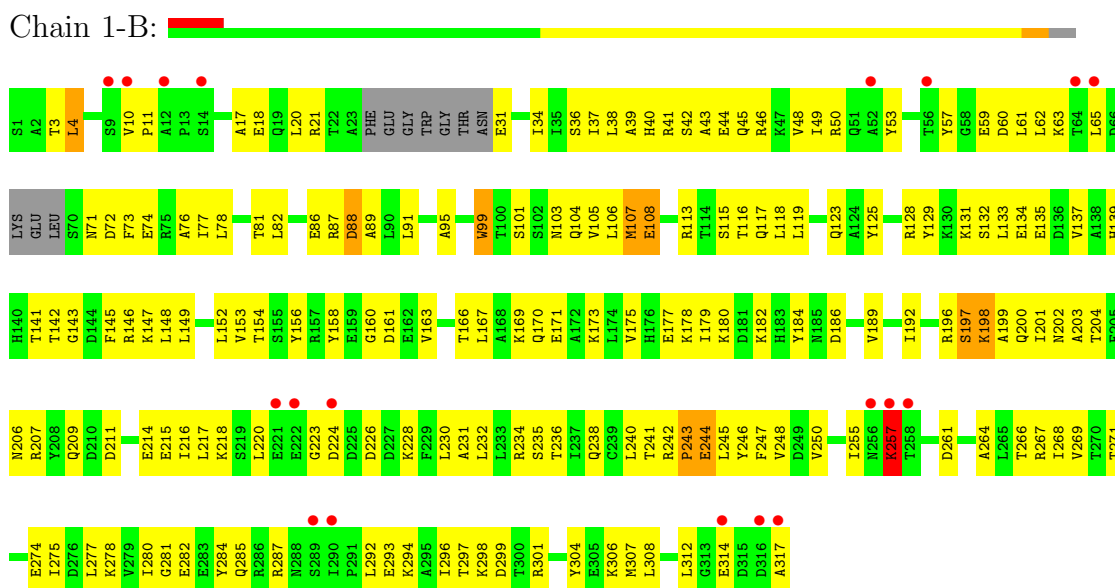
### 3 Residue-property plots

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

#### • Molecule 1: Annexin D1



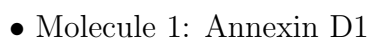
#### • Molecule 1: Annexin D1



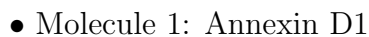
#### • Molecule 1: Annexin D1



Age Group	Percentage
18-24	10%
25-34	45%
35-44	40%
45-54	2%
55-64	1%
65-74	1%
75-84	1%
85+	1%



Age Group	Percentage
18-29	90%
30-49	85%
50-64	75%
65+	65%



Age Group	Percentage
18-24	2%
25-34	45%
35-44	50%
45-54	2%
55-64	1%
65-74	1%
75-84	1%
85+	1%

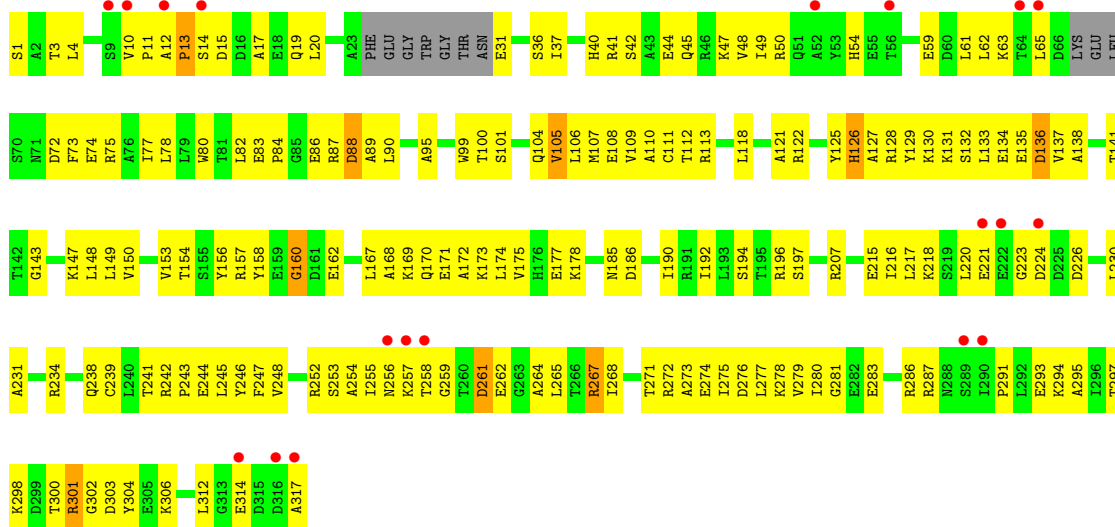






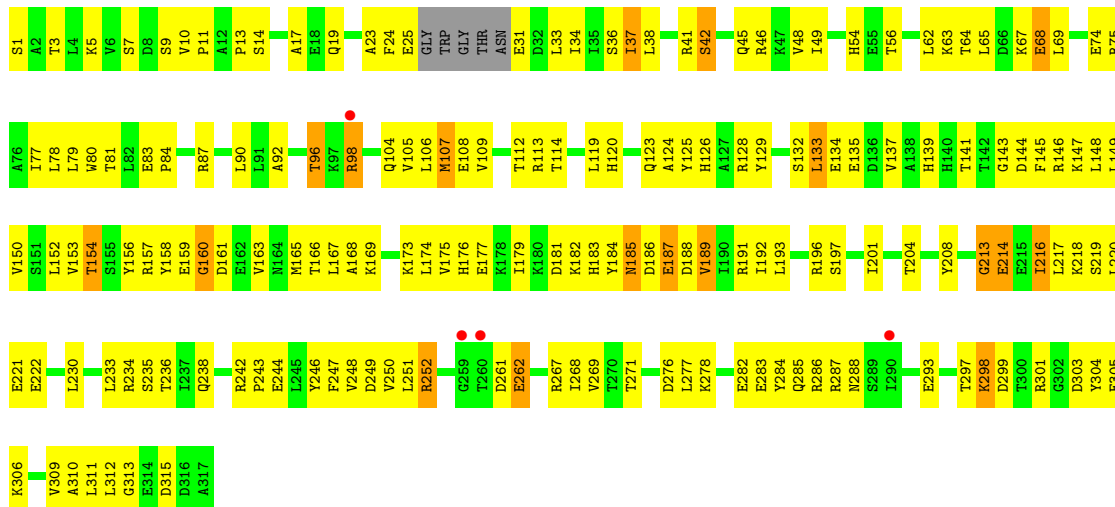
• Molecule 1: Annexin D1

Chain 3-B:



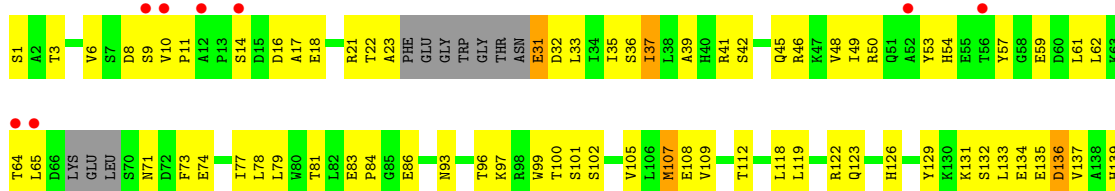
• Molecule 1: Annexin D1

Chain 4-A:

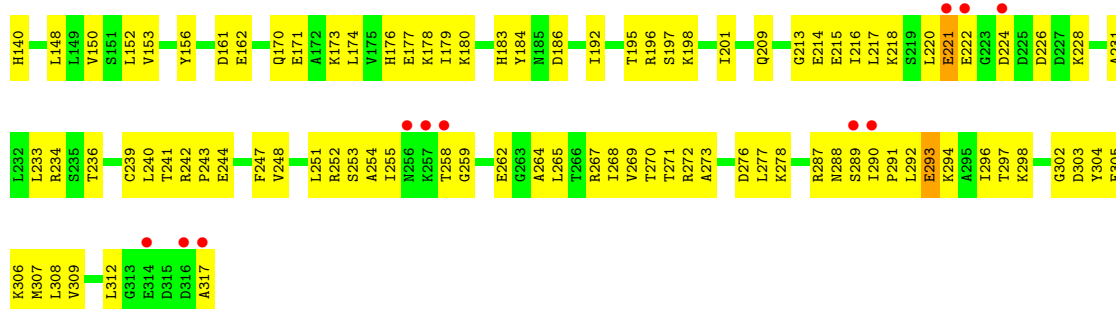


• Molecule 1: Annexin D1

Chain 4-B:

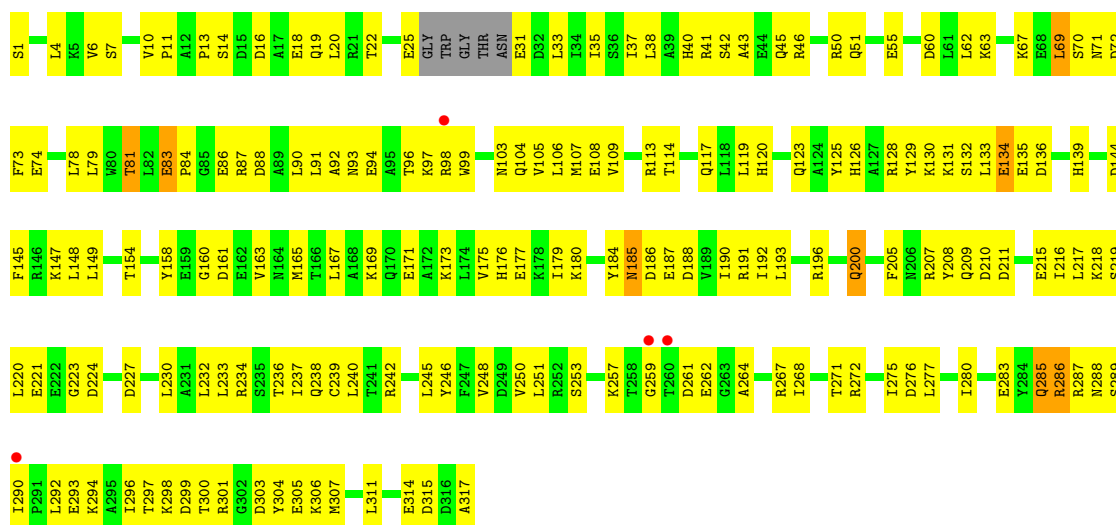






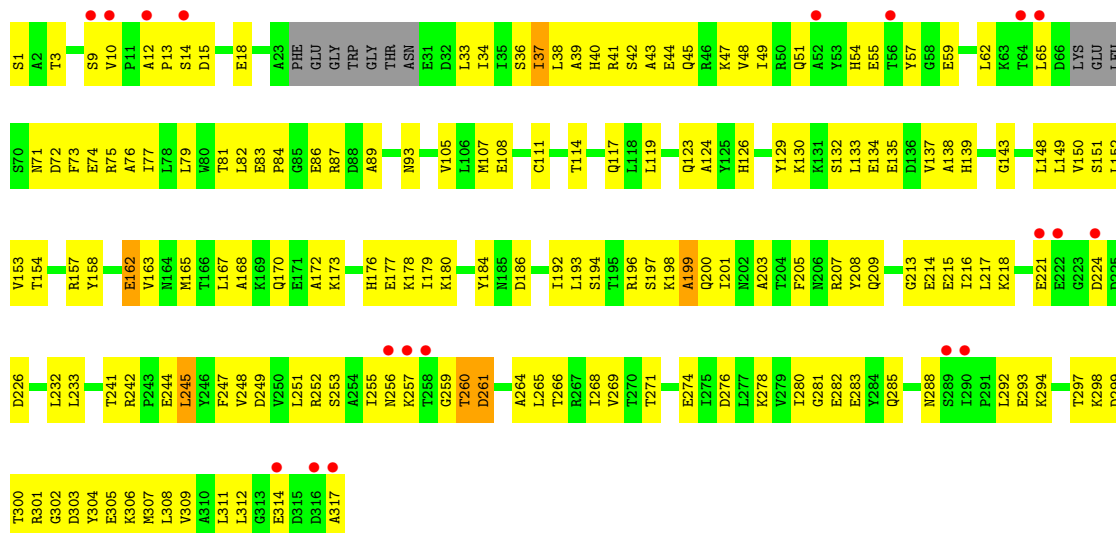
• Molecule 1: Annexin D1

Chain 5-A:



• Molecule 1: Annexin D1

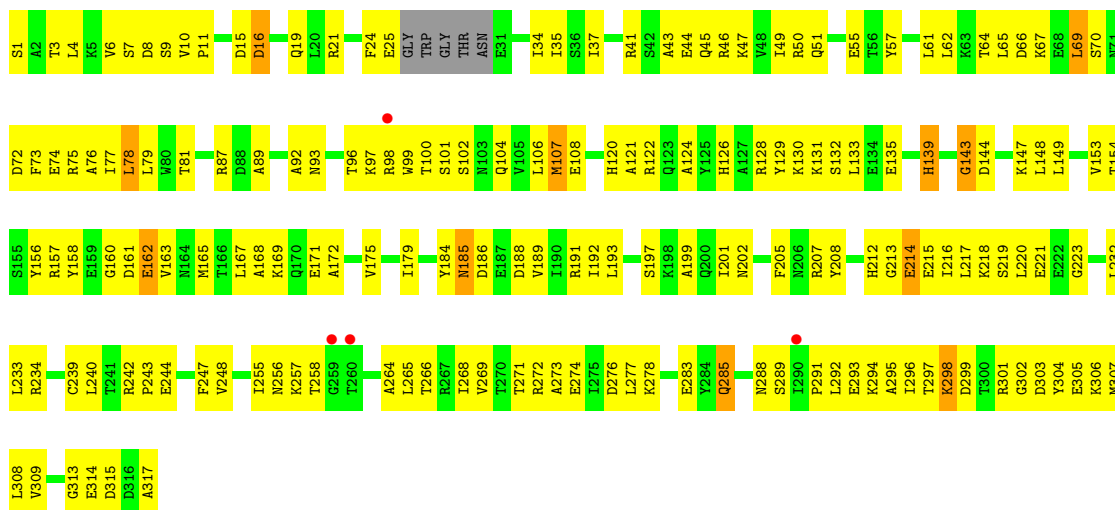
Chain 5-B:



• Molecule 1: Annexin D1

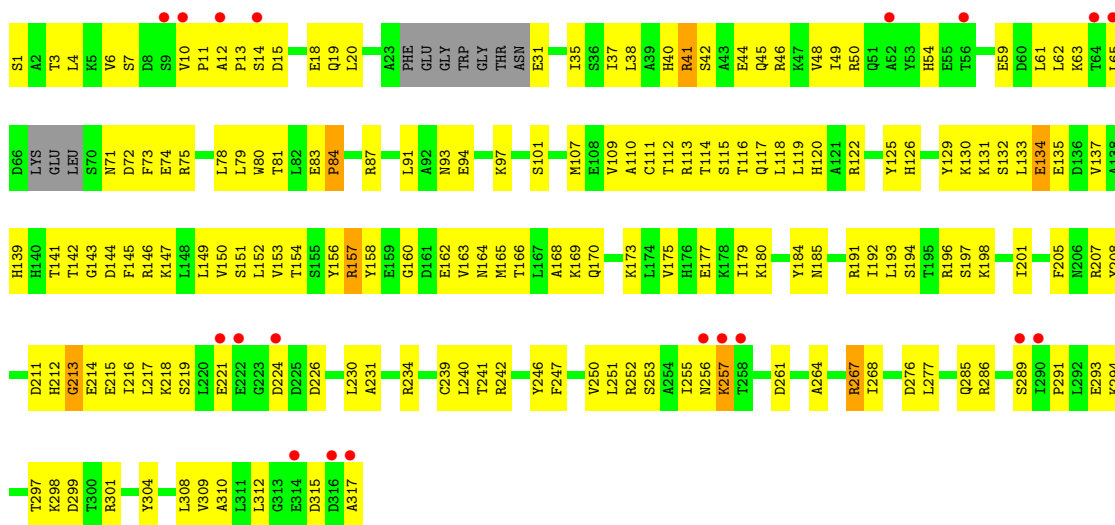


Chain 6-A:



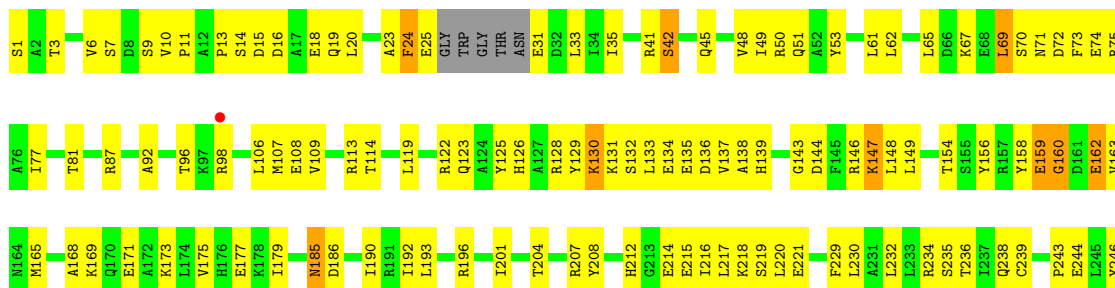
- Molecule 1: Annexin D1

Chain 6-B:



- Molecule 1: Annexin D1

Chain 7-A:

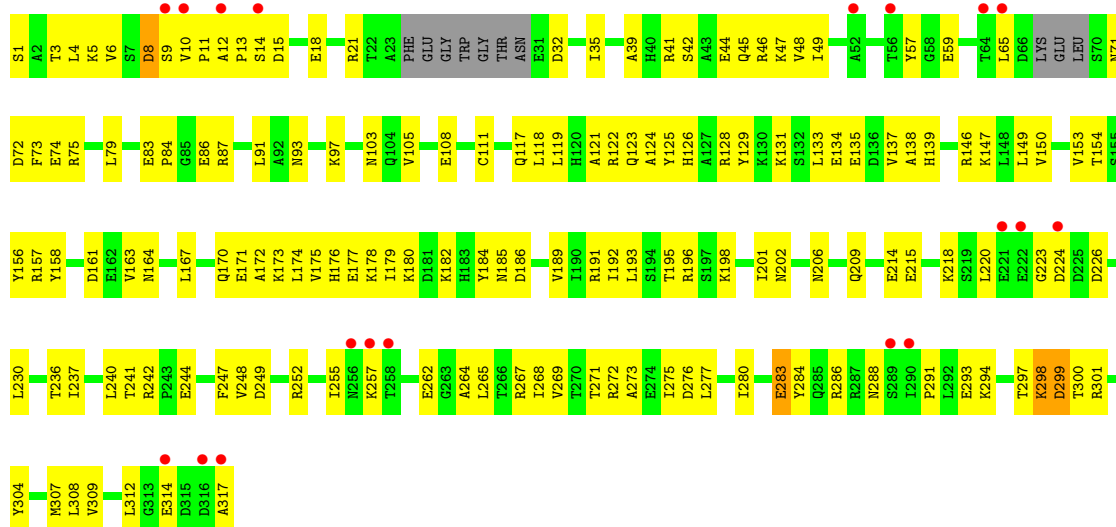






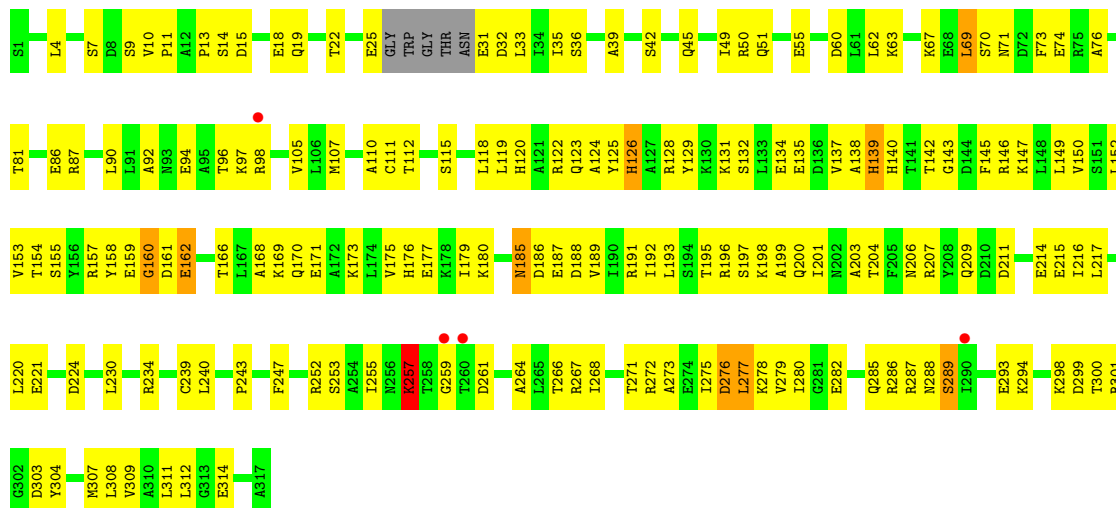
• Molecule 1: Annexin D1

Chain 7-B:



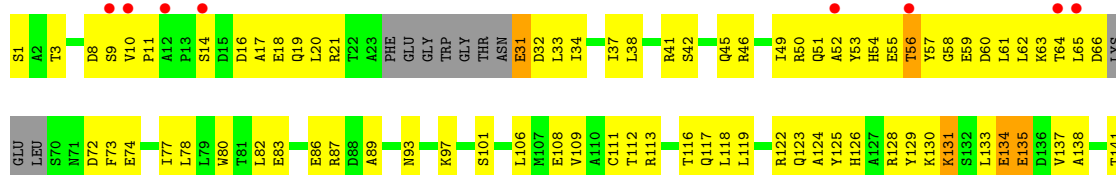
• Molecule 1: Annexin D1

Chain 8-A:

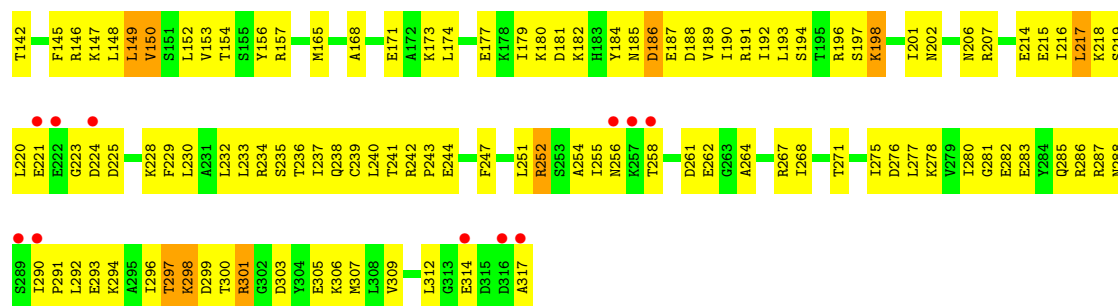


• Molecule 1: Annexin D1

Chain 8-B:









## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.54Å 96.94Å 226.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.51 33.12 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.6 (29.81-2.51) 93.5 (33.12-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.79 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.177 , 0.243 0.201 , 0.265	Depositor DCC
$R_{free}$ test set	1320 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27985 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	42008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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	0.32	0/2541	0.54	0/3428
1	1-B	0.29	0/2493	0.53	0/3363
1	2-A	0.32	0/2541	0.55	0/3428
1	2-B	0.29	0/2493	0.53	0/3363
1	3-A	0.31	0/2541	0.54	0/3428
1	3-B	0.29	0/2493	0.53	0/3363
1	4-A	0.33	0/2541	0.54	0/3428
1	4-B	0.29	0/2493	0.52	0/3363
1	5-A	0.32	0/2541	0.57	0/3428
1	5-B	0.30	0/2493	0.54	0/3363
1	6-A	0.33	0/2541	0.57	0/3428
1	6-B	0.30	0/2493	0.55	0/3363
1	7-A	0.34	0/2541	0.56	0/3428
1	7-B	0.31	0/2493	0.54	0/3363
1	8-A	0.34	0/2541	0.56	0/3428
1	8-B	0.31	0/2493	0.56	0/3363
All	All	0.31	0/40272	0.55	0/54328

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2508	0	2493	171	0
1	1-B	2462	0	2447	185	0
1	2-A	2508	0	2493	186	0
1	2-B	2462	0	2447	135	0
1	3-A	2508	0	2493	185	0
1	3-B	2462	0	2447	184	0
1	4-A	2508	0	2493	188	0
1	4-B	2462	0	2447	151	0
1	5-A	2508	0	2493	189	0
1	5-B	2462	0	2447	150	0
1	6-A	2508	0	2493	173	0
1	6-B	2462	0	2447	162	0
1	7-A	2508	0	2493	155	0
1	7-B	2462	0	2447	163	0
1	8-A	2508	0	2493	176	0
1	8-B	2462	0	2447	205	0
2	1-A	170	0	0	14	0
2	1-B	111	0	0	7	0
2	2-A	167	0	0	14	0
2	2-B	114	0	0	4	0
2	3-A	164	0	0	13	0
2	3-B	117	0	0	5	0
2	4-A	167	0	0	14	0
2	4-B	114	0	0	12	0
2	5-A	171	0	0	19	0
2	5-B	110	0	0	3	0
2	6-A	165	0	0	12	0
2	6-B	116	0	0	15	0
2	7-A	165	0	0	11	0
2	7-B	116	0	0	10	0
2	8-A	165	0	0	17	0
2	8-B	116	0	0	14	0
All	All	42008	0	39520	2690	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

All (2690) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:134:GLU:HG2	1:B:154:THR:HG22	1.28	1.15
1:B:90:LEU:HD13	1:B:128:ARG:HH21	1.12	1.10
1:A:134:GLU:HG2	1:A:154:THR:HG22	1.33	1.09
1:A:272:ARG:HA	1:A:272:ARG:HH11	1.14	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:267:ARG:HB3	1:B:267:ARG:HH11	1.11	1.06
1:A:12:ALA:HB1	1:A:13:PRO:HD2	1.36	1.04
1:A:267:ARG:HB3	1:A:267:ARG:HH11	1.17	1.02
1:B:248:VAL:HG21	1:B:283:GLU:HB3	1.45	0.98
1:B:80:TRP:HA	1:B:87:ARG:HH21	1.29	0.97
1:A:301:ARG:HH22	1:A:306:LYS:HD3	1.29	0.96
1:B:12:ALA:HB1	1:B:13:PRO:HD2	1.48	0.95
1:A:134:GLU:HG3	1:A:154:THR:HG22	1.47	0.95
1:A:71:ASN:HD21	1:A:73:PHE:HB3	1.32	0.94
1:A:252:ARG:HE	1:A:288:ASN:HD21	1.15	0.94
1:B:134:GLU:HG3	1:B:154:THR:HG22	1.49	0.93
1:B:291:PRO:HB2	1:B:294:LYS:HB2	1.50	0.93
1:A:191:ARG:HH12	1:A:196:ARG:HH21	1.16	0.93
1:A:301:ARG:HH11	1:A:301:ARG:HB3	1.32	0.92
1:B:65:LEU:HD22	1:B:74:GLU:HB3	1.51	0.92
1:A:196:ARG:HD2	1:A:200:GLN:HE21	1.34	0.92
1:A:252:ARG:HG2	1:A:288:ASN:HD21	1.30	0.92
1:A:59:GLU:HG3	1:A:63:LYS:HG3	1.50	0.92
1:B:191:ARG:HH12	1:B:196:ARG:NH2	1.67	0.92
1:B:277:LEU:HD21	1:B:312:LEU:HD23	1.50	0.92
1:A:294:LYS:HD2	1:A:317:ALA:HB1	1.52	0.92
1:A:35:ILE:HD12	1:A:307:MET:HB2	1.51	0.91
1:B:71:ASN:HD22	1:B:74:GLU:H	1.17	0.91
1:B:267:ARG:HH11	1:B:267:ARG:CB	1.84	0.90
1:A:272:ARG:HA	1:A:272:ARG:NH1	1.87	0.90
1:B:106:LEU:HD13	1:B:149:LEU:HD13	1.53	0.88
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.55	0.88
1:B:296:ILE:HG22	1:B:305:GLU:HG3	1.55	0.88
1:B:303:ASP:HA	1:B:306:LYS:HD3	1.56	0.87
1:A:69:LEU:HD23	1:A:69:LEU:H	1.35	0.87
1:A:165:MET:HE1	1:A:207:ARG:HD3	1.56	0.87
1:B:80:TRP:HA	1:B:87:ARG:HH21	1.39	0.87
1:A:169:LYS:HD2	1:A:207:ARG:HH21	1.39	0.87
1:A:244:GLU:HB3	2:A:468:HOH:O	1.75	0.87
1:B:215:GLU:H	1:B:218:LYS:HD2	1.37	0.87
1:A:252:ARG:HE	1:A:288:ASN:ND2	1.71	0.87
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.57	0.87
1:A:35:ILE:H	1:A:35:ILE:HD12	1.38	0.86
1:B:225:ASP:HA	1:B:234:ARG:HH12	1.39	0.86
1:A:1:SER:HB3	1:A:276:ASP:HA	1.55	0.86
1:A:301:ARG:HB3	1:A:301:ARG:NH1	1.90	0.86
1:B:119:LEU:HD22	1:B:156:TYR:CE1	2.09	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:244:GLU:HA	1:B:280:ILE:HG12	1.57	0.86
1:B:267:ARG:HB3	1:B:267:ARG:HH11	1.39	0.86
1:A:1:SER:HB3	1:A:276:ASP:HA	1.56	0.86
1:B:184:TYR:HB3	1:B:233:LEU:HD22	1.57	0.86
1:B:20:LEU:HD22	1:B:34:ILE:HG23	1.58	0.85
1:B:254:ALA:HB1	1:B:265:LEU:HB2	1.57	0.85
1:B:261:ASP:HB3	1:B:264:ALA:HB2	1.55	0.85
1:B:267:ARG:HB3	1:B:267:ARG:NH1	1.92	0.85
1:A:71:ASN:HD22	1:A:74:GLU:HG3	1.39	0.85
1:A:62:LEU:HD21	1:A:81:THR:HB	1.59	0.84
1:A:179:ILE:HD12	1:A:220:LEU:HD21	1.59	0.84
1:A:169:LYS:HD2	1:A:207:ARG:HH21	1.42	0.84
1:B:148:LEU:HD13	1:B:190:ILE:HG23	1.57	0.84
1:B:71:ASN:ND2	1:B:74:GLU:H	1.75	0.84
1:A:96:THR:HG22	1:A:106:LEU:HD11	1.60	0.84
1:B:87:ARG:HD3	1:B:271:THR:HG22	1.58	0.84
1:B:42:SER:HB2	1:B:45:GLN:HG3	1.60	0.84
1:A:169:LYS:HD2	1:A:207:ARG:HH21	1.42	0.84
1:B:247:PHE:HD1	1:B:268:ILE:HD12	1.43	0.84
1:A:1:SER:HB3	1:A:276:ASP:HA	1.57	0.83
1:A:144:ASP:HA	1:A:147:LYS:HD3	1.59	0.83
1:B:106:LEU:HD22	1:B:149:LEU:HD22	1.60	0.83
1:B:251:LEU:HD21	1:B:268:ILE:HG21	1.60	0.83
1:B:130:LYS:HA	1:B:130:LYS:HE2	1.61	0.83
1:B:65:LEU:HD13	1:B:77:ILE:HG21	1.62	0.82
1:B:191:ARG:HH12	1:B:196:ARG:HH21	1.27	0.82
1:A:39:ALA:HB2	1:A:307:MET:SD	2.20	0.82
1:A:286:ARG:HB2	1:A:286:ARG:HH11	1.43	0.82
1:B:309:VAL:HA	1:B:312:LEU:HD12	1.62	0.82
1:B:110:ALA:HA	1:B:118:LEU:HD13	1.60	0.82
1:A:23:ALA:HB1	1:A:34:ILE:HD11	1.61	0.82
1:B:3:THR:HG21	1:B:312:LEU:HD23	1.62	0.81
1:B:50:ARG:HD2	1:B:81:THR:HG22	1.62	0.81
1:A:69:LEU:HD23	1:A:69:LEU:H	1.45	0.81
1:B:87:ARG:HD3	1:B:271:THR:HG22	1.61	0.81
1:B:75:ARG:HH12	1:B:90:LEU:HD21	1.45	0.81
1:B:215:GLU:HB3	1:B:218:LYS:HG3	1.63	0.81
1:A:272:ARG:HB3	1:A:276:ASP:OD1	1.81	0.81
1:B:87:ARG:HD3	1:B:271:THR:HG22	1.60	0.81
1:A:134:GLU:HG3	1:A:154:THR:HG22	1.63	0.80
1:B:179:ILE:HD13	1:B:220:LEU:HD21	1.64	0.80
1:B:296:ILE:HG22	1:B:305:GLU:HG3	1.61	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:134:GLU:HG2	1:B:154:THR:HG22	1.64	0.80
1:B:62:LEU:HD13	1:B:78:LEU:HD12	1.63	0.80
1:B:171:GLU:OE1	1:B:192:ILE:HG12	1.81	0.80
1:B:152:LEU:HD23	1:B:194:SER:HB3	1.64	0.80
1:A:221:GLU:HA	1:A:234:ARG:NH2	1.96	0.80
1:A:180:LYS:HA	1:A:180:LYS:HE2	1.63	0.80
1:A:69:LEU:H	1:A:69:LEU:HD23	1.48	0.79
1:B:20:LEU:HD11	1:B:38:LEU:HD21	1.63	0.79
1:A:209:GLN:HE21	1:A:215:GLU:HA	1.46	0.79
1:A:35:ILE:HG13	1:A:306:LYS:HE3	1.63	0.79
1:A:286:ARG:HD2	2:A:365:HOH:O	1.80	0.79
1:B:152:LEU:HD23	1:B:194:SER:HB3	1.64	0.79
1:B:87:ARG:HD3	1:B:271:THR:HG22	1.63	0.79
1:A:267:ARG:NH1	1:A:267:ARG:HB3	1.96	0.79
1:B:62:LEU:HD11	1:B:81:THR:HB	1.63	0.79
1:B:65:LEU:HD22	1:B:74:GLU:HB3	1.65	0.79
1:A:248:VAL:HG21	1:A:283:GLU:HB3	1.63	0.79
1:B:1:SER:HB2	1:B:278:LYS:HB3	1.65	0.78
1:B:134:GLU:HG2	1:B:154:THR:HG22	1.64	0.78
1:B:90:LEU:HD13	1:B:128:ARG:NH2	1.95	0.78
1:B:50:ARG:HH12	1:B:82:LEU:HD23	1.47	0.78
1:A:78:LEU:O	1:A:80:TRP:N	2.16	0.78
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.18	0.78
1:A:158:TYR:O	1:A:197:SER:HB2	1.84	0.78
1:B:291:PRO:HD2	1:B:294:LYS:HD3	1.65	0.78
1:A:216:ILE:HA	1:A:219:SER:HB3	1.65	0.78
1:A:158:TYR:CE2	1:A:160:GLY:HA3	2.19	0.78
1:B:134:GLU:HG2	1:B:154:THR:HG23	1.65	0.78
1:A:23:ALA:HB2	1:A:33:LEU:HD22	1.65	0.78
1:B:10:VAL:HG22	1:B:45:GLN:HE21	1.47	0.78
1:B:144:ASP:HA	1:B:147:LYS:HD2	1.63	0.77
1:A:191:ARG:HH12	1:A:196:ARG:NH2	1.81	0.77
1:A:114:THR:HG22	2:A:344:HOH:O	1.84	0.77
1:B:165:MET:HE1	1:B:207:ARG:HD3	1.65	0.77
1:B:133:LEU:HD23	1:B:153:VAL:HB	1.66	0.77
1:B:255:ILE:HG21	1:B:295:ALA:HB1	1.66	0.77
1:B:34:ILE:HG21	1:B:77:ILE:HD12	1.66	0.77
1:B:1:SER:H3	1:B:279:VAL:H	1.32	0.77
1:A:301:ARG:HH11	1:A:301:ARG:CB	1.96	0.77
1:A:255:ILE:HG12	1:A:295:ALA:HB1	1.66	0.77
1:A:248:VAL:HG21	1:A:283:GLU:HB3	1.66	0.77
1:B:134:GLU:HG3	1:B:154:THR:CG2	2.15	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:285:GLN:HG2	1:A:291:PRO:HG3	1.67	0.76
1:B:39:ALA:HB2	1:B:307:MET:SD	2.25	0.76
1:A:255:ILE:HG21	1:A:295:ALA:HB1	1.66	0.76
1:B:79:LEU:HB3	1:B:270:THR:HG21	1.68	0.76
1:A:150:VAL:HA	1:A:153:VAL:HG22	1.67	0.76
1:A:179:ILE:HD12	1:A:220:LEU:HD21	1.66	0.76
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.21	0.76
1:A:277:LEU:HD21	1:A:312:LEU:HD23	1.67	0.76
1:B:87:ARG:NH1	1:B:271:THR:HA	2.01	0.75
1:A:172:ALA:HB1	1:A:208:TYR:HB2	1.68	0.75
1:B:267:ARG:HB3	1:B:267:ARG:NH1	1.96	0.75
1:B:264:ALA:HA	1:B:267:ARG:NH1	2.01	0.75
1:A:164:ASN:CG	1:A:167:LEU:HD13	2.07	0.75
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.66	0.75
1:A:278:LYS:O	1:A:282:GLU:HG3	1.87	0.75
1:B:65:LEU:HD22	1:B:77:ILE:HB	1.69	0.75
1:B:14:SER:HA	1:B:17:ALA:HB3	1.69	0.75
1:A:60:ASP:HB3	1:A:63:LYS:HG2	1.66	0.75
1:A:135:GLU:HB3	1:B:195:THR:HB	1.68	0.75
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.52	0.75
1:A:35:ILE:CD1	1:A:307:MET:HB2	2.16	0.74
1:B:179:ILE:HD11	1:B:220:LEU:HD21	1.69	0.74
1:A:14:SER:HA	1:A:17:ALA:HB3	1.70	0.74
1:A:221:GLU:HA	1:A:234:ARG:NH2	2.02	0.74
1:B:14:SER:HA	1:B:52:ALA:HB1	1.69	0.74
1:B:80:TRP:CA	1:B:87:ARG:HH21	2.00	0.74
1:A:193:LEU:HD22	1:A:240:LEU:HD12	1.68	0.74
1:B:53:TYR:O	1:B:57:TYR:HB2	1.87	0.74
1:B:202:ASN:HD21	1:B:206:ASN:HD21	1.34	0.74
1:B:251:LEU:HD11	1:B:268:ILE:HG21	1.69	0.74
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.52	0.74
1:B:309:VAL:HG23	1:B:315:ASP:HA	1.69	0.74
1:A:158:TYR:OH	1:B:130:LYS:HD2	1.87	0.74
1:A:137:VAL:HG21	1:A:153:VAL:HG21	1.69	0.74
1:A:179:ILE:HD12	1:A:220:LEU:HD21	1.70	0.74
1:B:75:ARG:HE	1:B:79:LEU:HD11	1.53	0.74
1:A:83:GLU:HG2	1:A:84:PRO:HD2	1.69	0.73
1:A:165:MET:HE1	1:A:207:ARG:HD3	1.70	0.73
1:B:303:ASP:HA	1:B:306:LYS:HD3	1.71	0.73
1:A:173:LYS:O	1:A:177:GLU:HG3	1.88	0.73
1:A:292:LEU:O	1:A:296:ILE:HG13	1.89	0.73
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.68	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:ALA:HA	1:A:277:LEU:HB2	1.70	0.73
1:B:148:LEU:HD13	1:B:190:ILE:HG12	1.69	0.73
1:A:1:SER:OG	1:A:278:LYS:HB3	1.89	0.73
1:A:134:GLU:HG3	1:A:154:THR:CG2	2.18	0.73
1:B:134:GLU:HG2	1:B:154:THR:CG2	2.19	0.73
1:A:196:ARG:NH1	1:B:135:GLU:HB2	2.03	0.73
1:B:167:LEU:O	1:B:171:GLU:HG2	1.88	0.73
1:A:51:GLN:HG2	2:A:472:HOH:O	1.88	0.73
1:B:297:THR:HG21	1:B:317:ALA:OXT	1.88	0.72
1:A:90:LEU:O	1:A:94:GLU:HG3	1.88	0.72
1:A:179:ILE:HD12	1:A:220:LEU:HD21	1.70	0.72
1:B:277:LEU:HD21	1:B:312:LEU:HD23	1.69	0.72
1:A:87:ARG:HD3	1:A:271:THR:HG22	1.70	0.72
1:A:244:GLU:HG3	1:A:279:VAL:HG12	1.71	0.72
1:A:83:GLU:HG3	1:A:84:PRO:HD2	1.70	0.72
1:B:97:LYS:HA	1:B:97:LYS:HE2	1.70	0.72
1:A:179:ILE:HD12	1:A:220:LEU:HD21	1.71	0.72
1:B:71:ASN:HD21	1:B:73:PHE:HB3	1.54	0.71
1:B:293:GLU:O	1:B:297:THR:HG22	1.90	0.71
1:B:157:ARG:HA	2:B:361:HOH:O	1.90	0.71
1:B:171:GLU:HG3	2:B:332:HOH:O	1.89	0.71
1:B:14:SER:O	1:B:18:GLU:HG3	1.89	0.71
1:A:70:SER:HB3	2:A:478:HOH:O	1.91	0.71
1:A:277:LEU:HD21	1:A:312:LEU:HD23	1.71	0.71
1:A:226:ASP:HB3	1:A:228:LYS:NZ	2.05	0.71
1:A:186:ASP:HB3	1:A:189:VAL:HG23	1.73	0.70
1:B:80:TRP:HA	1:B:87:ARG:NH2	2.04	0.70
1:A:34:ILE:N	1:A:34:ILE:HD12	2.06	0.70
1:A:188:ASP:HA	1:A:191:ARG:HB3	1.72	0.70
1:A:293:GLU:HB3	1:A:312:LEU:HD13	1.73	0.70
1:A:104:GLN:HG2	1:A:232:LEU:HD13	1.71	0.70
1:A:169:LYS:HD2	2:A:396:HOH:O	1.90	0.70
1:B:80:TRP:CA	1:B:87:ARG:HH21	2.04	0.70
1:A:109:VAL:HA	1:A:113:ARG:NH1	2.05	0.70
1:A:35:ILE:N	1:A:35:ILE:HD12	2.07	0.70
1:B:157:ARG:HD3	1:B:196:ARG:O	1.91	0.70
1:B:105:VAL:HG22	1:B:267:ARG:NH2	2.06	0.70
1:B:42:SER:OG	1:B:45:GLN:HG3	1.92	0.70
1:B:277:LEU:HD21	1:B:312:LEU:HD23	1.74	0.70
1:A:147:LYS:H	1:A:147:LYS:HD2	1.57	0.70
1:A:272:ARG:CA	1:A:272:ARG:HH11	1.99	0.70
1:A:87:ARG:HD3	1:A:271:THR:HG22	1.74	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:177:GLU:HA	1:B:180:LYS:HE2	1.73	0.70
1:B:109:VAL:O	1:B:113:ARG:HB2	1.91	0.69
1:B:264:ALA:O	1:B:268:ILE:HG12	1.91	0.69
1:B:255:ILE:C	1:B:257:LYS:H	1.93	0.69
1:B:134:GLU:CG	1:B:154:THR:HG22	2.21	0.69
1:A:1:SER:CB	1:A:276:ASP:HA	2.22	0.69
1:B:301:ARG:NH2	1:B:317:ALA:HB3	2.07	0.69
1:B:215:GLU:H	1:B:218:LYS:HD2	1.56	0.69
1:B:300:THR:HG22	1:B:301:ARG:H	1.57	0.69
1:A:224:ASP:O	1:A:230:LEU:HD23	1.91	0.69
1:A:134:GLU:HG3	1:A:154:THR:HG22	1.73	0.69
1:B:198:LYS:HD3	2:B:348:HOH:O	1.92	0.69
1:A:12:ALA:HB1	1:A:13:PRO:CD	2.18	0.69
1:A:79:LEU:O	1:A:87:ARG:HG3	1.92	0.69
1:A:168:ALA:HB1	1:A:204:THR:HA	1.72	0.69
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.74	0.69
1:A:175:VAL:O	1:A:179:ILE:HG12	1.93	0.69
1:B:38:LEU:HD13	1:B:77:ILE:HD12	1.74	0.69
1:A:303:ASP:HA	1:A:306:LYS:HD3	1.74	0.69
1:B:1:SER:HB3	1:B:276:ASP:HA	1.73	0.69
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.27	0.69
1:A:90:LEU:O	1:A:94:GLU:HG3	1.92	0.69
1:A:22:THR:O	1:A:25:GLU:HG2	1.93	0.69
1:B:169:LYS:HD2	1:B:207:ARG:HH21	1.56	0.69
1:B:107:MET:HE1	1:B:108:GLU:HA	1.75	0.69
1:A:111:CYS:HB3	1:A:239:CYS:HB3	1.75	0.69
1:A:209:GLN:NE2	1:A:215:GLU:HB2	2.08	0.69
1:A:156:TYR:HB3	2:B:323:HOH:O	1.93	0.69
1:A:252:ARG:NE	1:A:288:ASN:HD21	1.91	0.69
1:B:97:LYS:HE2	1:B:97:LYS:HA	1.74	0.69
1:A:186:ASP:HB3	1:A:189:VAL:HG23	1.74	0.69
1:B:71:ASN:HD22	1:B:74:GLU:HG3	1.58	0.69
1:B:10:VAL:HG21	1:B:41:ARG:NH1	2.08	0.68
1:B:193:LEU:HD23	1:B:201:ILE:HD13	1.75	0.68
1:A:119:LEU:O	1:A:123:GLN:HG3	1.92	0.68
1:B:253:SER:HB3	1:B:259:GLY:H	1.57	0.68
1:A:169:LYS:HD2	1:A:207:ARG:NH2	2.07	0.68
1:B:147:LYS:HE3	2:B:422:HOH:O	1.91	0.68
1:A:277:LEU:HA	1:A:280:ILE:HD12	1.76	0.68
1:B:248:VAL:HG21	1:B:283:GLU:HB2	1.75	0.68
1:A:67:LYS:HB2	1:A:69:LEU:HD13	1.75	0.68
1:A:220:LEU:HD22	1:A:230:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:ASN:OD1	1:A:97:LYS:HE2	1.94	0.68
1:A:1:SER:HB3	1:A:276:ASP:HA	1.74	0.68
1:B:198:LYS:HE2	1:B:240:LEU:HD23	1.74	0.68
1:A:157:ARG:HH22	1:A:194:SER:HA	1.59	0.68
1:B:71:ASN:HB3	1:B:74:GLU:HG3	1.76	0.68
1:A:129:TYR:O	1:A:131:LYS:HG3	1.93	0.68
1:A:103:ASN:ND2	2:A:340:HOH:O	2.24	0.68
1:A:293:GLU:HG2	1:A:294:LYS:HD2	1.75	0.67
1:A:209:GLN:HE21	1:A:215:GLU:HB2	1.57	0.67
1:A:65:LEU:HD22	1:A:74:GLU:O	1.93	0.67
1:B:1:SER:N	1:B:279:VAL:H	1.92	0.67
1:A:135:GLU:O	1:A:139:HIS:HB2	1.93	0.67
1:B:118:LEU:O	1:B:122:ARG:HG3	1.93	0.67
1:B:314:GLU:HB3	1:B:317:ALA:HB2	1.76	0.67
1:A:248:VAL:HG21	1:A:283:GLU:HB3	1.77	0.67
1:B:235:SER:HA	1:B:238:GLN:HE21	1.59	0.67
1:B:296:ILE:HD12	1:B:312:LEU:HD11	1.76	0.67
1:B:80:TRP:HA	1:B:87:ARG:NH2	2.10	0.67
1:A:92:ALA:HB1	1:A:106:LEU:CD2	2.24	0.67
1:B:166:THR:HG22	1:B:170:GLN:HE21	1.60	0.67
1:B:171:GLU:HB3	1:B:192:ILE:HD13	1.77	0.67
1:A:6:VAL:HG12	1:A:7:SER:N	2.09	0.67
1:B:247:PHE:CD1	1:B:268:ILE:HG23	2.29	0.67
1:A:314:GLU:HB3	1:A:317:ALA:HB3	1.75	0.67
1:A:71:ASN:HD22	1:A:74:GLU:HG3	1.60	0.67
1:A:51:GLN:HG2	2:A:473:HOH:O	1.95	0.67
1:A:98:ARG:HE	1:A:98:ARG:HA	1.58	0.67
1:B:264:ALA:HA	1:B:267:ARG:HH12	1.58	0.67
1:A:252:ARG:HH22	1:A:287:ARG:NH1	1.93	0.67
1:B:39:ALA:HB2	1:B:307:MET:SD	2.35	0.67
1:B:202:ASN:HB3	2:B:374:HOH:O	1.95	0.67
1:B:134:GLU:HG3	1:B:154:THR:CG2	2.24	0.67
1:A:221:GLU:HA	1:A:234:ARG:HH21	1.59	0.67
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.60	0.67
1:A:252:ARG:HG2	1:A:288:ASN:ND2	2.07	0.67
1:A:158:TYR:CE2	1:A:160:GLY:HA3	2.29	0.67
1:A:162:GLU:CD	1:B:130:LYS:HD3	2.16	0.67
1:A:51:GLN:O	1:A:55:GLU:HG3	1.95	0.67
1:B:192:ILE:O	1:B:196:ARG:HB2	1.93	0.67
1:B:10:VAL:HG22	1:B:41:ARG:NH1	2.10	0.67
1:A:215:GLU:OE1	1:A:218:LYS:HE3	1.95	0.67
1:A:216:ILE:HG23	1:A:217:LEU:N	2.10	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:ASN:ND2	1:A:74:GLU:HG3	2.10	0.66
1:B:297:THR:HG21	1:B:317:ALA:OXT	1.95	0.66
1:B:6:VAL:HA	1:B:40:HIS:O	1.96	0.66
1:B:216:ILE:HG23	1:B:217:LEU:N	2.09	0.66
1:B:253:SER:HB3	1:B:259:GLY:N	2.10	0.66
1:B:230:LEU:HG	1:B:234:ARG:HD2	1.76	0.66
1:A:196:ARG:CD	1:A:200:GLN:HE21	2.08	0.66
1:A:90:LEU:HA	1:A:129:TYR:OH	1.94	0.66
1:A:186:ASP:CG	1:A:187:GLU:H	1.99	0.66
1:B:59:GLU:OE2	1:B:63:LYS:HD3	1.95	0.66
1:A:220:LEU:HB3	1:A:230:LEU:HD11	1.76	0.66
1:A:37:ILE:HA	1:A:41:ARG:HH12	1.60	0.66
1:A:14:SER:O	1:A:18:GLU:HG3	1.95	0.66
1:B:169:LYS:HE3	1:B:211:ASP:OD1	1.96	0.66
1:B:188:ASP:O	1:B:192:ILE:HG13	1.94	0.66
1:B:239:CYS:O	1:B:243:PRO:HG3	1.95	0.66
1:A:200:GLN:CD	2:A:327:HOH:O	2.33	0.66
1:B:303:ASP:HA	1:B:306:LYS:HE2	1.78	0.66
1:A:98:ARG:HA	1:A:98:ARG:NE	2.10	0.66
1:B:12:ALA:HB3	1:B:15:ASP:OD2	1.96	0.66
1:B:214:GLU:OE1	1:B:219:SER:HA	1.95	0.66
1:B:89:ALA:HB1	1:B:125:TYR:HB2	1.75	0.66
1:B:216:ILE:HG23	1:B:217:LEU:H	1.60	0.66
1:B:147:LYS:HD3	2:B:404:HOH:O	1.96	0.66
1:B:173:LYS:O	1:B:177:GLU:HG3	1.96	0.66
1:B:171:GLU:HB3	1:B:192:ILE:HD13	1.76	0.66
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.78	0.66
1:A:285:GLN:CG	1:A:291:PRO:HG3	2.26	0.66
1:B:113:ARG:HB3	1:B:117:GLN:HB2	1.78	0.66
1:B:216:ILE:HG23	1:B:217:LEU:N	2.11	0.66
1:A:67:LYS:HD2	1:A:69:LEU:HB2	1.76	0.66
1:A:42:SER:OG	1:A:45:GLN:HB2	1.96	0.66
1:B:134:GLU:CD	1:B:134:GLU:H	1.96	0.66
1:B:65:LEU:CD1	1:B:77:ILE:HG21	2.26	0.66
1:A:269:VAL:HG12	1:A:311:LEU:HD12	1.78	0.66
1:A:205:PHE:HA	1:A:208:TYR:HB3	1.77	0.66
1:A:148:LEU:HD12	1:A:190:ILE:HG12	1.78	0.66
1:A:156:TYR:HD2	2:A:327:HOH:O	1.78	0.65
1:B:119:LEU:O	1:B:123:GLN:HG3	1.95	0.65
1:B:13:PRO:HB3	1:B:48:VAL:HG12	1.78	0.65
1:B:38:LEU:CD1	1:B:77:ILE:HD12	2.26	0.65
1:A:288:ASN:O	1:A:289:SER:HB2	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:GLU:HA	1:A:280:ILE:HG12	1.77	0.65
1:A:75:ARG:HH12	1:A:79:LEU:HD11	1.61	0.65
1:B:231:ALA:HA	1:B:234:ARG:HH21	1.61	0.65
1:A:107:MET:HE2	1:A:107:MET:C	2.17	0.65
1:A:175:VAL:O	1:A:179:ILE:HG12	1.97	0.65
1:A:169:LYS:HD2	1:A:207:ARG:NH2	2.10	0.65
1:B:105:VAL:O	1:B:108:GLU:N	2.29	0.65
1:B:3:THR:HG21	1:B:312:LEU:HD23	1.78	0.65
1:B:176:HIS:O	1:B:180:LYS:HB2	1.97	0.65
1:A:107:MET:HE1	1:A:108:GLU:HA	1.79	0.65
1:B:42:SER:OG	1:B:45:GLN:HG3	1.97	0.65
1:B:216:ILE:HG23	1:B:217:LEU:H	1.59	0.65
1:B:249:ASP:O	1:B:252:ARG:HB3	1.97	0.65
1:B:223:GLY:HA3	1:B:230:LEU:HD21	1.77	0.65
1:A:117:GLN:NE2	2:A:443:HOH:O	2.28	0.65
1:A:132:SER:OG	1:A:135:GLU:HB3	1.97	0.65
1:B:89:ALA:HB2	1:B:124:ALA:HB3	1.79	0.65
1:B:18:GLU:HA	1:B:57:TYR:OH	1.96	0.65
1:B:107:MET:HE3	1:B:107:MET:C	2.16	0.65
1:A:175:VAL:O	1:A:179:ILE:HG12	1.97	0.65
1:B:1:SER:HB3	1:B:278:LYS:HB3	1.79	0.65
1:B:51:GLN:HA	1:B:54:HIS:HB3	1.78	0.65
1:B:65:LEU:HD22	1:B:74:GLU:HB3	1.77	0.65
1:B:61:LEU:HD23	1:B:62:LEU:HD23	1.79	0.65
1:B:215:GLU:OE2	1:B:216:ILE:HG22	1.97	0.65
1:B:84:PRO:HG2	2:B:404:HOH:O	1.96	0.65
1:A:209:GLN:HG3	1:A:215:GLU:N	2.12	0.65
1:A:69:LEU:H	1:A:69:LEU:HD23	1.62	0.65
1:B:42:SER:OG	1:B:45:GLN:HG3	1.96	0.65
1:B:198:LYS:C	1:B:200:GLN:H	2.00	0.65
1:B:261:ASP:HB3	1:B:264:ALA:HB2	1.77	0.65
1:B:41:ARG:HA	1:B:41:ARG:NH1	2.12	0.65
1:B:178:LYS:HG3	1:B:186:ASP:OD2	1.97	0.65
1:B:10:VAL:HG21	1:B:45:GLN:HE22	1.61	0.65
1:B:105:VAL:HG22	1:B:267:ARG:NH2	2.12	0.65
1:A:205:PHE:O	1:A:208:TYR:HB3	1.97	0.65
1:B:41:ARG:HD2	1:B:49:ILE:HD11	1.79	0.65
1:B:300:THR:HG22	1:B:301:ARG:N	2.12	0.65
1:B:167:LEU:HA	1:B:170:GLN:NE2	2.11	0.65
1:A:215:GLU:H	1:A:218:LYS:HD2	1.61	0.64
1:A:3:THR:HG23	1:A:277:LEU:HB3	1.77	0.64
1:B:178:LYS:HG3	1:B:186:ASP:CG	2.17	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:GLU:HG2	1:A:154:THR:HG22	1.79	0.64
1:B:300:THR:HG22	1:B:301:ARG:H	1.61	0.64
2:A:361:HOH:O	1:B:126:HIS:HD2	1.80	0.64
1:A:273:ALA:HA	1:A:277:LEU:HB2	1.79	0.64
1:B:177:GLU:HA	1:B:180:LYS:HE3	1.77	0.64
1:B:1:SER:HB3	1:B:276:ASP:HA	1.77	0.64
1:A:216:ILE:HG23	1:A:217:LEU:N	2.13	0.64
1:B:87:ARG:HD2	2:B:321:HOH:O	1.97	0.64
1:A:269:VAL:HG11	1:A:308:LEU:HD22	1.80	0.64
1:B:135:GLU:O	1:B:139:HIS:HB2	1.98	0.64
1:A:197:SER:O	1:A:201:ILE:HG13	1.97	0.64
1:B:99:TRP:CZ3	1:B:141:THR:HA	2.32	0.64
1:A:51:GLN:O	1:A:55:GLU:HG3	1.98	0.64
1:A:272:ARG:HH12	1:A:275:ILE:HB	1.63	0.64
1:A:197:SER:O	1:A:201:ILE:HG13	1.97	0.64
1:A:92:ALA:O	1:A:96:THR:HG23	1.97	0.64
1:A:264:ALA:O	1:A:268:ILE:HG12	1.97	0.64
1:B:169:LYS:HE3	1:B:211:ASP:OD1	1.97	0.64
1:A:37:ILE:HG23	1:A:41:ARG:CZ	2.27	0.64
1:A:218:LYS:HA	1:A:221:GLU:OE2	1.98	0.64
1:A:141:THR:O	1:A:146:ARG:HD3	1.98	0.64
1:A:234:ARG:HD3	2:A:430:HOH:O	1.98	0.64
1:A:104:GLN:O	1:A:107:MET:HB3	1.98	0.64
1:B:152:LEU:HD23	1:B:194:SER:CB	2.28	0.64
1:B:297:THR:HG21	1:B:317:ALA:OXT	1.98	0.64
1:B:45:GLN:O	1:B:49:ILE:HG13	1.98	0.64
1:B:61:LEU:HD23	1:B:62:LEU:HD23	1.80	0.64
1:A:290:ILE:HD12	1:A:290:ILE:H	1.63	0.64
1:A:244:GLU:HA	1:A:280:ILE:HG12	1.80	0.64
1:B:77:ILE:HG22	1:B:78:LEU:N	2.14	0.63
1:B:90:LEU:O	1:B:94:GLU:HG3	1.98	0.63
1:A:1:SER:HB3	1:A:275:ILE:O	1.98	0.63
1:B:173:LYS:NZ	1:B:173:LYS:HB2	2.13	0.63
1:A:293:GLU:N	1:A:293:GLU:OE1	2.30	0.63
1:A:286:ARG:NH1	1:A:286:ARG:HB2	2.13	0.63
1:B:146:ARG:HG3	1:B:150:VAL:CG2	2.28	0.63
1:B:62:LEU:HD21	1:B:81:THR:HG21	1.81	0.63
1:B:217:LEU:HD21	1:B:237:ILE:HB	1.79	0.63
1:A:161:ASP:HA	1:A:199:ALA:CB	2.28	0.63
1:B:216:ILE:HG23	1:B:217:LEU:N	2.14	0.63
1:A:178:LYS:HB3	1:A:183:HIS:HB2	1.79	0.63
1:B:142:THR:O	1:B:145:PHE:HB2	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:ASP:HB3	1:A:264:ALA:HB2	1.80	0.63
1:B:293:GLU:OE2	1:B:314:GLU:HG3	1.98	0.63
1:A:6:VAL:HG21	1:A:42:SER:HB3	1.81	0.63
1:B:169:LYS:HG2	1:B:173:LYS:NZ	2.14	0.63
1:B:127:ALA:O	1:B:130:LYS:HE3	1.98	0.63
1:B:169:LYS:HD3	1:B:207:ARG:HH21	1.63	0.63
1:A:298:LYS:HE3	1:A:299:ASP:OD2	1.97	0.63
1:A:130:LYS:HD2	1:B:158:TYR:OH	1.98	0.63
1:B:134:GLU:HG3	1:B:154:THR:HG22	1.81	0.63
1:B:73:PHE:O	1:B:77:ILE:HG12	1.99	0.63
1:A:92:ALA:HB1	1:A:106:LEU:HD21	1.80	0.63
1:B:247:PHE:HD1	1:B:268:ILE:HD12	1.63	0.63
1:A:90:LEU:O	1:A:94:GLU:HG3	1.99	0.63
1:A:111:CYS:SG	1:A:152:LEU:HD22	2.39	0.63
1:A:129:TYR:O	1:A:131:LYS:N	2.32	0.63
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.63	0.63
1:A:198:LYS:HA	1:A:201:ILE:HD12	1.81	0.62
1:A:88:ASP:HA	1:A:91:LEU:HD12	1.82	0.62
1:A:218:LYS:HA	1:A:221:GLU:OE2	1.99	0.62
1:B:133:LEU:O	1:B:137:VAL:HG23	1.99	0.62
1:B:37:ILE:O	1:B:41:ARG:HG2	1.98	0.62
1:B:127:ALA:HA	1:B:130:LYS:NZ	2.13	0.62
1:B:215:GLU:HG3	2:B:366:HOH:O	1.99	0.62
1:B:198:LYS:HE2	1:B:240:LEU:HD23	1.81	0.62
1:B:4:LEU:HD22	1:B:274:GLU:HG2	1.81	0.62
1:B:10:VAL:HG22	1:B:45:GLN:NE2	2.15	0.62
1:B:44:GLU:O	1:B:48:VAL:HG23	1.98	0.62
1:B:135:GLU:O	1:B:139:HIS:HB2	2.00	0.62
1:A:216:ILE:HG23	1:A:217:LEU:N	2.14	0.62
1:A:216:ILE:HG23	1:A:217:LEU:H	1.64	0.62
1:B:87:ARG:HD2	2:B:322:HOH:O	1.98	0.62
1:A:298:LYS:HE3	1:A:299:ASP:OD2	1.99	0.62
1:A:191:ARG:HG2	1:A:191:ARG:HH11	1.63	0.62
1:A:62:LEU:HD22	1:A:65:LEU:HD12	1.82	0.62
1:B:14:SER:O	1:B:18:GLU:HG3	2.00	0.62
1:B:77:ILE:HD13	1:B:307:MET:SD	2.39	0.62
1:B:1:SER:H3	1:B:279:VAL:HG23	1.64	0.62
1:A:135:GLU:O	1:A:139:HIS:HB2	1.99	0.62
1:A:86:GLU:OE2	1:A:128:ARG:NH1	2.32	0.62
1:A:50:ARG:O	1:A:53:TYR:HB3	1.98	0.62
1:B:23:ALA:HB2	1:B:33:LEU:HD23	1.82	0.62
1:A:201:ILE:O	1:A:204:THR:N	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:ALA:HA	1:A:277:LEU:HD22	1.82	0.62
1:B:39:ALA:HB2	1:B:307:MET:SD	2.40	0.62
1:A:3:THR:HB	1:A:312:LEU:O	1.98	0.62
1:A:193:LEU:HD12	1:A:233:LEU:HD11	1.81	0.62
1:B:186:ASP:O	1:B:188:ASP:N	2.33	0.62
1:A:309:VAL:HA	1:A:312:LEU:HD12	1.82	0.62
1:A:60:ASP:HB3	1:A:63:LYS:HG2	1.82	0.62
1:A:46:ARG:HH11	1:A:46:ARG:HG3	1.64	0.62
1:B:134:GLU:CG	1:B:154:THR:HG22	2.30	0.62
1:B:11:PRO:HG2	1:B:16:ASP:OD2	1.98	0.62
1:A:31:GLU:HG2	1:A:303:ASP:OD1	2.00	0.62
1:B:169:LYS:HD3	1:B:207:ARG:NH2	2.15	0.62
1:B:73:PHE:HB2	1:B:304:TYR:HB2	1.82	0.62
1:B:209:GLN:HA	1:B:214:GLU:O	1.99	0.62
1:B:44:GLU:O	1:B:48:VAL:HG23	2.00	0.61
1:A:124:ALA:O	1:A:128:ARG:HB2	2.00	0.61
1:A:98:ARG:HA	1:A:98:ARG:NE	2.14	0.61
1:B:173:LYS:HZ2	1:B:173:LYS:HB2	1.65	0.61
1:B:50:ARG:NH1	1:B:82:LEU:HD23	2.14	0.61
1:B:215:GLU:OE1	1:B:218:LYS:HE3	2.00	0.61
1:A:23:ALA:HB1	1:A:34:ILE:CD1	2.29	0.61
1:A:186:ASP:HB3	1:A:189:VAL:HG23	1.81	0.61
1:B:238:GLN:HG2	1:B:246:TYR:HB2	1.81	0.61
1:A:286:ARG:CB	1:A:286:ARG:HH11	2.13	0.61
1:B:134:GLU:HG3	1:B:154:THR:HG22	1.82	0.61
1:B:119:LEU:O	1:B:123:GLN:HG3	2.00	0.61
1:B:277:LEU:HD21	1:B:312:LEU:HD23	1.83	0.61
1:A:220:LEU:HB2	1:A:234:ARG:NH1	2.15	0.61
1:A:19:GLN:HG2	2:A:392:HOH:O	2.00	0.61
1:A:119:LEU:O	1:A:123:GLN:HG3	1.99	0.61
1:B:149:LEU:O	1:B:152:LEU:N	2.34	0.61
1:A:293:GLU:OE2	1:A:314:GLU:HG3	1.99	0.61
1:A:107:MET:HE1	1:A:235:SER:HB3	1.83	0.61
1:A:186:ASP:O	1:A:190:ILE:HG13	2.01	0.61
1:B:64:THR:O	1:B:65:LEU:HG	2.01	0.61
1:A:51:GLN:O	1:A:55:GLU:HG3	2.00	0.61
1:B:220:LEU:HD22	1:B:230:LEU:HD11	1.82	0.61
1:A:256:ASN:O	1:A:258:THR:HG23	2.00	0.61
1:A:105:VAL:HG22	1:A:267:ARG:NH1	2.15	0.61
1:B:42:SER:HB2	2:B:344:HOH:O	1.99	0.61
1:B:198:LYS:HE2	1:B:240:LEU:HD23	1.83	0.61
1:B:147:LYS:HD3	2:B:407:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:162:GLU:O	1:A:163:VAL:HG23	2.01	0.61
1:B:255:ILE:C	1:B:257:LYS:H	2.04	0.61
1:B:300:THR:HG22	1:B:301:ARG:N	2.15	0.61
1:A:15:ASP:O	1:A:19:GLN:HG3	2.01	0.61
1:A:209:GLN:HE21	1:A:215:GLU:CA	2.14	0.61
1:B:133:LEU:CD2	1:B:153:VAL:HB	2.31	0.61
1:A:134:GLU:CG	1:A:154:THR:HG22	2.28	0.61
1:B:290:ILE:HD11	1:B:294:LYS:O	2.00	0.61
1:A:264:ALA:O	1:A:268:ILE:HG12	2.01	0.61
1:B:297:THR:HG21	1:B:317:ALA:O	2.01	0.61
1:B:71:ASN:ND2	1:B:74:GLU:HG3	2.16	0.61
1:B:196:ARG:HH11	1:B:196:ARG:HG2	1.66	0.60
1:B:169:LYS:HE3	1:B:211:ASP:OD1	2.01	0.60
1:B:73:PHE:HB2	1:B:303:ASP:O	2.01	0.60
1:A:207:ARG:HB3	1:A:211:ASP:OD2	2.00	0.60
1:B:133:LEU:HD12	1:B:137:VAL:HG23	1.83	0.60
1:B:126:HIS:HE1	1:B:132:SER:HA	1.66	0.60
1:A:304:TYR:CZ	1:A:308:LEU:HD11	2.35	0.60
1:B:150:VAL:HA	1:B:153:VAL:HG22	1.83	0.60
1:B:125:TYR:O	1:B:129:TYR:HB2	2.01	0.60
1:B:130:LYS:HA	1:B:130:LYS:HE2	1.83	0.60
1:A:73:PHE:O	1:A:77:ILE:HG13	2.02	0.60
1:A:234:ARG:HD3	2:A:431:HOH:O	2.02	0.60
1:A:161:ASP:O	1:A:163:VAL:HG23	2.01	0.60
1:B:78:LEU:O	1:B:82:LEU:HB2	2.02	0.60
1:A:35:ILE:CD1	1:A:35:ILE:H	2.13	0.60
1:A:290:ILE:HD12	1:A:290:ILE:N	2.15	0.60
1:A:51:GLN:C	1:A:53:TYR:H	2.05	0.60
1:B:193:LEU:HD22	1:B:236:THR:HG22	1.82	0.60
1:B:179:ILE:HD13	1:B:220:LEU:HD21	1.81	0.60
1:A:309:VAL:HA	1:A:312:LEU:HD12	1.83	0.60
1:A:184:TYR:HB3	1:A:233:LEU:HD22	1.82	0.60
1:A:165:MET:SD	1:A:207:ARG:HD3	2.42	0.60
1:A:13:PRO:HB3	1:A:48:VAL:HG12	1.83	0.60
1:A:78:LEU:O	1:A:82:LEU:HG	2.01	0.60
1:A:271:THR:O	1:A:272:ARG:HD2	2.01	0.60
1:A:201:ILE:O	1:A:204:THR:N	2.35	0.60
1:A:297:THR:HG23	1:A:309:VAL:HG11	1.82	0.60
1:A:71:ASN:HB3	1:A:74:GLU:OE1	2.02	0.60
1:B:3:THR:HG21	1:B:312:LEU:HD23	1.82	0.60
1:A:122:ARG:O	1:A:126:HIS:HB2	2.02	0.60
1:B:12:ALA:HB3	1:B:15:ASP:OD2	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:304:TYR:CZ	1:B:308:LEU:HD11	2.37	0.60
1:B:12:ALA:HB3	1:B:15:ASP:OD2	2.01	0.60
1:A:168:ALA:HB3	1:A:207:ARG:HG3	1.83	0.60
1:B:60:ASP:OD2	1:B:62:LEU:HB2	2.01	0.60
1:B:10:VAL:HG21	1:B:45:GLN:HE22	1.66	0.60
1:B:167:LEU:HA	1:B:170:GLN:NE2	2.16	0.60
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.66	0.60
1:A:186:ASP:O	1:A:190:ILE:HG13	2.02	0.60
1:A:22:THR:O	1:A:25:GLU:HG2	2.02	0.60
1:A:68:GLU:OE1	1:A:68:GLU:HA	2.01	0.60
1:A:98:ARG:HA	1:A:98:ARG:HE	1.67	0.60
1:B:217:LEU:HD13	1:B:238:GLN:HG2	1.84	0.60
1:A:165:MET:O	1:A:168:ALA:HB3	2.01	0.60
1:A:135:GLU:O	1:A:139:HIS:HB2	2.01	0.60
1:A:75:ARG:HE	1:A:79:LEU:HD11	1.67	0.60
1:B:71:ASN:HD22	1:B:74:GLU:N	1.95	0.60
1:B:109:VAL:HA	1:B:113:ARG:HD3	1.84	0.59
1:B:264:ALA:O	1:B:268:ILE:HG12	2.01	0.59
1:B:239:CYS:O	1:B:243:PRO:HG3	2.02	0.59
1:A:254:ALA:HB1	1:A:265:LEU:HB2	1.84	0.59
1:A:297:THR:HG22	1:A:305:GLU:HB3	1.83	0.59
1:A:165:MET:CE	1:A:207:ARG:HD3	2.32	0.59
1:A:288:ASN:O	1:A:289:SER:HB2	2.02	0.59
1:B:106:LEU:HD22	1:B:149:LEU:HB3	1.84	0.59
1:B:87:ARG:HD2	1:B:271:THR:HG22	1.83	0.59
1:B:126:HIS:HA	1:B:131:LYS:O	2.03	0.59
1:B:253:SER:HB3	1:B:259:GLY:N	2.17	0.59
1:B:175:VAL:CG2	1:B:192:ILE:HD12	2.33	0.59
1:B:54:HIS:C	1:B:56:THR:H	2.05	0.59
1:A:171:GLU:HB3	1:A:192:ILE:CD1	2.32	0.59
1:A:145:PHE:HD1	1:A:232:LEU:HD22	1.67	0.59
1:A:216:ILE:HG23	1:A:217:LEU:H	1.65	0.59
1:A:37:ILE:O	1:A:41:ARG:HG2	2.02	0.59
1:B:171:GLU:HB3	1:B:192:ILE:HD13	1.84	0.59
1:B:173:LYS:O	1:B:177:GLU:HG3	2.02	0.59
1:A:185:ASN:HD22	1:A:185:ASN:H	1.49	0.59
1:A:144:ASP:HA	1:A:147:LYS:NZ	2.18	0.59
1:A:156:TYR:HB3	2:B:324:HOH:O	2.01	0.59
1:A:304:TYR:CZ	1:A:308:LEU:HD11	2.37	0.59
1:A:134:GLU:CG	1:A:154:THR:HG22	2.32	0.59
1:B:107:MET:SD	1:B:236:THR:HA	2.41	0.59
1:B:59:GLU:OE2	1:B:63:LYS:HD3	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:THR:O	1:A:65:LEU:HD23	2.02	0.59
1:A:35:ILE:HD11	1:A:73:PHE:CE1	2.37	0.59
1:A:86:GLU:HA	1:A:124:ALA:HB1	1.84	0.59
1:A:253:SER:HB3	1:A:259:GLY:N	2.17	0.59
1:B:264:ALA:O	1:B:268:ILE:HG12	2.02	0.59
1:B:264:ALA:O	1:B:268:ILE:HG12	2.02	0.59
1:B:54:HIS:HA	1:B:59:GLU:O	2.01	0.59
1:A:77:ILE:O	1:A:80:TRP:HB3	2.03	0.59
1:A:158:TYR:HA	2:A:366:HOH:O	2.01	0.59
1:A:173:LYS:O	1:A:177:GLU:HG3	2.02	0.59
1:A:119:LEU:O	1:A:123:GLN:HG3	2.03	0.59
1:B:173:LYS:O	1:B:177:GLU:HG3	2.02	0.59
1:B:1:SER:HB3	1:B:276:ASP:HA	1.85	0.59
1:A:251:LEU:O	1:A:251:LEU:HD23	2.03	0.59
1:B:197:SER:O	1:B:201:ILE:HG13	2.01	0.59
1:A:35:ILE:HG23	1:A:307:MET:HA	1.85	0.59
1:B:253:SER:HA	1:B:258:THR:HB	1.84	0.59
1:A:175:VAL:O	1:A:179:ILE:HG12	2.02	0.59
1:A:111:CYS:HB3	1:A:240:LEU:HG	1.83	0.59
1:B:178:LYS:HG3	1:B:186:ASP:OD2	2.03	0.59
1:B:86:GLU:HA	1:B:124:ALA:HB1	1.85	0.59
1:B:1:SER:HB3	1:B:276:ASP:HA	1.85	0.59
1:B:84:PRO:HG2	2:B:408:HOH:O	2.02	0.59
1:B:149:LEU:O	1:B:153:VAL:HG22	2.03	0.59
1:B:118:LEU:O	1:B:122:ARG:HG3	2.03	0.59
1:A:35:ILE:HD12	1:A:307:MET:CB	2.29	0.59
1:B:244:GLU:HA	1:B:280:ILE:HG12	1.83	0.59
1:B:273:ALA:HA	1:B:277:LEU:HB2	1.85	0.58
1:A:91:LEU:HD22	1:A:267:ARG:HD3	1.85	0.58
1:A:215:GLU:CD	1:A:217:LEU:HD12	2.22	0.58
1:A:41:ARG:HH11	1:A:41:ARG:HG2	1.67	0.58
1:A:297:THR:CG2	1:A:305:GLU:HB3	2.32	0.58
1:B:18:GLU:HA	1:B:57:TYR:OH	2.03	0.58
1:B:193:LEU:HA	1:B:201:ILE:CD1	2.33	0.58
1:B:285:GLN:OE1	1:B:291:PRO:HG3	2.03	0.58
1:B:158:TYR:CE2	1:B:160:GLY:HA3	2.38	0.58
1:A:220:LEU:HB2	1:A:234:ARG:HH11	1.67	0.58
1:A:156:TYR:OH	1:B:123:GLN:HG2	2.03	0.58
1:A:134:GLU:OE2	2:A:320:HOH:O	2.17	0.58
1:A:171:GLU:HB3	1:A:192:ILE:HD13	1.85	0.58
1:B:19:GLN:HG2	1:B:33:LEU:HD21	1.84	0.58
1:A:264:ALA:O	1:A:268:ILE:HG12	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:SER:HA	1:B:40:HIS:ND1	2.19	0.58
1:A:186:ASP:HB3	1:A:189:VAL:CG2	2.32	0.58
1:B:296:ILE:HD12	1:B:312:LEU:HD11	1.85	0.58
1:A:286:ARG:NH1	1:A:286:ARG:HB2	2.19	0.58
1:B:304:TYR:OH	1:B:308:LEU:HD11	2.03	0.58
1:A:175:VAL:HG13	1:A:189:VAL:HG22	1.85	0.58
1:A:278:LYS:HD2	2:A:408:HOH:O	2.03	0.58
1:B:300:THR:HG22	1:B:301:ARG:N	2.18	0.58
1:A:34:ILE:HG22	1:A:34:ILE:O	2.03	0.58
1:A:3:THR:OG1	1:A:277:LEU:HD23	2.03	0.58
1:A:3:THR:HB	1:A:312:LEU:HA	1.84	0.58
1:A:74:GLU:HA	1:A:77:ILE:HD12	1.86	0.58
1:B:264:ALA:O	1:B:268:ILE:HG12	2.03	0.58
1:B:37:ILE:O	1:B:41:ARG:HG2	2.03	0.58
1:A:37:ILE:O	1:A:41:ARG:HG2	2.04	0.58
1:B:33:LEU:HD12	1:B:36:SER:HB3	1.84	0.58
1:B:304:TYR:CZ	1:B:308:LEU:HD11	2.38	0.58
1:B:215:GLU:H	1:B:218:LYS:HD2	1.68	0.58
1:A:272:ARG:HB3	1:A:276:ASP:OD1	2.03	0.58
1:B:149:LEU:O	1:B:153:VAL:HG22	2.04	0.58
1:B:71:ASN:HB3	1:B:74:GLU:CG	2.33	0.58
1:B:231:ALA:HA	1:B:234:ARG:HE	1.67	0.58
1:A:255:ILE:C	1:A:257:LYS:H	2.07	0.58
1:B:256:ASN:O	1:B:258:THR:HG23	2.03	0.58
1:B:73:PHE:O	1:B:77:ILE:HG12	2.03	0.58
1:B:135:GLU:O	1:B:139:HIS:HB2	2.03	0.58
1:B:89:ALA:HB1	1:B:125:TYR:CD2	2.39	0.58
1:B:303:ASP:HA	1:B:306:LYS:CD	2.33	0.58
1:B:239:CYS:O	1:B:243:PRO:HG3	2.04	0.58
1:A:129:TYR:O	1:A:131:LYS:HG3	2.03	0.58
1:B:65:LEU:HD22	1:B:74:GLU:CD	2.24	0.58
1:B:193:LEU:HA	1:B:201:ILE:HD13	1.86	0.58
1:B:42:SER:OG	1:B:45:GLN:HG3	2.04	0.58
1:A:197:SER:O	1:A:201:ILE:HG13	2.03	0.58
1:A:171:GLU:HB3	1:A:192:ILE:CD1	2.34	0.58
1:B:64:THR:O	1:B:65:LEU:HD23	2.04	0.58
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.67	0.58
1:B:138:ALA:O	1:B:146:ARG:HD3	2.04	0.58
1:B:18:GLU:HG2	1:B:57:TYR:CE2	2.39	0.58
1:B:302:GLY:O	1:B:306:LYS:HD3	2.04	0.58
1:A:129:TYR:O	1:A:131:LYS:HG3	2.04	0.58
1:A:71:ASN:ND2	1:A:73:PHE:HB3	2.13	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:THR:OG1	1:B:135:GLU:HB3	2.04	0.58
1:A:78:LEU:C	1:A:80:TRP:N	2.57	0.58
1:A:198:LYS:HB2	2:A:330:HOH:O	2.04	0.58
1:A:125:TYR:CD2	1:A:133:LEU:HD13	2.39	0.58
1:B:129:TYR:O	1:B:131:LYS:HG3	2.03	0.57
1:B:79:LEU:CB	1:B:270:THR:HG21	2.33	0.57
1:A:90:LEU:HD13	1:A:128:ARG:NH2	2.19	0.57
1:A:78:LEU:C	1:A:80:TRP:H	2.07	0.57
1:A:38:LEU:HD13	1:A:81:THR:OG1	2.03	0.57
1:A:139:HIS:HD2	2:B:335:HOH:O	1.85	0.57
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.05	0.57
1:A:77:ILE:HG12	1:A:307:MET:CE	2.34	0.57
1:A:149:LEU:O	1:A:153:VAL:HG13	2.04	0.57
1:A:216:ILE:HG23	1:A:217:LEU:N	2.19	0.57
1:B:110:ALA:HB1	1:B:152:LEU:O	2.04	0.57
1:A:185:ASN:HD22	1:A:185:ASN:N	2.02	0.57
1:B:177:GLU:O	1:B:180:LYS:HB3	2.04	0.57
1:A:169:LYS:HD2	1:A:207:ARG:HH21	1.69	0.57
1:A:247:PHE:CD1	1:A:268:ILE:HD12	2.39	0.57
1:A:107:MET:HE2	1:A:107:MET:O	2.04	0.57
1:B:35:ILE:HG22	1:B:35:ILE:O	2.03	0.57
1:B:252:ARG:HG3	1:B:253:SER:H	1.69	0.57
1:A:276:ASP:OD2	1:A:280:ILE:HD11	2.05	0.57
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.85	0.57
1:B:216:ILE:HG23	1:B:217:LEU:N	2.19	0.57
1:A:122:ARG:HH21	1:B:156:TYR:HB3	1.68	0.57
1:A:45:GLN:O	1:A:49:ILE:HG13	2.04	0.57
1:A:298:LYS:HE3	1:A:299:ASP:OD2	2.03	0.57
1:A:293:GLU:HB3	1:A:312:LEU:CD1	2.33	0.57
1:B:105:VAL:HG21	2:B:342:HOH:O	2.03	0.57
1:A:165:MET:O	1:A:168:ALA:HB3	2.05	0.57
1:A:15:ASP:O	1:A:19:GLN:HG3	2.04	0.57
1:B:216:ILE:HG23	1:B:217:LEU:H	1.68	0.57
1:B:143:GLY:HA3	2:B:355:HOH:O	2.05	0.57
1:A:122:ARG:NH2	1:A:154:THR:HA	2.19	0.57
1:A:267:ARG:NH1	1:A:268:ILE:HD11	2.20	0.57
1:B:61:LEU:O	1:B:64:THR:HG22	2.05	0.57
1:B:281:GLY:C	1:B:283:GLU:H	2.07	0.57
1:A:234:ARG:HD3	2:A:428:HOH:O	2.05	0.57
1:B:6:VAL:HG13	1:B:41:ARG:HA	1.86	0.57
1:B:202:ASN:ND2	1:B:206:ASN:ND2	2.52	0.57
1:B:45:GLN:O	1:B:49:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:ARG:HH21	1:B:156:TYR:HB3	1.69	0.57
1:B:106:LEU:O	1:B:106:LEU:HD23	2.05	0.57
1:B:21:ARG:HG2	1:B:57:TYR:CZ	2.40	0.57
1:A:250:VAL:HG11	1:A:268:ILE:HD11	1.87	0.57
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.39	0.57
1:B:202:ASN:ND2	1:B:206:ASN:HD21	2.01	0.57
1:A:108:GLU:OE2	2:A:318:HOH:O	2.17	0.57
1:A:139:HIS:HD2	2:A:341:HOH:O	1.87	0.57
1:B:111:CYS:HB3	1:B:240:LEU:HG	1.85	0.57
1:A:197:SER:O	1:A:201:ILE:HG13	2.04	0.57
1:A:99:TRP:CZ3	1:A:141:THR:HA	2.40	0.57
1:A:92:ALA:O	1:A:96:THR:HG23	2.05	0.57
1:A:242:ARG:HB2	1:A:245:LEU:HD12	1.87	0.57
1:A:239:CYS:O	1:A:243:PRO:HG3	2.05	0.57
1:A:75:ARG:O	1:A:78:LEU:HB3	2.05	0.57
1:A:175:VAL:O	1:A:179:ILE:HG12	2.04	0.57
1:A:122:ARG:HH21	1:A:134:GLU:CD	2.08	0.57
1:B:148:LEU:HA	1:B:190:ILE:HG21	1.87	0.57
1:B:19:GLN:CD	1:B:37:ILE:HD11	2.25	0.57
1:A:132:SER:N	1:A:135:GLU:OE2	2.30	0.57
1:A:114:THR:OG1	1:A:117:GLN:HG3	2.05	0.57
1:B:215:GLU:N	1:B:218:LYS:HD2	2.20	0.57
1:B:113:ARG:HG3	2:B:376:HOH:O	2.05	0.57
1:B:65:LEU:HD22	1:B:74:GLU:CB	2.35	0.57
1:A:156:TYR:HB3	1:B:122:ARG:NH2	2.20	0.57
1:A:171:GLU:O	1:A:175:VAL:HG23	2.04	0.57
1:B:3:THR:HG23	1:B:278:LYS:N	2.19	0.57
1:A:142:THR:HB	2:A:372:HOH:O	2.05	0.57
1:A:148:LEU:HD23	1:A:232:LEU:HG	1.86	0.56
1:A:60:ASP:HB3	1:A:63:LYS:HG2	1.86	0.56
1:A:125:TYR:O	1:A:129:TYR:HB2	2.05	0.56
1:A:165:MET:HB3	2:A:397:HOH:O	2.04	0.56
1:A:119:LEU:HD21	1:B:119:LEU:HD21	1.87	0.56
1:A:161:ASP:HA	1:A:199:ALA:HB2	1.86	0.56
1:A:188:ASP:HA	1:A:191:ARG:HB3	1.85	0.56
1:B:260:THR:O	1:B:260:THR:HG22	2.05	0.56
1:B:84:PRO:HG2	2:B:405:HOH:O	2.04	0.56
1:A:168:ALA:O	1:A:172:ALA:HB2	2.04	0.56
1:A:301:ARG:CZ	2:A:368:HOH:O	2.52	0.56
1:A:242:ARG:HD3	2:A:386:HOH:O	2.05	0.56
1:B:3:THR:OG1	1:B:277:LEU:HB3	2.05	0.56
1:A:132:SER:N	1:A:135:GLU:OE2	2.30	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:LEU:HD12	1:A:266:THR:HG22	1.87	0.56
1:A:196:ARG:HB3	1:A:200:GLN:HG2	1.87	0.56
1:A:1:SER:CB	1:A:276:ASP:HA	2.32	0.56
1:A:122:ARG:HG2	1:A:133:LEU:HB3	1.88	0.56
1:B:34:ILE:HG22	1:B:38:LEU:HD12	1.86	0.56
1:B:202:ASN:HD21	1:B:206:ASN:HD21	1.53	0.56
1:A:191:ARG:NH1	1:A:196:ARG:HH21	1.95	0.56
1:B:119:LEU:O	1:B:123:GLN:HG3	2.06	0.56
1:A:154:THR:HB	1:B:154:THR:OG1	2.04	0.56
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.06	0.56
1:A:165:MET:CE	1:A:207:ARG:HD3	2.34	0.56
1:A:159:GLU:N	2:A:366:HOH:O	2.38	0.56
1:A:173:LYS:O	1:A:177:GLU:HG3	2.05	0.56
1:A:66:ASP:HA	1:A:78:LEU:HD22	1.88	0.56
1:A:14:SER:O	1:A:18:GLU:HG3	2.04	0.56
1:B:169:LYS:CE	1:B:207:ARG:HH21	2.18	0.56
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.86	0.56
1:A:103:ASN:O	1:A:104:GLN:HG3	2.05	0.56
1:B:44:GLU:H	1:B:44:GLU:CD	2.07	0.56
1:B:146:ARG:HG3	1:B:150:VAL:HG21	1.88	0.56
1:B:198:LYS:O	1:B:201:ILE:N	2.39	0.56
1:B:71:ASN:HB3	1:B:74:GLU:HG3	1.88	0.56
1:A:101:SER:HB2	1:A:145:PHE:CZ	2.40	0.56
1:B:82:LEU:HD22	1:B:87:ARG:N	2.21	0.56
1:B:84:PRO:HG2	2:B:402:HOH:O	2.06	0.56
1:A:104:GLN:NE2	1:A:246:TYR:HE1	2.04	0.56
1:B:255:ILE:HD12	1:B:284:TYR:OH	2.05	0.56
1:A:171:GLU:O	1:A:175:VAL:HG23	2.05	0.56
1:B:293:GLU:HG3	1:B:314:GLU:HG3	1.88	0.56
1:A:301:ARG:NH2	1:A:306:LYS:HD3	2.11	0.56
1:A:62:LEU:HD21	1:A:81:THR:HB	1.86	0.56
1:B:93:ASN:HB2	1:B:129:TYR:CE2	2.41	0.56
1:B:304:TYR:CZ	1:B:308:LEU:HD11	2.40	0.56
1:B:8:ASP:CG	1:B:9:SER:H	2.07	0.56
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.87	0.56
1:B:133:LEU:O	1:B:137:VAL:HG23	2.05	0.56
1:B:50:ARG:HG2	1:B:61:LEU:HD21	1.87	0.56
1:A:92:ALA:O	1:A:96:THR:HG22	2.06	0.56
1:A:217:LEU:HD11	1:A:238:GLN:HG2	1.88	0.56
2:A:362:HOH:O	1:B:126:HIS:HD2	1.88	0.56
1:B:225:ASP:HA	1:B:234:ARG:NH1	2.17	0.56
1:B:191:ARG:HD3	2:B:320:HOH:O	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:GLU:O	1:A:180:LYS:HB2	2.06	0.56
1:A:171:GLU:O	1:A:175:VAL:HG23	2.06	0.56
1:A:122:ARG:HB3	2:A:322:HOH:O	2.06	0.56
1:A:76:ALA:HA	1:A:266:THR:HG23	1.87	0.56
1:A:186:ASP:OD2	1:A:188:ASP:HB2	2.05	0.56
1:A:158:TYR:CZ	1:A:160:GLY:HA3	2.40	0.56
1:A:134:GLU:HB3	1:B:195:THR:HG22	1.88	0.56
1:A:107:MET:SD	1:A:236:THR:HA	2.46	0.56
1:B:175:VAL:HG23	1:B:192:ILE:CD1	2.36	0.56
1:A:19:GLN:HB3	1:A:33:LEU:HD21	1.86	0.56
1:B:78:LEU:O	1:B:82:LEU:HG	2.06	0.56
1:B:71:ASN:HB3	1:B:74:GLU:HB2	1.87	0.56
1:B:220:LEU:HD11	1:B:237:ILE:HD12	1.87	0.56
1:B:309:VAL:CG2	1:B:315:ASP:HA	2.36	0.56
1:B:125:TYR:O	1:B:129:TYR:HB2	2.06	0.56
1:A:3:THR:CB	1:A:312:LEU:HA	2.36	0.56
1:B:12:ALA:HB1	1:B:13:PRO:CD	2.30	0.56
1:B:19:GLN:OE1	1:B:37:ILE:HD11	2.06	0.56
1:A:301:ARG:HH22	1:A:306:LYS:CD	2.13	0.56
1:A:297:THR:HG22	1:A:305:GLU:HB3	1.88	0.56
1:B:272:ARG:O	1:B:277:LEU:HB2	2.06	0.56
1:A:275:ILE:HD12	2:A:333:HOH:O	2.05	0.56
1:A:171:GLU:O	1:A:175:VAL:HG23	2.06	0.56
1:A:122:ARG:CZ	1:A:154:THR:HA	2.36	0.56
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.88	0.56
1:B:268:ILE:O	1:B:272:ARG:HG2	2.06	0.56
1:A:119:LEU:O	1:A:123:GLN:HG3	2.06	0.56
1:A:11:PRO:HG2	1:A:16:ASP:OD1	2.06	0.56
1:A:31:GLU:HG2	1:A:303:ASP:OD1	2.04	0.56
1:A:158:TYR:HD1	1:B:126:HIS:HB3	1.71	0.56
1:A:125:TYR:CE2	1:A:133:LEU:HD13	2.41	0.56
1:A:165:MET:CE	1:A:207:ARG:HD3	2.32	0.55
1:A:158:TYR:CZ	1:A:160:GLY:HA3	2.41	0.55
1:B:239:CYS:O	1:B:243:PRO:HG3	2.06	0.55
1:A:293:GLU:HG2	1:A:294:LYS:H	1.71	0.55
1:B:297:THR:HG21	1:B:317:ALA:OXT	2.04	0.55
1:B:122:ARG:HD2	2:B:356:HOH:O	2.07	0.55
1:B:179:ILE:HD11	1:B:220:LEU:CD2	2.36	0.55
1:B:45:GLN:O	1:B:49:ILE:HG13	2.06	0.55
1:B:119:LEU:O	1:B:123:GLN:HG3	2.07	0.55
1:A:62:LEU:HD21	1:A:81:THR:CB	2.33	0.55
1:B:96:THR:HG21	1:B:136:ASP:O	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:248:VAL:HG21	1:B:283:GLU:HB3	1.88	0.55
1:B:254:ALA:HB1	1:B:265:LEU:HB2	1.89	0.55
1:A:96:THR:HA	1:A:99:TRP:HB2	1.88	0.55
1:B:119:LEU:O	1:B:123:GLN:HG3	2.06	0.55
1:A:161:ASP:O	1:A:163:VAL:HG23	2.06	0.55
1:B:309:VAL:HA	1:B:312:LEU:HD12	1.88	0.55
1:A:35:ILE:HD12	1:A:307:MET:HA	1.88	0.55
1:B:220:LEU:HD12	1:B:234:ARG:HG2	1.87	0.55
1:B:148:LEU:HA	1:B:190:ILE:CG2	2.36	0.55
1:B:145:PHE:HZ	1:B:228:LYS:HB2	1.71	0.55
1:B:73:PHE:CE1	1:B:77:ILE:HD11	2.42	0.55
1:A:67:LYS:HD3	1:A:70:SER:HB3	1.88	0.55
1:A:162:GLU:CD	1:A:162:GLU:H	2.10	0.55
1:B:50:ARG:CZ	1:B:62:LEU:HD12	2.37	0.55
1:A:293:GLU:O	1:A:297:THR:HG23	2.06	0.55
1:B:158:TYR:O	1:B:197:SER:OG	2.23	0.55
1:A:148:LEU:HG	1:A:152:LEU:HD12	1.88	0.55
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.88	0.55
1:A:179:ILE:HD12	1:A:220:LEU:CD2	2.36	0.55
1:B:261:ASP:OD1	1:B:264:ALA:HB2	2.06	0.55
1:A:6:VAL:HG12	1:A:7:SER:H	1.72	0.55
1:A:89:ALA:HB2	1:A:121:ALA:O	2.07	0.55
1:A:173:LYS:O	1:A:177:GLU:HG3	2.07	0.55
1:B:273:ALA:HA	1:B:277:LEU:HB2	1.89	0.55
1:B:74:GLU:O	1:B:77:ILE:HB	2.06	0.55
1:B:43:ALA:HB2	1:B:274:GLU:OE2	2.07	0.55
1:A:235:SER:HA	1:A:238:GLN:OE1	2.07	0.55
1:A:166:THR:HB	2:A:350:HOH:O	2.05	0.55
1:B:75:ARG:NH1	1:B:90:LEU:HD21	2.19	0.55
1:A:4:LEU:HD12	1:A:311:LEU:HA	1.89	0.55
1:A:168:ALA:HA	2:A:327:HOH:O	2.06	0.55
1:B:109:VAL:HG12	1:B:109:VAL:O	2.07	0.55
1:A:95:ALA:HB1	1:A:103:ASN:ND2	2.21	0.55
1:A:58:GLY:O	1:A:59:GLU:HG3	2.06	0.55
1:B:205:PHE:O	1:B:208:TYR:HB3	2.07	0.55
1:A:184:TYR:OH	1:A:223:GLY:HA3	2.07	0.55
1:A:137:VAL:HG13	1:A:141:THR:HG21	1.89	0.55
1:B:1:SER:OG	1:B:279:VAL:HG23	2.06	0.55
1:B:128:ARG:HD3	1:B:129:TYR:CZ	2.41	0.55
1:A:135:GLU:C	1:A:137:VAL:H	2.11	0.55
1:A:154:THR:HB	1:B:154:THR:O	2.06	0.55
1:B:132:SER:OG	1:B:135:GLU:HB3	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:244:GLU:O	1:B:248:VAL:HG23	2.07	0.55
1:A:193:LEU:HD22	1:A:240:LEU:HD12	1.89	0.55
1:B:255:ILE:C	1:B:257:LYS:H	2.08	0.55
1:B:173:LYS:HE2	2:B:413:HOH:O	2.07	0.55
1:A:19:GLN:HG2	2:A:393:HOH:O	2.05	0.55
1:B:256:ASN:O	1:B:257:LYS:HB3	2.06	0.55
1:A:300:THR:HG22	1:A:301:ARG:N	2.22	0.55
1:A:162:GLU:HG2	1:B:130:LYS:HB3	1.89	0.55
1:A:208:TYR:HA	1:A:212:HIS:HD2	1.71	0.55
1:A:50:ARG:CZ	1:A:62:LEU:HD12	2.37	0.54
1:A:1:SER:OG	1:A:276:ASP:HA	2.07	0.54
1:A:191:ARG:HG2	1:A:191:ARG:NH1	2.22	0.54
2:A:364:HOH:O	1:B:126:HIS:HD2	1.88	0.54
1:A:203:ALA:HA	1:A:206:ASN:ND2	2.22	0.54
1:B:127:ALA:HA	1:B:130:LYS:CE	2.36	0.54
1:A:47:LYS:HG3	1:A:83:GLU:OE2	2.07	0.54
1:A:216:ILE:HG23	1:A:217:LEU:H	1.71	0.54
1:A:4:LEU:HG	1:A:6:VAL:HG23	1.89	0.54
1:A:241:THR:HG22	1:A:242:ARG:HG3	1.88	0.54
1:A:92:ALA:O	1:A:125:TYR:HE2	1.88	0.54
1:A:58:GLY:O	1:A:59:GLU:HB2	2.08	0.54
1:B:202:ASN:HD21	1:B:206:ASN:ND2	2.05	0.54
1:A:13:PRO:HA	1:A:16:ASP:OD2	2.07	0.54
1:A:198:LYS:HE2	1:A:240:LEU:HD22	1.90	0.54
1:B:278:LYS:O	1:B:282:GLU:HG3	2.07	0.54
1:B:249:ASP:O	1:B:252:ARG:HB3	2.07	0.54
1:B:267:ARG:NH1	1:B:268:ILE:HD11	2.21	0.54
1:B:291:PRO:HB2	1:B:294:LYS:HG3	1.87	0.54
1:B:11:PRO:HD2	1:B:41:ARG:HH21	1.72	0.54
1:B:192:ILE:O	1:B:201:ILE:HD11	2.07	0.54
1:A:107:MET:HE2	1:A:107:MET:C	2.28	0.54
1:B:209:GLN:HA	1:B:214:GLU:O	2.07	0.54
1:A:234:ARG:HD3	2:A:433:HOH:O	2.07	0.54
1:A:122:ARG:NH2	1:B:156:TYR:HB2	2.22	0.54
1:A:134:GLU:HG3	1:A:154:THR:HG22	1.89	0.54
1:B:157:ARG:HH22	1:B:194:SER:HA	1.72	0.54
1:B:176:HIS:O	1:B:180:LYS:HG2	2.07	0.54
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.42	0.54
1:B:241:THR:HG22	1:B:242:ARG:N	2.22	0.54
1:B:87:ARG:HH11	1:B:271:THR:HG22	1.70	0.54
1:A:104:GLN:NE2	1:A:246:TYR:CE1	2.76	0.54
1:A:118:LEU:O	1:A:122:ARG:HG3	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:139:HIS:CD2	1:B:196:ARG:HH22	2.25	0.54
1:B:73:PHE:CZ	1:B:77:ILE:HD11	2.42	0.54
1:B:230:LEU:HG	1:B:234:ARG:CD	2.37	0.54
1:A:43:ALA:HA	1:A:46:ARG:CZ	2.38	0.54
1:A:271:THR:O	1:A:272:ARG:HD2	2.08	0.54
1:A:87:ARG:HD3	1:A:271:THR:HG22	1.90	0.54
1:A:62:LEU:CD1	1:A:82:LEU:HD23	2.38	0.54
1:B:178:LYS:HG3	1:B:186:ASP:OD2	2.07	0.54
1:B:42:SER:O	1:B:46:ARG:HG3	2.08	0.54
1:B:47:LYS:HE2	1:B:83:GLU:OE2	2.08	0.54
1:B:218:LYS:HA	1:B:221:GLU:OE2	2.07	0.54
1:A:98:ARG:HA	1:A:98:ARG:NE	2.22	0.54
1:B:45:GLN:O	1:B:49:ILE:HG13	2.08	0.54
1:A:135:GLU:HB2	1:B:196:ARG:NH1	2.22	0.54
1:A:185:ASN:ND2	1:A:185:ASN:H	2.05	0.54
1:B:248:VAL:HG23	1:B:280:ILE:HG23	1.89	0.54
1:A:13:PRO:CB	1:A:48:VAL:HG12	2.37	0.54
1:B:86:GLU:HA	1:B:124:ALA:HB1	1.90	0.54
1:A:134:GLU:OE1	1:A:134:GLU:N	2.41	0.54
1:A:186:ASP:HB3	1:A:189:VAL:HG23	1.90	0.54
1:B:175:VAL:HG23	1:B:192:ILE:HD12	1.90	0.54
1:B:156:TYR:HD1	2:B:354:HOH:O	1.90	0.54
1:B:291:PRO:HB2	1:B:294:LYS:HG3	1.90	0.54
1:B:259:GLY:O	1:B:261:ASP:N	2.39	0.54
1:A:158:TYR:C	1:A:160:GLY:H	2.10	0.54
1:A:35:ILE:HD11	1:A:73:PHE:CE1	2.40	0.54
1:B:262:GLU:OE1	1:B:262:GLU:HA	2.07	0.54
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.90	0.54
1:A:107:MET:HE2	1:A:107:MET:O	2.06	0.54
1:A:99:TRP:CD1	1:A:103:ASN:HB3	2.43	0.54
1:B:134:GLU:CG	1:B:154:THR:HG22	2.19	0.54
1:A:132:SER:N	1:A:135:GLU:OE2	2.39	0.54
1:A:11:PRO:HG2	1:A:16:ASP:OD2	2.08	0.54
1:B:293:GLU:OE2	1:B:314:GLU:HG3	2.07	0.54
1:B:269:VAL:O	1:B:273:ALA:HB2	2.08	0.54
1:A:150:VAL:HA	1:A:153:VAL:CG2	2.37	0.54
1:B:107:MET:HE3	1:B:239:CYS:HB2	1.88	0.54
1:B:132:SER:HA	2:B:318:HOH:O	2.08	0.54
1:A:310:ALA:O	1:A:313:GLY:N	2.39	0.54
1:B:248:VAL:HG21	1:B:283:GLU:HB3	1.89	0.54
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.08	0.54
1:A:19:GLN:HG2	2:A:392:HOH:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:LYS:HE3	2:B:325:HOH:O	2.07	0.54
1:B:215:GLU:H	1:B:218:LYS:HD2	1.72	0.54
1:B:303:ASP:HA	1:B:306:LYS:CE	2.37	0.54
1:B:75:ARG:CZ	1:B:79:LEU:HD11	2.38	0.54
1:A:46:ARG:O	1:A:49:ILE:HB	2.09	0.54
1:B:116:THR:O	1:B:119:LEU:N	2.41	0.54
1:A:115:SER:OG	1:A:159:GLU:HG3	2.08	0.54
1:A:122:ARG:NH2	1:B:156:TYR:HB3	2.23	0.54
1:A:108:GLU:OE2	1:A:267:ARG:NH1	2.40	0.54
1:B:173:LYS:HG2	1:B:173:LYS:O	2.08	0.54
1:A:16:ASP:O	1:A:20:LEU:HG	2.08	0.54
1:B:113:ARG:HG3	1:B:117:GLN:HB3	1.90	0.53
1:A:265:LEU:HG	1:A:308:LEU:HD13	1.90	0.53
1:B:45:GLN:O	1:B:49:ILE:HG13	2.08	0.53
1:A:215:GLU:HG2	1:A:216:ILE:H	1.72	0.53
1:A:298:LYS:HE3	1:A:299:ASP:OD2	2.08	0.53
1:A:308:LEU:O	1:A:312:LEU:HG	2.08	0.53
1:B:118:LEU:O	1:B:122:ARG:HG3	2.07	0.53
1:B:1:SER:HB2	1:B:278:LYS:HD3	1.89	0.53
1:B:191:ARG:NH1	1:B:196:ARG:NH2	2.48	0.53
1:A:144:ASP:HA	1:A:147:LYS:CD	2.36	0.53
1:A:192:ILE:HA	1:A:196:ARG:HG2	1.88	0.53
1:A:286:ARG:HH11	1:A:286:ARG:CB	2.21	0.53
1:A:109:VAL:HG12	1:A:109:VAL:O	2.07	0.53
1:A:167:LEU:HD23	1:A:200:GLN:HE22	1.73	0.53
1:B:72:ASP:HB3	1:B:304:TYR:CG	2.43	0.53
1:A:4:LEU:HD22	1:A:274:GLU:HG2	1.89	0.53
1:A:33:LEU:O	1:A:37:ILE:HG12	2.08	0.53
1:B:242:ARG:HB3	1:B:244:GLU:OE2	2.09	0.53
1:A:186:ASP:CG	1:A:187:GLU:N	2.62	0.53
1:A:87:ARG:HD3	1:A:271:THR:HG22	1.90	0.53
1:B:238:GLN:NE2	1:B:245:LEU:HB2	2.23	0.53
1:B:276:ASP:O	1:B:280:ILE:HG13	2.08	0.53
1:B:252:ARG:NE	1:B:288:ASN:OD1	2.41	0.53
1:B:115:SER:HA	2:B:327:HOH:O	2.07	0.53
1:B:177:GLU:HA	1:B:180:LYS:HE3	1.89	0.53
1:A:300:THR:HG22	1:A:301:ARG:N	2.24	0.53
1:B:126:HIS:CE1	1:B:132:SER:HA	2.43	0.53
1:A:239:CYS:O	1:A:243:PRO:HG3	2.09	0.53
1:A:177:GLU:O	1:A:180:LYS:HB2	2.08	0.53
1:A:253:SER:O	1:A:256:ASN:N	2.39	0.53
1:A:207:ARG:CZ	2:A:397:HOH:O	2.57	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:MET:HG2	1:A:111:CYS:SG	2.48	0.53
1:B:261:ASP:OD2	1:B:264:ALA:HB2	2.09	0.53
1:B:42:SER:O	1:B:46:ARG:HG3	2.08	0.53
1:B:73:PHE:O	1:B:77:ILE:HG12	2.08	0.53
1:A:83:GLU:HB3	1:A:84:PRO:HD2	1.89	0.53
1:A:131:LYS:HD2	1:A:136:ASP:OD1	2.08	0.53
1:B:14:SER:O	1:B:18:GLU:HG3	2.09	0.53
1:A:87:ARG:HD2	1:A:271:THR:HG22	1.90	0.53
1:A:302:GLY:O	1:A:306:LYS:HG3	2.07	0.53
1:A:162:GLU:N	2:A:321:HOH:O	2.40	0.53
1:B:130:LYS:CA	1:B:130:LYS:HE2	2.37	0.53
1:B:44:GLU:O	1:B:48:VAL:HG23	2.08	0.53
1:B:264:ALA:O	1:B:268:ILE:HG12	2.08	0.53
1:A:139:HIS:ND1	2:A:433:HOH:O	2.34	0.53
1:A:171:GLU:HB3	1:A:192:ILE:HD13	1.91	0.53
1:A:3:THR:HG23	1:A:277:LEU:HB3	1.90	0.53
1:B:301:ARG:HH21	1:B:317:ALA:HB3	1.74	0.53
1:A:196:ARG:HH11	1:B:135:GLU:HB2	1.72	0.53
1:B:166:THR:HG22	1:B:170:GLN:NE2	2.23	0.53
1:A:169:LYS:HD2	2:A:396:HOH:O	2.08	0.53
1:B:125:TYR:CD2	1:B:133:LEU:HB2	2.44	0.53
1:A:1:SER:HB2	1:A:275:ILE:O	2.08	0.53
1:A:119:LEU:O	1:A:123:GLN:HG3	2.09	0.53
1:B:101:SER:HB2	1:B:145:PHE:CZ	2.44	0.53
1:A:224:ASP:HB3	1:A:227:ASP:HB2	1.91	0.53
1:B:45:GLN:O	1:B:49:ILE:HG13	2.09	0.53
1:A:161:ASP:O	1:A:163:VAL:HG23	2.09	0.53
1:B:119:LEU:HD22	1:B:156:TYR:HE1	1.68	0.53
1:B:310:ALA:HA	1:B:315:ASP:HB2	1.91	0.53
1:A:46:ARG:NE	1:A:80:TRP:O	2.42	0.53
1:B:8:ASP:O	1:B:9:SER:HB3	2.09	0.53
1:A:175:VAL:O	1:A:179:ILE:HG12	2.08	0.53
1:A:249:ASP:O	1:A:252:ARG:HB3	2.09	0.53
1:A:77:ILE:HG12	1:A:307:MET:HE2	1.91	0.52
1:A:215:GLU:N	1:A:218:LYS:HD2	2.24	0.52
1:A:154:THR:HB	1:B:154:THR:HB	1.90	0.52
1:A:185:ASN:C	1:A:185:ASN:HD22	2.11	0.52
1:B:95:ALA:O	1:B:99:TRP:HB2	2.09	0.52
1:A:293:GLU:HG2	1:A:294:LYS:H	1.74	0.52
1:B:276:ASP:O	1:B:280:ILE:HG13	2.09	0.52
1:B:83:GLU:HB2	1:B:86:GLU:HG3	1.91	0.52
1:A:215:GLU:O	1:A:219:SER:N	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:VAL:CG1	1:A:7:SER:N	2.72	0.52
1:B:54:HIS:HA	1:B:59:GLU:O	2.09	0.52
1:A:192:ILE:O	1:A:201:ILE:HD11	2.09	0.52
1:A:297:THR:HG22	1:A:301:ARG:HE	1.74	0.52
1:A:247:PHE:CD1	1:A:268:ILE:HD12	2.44	0.52
1:A:247:PHE:CD1	1:A:268:ILE:HD12	2.44	0.52
1:B:148:LEU:O	1:B:152:LEU:HG	2.10	0.52
1:A:51:GLN:O	1:A:55:GLU:HG3	2.09	0.52
1:A:71:ASN:OD1	1:A:74:GLU:HG3	2.08	0.52
1:A:165:MET:HE1	1:A:207:ARG:HD3	1.89	0.52
1:A:253:SER:O	1:A:259:GLY:N	2.42	0.52
1:A:92:ALA:HB1	1:A:106:LEU:CD2	2.39	0.52
1:A:3:THR:OG1	1:A:277:LEU:HD23	2.09	0.52
1:A:134:GLU:OE2	1:B:156:TYR:HB3	2.10	0.52
1:A:143:GLY:O	1:A:146:ARG:HB3	2.09	0.52
1:A:158:TYR:O	1:A:160:GLY:N	2.42	0.52
1:B:73:PHE:C	1:B:75:ARG:H	2.12	0.52
1:B:184:TYR:HB3	1:B:233:LEU:CD2	2.36	0.52
1:B:244:GLU:O	1:B:248:VAL:HG23	2.09	0.52
1:B:114:THR:HG23	1:B:117:GLN:NE2	2.24	0.52
1:A:169:LYS:CD	1:A:207:ARG:HH21	2.18	0.52
1:A:145:PHE:O	1:A:149:LEU:HG	2.10	0.52
1:B:132:SER:O	1:B:135:GLU:HG2	2.09	0.52
1:A:261:ASP:HB3	1:A:264:ALA:HB2	1.92	0.52
1:A:71:ASN:HB3	1:A:74:GLU:OE1	2.10	0.52
1:B:255:ILE:C	1:B:257:LYS:N	2.63	0.52
1:B:83:GLU:HG2	2:B:396:HOH:O	2.10	0.52
1:A:207:ARG:CZ	2:A:397:HOH:O	2.57	0.52
1:B:107:MET:HE2	1:B:108:GLU:HA	1.91	0.52
1:A:111:CYS:SG	1:A:152:LEU:HD22	2.50	0.52
1:B:214:GLU:HB2	1:B:218:LYS:HD2	1.92	0.52
1:A:186:ASP:OD2	1:A:188:ASP:HB2	2.08	0.52
1:A:107:MET:C	1:A:107:MET:SD	2.88	0.52
1:A:111:CYS:HB3	1:A:239:CYS:CB	2.38	0.52
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.74	0.52
1:B:281:GLY:HA3	2:B:410:HOH:O	2.09	0.52
1:A:105:VAL:O	1:A:109:VAL:HG23	2.10	0.52
1:A:185:ASN:C	1:A:185:ASN:HD22	2.13	0.52
1:A:67:LYS:HD3	2:A:355:HOH:O	2.09	0.52
1:B:198:LYS:HA	1:B:201:ILE:HD12	1.92	0.52
1:A:189:VAL:O	1:A:193:LEU:HG	2.10	0.52
1:B:38:LEU:HD13	1:B:77:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:305:GLU:O	1:B:309:VAL:HG22	2.09	0.52
1:B:181:ASP:O	1:B:182:LYS:HB2	2.07	0.52
1:B:99:TRP:CE3	1:B:141:THR:HA	2.44	0.52
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.92	0.52
1:B:179:ILE:HD12	1:B:184:TYR:HD1	1.74	0.52
1:A:15:ASP:O	1:A:19:GLN:HG3	2.09	0.52
1:B:46:ARG:O	1:B:50:ARG:HG3	2.10	0.52
1:B:306:LYS:HA	1:B:309:VAL:HG22	1.91	0.52
1:A:261:ASP:CB	1:A:264:ALA:HB2	2.40	0.52
1:B:1:SER:HB3	1:B:276:ASP:HA	1.92	0.52
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.75	0.52
1:B:269:VAL:HG21	1:B:308:LEU:HD22	1.90	0.52
1:B:65:LEU:O	1:B:78:LEU:HD22	2.09	0.52
1:A:1:SER:CB	1:A:276:ASP:HA	2.36	0.52
1:B:157:ARG:HH22	1:B:194:SER:HA	1.75	0.52
1:B:13:PRO:HG2	1:B:14:SER:H	1.74	0.52
1:B:301:ARG:HG2	2:B:406:HOH:O	2.10	0.52
1:A:107:MET:O	1:A:111:CYS:HB2	2.09	0.52
1:A:234:ARG:HD3	2:A:399:HOH:O	2.10	0.52
1:B:276:ASP:O	1:B:280:ILE:HG13	2.07	0.52
1:B:50:ARG:CZ	1:B:62:LEU:HD12	2.40	0.52
1:A:247:PHE:CE1	1:A:268:ILE:HD12	2.45	0.52
1:B:62:LEU:HD13	1:B:78:LEU:HD12	1.92	0.52
1:A:19:GLN:HG2	2:A:393:HOH:O	2.10	0.52
1:B:199:ALA:O	1:B:202:ASN:HB2	2.10	0.52
1:A:31:GLU:C	1:A:33:LEU:H	2.13	0.52
1:B:230:LEU:O	1:B:234:ARG:HG3	2.09	0.52
1:A:168:ALA:HB1	1:A:204:THR:HA	1.92	0.52
1:A:215:GLU:HG2	1:A:216:ILE:H	1.75	0.52
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.10	0.52
1:A:187:GLU:HA	1:A:190:ILE:HD12	1.92	0.52
1:B:298:LYS:HE3	1:B:299:ASP:OD2	2.09	0.52
1:A:171:GLU:HB3	1:A:192:ILE:CD1	2.40	0.52
1:A:133:LEU:O	1:A:137:VAL:HG23	2.10	0.51
1:B:133:LEU:O	1:B:137:VAL:HG23	2.10	0.51
1:A:108:GLU:OE2	2:A:318:HOH:O	2.19	0.51
1:B:114:THR:H	1:B:117:GLN:HE21	1.58	0.51
1:B:20:LEU:HD13	1:B:61:LEU:HD13	1.92	0.51
1:B:114:THR:HG23	1:B:117:GLN:OE1	2.10	0.51
1:A:65:LEU:HD22	1:A:74:GLU:HG2	1.92	0.51
1:A:248:VAL:HA	1:A:251:LEU:HD12	1.92	0.51
1:A:252:ARG:NH2	1:A:287:ARG:HG3	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:150:VAL:HA	1:B:153:VAL:CG2	2.40	0.51
1:A:60:ASP:HB3	1:A:63:LYS:HG2	1.92	0.51
1:B:171:GLU:O	1:B:175:VAL:HG23	2.10	0.51
1:B:253:SER:HB3	1:B:259:GLY:CA	2.40	0.51
1:A:143:GLY:O	1:A:147:LYS:HD2	2.10	0.51
1:A:247:PHE:CD2	1:A:280:ILE:HD11	2.45	0.51
1:A:92:ALA:O	1:A:96:THR:HG23	2.10	0.51
1:B:158:TYR:HA	2:B:347:HOH:O	2.10	0.51
2:A:362:HOH:O	1:B:126:HIS:HD2	1.92	0.51
1:B:133:LEU:N	2:B:318:HOH:O	2.23	0.51
1:A:5:LYS:HE3	1:A:313:GLY:HA3	1.93	0.51
1:A:110:ALA:HB2	1:A:153:VAL:HG12	1.91	0.51
1:A:7:SER:C	1:A:9:SER:H	2.13	0.51
1:B:292:LEU:HD12	1:B:292:LEU:O	2.10	0.51
1:A:45:GLN:O	1:A:49:ILE:HG13	2.11	0.51
1:A:67:LYS:HG3	1:A:69:LEU:O	2.11	0.51
1:A:293:GLU:OE2	1:A:314:GLU:HG3	2.09	0.51
1:B:215:GLU:HB3	1:B:218:LYS:HG3	1.92	0.51
1:B:13:PRO:CB	1:B:48:VAL:HG12	2.41	0.51
1:A:154:THR:OG1	1:B:154:THR:HB	2.10	0.51
1:B:169:LYS:CE	1:B:207:ARG:HH21	2.23	0.51
1:A:166:THR:CB	2:A:350:HOH:O	2.57	0.51
1:B:71:ASN:HB3	1:B:74:GLU:HG3	1.91	0.51
1:B:175:VAL:HG22	1:B:189:VAL:HG22	1.91	0.51
1:B:187:GLU:H	1:B:187:GLU:CD	2.12	0.51
1:B:31:GLU:N	1:B:31:GLU:OE1	2.44	0.51
1:A:191:ARG:HG3	1:B:138:ALA:HB1	1.93	0.51
1:B:62:LEU:CD2	1:B:65:LEU:HD12	2.39	0.51
1:A:107:MET:HG3	1:A:236:THR:OG1	2.11	0.51
1:B:21:ARG:HD3	1:B:57:TYR:CE2	2.45	0.51
1:B:112:THR:HB	1:B:272:ARG:NH1	2.25	0.51
1:B:305:GLU:O	1:B:309:VAL:HG22	2.11	0.51
1:B:33:LEU:HA	1:B:36:SER:OG	2.10	0.51
1:A:35:ILE:HD13	1:A:307:MET:SD	2.51	0.51
1:A:145:PHE:O	1:A:149:LEU:HG	2.11	0.51
1:B:21:ARG:HG2	1:B:57:TYR:CZ	2.45	0.51
1:A:238:GLN:O	1:A:242:ARG:N	2.44	0.51
1:A:128:ARG:O	1:A:128:ARG:HG2	2.11	0.51
1:A:300:THR:HG22	1:A:301:ARG:N	2.26	0.51
1:A:91:LEU:CD2	1:A:267:ARG:HD3	2.39	0.51
1:B:193:LEU:HA	1:B:201:ILE:CD1	2.41	0.51
1:A:218:LYS:HA	1:A:221:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:261:ASP:CB	1:B:264:ALA:HB2	2.39	0.51
1:A:122:ARG:NH1	1:A:154:THR:HA	2.25	0.51
1:A:297:THR:HG21	1:A:317:ALA:OXT	2.11	0.51
1:A:220:LEU:C	1:A:234:ARG:HH21	2.12	0.51
1:B:133:LEU:HG	1:B:153:VAL:HG21	1.92	0.51
1:A:167:LEU:CD2	1:A:200:GLN:HE22	2.24	0.51
1:A:216:ILE:HG22	2:A:362:HOH:O	2.11	0.51
1:A:46:ARG:NH1	1:A:46:ARG:HG3	2.25	0.51
1:B:132:SER:O	1:B:135:GLU:HG2	2.10	0.51
1:B:307:MET:O	1:B:311:LEU:HG	2.11	0.51
1:A:244:GLU:O	1:A:248:VAL:HG23	2.11	0.51
1:A:167:LEU:HB3	2:A:326:HOH:O	2.11	0.51
1:A:135:GLU:CA	1:B:195:THR:HB	2.40	0.51
1:B:77:ILE:HD13	1:B:307:MET:CE	2.41	0.51
1:B:168:ALA:O	1:B:172:ALA:HB2	2.11	0.51
1:A:285:GLN:OE1	1:A:285:GLN:O	2.28	0.51
1:A:293:GLU:OE2	1:A:314:GLU:HG3	2.11	0.51
1:B:103:ASN:OD1	1:B:105:VAL:HG23	2.10	0.51
1:A:107:MET:SD	1:A:236:THR:HA	2.51	0.51
1:A:255:ILE:C	1:A:257:LYS:H	2.13	0.51
1:A:1:SER:HG	1:A:278:LYS:HB3	1.75	0.51
1:B:38:LEU:O	1:B:80:TRP:NE1	2.44	0.51
1:B:286:ARG:HH11	1:B:286:ARG:HG2	1.76	0.51
1:A:223:GLY:HA3	1:A:230:LEU:HD21	1.93	0.51
1:B:249:ASP:O	1:B:252:ARG:HB3	2.10	0.51
1:B:197:SER:HB2	2:B:329:HOH:O	2.10	0.51
1:A:69:LEU:N	1:A:69:LEU:HD12	2.26	0.51
1:A:36:SER:HB2	2:A:471:HOH:O	2.11	0.51
1:A:129:TYR:C	1:A:131:LYS:H	2.13	0.51
1:A:46:ARG:HE	1:A:81:THR:HA	1.76	0.51
1:B:177:GLU:HA	1:B:180:LYS:NZ	2.26	0.51
1:B:209:GLN:HG3	1:B:214:GLU:N	2.26	0.51
1:B:1:SER:HB2	1:B:275:ILE:O	2.11	0.51
1:A:188:ASP:O	1:A:192:ILE:HG13	2.11	0.51
1:B:106:LEU:HD13	1:B:137:VAL:HG22	1.92	0.51
1:B:117:GLN:HE22	1:B:275:ILE:HD11	1.76	0.51
1:B:146:ARG:HG3	1:B:150:VAL:HG23	1.92	0.50
1:A:158:TYR:O	1:A:197:SER:HB2	2.11	0.50
1:B:171:GLU:HB3	1:B:192:ILE:CD1	2.40	0.50
1:B:215:GLU:HA	2:B:365:HOH:O	2.10	0.50
1:A:157:ARG:CG	1:A:197:SER:HA	2.41	0.50
1:A:158:TYR:OH	1:A:160:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:GLU:HB2	1:B:86:GLU:HG3	1.92	0.50
1:A:300:THR:HG22	1:A:301:ARG:N	2.26	0.50
1:A:115:SER:HB2	1:A:159:GLU:CD	2.31	0.50
1:A:145:PHE:O	1:A:149:LEU:HG	2.10	0.50
1:B:150:VAL:HA	1:B:153:VAL:HG22	1.93	0.50
1:A:205:PHE:CE2	1:A:237:ILE:HG23	2.46	0.50
1:B:300:THR:HG22	1:B:301:ARG:H	1.76	0.50
1:A:107:MET:HE1	1:A:235:SER:HB3	1.94	0.50
1:B:157:ARG:HB3	2:B:319:HOH:O	2.11	0.50
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.12	0.50
1:B:198:LYS:NZ	2:B:336:HOH:O	2.44	0.50
1:A:309:VAL:HB	1:A:314:GLU:O	2.11	0.50
1:B:216:ILE:C	1:B:218:LYS:H	2.14	0.50
1:A:7:SER:O	1:A:10:VAL:HG23	2.11	0.50
1:A:148:LEU:HD22	1:A:232:LEU:HD21	1.94	0.50
1:B:45:GLN:O	1:B:49:ILE:HG13	2.12	0.50
1:A:15:ASP:HA	1:A:18:GLU:OE1	2.11	0.50
1:B:196:ARG:O	1:B:201:ILE:HD11	2.12	0.50
1:B:150:VAL:HA	1:B:153:VAL:HG22	1.94	0.50
1:B:182:LYS:HG2	1:B:184:TYR:OH	2.11	0.50
1:B:309:VAL:HB	1:B:314:GLU:O	2.10	0.50
1:A:118:LEU:O	1:A:121:ALA:N	2.45	0.50
1:B:251:LEU:HD21	1:B:268:ILE:HB	1.94	0.50
1:B:231:ALA:CB	1:B:234:ARG:HH21	2.24	0.50
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.92	0.50
1:B:109:VAL:HA	1:B:113:ARG:HH21	1.77	0.50
1:B:197:SER:O	1:B:201:ILE:HG13	2.11	0.50
1:A:260:THR:O	1:A:260:THR:HG22	2.12	0.50
1:B:253:SER:HB3	1:B:259:GLY:HA3	1.92	0.50
1:B:162:GLU:OE1	1:B:162:GLU:N	2.44	0.50
1:B:297:THR:HB	1:B:305:GLU:HG2	1.92	0.50
1:B:288:ASN:O	1:B:290:ILE:HG22	2.11	0.50
1:A:15:ASP:O	1:A:19:GLN:HG3	2.12	0.50
1:A:69:LEU:HD12	1:A:69:LEU:H	1.76	0.50
1:A:49:ILE:HG22	1:A:50:ARG:N	2.26	0.50
1:A:1:SER:HB2	1:A:276:ASP:HA	1.94	0.50
1:A:238:GLN:OE1	1:A:246:TYR:HA	2.11	0.50
1:B:62:LEU:HD21	1:B:81:THR:HB	1.94	0.50
1:A:161:ASP:O	1:A:163:VAL:HG23	2.10	0.50
1:A:35:ILE:HD12	1:A:307:MET:SD	2.52	0.50
1:A:34:ILE:HD12	1:A:34:ILE:H	1.77	0.50
1:A:50:ARG:O	1:A:53:TYR:HB3	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:LEU:HA	1:A:280:ILE:HB	1.94	0.50
1:A:71:ASN:ND2	1:A:74:GLU:HG3	2.25	0.50
1:B:146:ARG:HG3	1:B:150:VAL:CG2	2.42	0.50
1:A:11:PRO:HG2	1:A:16:ASP:OD1	2.12	0.50
1:B:20:LEU:HD13	1:B:61:LEU:CD1	2.42	0.50
1:A:95:ALA:HB1	1:A:103:ASN:HD21	1.76	0.50
1:B:107:MET:HG2	1:B:111:CYS:SG	2.52	0.50
1:B:200:GLN:O	1:B:203:ALA:HB3	2.12	0.50
1:B:267:ARG:HD2	1:B:267:ARG:C	2.32	0.50
1:A:139:HIS:CD2	1:B:196:ARG:HH22	2.30	0.50
1:A:128:ARG:HG2	1:A:128:ARG:O	2.12	0.50
1:B:37:ILE:O	1:B:41:ARG:HG2	2.11	0.50
1:B:93:ASN:O	1:B:97:LYS:HG2	2.12	0.50
1:B:31:GLU:N	1:B:31:GLU:OE1	2.45	0.50
1:A:242:ARG:HB2	1:A:245:LEU:HD12	1.93	0.50
1:A:90:LEU:HD13	1:A:128:ARG:NH2	2.27	0.50
1:B:232:LEU:O	1:B:236:THR:OG1	2.24	0.50
1:B:245:LEU:HD23	1:B:283:GLU:HG3	1.94	0.50
1:B:110:ALA:HB1	1:B:118:LEU:HD22	1.94	0.50
1:A:186:ASP:OD2	1:A:188:ASP:HB2	2.12	0.50
1:A:67:LYS:HD3	2:A:358:HOH:O	2.11	0.50
1:B:186:ASP:HB3	1:B:189:VAL:HG23	1.94	0.50
1:B:8:ASP:O	1:B:9:SER:HB3	2.12	0.50
1:B:314:GLU:HB3	1:B:317:ALA:HB2	1.94	0.50
1:A:220:LEU:HB3	1:A:230:LEU:HD11	1.93	0.50
1:B:18:GLU:HA	1:B:57:TYR:HE2	1.76	0.50
1:A:243:PRO:HG3	2:A:415:HOH:O	2.12	0.49
1:B:105:VAL:HG22	1:B:267:ARG:NH1	2.26	0.49
1:A:7:SER:C	1:A:9:SER:H	2.15	0.49
1:A:164:ASN:OD1	1:A:167:LEU:HD13	2.11	0.49
1:A:112:THR:HG23	1:A:239:CYS:HB3	1.93	0.49
1:A:75:ARG:O	1:A:78:LEU:HB3	2.12	0.49
1:B:108:GLU:O	1:B:113:ARG:NH1	2.45	0.49
1:A:246:TYR:CZ	1:A:250:VAL:HG21	2.46	0.49
1:B:1:SER:HB2	1:B:276:ASP:HA	1.93	0.49
1:B:157:ARG:NH2	1:B:194:SER:HA	2.27	0.49
1:A:7:SER:C	1:A:9:SER:N	2.65	0.49
1:B:193:LEU:HD13	1:B:236:THR:HG21	1.94	0.49
1:A:13:PRO:HA	1:A:16:ASP:OD2	2.11	0.49
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.76	0.49
1:A:248:VAL:HG13	1:A:284:TYR:HD1	1.77	0.49
1:B:277:LEU:CD2	1:B:312:LEU:HD23	2.41	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:LEU:O	1:A:234:ARG:HG3	2.11	0.49
1:A:191:ARG:HH22	1:A:192:ILE:HD11	1.77	0.49
1:B:261:ASP:CG	1:B:267:ARG:HH22	2.15	0.49
1:B:142:THR:O	1:B:145:PHE:HB2	2.12	0.49
1:B:174:LEU:HD23	1:B:188:ASP:HB3	1.95	0.49
1:B:105:VAL:O	1:B:106:LEU:C	2.50	0.49
1:B:216:ILE:HG23	1:B:217:LEU:H	1.77	0.49
1:B:293:GLU:O	1:B:297:THR:HG22	2.12	0.49
1:A:38:LEU:C	1:A:40:HIS:H	2.15	0.49
1:B:118:LEU:HD12	1:B:121:ALA:HB3	1.95	0.49
1:B:192:ILE:HG23	1:B:196:ARG:CG	2.43	0.49
1:A:50:ARG:NH2	1:A:62:LEU:HD12	2.27	0.49
1:A:105:VAL:O	1:A:109:VAL:HG23	2.12	0.49
1:A:126:HIS:HB3	2:A:468:HOH:O	2.12	0.49
1:A:135:GLU:OE1	1:B:196:ARG:HD2	2.12	0.49
1:B:104:GLN:NE2	1:B:231:ALA:O	2.45	0.49
1:B:178:LYS:HE3	1:B:186:ASP:OD1	2.12	0.49
1:B:172:ALA:C	1:B:174:LEU:H	2.15	0.49
1:A:300:THR:HG22	1:A:301:ARG:N	2.28	0.49
1:A:46:ARG:O	1:A:49:ILE:HB	2.12	0.49
1:A:33:LEU:O	1:A:33:LEU:HD23	2.13	0.49
1:B:217:LEU:O	1:B:221:GLU:HG3	2.12	0.49
1:B:82:LEU:HD23	1:B:83:GLU:N	2.28	0.49
1:B:119:LEU:O	1:B:123:GLN:HG3	2.11	0.49
1:A:193:LEU:HD11	1:A:233:LEU:CD1	2.43	0.49
1:A:239:CYS:O	1:A:243:PRO:HG3	2.12	0.49
1:A:107:MET:SD	1:A:239:CYS:SG	3.11	0.49
1:A:14:SER:O	1:A:18:GLU:HG3	2.11	0.49
1:A:171:GLU:HB3	1:A:192:ILE:HD13	1.94	0.49
1:A:301:ARG:HD2	2:A:369:HOH:O	2.12	0.49
1:A:132:SER:HB3	1:B:157:ARG:HA	1.94	0.49
1:A:286:ARG:HB2	1:A:286:ARG:HH11	1.76	0.49
1:B:243:PRO:O	1:B:246:TYR:N	2.41	0.49
1:B:148:LEU:O	1:B:152:LEU:HG	2.11	0.49
1:A:38:LEU:O	1:A:80:TRP:NE1	2.39	0.49
1:A:301:ARG:HD2	2:A:370:HOH:O	2.13	0.49
1:A:172:ALA:HB1	1:A:208:TYR:CB	2.41	0.49
1:A:122:ARG:NH2	1:A:154:THR:HA	2.26	0.49
1:A:123:GLN:HA	1:A:126:HIS:HB2	1.95	0.49
1:A:279:VAL:O	1:A:279:VAL:HG12	2.13	0.49
1:B:110:ALA:CB	1:B:118:LEU:HD22	2.42	0.49
1:B:294:LYS:HE3	1:B:317:ALA:OXT	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:183:HIS:HB3	1:A:186:ASP:HB2	1.95	0.49
1:A:45:GLN:O	1:A:49:ILE:HG13	2.12	0.49
1:B:150:VAL:O	1:B:153:VAL:HG22	2.13	0.49
1:B:53:TYR:CD1	1:B:53:TYR:C	2.86	0.49
1:A:175:VAL:O	1:A:179:ILE:HG12	2.13	0.49
1:A:224:ASP:O	1:A:230:LEU:HD23	2.13	0.49
1:A:75:ARG:NE	1:A:79:LEU:HD11	2.27	0.49
1:B:303:ASP:CG	1:B:306:LYS:HZ1	2.16	0.49
1:A:13:PRO:HA	1:A:16:ASP:OD2	2.13	0.49
1:A:148:LEU:HD23	1:A:232:LEU:CD2	2.42	0.49
1:A:4:LEU:HD22	1:A:274:GLU:HG2	1.94	0.49
1:B:133:LEU:CD1	1:B:137:VAL:HG23	2.43	0.49
1:B:62:LEU:HD11	1:B:81:THR:HB	1.95	0.49
1:B:76:ALA:HA	1:B:266:THR:CG2	2.43	0.49
1:A:185:ASN:HD22	1:A:185:ASN:C	2.17	0.49
1:B:42:SER:OG	1:B:45:GLN:HG3	2.12	0.49
1:A:220:LEU:HD13	1:A:234:ARG:HG2	1.94	0.49
1:A:69:LEU:H	1:A:69:LEU:HD12	1.78	0.49
1:A:302:GLY:HA3	2:A:382:HOH:O	2.12	0.49
1:A:34:ILE:N	1:A:34:ILE:CD1	2.76	0.49
1:A:65:LEU:HB3	1:A:78:LEU:HB2	1.94	0.49
1:A:264:ALA:HA	1:A:267:ARG:HD2	1.95	0.49
1:A:105:VAL:HG22	1:A:267:ARG:HD3	1.95	0.49
1:B:11:PRO:HB2	1:B:15:ASP:CB	2.42	0.49
1:A:252:ARG:HH22	1:A:287:ARG:CZ	2.25	0.49
1:A:220:LEU:HD11	1:A:237:ILE:HD12	1.94	0.49
1:B:255:ILE:C	1:B:257:LYS:N	2.61	0.49
1:A:227:ASP:HB3	1:A:230:LEU:HB3	1.94	0.49
1:A:297:THR:O	1:A:298:LYS:C	2.50	0.49
1:B:231:ALA:CA	1:B:234:ARG:HH21	2.25	0.49
1:A:104:GLN:HE22	1:A:235:SER:CB	2.24	0.49
1:B:189:VAL:O	1:B:193:LEU:HG	2.13	0.49
1:B:55:GLU:C	1:B:57:TYR:H	2.17	0.49
1:A:69:LEU:HD12	1:A:69:LEU:N	2.27	0.49
1:B:218:LYS:HA	1:B:221:GLU:OE2	2.12	0.49
1:A:130:LYS:HB3	1:B:162:GLU:HG2	1.94	0.49
1:A:6:VAL:CG1	1:A:7:SER:H	2.26	0.49
1:B:189:VAL:HA	1:B:192:ILE:HD12	1.95	0.49
1:A:51:GLN:O	1:A:55:GLU:HG3	2.13	0.48
1:B:244:GLU:HG2	1:B:245:LEU:N	2.26	0.48
1:B:61:LEU:HD11	2:B:350:HOH:O	2.12	0.48
1:A:216:ILE:HG23	1:A:217:LEU:N	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:251:LEU:HD21	1:B:268:ILE:CG2	2.39	0.48
1:A:125:TYR:CD2	1:A:133:LEU:HD13	2.48	0.48
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.11	0.48
1:A:215:GLU:OE1	1:A:217:LEU:HB2	2.13	0.48
1:B:73:PHE:O	1:B:77:ILE:HG12	2.12	0.48
1:A:161:ASP:O	1:A:163:VAL:HG23	2.12	0.48
1:A:62:LEU:HD21	1:A:81:THR:HB	1.94	0.48
1:B:126:HIS:CE1	1:B:132:SER:HA	2.46	0.48
1:A:264:ALA:HA	1:A:267:ARG:HH12	1.78	0.48
1:B:298:LYS:HE3	1:B:299:ASP:OD2	2.13	0.48
1:A:98:ARG:HH11	1:A:98:ARG:HG2	1.77	0.48
1:A:158:TYR:HD1	1:B:126:HIS:HB3	1.77	0.48
1:B:278:LYS:O	1:B:278:LYS:HD3	2.13	0.48
1:B:128:ARG:O	1:B:129:TYR:CG	2.65	0.48
1:A:114:THR:OG1	1:A:117:GLN:HG3	2.13	0.48
1:A:167:LEU:HD21	1:A:171:GLU:OE1	2.14	0.48
1:A:186:ASP:HB3	1:A:189:VAL:CG2	2.43	0.48
1:A:297:THR:HB	1:A:301:ARG:HD2	1.93	0.48
1:A:195:THR:HB	1:B:135:GLU:N	2.27	0.48
1:A:191:ARG:HG2	2:A:342:HOH:O	2.13	0.48
1:A:158:TYR:O	1:A:197:SER:HB2	2.13	0.48
1:B:43:ALA:HB2	1:B:274:GLU:OE2	2.13	0.48
1:A:4:LEU:HD22	1:A:274:GLU:HG2	1.94	0.48
1:A:125:TYR:HD1	1:A:131:LYS:O	1.97	0.48
1:A:105:VAL:HG22	1:A:267:ARG:CD	2.43	0.48
1:A:187:GLU:OE2	1:B:147:LYS:HE2	2.12	0.48
1:A:119:LEU:HD21	1:B:119:LEU:HD21	1.95	0.48
1:B:37:ILE:O	1:B:41:ARG:HG2	2.12	0.48
1:A:100:THR:HG22	1:A:102:SER:H	1.78	0.48
1:A:35:ILE:HD11	1:A:307:MET:HB2	1.96	0.48
1:A:220:LEU:HD22	1:A:230:LEU:HD11	1.95	0.48
1:A:293:GLU:OE2	2:A:388:HOH:O	2.20	0.48
1:A:157:ARG:CD	1:A:197:SER:HA	2.44	0.48
1:B:167:LEU:HD21	1:B:196:ARG:NH2	2.28	0.48
1:B:50:ARG:NH2	1:B:62:LEU:HD12	2.29	0.48
1:A:185:ASN:HD22	1:A:185:ASN:C	2.16	0.48
1:B:198:LYS:O	1:B:200:GLN:N	2.46	0.48
1:B:179:ILE:CD1	1:B:216:ILE:HD11	2.43	0.48
1:B:133:LEU:O	1:B:137:VAL:HG23	2.13	0.48
1:A:220:LEU:HD22	1:A:230:LEU:CD1	2.43	0.48
1:A:61:LEU:HD23	1:A:61:LEU:O	2.14	0.48
1:B:247:PHE:HD1	1:B:268:ILE:HG23	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:ALA:HA	1:A:266:THR:CG2	2.42	0.48
1:A:212:HIS:O	1:A:214:GLU:HG2	2.13	0.48
1:A:132:SER:C	1:A:134:GLU:H	2.16	0.48
1:A:135:GLU:HA	2:B:319:HOH:O	2.13	0.48
1:B:71:ASN:HB3	1:B:74:GLU:CG	2.43	0.48
1:B:37:ILE:O	1:B:41:ARG:HG2	2.13	0.48
1:B:61:LEU:H	1:B:61:LEU:HD23	1.79	0.48
1:A:263:GLY:O	1:A:267:ARG:HB3	2.12	0.48
1:B:148:LEU:HB2	1:B:190:ILE:CD1	2.43	0.48
1:A:67:LYS:CG	1:A:70:SER:HB3	2.43	0.48
1:A:261:ASP:CG	1:A:264:ALA:HB2	2.34	0.48
1:B:192:ILE:O	1:B:201:ILE:HD11	2.13	0.48
1:B:43:ALA:HB2	1:B:274:GLU:OE2	2.14	0.48
1:B:265:LEU:HG	1:B:308:LEU:HD13	1.96	0.48
1:B:293:GLU:HG3	1:B:294:LYS:N	2.28	0.48
1:B:82:LEU:HB3	1:B:86:GLU:HB2	1.96	0.48
1:A:150:VAL:CA	1:A:153:VAL:HG22	2.39	0.48
1:B:173:LYS:NZ	2:B:411:HOH:O	2.33	0.48
1:B:99:TRP:CZ2	1:B:101:SER:HA	2.48	0.48
1:B:112:THR:O	1:B:113:ARG:HD2	2.13	0.48
2:A:361:HOH:O	1:B:126:HIS:CD2	2.62	0.48
1:A:253:SER:HB3	1:A:259:GLY:H	1.77	0.48
1:A:122:ARG:HB3	2:A:323:HOH:O	2.13	0.48
1:A:145:PHE:O	1:A:149:LEU:HG	2.14	0.48
1:B:205:PHE:O	1:B:208:TYR:HB3	2.12	0.48
1:B:297:THR:HB	1:B:309:VAL:HG11	1.96	0.48
1:B:231:ALA:O	1:B:234:ARG:HB2	2.13	0.48
1:B:271:THR:O	1:B:272:ARG:HD2	2.14	0.48
1:A:92:ALA:O	1:A:96:THR:HG23	2.14	0.48
1:A:181:ASP:O	1:A:182:LYS:HB2	2.12	0.48
1:B:46:ARG:O	1:B:50:ARG:HG3	2.14	0.48
1:B:130:LYS:O	1:B:131:LYS:HG3	2.14	0.48
1:A:173:LYS:O	1:A:177:GLU:HG3	2.13	0.48
1:A:148:LEU:HD23	1:A:232:LEU:CD2	2.43	0.48
1:A:141:THR:O	1:A:146:ARG:HD3	2.14	0.48
1:A:87:ARG:NH1	1:A:271:THR:HA	2.29	0.48
1:A:158:TYR:CZ	1:A:160:GLY:HA3	2.48	0.48
1:A:294:LYS:NZ	1:A:317:ALA:HA	2.29	0.48
1:A:62:LEU:HD21	1:A:81:THR:CB	2.43	0.48
1:B:7:SER:H	1:B:41:ARG:HH22	1.60	0.48
1:A:45:GLN:O	1:A:49:ILE:HG13	2.14	0.48
1:B:54:HIS:HA	1:B:59:GLU:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:25:GLU:HB3	2:A:440:HOH:O	2.14	0.48
1:A:269:VAL:O	1:A:273:ALA:HB2	2.14	0.48
1:B:197:SER:O	1:B:200:GLN:N	2.46	0.48
2:A:320:HOH:O	1:B:156:TYR:HB3	2.13	0.48
1:B:6:VAL:HG21	1:B:42:SER:HB3	1.96	0.48
1:B:252:ARG:CD	1:B:256:ASN:HD21	2.27	0.48
1:A:134:GLU:CD	2:A:320:HOH:O	2.53	0.48
1:B:149:LEU:O	1:B:150:VAL:C	2.52	0.48
1:A:186:ASP:HB3	1:A:189:VAL:HB	1.95	0.48
1:A:253:SER:HB3	1:A:259:GLY:H	1.78	0.48
1:B:109:VAL:HA	1:B:113:ARG:CZ	2.42	0.48
1:A:281:GLY:O	1:A:285:GLN:HB2	2.14	0.48
1:B:209:GLN:O	1:B:213:GLY:N	2.47	0.48
1:A:175:VAL:O	1:A:179:ILE:HG12	2.13	0.48
1:A:295:ALA:O	1:A:298:LYS:HD3	2.14	0.48
1:B:261:ASP:OD2	1:B:264:ALA:HB2	2.14	0.48
1:B:42:SER:OG	1:B:45:GLN:HB2	2.14	0.48
1:B:258:THR:O	1:B:258:THR:HG22	2.13	0.48
1:A:35:ILE:HD12	1:A:307:MET:SD	2.54	0.48
1:B:223:GLY:HA3	1:B:230:LEU:CD2	2.44	0.48
1:A:247:PHE:CE1	1:A:268:ILE:HD12	2.49	0.48
1:B:109:VAL:O	1:B:109:VAL:CG1	2.61	0.48
1:B:40:HIS:O	1:B:41:ARG:HD3	2.13	0.48
1:B:293:GLU:O	1:B:297:THR:HG22	2.14	0.48
1:A:130:LYS:HD2	1:B:158:TYR:OH	2.14	0.48
1:A:66:ASP:HA	1:A:78:LEU:HD11	1.96	0.47
1:B:187:GLU:HG3	2:B:370:HOH:O	2.12	0.47
1:A:114:THR:HB	1:A:159:GLU:OE2	2.13	0.47
1:B:247:PHE:CE1	1:B:268:ILE:HD12	2.49	0.47
1:A:33:LEU:HD12	1:A:36:SER:OG	2.14	0.47
1:A:278:LYS:HG2	1:A:282:GLU:OE2	2.14	0.47
1:B:259:GLY:HA3	2:B:364:HOH:O	2.13	0.47
1:B:205:PHE:HA	1:B:208:TYR:HB3	1.96	0.47
1:B:163:VAL:HG22	1:B:199:ALA:O	2.13	0.47
1:B:247:PHE:HD1	1:B:268:ILE:HD12	1.79	0.47
1:A:185:ASN:HD22	1:A:185:ASN:C	2.16	0.47
1:A:104:GLN:O	1:A:107:MET:HB3	2.13	0.47
1:A:7:SER:C	1:A:9:SER:H	2.17	0.47
1:A:87:ARG:NH2	2:A:333:HOH:O	2.47	0.47
1:A:6:VAL:HA	1:A:40:HIS:O	2.14	0.47
1:A:168:ALA:HA	2:A:328:HOH:O	2.13	0.47
1:A:122:ARG:HD2	2:A:476:HOH:O	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:189:VAL:HG11	1:B:233:LEU:HD21	1.97	0.47
1:A:42:SER:OG	1:A:45:GLN:HG3	2.13	0.47
1:A:10:VAL:HG21	1:A:45:GLN:NE2	2.29	0.47
1:A:269:VAL:O	1:A:273:ALA:HB2	2.14	0.47
1:B:12:ALA:O	1:B:15:ASP:HB2	2.14	0.47
1:B:65:LEU:HD22	1:B:74:GLU:HG2	1.96	0.47
1:A:122:ARG:HH21	1:B:156:TYR:CB	2.27	0.47
1:B:248:VAL:HG13	1:B:284:TYR:HD1	1.79	0.47
1:A:37:ILE:O	1:A:41:ARG:HG2	2.14	0.47
1:A:107:MET:SD	1:A:239:CYS:SG	3.12	0.47
1:A:39:ALA:HB2	1:A:307:MET:CE	2.44	0.47
1:A:307:MET:O	1:A:311:LEU:HG	2.14	0.47
1:B:238:GLN:NE2	1:B:245:LEU:HD12	2.29	0.47
1:B:174:LEU:HD12	1:B:177:GLU:OE1	2.12	0.47
1:A:199:ALA:O	1:A:202:ASN:HB3	2.14	0.47
1:B:305:GLU:O	1:B:309:VAL:HG22	2.14	0.47
1:A:19:GLN:HB3	1:A:33:LEU:HD21	1.96	0.47
1:B:265:LEU:O	1:B:269:VAL:HG23	2.14	0.47
1:A:162:GLU:O	1:A:163:VAL:CG2	2.62	0.47
1:A:61:LEU:C	1:A:61:LEU:HD23	2.34	0.47
1:A:134:GLU:N	1:A:134:GLU:OE1	2.44	0.47
1:B:169:LYS:HG3	1:B:211:ASP:OD2	2.14	0.47
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.95	0.47
1:B:255:ILE:O	1:B:257:LYS:HD3	2.14	0.47
1:A:126:HIS:O	1:A:130:LYS:N	2.47	0.47
1:A:189:VAL:O	1:A:192:ILE:N	2.45	0.47
1:B:171:GLU:HB3	1:B:192:ILE:HD13	1.94	0.47
1:B:288:ASN:O	1:B:289:SER:HB2	2.15	0.47
1:A:87:ARG:HD3	1:A:271:THR:HG22	1.96	0.47
1:B:225:ASP:OD1	1:B:234:ARG:NH2	2.48	0.47
1:B:173:LYS:HE3	2:B:413:HOH:O	2.14	0.47
1:A:307:MET:O	1:A:311:LEU:HG	2.15	0.47
1:A:184:TYR:HB3	1:A:233:LEU:HD22	1.96	0.47
1:A:300:THR:HG22	1:A:301:ARG:N	2.30	0.47
1:B:272:ARG:O	1:B:277:LEU:HB2	2.14	0.47
1:A:128:ARG:HD3	1:A:129:TYR:CE2	2.49	0.47
1:A:24:PHE:O	1:A:25:GLU:HB3	2.15	0.47
1:B:109:VAL:HG13	1:B:113:ARG:NE	2.29	0.47
1:A:101:SER:HB2	1:A:145:PHE:CZ	2.49	0.47
1:B:158:TYR:CZ	1:B:160:GLY:HA3	2.49	0.47
1:B:34:ILE:CG2	1:B:38:LEU:HD12	2.44	0.47
1:B:75:ARG:O	1:B:79:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:250:VAL:CG1	1:A:268:ILE:HD11	2.45	0.47
1:A:1:SER:N	1:A:278:LYS:HB3	2.29	0.47
1:B:93:ASN:OD1	1:B:97:LYS:HE2	2.15	0.47
1:A:107:MET:HB2	1:A:149:LEU:HD21	1.95	0.47
1:B:116:THR:O	1:B:118:LEU:N	2.47	0.47
1:A:293:GLU:HA	1:A:296:ILE:HD12	1.96	0.47
1:B:288:ASN:C	1:B:290:ILE:H	2.18	0.47
1:A:247:PHE:HE2	1:A:272:ARG:NH2	2.12	0.47
1:B:291:PRO:CD	1:B:294:LYS:HD3	2.40	0.47
1:A:293:GLU:HG2	1:A:294:LYS:N	2.30	0.47
1:A:101:SER:O	1:A:228:LYS:HB3	2.15	0.47
1:A:62:LEU:HD21	1:A:81:THR:CG2	2.44	0.47
1:A:74:GLU:HA	1:A:77:ILE:HD12	1.95	0.47
1:B:78:LEU:C	1:B:80:TRP:H	2.18	0.47
1:B:165:MET:HA	1:B:168:ALA:HB3	1.96	0.47
1:B:267:ARG:O	1:B:271:THR:HG23	2.14	0.47
1:A:293:GLU:OE2	1:A:314:GLU:HG3	2.15	0.47
1:A:156:TYR:HB3	2:B:323:HOH:O	2.13	0.47
1:A:252:ARG:HE	1:A:288:ASN:CG	2.16	0.47
1:A:69:LEU:H	1:A:69:LEU:HD12	1.80	0.47
1:A:105:VAL:HG22	1:A:267:ARG:CZ	2.44	0.47
1:A:246:TYR:CZ	1:A:250:VAL:HG21	2.50	0.47
1:B:169:LYS:HG3	1:B:211:ASP:OD2	2.15	0.47
1:A:256:ASN:ND2	2:A:345:HOH:O	2.48	0.47
1:B:265:LEU:O	1:B:269:VAL:HG23	2.14	0.47
1:B:17:ALA:HB2	1:B:52:ALA:HB3	1.95	0.47
1:A:195:THR:O	2:A:324:HOH:O	2.20	0.47
1:A:10:VAL:HG21	1:A:45:GLN:HE22	1.80	0.47
1:A:221:GLU:HA	1:A:234:ARG:HH21	1.80	0.47
1:A:138:ALA:HB2	1:A:150:VAL:HG21	1.97	0.47
1:A:251:LEU:HD21	1:A:268:ILE:HB	1.97	0.47
1:B:314:GLU:HB3	1:B:317:ALA:HB2	1.97	0.47
1:B:57:TYR:O	1:B:59:GLU:HG3	2.13	0.47
1:A:216:ILE:CG2	1:A:217:LEU:N	2.77	0.47
1:B:101:SER:HB2	1:B:145:PHE:CZ	2.50	0.47
1:B:106:LEU:HD22	1:B:149:LEU:CD2	2.40	0.47
1:A:248:VAL:HG13	1:A:284:TYR:CD1	2.50	0.47
1:A:62:LEU:C	1:A:64:THR:N	2.68	0.47
1:A:247:PHE:CE1	1:A:268:ILE:HD12	2.50	0.47
1:A:288:ASN:O	1:A:289:SER:HB2	2.15	0.47
1:A:62:LEU:HD21	1:A:81:THR:HB	1.96	0.47
1:A:310:ALA:O	2:A:352:HOH:O	2.20	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:262:GLU:HB3	2:B:383:HOH:O	2.14	0.47
1:B:294:LYS:O	1:B:298:LYS:HB2	2.15	0.47
1:B:10:VAL:HG22	1:B:41:ARG:CZ	2.45	0.47
1:B:137:VAL:O	1:B:141:THR:HG23	2.15	0.47
1:A:171:GLU:O	1:A:175:VAL:HG23	2.14	0.47
1:A:179:ILE:HG23	1:A:220:LEU:HD23	1.97	0.47
1:A:242:ARG:HB3	1:A:244:GLU:CD	2.34	0.47
1:A:144:ASP:O	1:A:147:LYS:HB2	2.14	0.47
1:A:198:LYS:NZ	2:A:344:HOH:O	2.47	0.47
1:B:262:GLU:HB3	2:B:377:HOH:O	2.15	0.47
1:B:235:SER:O	1:B:238:GLN:N	2.48	0.47
1:B:262:GLU:HB3	2:B:380:HOH:O	2.14	0.47
1:B:20:LEU:HD13	1:B:61:LEU:HD13	1.96	0.47
1:B:293:GLU:HB3	1:B:314:GLU:HG3	1.97	0.47
1:A:105:VAL:HG22	1:A:267:ARG:NH2	2.30	0.47
1:B:215:GLU:HG2	1:B:217:LEU:H	1.79	0.47
1:B:294:LYS:HA	1:B:297:THR:HG22	1.96	0.47
1:A:70:SER:HB3	1:A:74:GLU:HB2	1.97	0.47
1:A:296:ILE:HG22	1:A:296:ILE:O	2.13	0.47
1:B:252:ARG:HG3	1:B:253:SER:N	2.30	0.47
1:B:116:THR:HG23	1:B:120:HIS:CE1	2.49	0.47
1:B:246:TYR:O	1:B:250:VAL:HG23	2.15	0.47
1:A:108:GLU:OE1	1:A:267:ARG:NH2	2.48	0.47
1:B:198:LYS:HA	1:B:201:ILE:HB	1.97	0.47
1:A:158:TYR:CZ	1:A:160:GLY:HA3	2.50	0.47
1:B:59:GLU:OE2	1:B:63:LYS:HD3	2.14	0.47
1:A:92:ALA:HB1	1:A:106:LEU:HD23	1.94	0.47
1:B:300:THR:HG22	1:B:302:GLY:H	1.80	0.47
1:A:122:ARG:NH2	1:B:156:TYR:HB3	2.30	0.46
1:B:277:LEU:HG	1:B:312:LEU:HD21	1.97	0.46
1:A:216:ILE:O	1:A:219:SER:HB3	2.16	0.46
1:B:298:LYS:HE3	1:B:299:ASP:OD2	2.14	0.46
1:A:195:THR:O	2:A:324:HOH:O	2.20	0.46
1:B:297:THR:CB	1:B:305:GLU:HG2	2.44	0.46
1:A:130:LYS:HA	1:B:158:TYR:CE1	2.49	0.46
1:B:150:VAL:CA	1:B:153:VAL:HG22	2.46	0.46
1:B:56:THR:O	1:B:56:THR:HG22	2.15	0.46
1:A:267:ARG:HB3	1:A:267:ARG:NH1	2.29	0.46
1:A:261:ASP:CG	1:A:264:ALA:HB2	2.36	0.46
1:B:10:VAL:HA	1:B:41:ARG:NH2	2.30	0.46
1:A:244:GLU:HA	1:A:280:ILE:CG1	2.44	0.46
1:B:71:ASN:OD1	1:B:73:PHE:N	2.47	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:19:GLN:HA	2:A:449:HOH:O	2.15	0.46
1:B:202:ASN:ND2	1:B:206:ASN:HD21	2.13	0.46
1:B:21:ARG:HG2	1:B:57:TYR:OH	2.14	0.46
1:B:112:THR:HB	1:B:272:ARG:HH12	1.80	0.46
1:A:141:THR:HB	1:A:146:ARG:HB2	1.98	0.46
1:A:184:TYR:O	1:A:189:VAL:HG11	2.16	0.46
1:B:17:ALA:HB1	1:B:53:TYR:HB2	1.98	0.46
1:A:168:ALA:CB	1:A:204:THR:HA	2.41	0.46
1:A:248:VAL:HA	1:A:251:LEU:HD12	1.97	0.46
1:B:157:ARG:NH1	1:B:193:LEU:O	2.45	0.46
1:B:185:ASN:HA	1:B:229:PHE:CE2	2.50	0.46
1:B:198:LYS:C	1:B:200:GLN:N	2.67	0.46
1:B:44:GLU:O	1:B:48:VAL:HG23	2.14	0.46
1:B:111:CYS:SG	1:B:152:LEU:HD22	2.55	0.46
1:B:244:GLU:HG2	1:B:245:LEU:N	2.30	0.46
1:B:10:VAL:HG13	1:B:41:ARG:CZ	2.46	0.46
1:A:216:ILE:CG2	1:A:217:LEU:H	2.28	0.46
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.14	0.46
1:A:24:PHE:O	1:A:25:GLU:C	2.52	0.46
1:A:243:PRO:HB2	1:A:247:PHE:HE2	1.81	0.46
1:A:87:ARG:NH1	1:A:271:THR:HG22	2.30	0.46
1:A:256:ASN:O	1:A:257:LYS:HB2	2.15	0.46
1:A:188:ASP:HA	1:A:191:ARG:NE	2.30	0.46
1:A:11:PRO:HG2	1:A:16:ASP:OD2	2.15	0.46
1:A:45:GLN:O	1:A:49:ILE:HG13	2.15	0.46
1:B:82:LEU:CD2	1:B:86:GLU:HB3	2.46	0.46
1:A:135:GLU:HB2	1:B:196:ARG:HH11	1.79	0.46
1:A:193:LEU:HD22	1:A:240:LEU:CD1	2.46	0.46
1:A:97:LYS:C	1:A:98:ARG:HE	2.19	0.46
1:A:209:GLN:HE21	1:A:215:GLU:CB	2.28	0.46
1:A:297:THR:HG21	1:A:317:ALA:OXT	2.14	0.46
1:A:1:SER:HB2	1:A:275:ILE:O	2.16	0.46
1:B:247:PHE:CE1	1:B:268:ILE:HD12	2.49	0.46
1:A:35:ILE:CD1	1:A:307:MET:HB2	2.46	0.46
1:A:245:LEU:HD11	2:A:389:HOH:O	2.15	0.46
1:A:31:GLU:O	1:A:34:ILE:HD13	2.16	0.46
1:B:231:ALA:HA	1:B:234:ARG:NH2	2.27	0.46
1:A:39:ALA:HB2	1:A:307:MET:HE1	1.98	0.46
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.97	0.46
1:B:111:CYS:C	1:B:113:ARG:H	2.19	0.46
1:B:88:ASP:HB3	1:B:121:ALA:HB2	1.97	0.46
1:A:3:THR:HG23	1:A:277:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:92:ALA:O	1:A:96:THR:HG23	2.15	0.46
1:B:148:LEU:HD23	1:B:232:LEU:CD2	2.46	0.46
1:A:125:TYR:O	1:A:126:HIS:C	2.53	0.46
1:B:12:ALA:O	1:B:15:ASP:HB2	2.14	0.46
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.98	0.46
1:B:184:TYR:CZ	1:B:230:LEU:HD13	2.49	0.46
1:B:149:LEU:O	1:B:153:VAL:HG22	2.16	0.46
1:B:105:VAL:O	1:B:105:VAL:HG12	2.15	0.46
1:A:209:GLN:NE2	1:A:215:GLU:HG3	2.31	0.46
1:A:178:LYS:O	1:A:183:HIS:N	2.44	0.46
1:A:195:THR:CB	1:B:135:GLU:HB3	2.45	0.46
1:A:23:ALA:HB2	1:A:33:LEU:HD23	1.96	0.46
1:A:300:THR:O	1:A:301:ARG:HG3	2.16	0.46
1:B:104:GLN:HG3	1:B:232:LEU:CD1	2.45	0.46
1:B:182:LYS:HD2	1:B:184:TYR:OH	2.14	0.46
1:A:139:HIS:CD2	1:B:196:ARG:HH22	2.33	0.46
1:A:181:ASP:O	1:A:182:LYS:HB2	2.15	0.46
1:B:72:ASP:HA	1:B:75:ARG:HB3	1.97	0.46
1:B:198:LYS:NZ	2:B:335:HOH:O	2.47	0.46
1:B:21:ARG:HG2	1:B:57:TYR:CE1	2.50	0.46
1:A:288:ASN:O	1:A:289:SER:CB	2.63	0.46
1:B:108:GLU:OE1	1:B:267:ARG:NH1	2.49	0.46
1:A:80:TRP:CH2	1:A:311:LEU:HD22	2.51	0.46
1:B:1:SER:N	1:B:279:VAL:HG23	2.30	0.46
1:B:88:ASP:OD1	1:B:109:VAL:HG13	2.14	0.46
1:A:41:ARG:HA	1:A:45:GLN:OE1	2.16	0.46
1:A:62:LEU:HD13	1:A:82:LEU:HD23	1.96	0.46
1:B:54:HIS:HA	1:B:59:GLU:O	2.15	0.46
1:A:91:LEU:O	1:A:92:ALA:C	2.53	0.46
1:B:148:LEU:HD23	1:B:232:LEU:HG	1.98	0.46
1:B:18:GLU:O	1:B:21:ARG:HB3	2.15	0.46
1:B:166:THR:O	1:B:170:GLN:HG3	2.16	0.46
1:A:44:GLU:O	1:A:47:LYS:HB3	2.15	0.46
1:A:231:ALA:HA	1:A:234:ARG:HD2	1.98	0.46
1:A:184:TYR:CE2	1:A:230:LEU:HD22	2.50	0.46
1:A:261:ASP:HB3	1:A:264:ALA:HB2	1.96	0.46
1:B:133:LEU:N	2:B:319:HOH:O	2.48	0.46
1:B:150:VAL:O	1:B:153:VAL:HG22	2.15	0.46
1:A:83:GLU:CG	1:A:84:PRO:HD2	2.43	0.46
1:A:97:LYS:O	1:A:98:ARG:HG2	2.16	0.46
1:A:138:ALA:O	1:A:146:ARG:HD3	2.16	0.46
1:B:202:ASN:ND2	1:B:206:ASN:HD21	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:ILE:HG21	1:A:295:ALA:HB1	1.98	0.46
1:B:231:ALA:O	1:B:234:ARG:HB2	2.15	0.46
1:A:275:ILE:HG22	1:A:276:ASP:N	2.31	0.46
1:B:192:ILE:O	1:B:196:ARG:HB2	2.16	0.46
1:A:72:ASP:HB3	1:A:304:TYR:CD1	2.51	0.46
1:A:185:ASN:HD22	1:A:185:ASN:C	2.19	0.46
1:A:128:ARG:HG2	1:A:128:ARG:NH1	2.28	0.46
1:A:10:VAL:HG21	1:A:45:GLN:NE2	2.31	0.46
1:B:12:ALA:HB1	1:B:13:PRO:HD2	1.96	0.46
1:A:173:LYS:O	1:A:176:HIS:HB3	2.16	0.46
1:A:203:ALA:HA	1:A:206:ASN:HD22	1.81	0.46
1:B:149:LEU:O	1:B:153:VAL:HG13	2.16	0.46
1:A:104:GLN:O	1:A:108:GLU:HB2	2.15	0.46
1:A:78:LEU:O	1:A:79:LEU:C	2.54	0.46
1:B:107:MET:SD	1:B:107:MET:C	2.95	0.46
1:B:293:GLU:OE1	1:B:293:GLU:N	2.38	0.46
1:B:151:SER:HB3	1:B:194:SER:OG	2.16	0.46
1:A:79:LEU:O	1:A:87:ARG:NE	2.49	0.46
1:A:21:ARG:HD3	1:A:57:TYR:CD2	2.50	0.46
1:A:247:PHE:HD1	1:A:268:ILE:HD12	1.80	0.46
1:B:296:ILE:CD1	1:B:312:LEU:HD11	2.43	0.46
1:A:216:ILE:O	1:A:219:SER:HB2	2.16	0.46
1:A:301:ARG:NH2	1:A:315:ASP:O	2.49	0.46
1:A:109:VAL:O	1:A:113:ARG:HD3	2.16	0.46
1:B:184:TYR:O	1:B:233:LEU:HD22	2.16	0.46
1:A:168:ALA:O	1:A:204:THR:HG23	2.15	0.46
1:A:155:SER:OG	1:A:157:ARG:HG3	2.16	0.46
1:B:84:PRO:O	1:B:88:ASP:HB2	2.16	0.46
1:A:37:ILE:HA	1:A:41:ARG:NH1	2.27	0.46
1:A:104:GLN:OE1	1:A:246:TYR:HE1	1.99	0.46
1:A:35:ILE:HD12	1:A:307:MET:HA	1.98	0.46
1:A:90:LEU:HD11	2:A:357:HOH:O	2.16	0.46
1:B:252:ARG:HE	1:B:288:ASN:HD21	1.61	0.46
1:B:4:LEU:HG	1:B:6:VAL:HG23	1.98	0.46
1:B:138:ALA:O	1:B:146:ARG:HD3	2.16	0.46
1:B:261:ASP:CG	1:B:264:ALA:HB2	2.36	0.46
1:B:113:ARG:N	1:B:113:ARG:HD2	2.30	0.46
1:A:193:LEU:HD12	1:A:233:LEU:CD1	2.45	0.46
1:A:134:GLU:OE1	1:A:134:GLU:N	2.49	0.46
1:A:135:GLU:HA	1:B:195:THR:HB	1.97	0.46
1:A:158:TYR:CE2	1:A:160:GLY:HA3	2.51	0.46
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:GLU:CD	1:A:134:GLU:H	2.18	0.46
1:B:273:ALA:HA	1:B:277:LEU:CB	2.45	0.46
1:A:192:ILE:HA	1:A:196:ARG:HG2	1.97	0.46
1:A:184:TYR:CD2	1:A:230:LEU:HD13	2.51	0.46
1:A:242:ARG:NH2	2:A:390:HOH:O	2.49	0.46
1:A:72:ASP:HB3	1:A:304:TYR:CD1	2.51	0.46
1:A:158:TYR:CD1	1:B:126:HIS:HB3	2.51	0.46
1:A:220:LEU:HD22	1:A:230:LEU:HD11	1.97	0.46
1:A:303:ASP:HA	1:A:306:LYS:HD3	1.97	0.45
1:A:220:LEU:HD13	1:A:234:ARG:CG	2.45	0.45
1:A:62:LEU:C	1:A:64:THR:H	2.19	0.45
1:B:161:ASP:O	1:B:163:VAL:HG23	2.16	0.45
1:A:173:LYS:O	1:A:177:GLU:HB2	2.15	0.45
1:B:293:GLU:HG2	1:B:294:LYS:H	1.81	0.45
1:B:109:VAL:HA	1:B:113:ARG:HE	1.82	0.45
1:A:171:GLU:HB3	1:A:192:ILE:HD13	1.98	0.45
1:A:96:THR:HG22	1:A:106:LEU:HD11	1.98	0.45
1:A:176:HIS:HB2	1:A:208:TYR:CE2	2.51	0.45
1:B:248:VAL:HG13	1:B:284:TYR:HA	1.98	0.45
1:A:87:ARG:CD	1:A:271:THR:HG22	2.44	0.45
1:A:192:ILE:HG23	1:A:196:ARG:HG3	1.98	0.45
1:B:19:GLN:OE1	1:B:37:ILE:HD11	2.16	0.45
1:A:304:TYR:O	1:A:308:LEU:HG	2.16	0.45
1:A:187:GLU:HA	1:A:190:ILE:HD12	1.98	0.45
1:A:139:HIS:HD2	2:B:334:HOH:O	1.99	0.45
1:B:71:ASN:OD1	1:B:73:PHE:N	2.46	0.45
1:A:188:ASP:O	1:A:192:ILE:HG13	2.15	0.45
1:B:216:ILE:CG2	1:B:217:LEU:N	2.78	0.45
1:A:35:ILE:HD11	1:A:73:PHE:CE1	2.51	0.45
1:B:87:ARG:HD3	1:B:271:THR:HG22	1.99	0.45
1:B:112:THR:HG22	1:B:243:PRO:CG	2.46	0.45
1:B:220:LEU:HB3	1:B:230:LEU:HD11	1.98	0.45
1:A:278:LYS:HE3	2:A:401:HOH:O	2.15	0.45
1:B:73:PHE:CZ	1:B:77:ILE:HD11	2.50	0.45
1:A:147:LYS:CD	1:A:147:LYS:H	2.26	0.45
1:B:128:ARG:HD3	1:B:129:TYR:CE2	2.51	0.45
1:A:132:SER:OG	1:A:135:GLU:HB2	2.17	0.45
1:A:19:GLN:HA	2:A:452:HOH:O	2.15	0.45
1:A:267:ARG:HD3	1:A:268:ILE:HD13	1.98	0.45
1:B:86:GLU:O	1:B:89:ALA:HB3	2.17	0.45
1:A:14:SER:O	1:A:18:GLU:HG3	2.16	0.45
1:B:75:ARG:HE	1:B:79:LEU:CD1	2.26	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:MET:HE3	1:A:207:ARG:HD3	1.97	0.45
1:B:265:LEU:O	1:B:269:VAL:HG23	2.17	0.45
1:A:255:ILE:HD13	1:A:295:ALA:HB1	1.99	0.45
1:B:216:ILE:O	1:B:219:SER:HB3	2.15	0.45
1:B:106:LEU:CD2	1:B:149:LEU:HB3	2.45	0.45
1:A:146:ARG:HG3	1:A:150:VAL:HG23	1.98	0.45
1:A:38:LEU:HD13	1:A:81:THR:OG1	2.17	0.45
1:A:7:SER:C	1:A:9:SER:H	2.19	0.45
1:A:205:PHE:CE2	1:A:237:ILE:HG23	2.51	0.45
1:B:298:LYS:HE3	1:B:299:ASP:OD2	2.16	0.45
1:B:93:ASN:O	1:B:97:LYS:HG2	2.17	0.45
1:A:19:GLN:HA	2:A:448:HOH:O	2.14	0.45
1:A:267:ARG:HB3	1:A:267:ARG:CZ	2.46	0.45
1:A:171:GLU:O	1:A:175:VAL:HG23	2.15	0.45
1:A:265:LEU:HB3	2:A:328:HOH:O	2.16	0.45
1:A:158:TYR:CZ	1:A:160:GLY:HA3	2.51	0.45
1:A:122:ARG:NH2	1:B:156:TYR:CB	2.80	0.45
1:B:192:ILE:HG22	1:B:201:ILE:HD11	1.99	0.45
1:A:195:THR:HG22	1:B:134:GLU:HB3	1.97	0.45
1:A:188:ASP:HB3	1:A:191:ARG:HH21	1.81	0.45
1:B:6:VAL:HG21	1:B:42:SER:HB3	1.99	0.45
1:A:142:THR:O	1:A:145:PHE:HB2	2.17	0.45
1:B:215:GLU:HB3	1:B:218:LYS:HG3	1.99	0.45
1:A:267:ARG:HG3	1:A:271:THR:CG2	2.46	0.45
1:B:247:PHE:HD1	1:B:268:ILE:HD12	1.77	0.45
1:A:287:ARG:O	1:A:287:ARG:NH1	2.46	0.45
1:A:69:LEU:H	1:A:69:LEU:CD2	2.15	0.45
1:B:116:THR:C	1:B:118:LEU:N	2.69	0.45
1:A:87:ARG:NH1	1:A:88:ASP:OD1	2.49	0.45
1:B:198:LYS:O	1:B:199:ALA:C	2.53	0.45
1:B:301:ARG:NH1	1:B:306:LYS:HG2	2.32	0.45
1:B:179:ILE:CD1	1:B:216:ILE:HD11	2.45	0.45
1:A:248:VAL:HG12	1:A:249:ASP:N	2.31	0.45
1:B:198:LYS:HE2	1:B:240:LEU:HD23	1.98	0.45
1:B:291:PRO:O	1:B:295:ALA:HB2	2.17	0.45
1:B:97:LYS:HE2	1:B:97:LYS:CA	2.45	0.45
1:A:257:LYS:N	1:A:257:LYS:HD3	2.32	0.45
1:A:128:ARG:HB2	2:A:445:HOH:O	2.15	0.45
1:A:75:ARG:CZ	1:A:79:LEU:HD21	2.46	0.45
1:A:202:ASN:HD21	1:A:206:ASN:HD21	1.65	0.45
1:B:100:THR:OG1	1:B:101:SER:N	2.50	0.45
1:B:252:ARG:HE	1:B:288:ASN:ND2	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:47:LYS:HE2	1:B:83:GLU:OE1	2.16	0.45
1:B:111:CYS:HB3	1:B:240:LEU:HG	1.99	0.45
1:A:50:ARG:HD2	1:A:81:THR:HG22	1.97	0.45
1:B:21:ARG:CZ	2:B:342:HOH:O	2.63	0.45
1:B:264:ALA:O	1:B:268:ILE:HG12	2.16	0.45
1:B:62:LEU:HD21	1:B:81:THR:CG2	2.45	0.45
1:B:290:ILE:HG23	1:B:290:ILE:O	2.15	0.45
1:A:172:ALA:HB2	1:A:204:THR:O	2.16	0.45
1:B:169:LYS:HE3	1:B:207:ARG:HH21	1.82	0.45
1:B:86:GLU:O	1:B:89:ALA:HB3	2.17	0.45
1:B:47:LYS:HE2	1:B:83:GLU:OE2	2.15	0.45
1:A:276:ASP:O	1:A:278:LYS:N	2.49	0.45
1:A:150:VAL:O	1:A:154:THR:OG1	2.16	0.45
1:B:1:SER:HB2	1:B:275:ILE:O	2.16	0.45
1:A:129:TYR:C	1:A:131:LYS:N	2.69	0.45
1:A:239:CYS:O	1:A:243:PRO:HG3	2.16	0.45
1:A:76:ALA:HA	1:A:266:THR:CG2	2.47	0.45
1:A:272:ARG:CA	1:A:272:ARG:NH1	2.70	0.45
1:B:1:SER:OG	1:B:279:VAL:HG23	2.15	0.45
1:A:158:TYR:CZ	1:B:130:LYS:HA	2.52	0.45
1:A:103:ASN:HB2	2:A:400:HOH:O	2.15	0.45
1:B:269:VAL:O	1:B:273:ALA:HB2	2.17	0.45
1:B:304:TYR:O	1:B:308:LEU:HG	2.17	0.45
1:B:91:LEU:HD22	1:B:267:ARG:HG3	1.99	0.45
1:A:10:VAL:CG1	1:A:11:PRO:HD2	2.45	0.45
1:A:276:ASP:O	1:A:280:ILE:HG13	2.16	0.45
1:B:215:GLU:HB3	1:B:218:LYS:HD2	1.98	0.45
1:A:79:LEU:HD23	1:A:79:LEU:N	2.32	0.45
1:A:112:THR:HG21	1:A:247:PHE:CE2	2.51	0.45
1:B:262:GLU:HB3	2:B:379:HOH:O	2.17	0.45
1:A:134:GLU:HG3	1:A:154:THR:CG2	2.47	0.45
1:B:184:TYR:HB3	1:B:233:LEU:HD22	1.99	0.45
1:B:237:ILE:O	1:B:237:ILE:HG22	2.15	0.45
1:A:119:LEU:O	1:A:123:GLN:HG3	2.17	0.45
1:A:35:ILE:HD11	1:A:307:MET:HB2	1.99	0.45
1:B:112:THR:HG22	1:B:239:CYS:HB3	1.98	0.45
1:B:71:ASN:OD1	1:B:73:PHE:N	2.49	0.45
1:B:87:ARG:HH12	1:B:271:THR:HA	1.76	0.45
1:A:7:SER:C	1:A:9:SER:N	2.70	0.45
1:B:95:ALA:O	1:B:99:TRP:HB2	2.16	0.45
1:B:76:ALA:HA	1:B:266:THR:CG2	2.47	0.45
1:A:298:LYS:HG2	1:A:299:ASP:N	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:12:ALA:HB3	1:A:15:ASP:OD2	2.17	0.45
1:A:112:THR:HG22	1:A:239:CYS:O	2.16	0.45
2:A:327:HOH:O	1:B:196:ARG:HB3	2.17	0.45
1:B:125:TYR:CG	1:B:133:LEU:HB2	2.51	0.45
1:B:41:ARG:HD2	1:B:49:ILE:CD1	2.47	0.45
1:B:18:GLU:HA	1:B:57:TYR:CE2	2.51	0.45
1:A:191:ARG:HH12	1:A:196:ARG:NH2	2.15	0.45
1:A:286:ARG:HG2	1:A:286:ARG:O	2.16	0.45
1:A:37:ILE:O	1:A:41:ARG:HG2	2.16	0.45
1:A:3:THR:OG1	1:A:277:LEU:HD23	2.16	0.45
1:B:293:GLU:CB	1:B:314:GLU:HG3	2.47	0.45
1:A:7:SER:O	1:A:10:VAL:HG23	2.16	0.45
1:B:14:SER:O	1:B:18:GLU:HG3	2.16	0.45
1:A:46:ARG:O	1:A:50:ARG:HG3	2.17	0.45
1:A:4:LEU:HD21	1:A:41:ARG:O	2.17	0.45
1:A:81:THR:HG22	1:A:81:THR:O	2.17	0.45
1:B:107:MET:HE3	1:B:108:GLU:N	2.32	0.45
1:A:282:GLU:O	1:A:285:GLN:HB2	2.17	0.45
1:B:192:ILE:HG23	1:B:196:ARG:HG3	1.99	0.45
1:B:142:THR:O	1:B:145:PHE:HB2	2.17	0.45
1:B:216:ILE:CG2	1:B:217:LEU:N	2.80	0.45
1:A:49:ILE:HG22	1:A:50:ARG:N	2.32	0.45
1:A:68:GLU:OE1	1:A:68:GLU:HA	2.17	0.45
1:B:141:THR:OG1	1:B:146:ARG:HB2	2.17	0.45
1:A:286:ARG:NH1	1:A:286:ARG:HB2	2.32	0.45
1:B:198:LYS:NZ	2:B:380:HOH:O	2.50	0.45
1:B:285:GLN:HG3	1:B:290:ILE:N	2.32	0.45
1:B:36:SER:HA	1:B:40:HIS:CE1	2.52	0.45
1:A:134:GLU:HB3	1:B:195:THR:HG22	1.98	0.45
1:A:304:TYR:CE1	1:A:308:LEU:HD11	2.51	0.44
1:A:89:ALA:HB2	1:A:124:ALA:HB3	1.99	0.44
1:A:144:ASP:HA	1:A:147:LYS:CG	2.48	0.44
1:B:256:ASN:C	1:B:258:THR:H	2.21	0.44
1:A:93:ASN:HB2	1:A:129:TYR:CE2	2.52	0.44
1:B:66:ASP:HA	1:B:78:LEU:HD13	1.98	0.44
1:B:116:THR:O	1:B:119:LEU:HB3	2.16	0.44
1:B:20:LEU:CD2	1:B:34:ILE:HA	2.47	0.44
1:B:261:ASP:OD2	1:B:264:ALA:HB2	2.18	0.44
1:B:95:ALA:O	1:B:99:TRP:HB2	2.17	0.44
1:B:71:ASN:ND2	1:B:73:PHE:HB3	2.25	0.44
1:A:113:ARG:HB3	1:A:117:GLN:HB2	1.99	0.44
1:B:292:LEU:O	1:B:292:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:72:ASP:HB3	1:B:304:TYR:CD1	2.53	0.44
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.82	0.44
1:A:25:GLU:HB3	2:A:441:HOH:O	2.16	0.44
1:B:261:ASP:CG	1:B:267:ARG:HH22	2.20	0.44
1:B:157:ARG:CB	2:B:319:HOH:O	2.65	0.44
1:A:87:ARG:HH11	1:A:271:THR:HA	1.82	0.44
1:A:3:THR:HG23	1:A:277:LEU:HB3	2.00	0.44
1:B:10:VAL:HG21	1:B:45:GLN:NE2	2.30	0.44
1:A:118:LEU:O	1:A:118:LEU:HD12	2.17	0.44
1:A:12:ALA:CB	1:A:13:PRO:HD2	2.26	0.44
1:A:15:ASP:O	1:A:19:GLN:HG3	2.17	0.44
1:B:244:GLU:O	1:B:248:VAL:HG23	2.18	0.44
1:A:277:LEU:O	1:A:280:ILE:HB	2.18	0.44
1:B:19:GLN:OE1	1:B:33:LEU:HD11	2.17	0.44
1:B:236:THR:O	1:B:240:LEU:HG	2.18	0.44
1:B:109:VAL:HG13	1:B:113:ARG:HE	1.81	0.44
1:B:128:ARG:HG2	1:B:128:ARG:O	2.17	0.44
1:A:233:LEU:O	1:A:237:ILE:HG13	2.17	0.44
1:A:191:ARG:HH12	1:A:196:ARG:NH2	2.15	0.44
1:A:92:ALA:CB	1:A:106:LEU:HD23	2.48	0.44
1:A:227:ASP:OD1	1:A:230:LEU:HB2	2.17	0.44
1:B:165:MET:CE	1:B:207:ARG:HD3	2.47	0.44
1:B:248:VAL:HG21	1:B:283:GLU:CB	2.32	0.44
1:B:277:LEU:O	1:B:280:ILE:N	2.50	0.44
1:A:217:LEU:HD11	1:A:238:GLN:HG2	1.99	0.44
1:A:293:GLU:HB2	1:A:317:ALA:OXT	2.17	0.44
1:B:71:ASN:OD1	1:B:72:ASP:N	2.51	0.44
1:A:302:GLY:HA3	2:A:378:HOH:O	2.15	0.44
1:B:169:LYS:HD2	1:B:207:ARG:HH21	1.81	0.44
1:B:16:ASP:OD1	1:B:37:ILE:HD13	2.18	0.44
1:B:158:TYR:O	1:B:197:SER:HB2	2.18	0.44
1:B:261:ASP:OD1	1:B:267:ARG:NH2	2.50	0.44
1:A:50:ARG:NH2	1:A:62:LEU:HD12	2.32	0.44
1:B:185:ASN:O	1:B:186:ASP:C	2.56	0.44
1:A:176:HIS:NE2	1:A:180:LYS:HE2	2.32	0.44
1:B:150:VAL:O	1:B:153:VAL:N	2.50	0.44
1:A:215:GLU:HG2	1:A:216:ILE:N	2.32	0.44
1:A:195:THR:HB	1:B:135:GLU:HB3	1.98	0.44
1:A:298:LYS:HG3	1:A:299:ASP:OD1	2.17	0.44
1:A:122:ARG:HH21	1:B:156:TYR:CB	2.30	0.44
1:A:201:ILE:O	1:A:204:THR:HB	2.18	0.44
1:B:165:MET:CE	1:B:207:ARG:HD3	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:107:MET:SD	1:B:107:MET:C	2.96	0.44
1:B:93:ASN:O	1:B:97:LYS:HG2	2.18	0.44
1:B:105:VAL:O	1:B:109:VAL:HG23	2.18	0.44
1:A:168:ALA:CB	1:A:207:ARG:HG3	2.45	0.44
1:A:130:LYS:HD2	1:B:158:TYR:OH	2.17	0.44
1:A:10:VAL:HG13	1:A:41:ARG:NE	2.32	0.44
1:B:51:GLN:HE21	1:B:55:GLU:HG3	1.82	0.44
1:A:144:ASP:O	1:A:147:LYS:HB2	2.17	0.44
1:A:154:THR:HB	1:B:154:THR:O	2.18	0.44
1:A:51:GLN:C	1:A:53:TYR:N	2.69	0.44
1:A:271:THR:O	1:A:272:ARG:HD2	2.17	0.44
1:A:10:VAL:HG13	1:A:11:PRO:HD2	2.00	0.44
1:A:291:PRO:HB2	1:A:293:GLU:CD	2.38	0.44
1:B:198:LYS:O	1:B:201:ILE:HB	2.17	0.44
1:A:171:GLU:HB3	1:A:192:ILE:HD11	2.00	0.44
1:A:244:GLU:HB2	1:A:283:GLU:HG3	1.98	0.44
1:B:42:SER:O	1:B:46:ARG:HG3	2.18	0.44
1:A:218:LYS:HG2	1:A:221:GLU:OE2	2.18	0.44
1:A:134:GLU:HG3	1:A:154:THR:CG2	2.33	0.44
1:A:156:TYR:HB3	2:B:323:HOH:O	2.17	0.44
1:B:73:PHE:CZ	1:B:77:ILE:HD11	2.53	0.44
1:A:15:ASP:OD1	1:A:18:GLU:OE1	2.35	0.44
1:A:117:GLN:HE22	1:A:275:ILE:HD11	1.81	0.44
1:A:207:ARG:NE	2:A:397:HOH:O	2.51	0.44
1:B:115:SER:O	1:B:118:LEU:HB3	2.18	0.44
1:B:261:ASP:CG	1:B:267:ARG:HH22	2.20	0.44
1:B:128:ARG:HD3	1:B:129:TYR:CE2	2.52	0.44
1:B:167:LEU:HA	1:B:170:GLN:NE2	2.33	0.44
1:B:158:TYR:CZ	1:B:160:GLY:HA3	2.52	0.44
1:B:103:ASN:HB2	2:B:368:HOH:O	2.17	0.44
1:B:35:ILE:HG12	1:B:307:MET:HB2	1.99	0.44
1:A:41:ARG:O	1:A:46:ARG:HG3	2.17	0.44
1:B:36:SER:O	1:B:40:HIS:ND1	2.51	0.44
1:B:65:LEU:HD23	1:B:74:GLU:HB3	1.99	0.44
1:B:137:VAL:O	1:B:137:VAL:HG12	2.17	0.44
1:B:294:LYS:HA	1:B:297:THR:HG22	1.98	0.44
1:A:199:ALA:O	1:A:202:ASN:N	2.46	0.44
1:A:288:ASN:O	1:A:289:SER:HB2	2.18	0.44
1:A:191:ARG:HH12	1:A:196:ARG:HH21	1.66	0.44
1:A:109:VAL:O	1:A:113:ARG:HD3	2.17	0.44
1:B:248:VAL:HG21	1:B:283:GLU:CB	2.45	0.44
1:A:298:LYS:HG3	2:A:415:HOH:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:44:GLU:O	1:B:48:VAL:HG23	2.17	0.44
1:A:108:GLU:HB2	1:A:246:TYR:OH	2.16	0.44
1:B:298:LYS:HG2	1:B:299:ASP:CG	2.38	0.44
1:B:256:ASN:C	1:B:257:LYS:HD3	2.38	0.44
1:B:178:LYS:HG3	1:B:186:ASP:CG	2.38	0.44
1:B:129:TYR:O	1:B:131:LYS:HG3	2.18	0.44
1:A:14:SER:HA	1:A:17:ALA:CB	2.45	0.44
1:B:293:GLU:HG2	1:B:294:LYS:N	2.32	0.44
1:B:42:SER:OG	1:B:45:GLN:HG3	2.18	0.44
1:B:51:GLN:H	1:B:51:GLN:CD	2.20	0.44
1:B:182:LYS:O	1:B:184:TYR:N	2.45	0.44
1:A:286:ARG:NH2	2:A:363:HOH:O	2.46	0.44
1:A:105:VAL:HG12	1:A:109:VAL:HG23	1.99	0.44
1:A:285:GLN:O	1:A:287:ARG:N	2.51	0.44
1:A:70:SER:OG	1:A:75:ARG:HB2	2.17	0.44
1:A:106:LEU:HB2	1:A:149:LEU:HD13	1.98	0.44
1:B:126:HIS:ND1	1:B:131:LYS:O	2.51	0.44
1:A:34:ILE:HG21	1:A:77:ILE:HD13	2.00	0.44
1:A:242:ARG:HG3	1:A:244:GLU:CD	2.37	0.44
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.82	0.44
1:B:166:THR:O	1:B:170:GLN:HG3	2.17	0.44
1:B:31:GLU:N	1:B:31:GLU:OE1	2.51	0.44
1:B:304:TYR:CZ	1:B:308:LEU:HD11	2.53	0.44
1:A:216:ILE:CG2	1:A:217:LEU:N	2.81	0.44
1:A:42:SER:OG	1:A:45:GLN:HG3	2.18	0.44
1:B:65:LEU:O	1:B:78:LEU:HB2	2.18	0.44
1:B:298:LYS:O	1:B:300:THR:N	2.51	0.44
1:B:238:GLN:HE22	1:B:245:LEU:HD12	1.82	0.44
1:B:247:PHE:CD1	1:B:268:ILE:HG23	2.53	0.44
1:A:278:LYS:HE3	1:A:282:GLU:OE2	2.18	0.44
1:A:214:GLU:HG3	1:A:219:SER:HB2	1.99	0.44
1:A:186:ASP:O	1:A:190:ILE:HG13	2.18	0.44
1:A:3:THR:HG23	1:A:277:LEU:HB3	1.99	0.44
1:B:134:GLU:CG	1:B:154:THR:HG22	2.48	0.44
1:A:304:TYR:O	1:A:308:LEU:HG	2.18	0.44
1:A:98:ARG:HA	1:A:98:ARG:HE	1.82	0.44
1:A:50:ARG:CZ	1:A:62:LEU:HD12	2.48	0.44
1:A:118:LEU:HD12	1:A:118:LEU:O	2.18	0.44
1:B:197:SER:O	1:B:201:ILE:HG13	2.16	0.44
1:B:165:MET:HB3	1:B:165:MET:HE2	1.78	0.44
1:A:300:THR:O	1:A:305:GLU:HG2	2.18	0.44
1:A:192:ILE:O	1:A:196:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:TYR:O	1:A:126:HIS:C	2.56	0.44
1:B:301:ARG:HG2	2:B:404:HOH:O	2.18	0.43
1:A:144:ASP:HA	1:A:147:LYS:HZ1	1.81	0.43
1:B:215:GLU:HG3	1:B:217:LEU:H	1.83	0.43
1:A:174:LEU:HD21	1:A:188:ASP:CB	2.48	0.43
1:A:3:THR:HB	1:A:312:LEU:CA	2.48	0.43
1:A:13:PRO:HB3	1:A:48:VAL:HG12	2.00	0.43
1:B:75:ARG:CZ	1:B:79:LEU:HD11	2.48	0.43
1:A:38:LEU:HD12	1:A:77:ILE:HD12	1.99	0.43
1:B:62:LEU:O	1:B:66:ASP:HB2	2.17	0.43
1:A:278:LYS:C	1:A:280:ILE:H	2.20	0.43
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.83	0.43
1:B:47:LYS:HE2	1:B:83:GLU:OE1	2.18	0.43
1:B:218:LYS:HA	1:B:221:GLU:HG3	2.00	0.43
1:B:33:LEU:O	1:B:33:LEU:HG	2.18	0.43
1:B:244:GLU:N	1:B:244:GLU:OE1	2.51	0.43
1:A:158:TYR:CA	2:A:366:HOH:O	2.63	0.43
1:A:195:THR:OG1	1:B:135:GLU:HB3	2.18	0.43
1:A:193:LEU:HD22	1:A:240:LEU:HD12	2.00	0.43
1:B:302:GLY:O	1:B:306:LYS:HG3	2.19	0.43
1:B:48:VAL:HB	2:B:357:HOH:O	2.17	0.43
1:A:185:ASN:HD22	1:A:186:ASP:N	2.16	0.43
1:B:4:LEU:CD2	1:B:274:GLU:HG2	2.46	0.43
1:B:233:LEU:O	1:B:236:THR:HB	2.18	0.43
1:A:159:GLU:N	2:A:368:HOH:O	2.50	0.43
1:A:87:ARG:NH1	1:A:271:THR:HA	2.34	0.43
1:A:11:PRO:CG	1:A:41:ARG:HH21	2.31	0.43
1:A:134:GLU:CG	1:A:154:THR:HG22	2.23	0.43
1:B:281:GLY:O	1:B:285:GLN:HB2	2.18	0.43
1:A:98:ARG:CA	1:A:98:ARG:HE	2.28	0.43
1:A:158:TYR:CE1	1:B:130:LYS:HA	2.53	0.43
1:A:99:TRP:CZ2	1:A:101:SER:HA	2.53	0.43
1:A:264:ALA:O	1:A:268:ILE:HG12	2.18	0.43
1:B:107:MET:O	1:B:108:GLU:C	2.56	0.43
1:A:157:ARG:HD3	1:A:196:ARG:O	2.18	0.43
1:B:102:SER:OG	1:B:228:LYS:HD2	2.18	0.43
1:A:191:ARG:NH1	1:A:196:ARG:NH2	2.60	0.43
1:A:255:ILE:HD11	1:A:296:ILE:HA	1.99	0.43
1:B:177:GLU:O	1:B:180:LYS:HB3	2.18	0.43
1:B:146:ARG:HG3	1:B:150:VAL:HG21	1.99	0.43
1:A:107:MET:HG2	1:A:111:CYS:SG	2.58	0.43
1:A:248:VAL:HG21	1:A:283:GLU:CB	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:GLU:HA	1:B:124:ALA:HB1	1.99	0.43
1:B:294:LYS:HB3	1:B:294:LYS:HE2	1.89	0.43
1:A:72:ASP:HB3	1:A:304:TYR:CG	2.53	0.43
1:B:117:GLN:NE2	2:B:377:HOH:O	2.51	0.43
1:B:252:ARG:HA	1:B:284:TYR:HE1	1.83	0.43
1:A:144:ASP:OD1	1:A:185:ASN:HB2	2.18	0.43
1:A:114:THR:HB	1:A:159:GLU:OE2	2.18	0.43
1:B:202:ASN:HD21	1:B:206:ASN:HD21	1.65	0.43
1:A:70:SER:HB2	1:A:74:GLU:HB2	2.00	0.43
1:B:255:ILE:C	1:B:257:LYS:N	2.71	0.43
1:B:18:GLU:O	1:B:21:ARG:HB3	2.19	0.43
1:A:191:ARG:NH2	1:A:192:ILE:HD11	2.34	0.43
1:B:178:LYS:C	1:B:180:LYS:N	2.69	0.43
1:B:75:ARG:NH1	1:B:79:LEU:HD11	2.33	0.43
1:B:51:GLN:N	1:B:51:GLN:CD	2.71	0.43
1:A:37:ILE:O	1:A:41:ARG:HG2	2.18	0.43
1:A:68:GLU:OE1	1:A:68:GLU:HA	2.19	0.43
1:B:65:LEU:HD23	1:B:74:GLU:CB	2.48	0.43
1:A:264:ALA:O	1:A:268:ILE:HG12	2.17	0.43
1:B:277:LEU:CD2	1:B:312:LEU:HD23	2.45	0.43
1:B:130:LYS:O	1:B:131:LYS:HB3	2.19	0.43
1:A:184:TYR:CE2	1:A:230:LEU:HD13	2.54	0.43
1:A:107:MET:SD	1:A:107:MET:C	2.96	0.43
1:B:71:ASN:OD1	1:B:73:PHE:N	2.51	0.43
1:B:161:ASP:O	1:B:163:VAL:HG23	2.17	0.43
1:A:287:ARG:O	1:A:287:ARG:NH1	2.41	0.43
1:A:50:ARG:NH2	1:A:62:LEU:HD12	2.33	0.43
1:B:13:PRO:HG3	1:B:48:VAL:HG12	1.99	0.43
1:A:41:ARG:HB2	1:A:46:ARG:HG2	2.01	0.43
1:A:43:ALA:N	1:A:46:ARG:NH1	2.66	0.43
1:A:64:THR:HG23	1:A:65:LEU:HG	2.01	0.43
1:A:143:GLY:HA2	2:A:319:HOH:O	2.19	0.43
1:B:169:LYS:HG2	1:B:173:LYS:HZ3	1.83	0.43
1:B:77:ILE:HD13	1:B:307:MET:HG2	2.00	0.43
1:B:298:LYS:HB3	1:B:298:LYS:HE2	1.80	0.43
1:B:123:GLN:O	1:B:126:HIS:N	2.50	0.43
1:B:165:MET:O	1:B:168:ALA:HB3	2.18	0.43
1:A:298:LYS:HG2	1:A:299:ASP:OD1	2.18	0.43
1:A:71:ASN:OD1	1:A:74:GLU:HG3	2.17	0.43
1:B:73:PHE:HD1	1:B:304:TYR:HA	1.84	0.43
1:A:4:LEU:HD22	1:A:274:GLU:HG2	2.00	0.43
1:A:200:GLN:O	1:A:200:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:215:GLU:HB3	1:B:218:LYS:CG	2.42	0.43
1:B:303:ASP:N	1:B:306:LYS:HZ3	2.17	0.43
1:B:244:GLU:HG2	1:B:245:LEU:H	1.84	0.43
1:B:267:ARG:HH11	1:B:268:ILE:HD11	1.84	0.43
1:A:107:MET:HB2	1:A:232:LEU:HD11	2.00	0.43
1:B:20:LEU:HD13	1:B:61:LEU:CD1	2.48	0.43
1:A:108:GLU:OE1	1:A:246:TYR:OH	2.35	0.43
1:B:284:TYR:CD2	1:B:292:LEU:HB2	2.53	0.43
1:B:17:ALA:HB1	1:B:53:TYR:HB2	2.00	0.43
1:B:132:SER:CA	2:B:318:HOH:O	2.66	0.43
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.53	0.43
1:A:216:ILE:O	1:A:220:LEU:HG	2.19	0.43
1:B:286:ARG:NH1	1:B:286:ARG:HG2	2.33	0.43
1:B:34:ILE:HG22	1:B:38:LEU:HD12	1.99	0.43
1:A:290:ILE:H	1:A:290:ILE:CD1	2.30	0.43
1:A:130:LYS:HA	1:B:158:TYR:CE1	2.53	0.43
1:B:51:GLN:HG3	1:B:55:GLU:OE2	2.19	0.43
1:B:87:ARG:HD2	2:B:322:HOH:O	2.18	0.43
1:A:67:LYS:HB2	1:A:69:LEU:CD2	2.49	0.43
1:B:297:THR:HG21	1:B:317:ALA:OXT	2.18	0.43
1:A:167:LEU:HD21	1:A:196:ARG:NH2	2.34	0.43
1:B:54:HIS:HA	1:B:59:GLU:O	2.19	0.43
1:A:220:LEU:C	1:A:222:GLU:H	2.19	0.43
1:B:265:LEU:HD21	1:B:296:ILE:HD13	2.00	0.43
1:A:56:THR:HG22	1:A:56:THR:O	2.19	0.43
1:B:191:ARG:HG2	1:B:191:ARG:O	2.19	0.43
1:B:101:SER:HB3	1:B:145:PHE:CZ	2.53	0.43
1:A:100:THR:C	1:A:102:SER:H	2.21	0.43
1:B:247:PHE:HB3	1:B:280:ILE:HD13	2.01	0.43
1:B:293:GLU:OE2	1:B:314:GLU:HG3	2.18	0.43
1:B:247:PHE:CD2	1:B:280:ILE:HD11	2.54	0.43
1:B:304:TYR:CE1	1:B:308:LEU:HD11	2.53	0.43
1:A:216:ILE:CG2	1:A:217:LEU:N	2.81	0.43
1:A:129:TYR:O	1:A:131:LYS:N	2.51	0.43
1:A:288:ASN:O	1:A:289:SER:HB2	2.19	0.43
1:A:105:VAL:HG22	1:A:267:ARG:NH2	2.33	0.43
1:B:278:LYS:O	1:B:282:GLU:HG3	2.18	0.43
1:B:246:TYR:O	1:B:250:VAL:HG23	2.19	0.43
1:B:298:LYS:HG2	1:B:299:ASP:OD1	2.18	0.43
1:A:132:SER:C	1:A:134:GLU:N	2.71	0.43
1:A:137:VAL:HG13	1:A:141:THR:CG2	2.48	0.43
1:A:185:ASN:C	1:A:185:ASN:HD22	2.22	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:248:VAL:HG13	1:A:284:TYR:HD1	1.84	0.43
1:B:193:LEU:HD22	1:B:240:LEU:CD1	2.48	0.43
1:A:278:LYS:C	1:A:280:ILE:N	2.72	0.43
1:A:209:GLN:HG3	1:A:215:GLU:CA	2.49	0.43
1:A:307:MET:CE	1:A:311:LEU:HD21	2.49	0.43
1:B:122:ARG:O	1:B:125:TYR:HB3	2.18	0.43
1:A:111:CYS:SG	1:A:240:LEU:HD21	2.59	0.43
1:B:298:LYS:HG2	1:B:299:ASP:N	2.34	0.43
1:A:135:GLU:HB3	1:B:195:THR:CB	2.45	0.43
1:A:286:ARG:NH1	1:A:286:ARG:HB2	2.34	0.43
1:A:288:ASN:O	1:A:289:SER:CB	2.66	0.43
1:A:107:MET:HB2	1:A:232:LEU:HD11	2.00	0.43
1:A:216:ILE:HG23	1:A:217:LEU:H	1.82	0.43
1:A:92:ALA:HB1	1:A:106:LEU:CD2	2.49	0.43
1:A:114:THR:HG23	1:A:159:GLU:OE2	2.19	0.43
1:A:297:THR:O	1:A:299:ASP:N	2.51	0.43
1:A:50:ARG:HE	1:A:60:ASP:CG	2.20	0.43
1:B:150:VAL:O	1:B:154:THR:OG1	2.21	0.43
1:B:275:ILE:HG22	1:B:276:ASP:N	2.34	0.43
1:B:179:ILE:CD1	1:B:216:ILE:HD11	2.49	0.43
1:A:67:LYS:HB2	1:A:69:LEU:CD2	2.49	0.43
1:A:205:PHE:CE1	1:A:216:ILE:HD13	2.54	0.43
1:A:62:LEU:HD21	1:A:81:THR:HG21	2.00	0.43
1:A:122:ARG:NH1	1:A:154:THR:HA	2.34	0.43
1:A:71:ASN:HD22	1:A:74:GLU:HG3	1.83	0.43
1:A:41:ARG:HA	1:A:45:GLN:OE1	2.19	0.43
1:B:175:VAL:O	1:B:179:ILE:HG13	2.19	0.43
1:A:199:ALA:O	1:A:202:ASN:HB3	2.19	0.43
1:B:34:ILE:CG2	1:B:38:LEU:HD12	2.48	0.43
1:A:135:GLU:O	1:A:139:HIS:CB	2.65	0.43
1:A:42:SER:O	1:A:46:ARG:HG3	2.19	0.43
1:B:236:THR:O	1:B:240:LEU:HG	2.18	0.43
1:A:14:SER:O	1:A:17:ALA:HB3	2.19	0.43
1:B:129:TYR:O	1:B:131:LYS:HG3	2.19	0.43
1:A:200:GLN:O	1:A:203:ALA:N	2.52	0.43
1:B:293:GLU:CG	1:B:314:GLU:HG3	2.48	0.43
1:A:248:VAL:CG2	1:A:283:GLU:HB3	2.48	0.43
1:B:223:GLY:HA3	1:B:230:LEU:HD21	2.00	0.43
1:A:7:SER:C	1:A:9:SER:N	2.72	0.43
1:A:24:PHE:CZ	1:A:61:LEU:HD11	2.54	0.42
1:A:99:TRP:CG	1:A:100:THR:N	2.86	0.42
1:A:21:ARG:HG2	1:A:57:TYR:CZ	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:24:PHE:CE2	1:A:61:LEU:HD11	2.54	0.42
1:A:157:ARG:HG2	1:A:197:SER:HA	2.00	0.42
1:B:99:TRP:CG	1:B:100:THR:N	2.86	0.42
1:B:162:GLU:N	1:B:162:GLU:OE1	2.52	0.42
1:B:139:HIS:HB3	1:B:140:HIS:CE1	2.54	0.42
1:A:176:HIS:HB2	1:A:208:TYR:CE2	2.54	0.42
1:A:247:PHE:CD1	1:A:268:ILE:HG23	2.55	0.42
1:B:82:LEU:HD11	1:B:90:LEU:HD22	2.01	0.42
1:B:131:LYS:HD3	1:B:136:ASP:OD1	2.18	0.42
1:A:215:GLU:OE2	1:A:217:LEU:HD12	2.19	0.42
1:B:35:ILE:O	1:B:39:ALA:HB3	2.19	0.42
1:B:3:THR:O	1:B:5:LYS:HG3	2.19	0.42
1:A:19:GLN:HG2	2:A:390:HOH:O	2.18	0.42
1:A:309:VAL:HA	1:A:312:LEU:HD12	2.01	0.42
1:B:169:LYS:HE3	1:B:211:ASP:CG	2.39	0.42
1:A:236:THR:HG22	1:A:236:THR:O	2.18	0.42
1:B:53:TYR:C	1:B:53:TYR:CD1	2.92	0.42
1:A:23:ALA:C	1:A:25:GLU:H	2.23	0.42
1:A:304:TYR:HD2	1:A:305:GLU:OE2	2.02	0.42
1:A:164:ASN:N	1:A:200:GLN:OE1	2.50	0.42
1:A:128:ARG:HD3	1:A:129:TYR:CE2	2.55	0.42
1:A:44:GLU:O	1:A:47:LYS:HB3	2.19	0.42
1:B:11:PRO:HG3	1:B:41:ARG:HH21	1.84	0.42
1:B:178:LYS:HG3	1:B:186:ASP:CG	2.39	0.42
1:A:229:PHE:O	1:A:232:LEU:HB3	2.18	0.42
1:B:113:ARG:CG	1:B:117:GLN:HB3	2.50	0.42
1:A:265:LEU:CD2	1:A:308:LEU:HD13	2.49	0.42
1:A:21:ARG:HG2	1:A:57:TYR:CZ	2.54	0.42
1:A:135:GLU:N	1:B:195:THR:HB	2.34	0.42
1:B:231:ALA:HA	1:B:234:ARG:NE	2.33	0.42
1:B:18:GLU:HA	1:B:57:TYR:OH	2.19	0.42
1:B:33:LEU:O	1:B:37:ILE:HG13	2.19	0.42
1:A:261:ASP:O	1:A:262:GLU:C	2.57	0.42
1:B:122:ARG:CZ	1:B:154:THR:HA	2.50	0.42
1:B:54:HIS:C	1:B:56:THR:N	2.71	0.42
1:A:246:TYR:O	1:A:250:VAL:HG23	2.19	0.42
1:B:230:LEU:HG	1:B:234:ARG:HD2	2.01	0.42
1:B:157:ARG:CA	2:B:361:HOH:O	2.60	0.42
1:B:108:GLU:OE2	1:B:267:ARG:HD2	2.19	0.42
1:A:105:VAL:HG22	1:A:267:ARG:HH12	1.84	0.42
1:A:37:ILE:HG23	1:A:41:ARG:NH1	2.33	0.42
1:B:33:LEU:O	1:B:37:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:105:VAL:O	1:B:108:GLU:HB3	2.19	0.42
1:B:168:ALA:O	1:B:172:ALA:HB2	2.19	0.42
1:B:286:ARG:NH1	1:B:286:ARG:HG2	2.34	0.42
1:A:293:GLU:HA	1:A:296:ILE:HD12	2.01	0.42
1:B:132:SER:OG	1:B:135:GLU:N	2.51	0.42
1:A:35:ILE:HD12	1:A:307:MET:SD	2.59	0.42
1:B:113:ARG:HH22	1:B:271:THR:HG21	1.85	0.42
1:B:201:ILE:O	1:B:204:THR:HB	2.20	0.42
1:B:4:LEU:HD23	1:B:4:LEU:C	2.39	0.42
1:A:246:TYR:C	1:A:248:VAL:H	2.22	0.42
1:B:54:HIS:O	1:B:56:THR:N	2.50	0.42
1:B:18:GLU:O	1:B:21:ARG:HB3	2.20	0.42
1:A:35:ILE:HG23	1:A:307:MET:HA	2.02	0.42
1:A:276:ASP:OD1	1:A:276:ASP:N	2.51	0.42
1:A:186:ASP:HB3	1:A:189:VAL:CG2	2.48	0.42
1:A:161:ASP:OD1	1:A:199:ALA:HB2	2.19	0.42
1:A:22:THR:O	1:A:25:GLU:HG2	2.19	0.42
1:A:79:LEU:HD12	1:A:266:THR:CG2	2.48	0.42
1:B:106:LEU:HD22	1:B:133:LEU:HD11	2.01	0.42
1:B:294:LYS:HB3	1:B:294:LYS:HE2	1.88	0.42
1:B:65:LEU:HD22	1:B:74:GLU:CG	2.50	0.42
1:B:3:THR:HB	1:B:312:LEU:O	2.20	0.42
1:A:72:ASP:HB3	1:A:304:TYR:CD1	2.54	0.42
1:B:218:LYS:O	1:B:221:GLU:HB2	2.18	0.42
1:A:185:ASN:C	1:A:185:ASN:ND2	2.73	0.42
1:A:130:LYS:HB3	1:B:162:GLU:OE2	2.19	0.42
1:A:71:ASN:OD1	1:A:74:GLU:HG3	2.18	0.42
1:B:284:TYR:O	1:B:288:ASN:HB2	2.19	0.42
1:A:267:ARG:O	1:A:271:THR:HG23	2.19	0.42
1:B:133:LEU:O	1:B:137:VAL:HG23	2.19	0.42
1:B:119:LEU:O	1:B:122:ARG:N	2.52	0.42
1:A:61:LEU:O	1:A:64:THR:HG22	2.20	0.42
1:B:163:VAL:HG12	1:B:164:ASN:N	2.35	0.42
1:B:63:LYS:HA	2:B:350:HOH:O	2.18	0.42
1:B:220:LEU:C	1:B:222:GLU:H	2.22	0.42
1:B:73:PHE:CE1	1:B:77:ILE:HD11	2.55	0.42
1:A:312:LEU:HB3	2:A:458:HOH:O	2.18	0.42
1:A:54:HIS:C	1:A:56:THR:H	2.23	0.42
1:A:118:LEU:O	1:A:122:ARG:HB2	2.20	0.42
1:B:56:THR:O	1:B:57:TYR:CG	2.72	0.42
1:B:300:THR:CG2	1:B:301:ARG:H	2.29	0.42
1:B:235:SER:O	1:B:238:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:286:ARG:NH2	2:A:366:HOH:O	2.53	0.42
1:A:105:VAL:HG22	1:A:267:ARG:NH1	2.34	0.42
1:B:304:TYR:CZ	1:B:308:LEU:HD11	2.54	0.42
1:B:75:ARG:HG2	1:B:75:ARG:HH11	1.84	0.42
1:A:298:LYS:HE2	1:A:298:LYS:HB3	1.80	0.42
1:A:122:ARG:HD2	1:A:153:VAL:O	2.19	0.42
1:A:301:ARG:NE	2:A:372:HOH:O	2.52	0.42
1:B:203:ALA:O	1:B:207:ARG:HG2	2.19	0.42
1:A:168:ALA:HB1	1:A:204:THR:HA	2.00	0.42
1:A:303:ASP:CA	1:A:306:LYS:HD3	2.47	0.42
1:A:157:ARG:HH12	1:A:194:SER:HA	1.84	0.42
1:B:301:ARG:HG2	1:B:301:ARG:NH1	2.34	0.42
1:B:300:THR:CG2	1:B:301:ARG:N	2.81	0.42
1:B:216:ILE:HG23	1:B:217:LEU:N	2.34	0.42
1:A:161:ASP:CA	1:A:199:ALA:CB	2.96	0.42
1:A:32:ASP:O	1:A:36:SER:HB3	2.19	0.42
1:A:264:ALA:HA	1:A:267:ARG:HH12	1.84	0.42
1:B:125:TYR:CD1	1:B:125:TYR:O	2.72	0.42
1:A:148:LEU:HD13	1:A:229:PHE:CE1	2.55	0.42
1:A:188:ASP:O	1:A:192:ILE:HG13	2.20	0.42
1:B:12:ALA:HA	1:B:13:PRO:HD2	1.88	0.42
1:A:154:THR:HB	1:B:154:THR:HB	2.00	0.42
1:B:150:VAL:O	1:B:154:THR:HG23	2.19	0.42
1:B:134:GLU:HG3	1:B:154:THR:HG22	2.01	0.42
1:A:204:THR:HG22	1:A:204:THR:O	2.19	0.42
1:A:72:ASP:HB3	1:A:304:TYR:CE1	2.54	0.42
1:A:168:ALA:O	1:A:172:ALA:HB2	2.19	0.42
1:A:242:ARG:NE	1:A:244:GLU:OE2	2.53	0.42
1:A:248:VAL:CG2	1:A:283:GLU:HB3	2.49	0.42
1:A:112:THR:HG21	1:A:247:PHE:CZ	2.54	0.42
1:A:98:ARG:CA	1:A:98:ARG:HE	2.31	0.42
1:A:133:LEU:O	1:A:137:VAL:HG23	2.20	0.42
1:B:138:ALA:O	1:B:146:ARG:NH1	2.48	0.42
1:B:157:ARG:HD3	1:B:196:ARG:O	2.20	0.42
1:A:304:TYR:CZ	1:A:308:LEU:HD11	2.55	0.42
1:A:215:GLU:HG3	2:A:363:HOH:O	2.19	0.42
1:A:158:TYR:OH	1:B:130:LYS:NZ	2.52	0.42
1:A:122:ARG:O	1:A:123:GLN:C	2.58	0.42
1:A:191:ARG:HD2	1:B:138:ALA:HB1	2.02	0.42
1:A:307:MET:O	1:A:311:LEU:HG	2.19	0.42
1:A:250:VAL:HG11	1:A:268:ILE:HD11	2.00	0.42
1:A:218:LYS:HA	1:A:221:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:ARG:NH2	1:B:156:TYR:CB	2.82	0.42
1:B:216:ILE:CG2	1:B:217:LEU:N	2.82	0.42
1:A:72:ASP:HB3	1:A:304:TYR:CD1	2.55	0.42
1:B:91:LEU:O	1:B:94:GLU:HG2	2.19	0.42
1:B:251:LEU:O	1:B:255:ILE:HG13	2.20	0.42
1:A:33:LEU:C	1:A:33:LEU:HD23	2.40	0.42
1:B:178:LYS:O	1:B:180:LYS:N	2.52	0.42
1:B:131:LYS:HZ1	1:B:135:GLU:CD	2.23	0.42
1:B:302:GLY:O	1:B:306:LYS:HG3	2.19	0.42
1:B:294:LYS:HA	1:B:297:THR:HG22	2.02	0.42
1:A:3:THR:HG22	1:A:278:LYS:HA	2.02	0.42
1:B:196:ARG:HD3	1:B:200:GLN:HG2	2.02	0.42
1:A:126:HIS:HE1	1:A:132:SER:HB3	1.85	0.42
1:B:16:ASP:OD1	1:B:37:ILE:HD13	2.20	0.42
1:A:7:SER:O	1:A:9:SER:N	2.53	0.42
1:B:245:LEU:O	1:B:248:VAL:N	2.52	0.42
1:A:46:ARG:O	1:A:50:ARG:HG3	2.20	0.42
1:B:272:ARG:HH21	1:B:276:ASP:CG	2.23	0.42
1:B:182:LYS:HA	1:B:184:TYR:CE1	2.54	0.42
1:B:198:LYS:NZ	2:B:335:HOH:O	2.53	0.42
1:A:264:ALA:O	1:A:268:ILE:HG12	2.19	0.42
1:A:244:GLU:OE1	1:A:245:LEU:N	2.51	0.42
1:B:131:LYS:HB3	1:B:135:GLU:CD	2.40	0.42
2:A:362:HOH:O	1:B:126:HIS:CD2	2.72	0.42
1:B:13:PRO:HB2	1:B:52:ALA:HB2	2.02	0.42
1:B:304:TYR:CZ	1:B:308:LEU:HD11	2.54	0.42
1:A:119:LEU:O	1:A:119:LEU:HG	2.19	0.42
1:B:255:ILE:HG22	1:B:255:ILE:O	2.19	0.42
1:A:35:ILE:HG13	1:A:73:PHE:CE1	2.54	0.42
1:B:301:ARG:HG2	1:B:301:ARG:O	2.20	0.42
1:B:38:LEU:O	1:B:46:ARG:HD3	2.20	0.42
1:A:215:GLU:OE1	1:A:218:LYS:HG3	2.20	0.42
1:B:13:PRO:HB3	2:B:359:HOH:O	2.19	0.42
1:B:285:GLN:HG3	1:B:289:SER:O	2.20	0.42
1:B:298:LYS:HB3	1:B:298:LYS:HE2	1.84	0.42
1:B:294:LYS:HB3	1:B:294:LYS:HE2	1.90	0.42
1:B:281:GLY:O	1:B:285:GLN:N	2.49	0.42
1:B:287:ARG:O	1:B:287:ARG:HG3	2.19	0.42
1:A:188:ASP:O	1:A:192:ILE:HG13	2.20	0.42
1:A:148:LEU:HD23	1:A:148:LEU:C	2.40	0.42
1:B:150:VAL:O	1:B:154:THR:HG23	2.19	0.42
1:A:200:GLN:OE1	2:A:327:HOH:O	2.21	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:196:ARG:HB2	1:B:201:ILE:HG13	2.02	0.42
1:A:65:LEU:HD13	1:A:77:ILE:HB	2.01	0.42
1:A:132:SER:O	1:A:133:LEU:C	2.58	0.42
1:A:255:ILE:HD13	1:A:295:ALA:CB	2.49	0.41
1:A:313:GLY:O	1:A:315:ASP:N	2.53	0.41
1:B:304:TYR:O	1:B:307:MET:HB3	2.19	0.41
1:B:46:ARG:O	1:B:49:ILE:HB	2.20	0.41
1:A:220:LEU:HB3	1:A:230:LEU:HD11	2.02	0.41
1:B:131:LYS:NZ	1:B:135:GLU:OE1	2.50	0.41
1:A:167:LEU:O	1:A:171:GLU:HB2	2.19	0.41
1:A:79:LEU:O	1:A:87:ARG:HG3	2.20	0.41
1:B:252:ARG:O	1:B:256:ASN:HB2	2.20	0.41
1:B:71:ASN:HD22	1:B:74:GLU:CG	2.28	0.41
1:A:86:GLU:HG3	1:A:128:ARG:HD2	2.01	0.41
1:A:19:GLN:HG2	2:A:394:HOH:O	2.19	0.41
1:B:125:TYR:HD1	1:B:131:LYS:O	2.03	0.41
1:B:72:ASP:CG	1:B:72:ASP:O	2.57	0.41
1:B:132:SER:O	1:B:135:GLU:HG2	2.19	0.41
1:B:143:GLY:O	1:B:147:LYS:HG3	2.19	0.41
1:B:215:GLU:OE1	1:B:218:LYS:HG3	2.20	0.41
1:A:62:LEU:O	1:A:64:THR:N	2.52	0.41
1:B:247:PHE:HD1	1:B:268:ILE:HD12	1.85	0.41
1:B:35:ILE:HG23	1:B:307:MET:HA	2.01	0.41
1:A:213:GLY:O	1:A:214:GLU:HB3	2.20	0.41
1:B:186:ASP:O	1:B:187:GLU:C	2.58	0.41
1:A:301:ARG:HD2	2:A:371:HOH:O	2.20	0.41
1:A:87:ARG:CD	1:A:271:THR:HG22	2.50	0.41
1:B:87:ARG:NH1	2:B:322:HOH:O	2.28	0.41
1:A:252:ARG:HH21	1:A:287:ARG:HG3	1.84	0.41
1:A:135:GLU:HB2	1:B:196:ARG:HD3	2.02	0.41
1:A:115:SER:O	1:A:118:LEU:HB3	2.20	0.41
1:B:277:LEU:O	1:B:281:GLY:N	2.46	0.41
1:B:4:LEU:HD22	1:B:274:GLU:HG2	2.02	0.41
1:A:103:ASN:HA	2:A:442:HOH:O	2.21	0.41
1:B:108:GLU:OE1	1:B:267:ARG:NH1	2.53	0.41
1:A:171:GLU:O	1:A:175:VAL:HG23	2.20	0.41
1:A:107:MET:HE3	1:A:239:CYS:HB2	2.02	0.41
1:A:1:SER:HA	1:A:278:LYS:HB3	2.02	0.41
1:A:126:HIS:HA	1:A:131:LYS:O	2.20	0.41
1:A:205:PHE:HA	1:A:208:TYR:HB3	2.02	0.41
1:A:3:THR:HG23	1:A:278:LYS:N	2.35	0.41
1:B:87:ARG:CD	1:B:271:THR:HG22	2.47	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:ILE:O	1:A:53:TYR:N	2.52	0.41
1:B:133:LEU:HD12	1:B:137:VAL:HG23	2.01	0.41
1:B:251:LEU:O	1:B:254:ALA:HB3	2.20	0.41
1:A:192:ILE:HG23	1:A:196:ARG:HG3	2.02	0.41
1:B:107:MET:O	1:B:110:ALA:N	2.52	0.41
1:A:112:THR:HB	1:A:272:ARG:HH22	1.86	0.41
1:B:287:ARG:HG3	1:B:287:ARG:O	2.20	0.41
1:A:65:LEU:O	1:A:78:LEU:HD13	2.21	0.41
1:B:176:HIS:O	1:B:180:LYS:HG2	2.20	0.41
1:B:93:ASN:O	1:B:97:LYS:HG2	2.20	0.41
1:A:309:VAL:HB	1:A:314:GLU:O	2.20	0.41
1:A:3:THR:HG23	1:A:277:LEU:HB3	2.01	0.41
1:B:192:ILE:C	1:B:201:ILE:HD11	2.41	0.41
1:B:104:GLN:C	1:B:106:LEU:N	2.73	0.41
1:A:242:ARG:HB3	1:A:244:GLU:OE1	2.20	0.41
1:B:38:LEU:C	1:B:40:HIS:H	2.23	0.41
1:B:242:ARG:HD3	1:B:245:LEU:HD12	2.01	0.41
1:B:255:ILE:HG12	1:B:265:LEU:HD22	2.02	0.41
1:B:97:LYS:CA	1:B:97:LYS:HE2	2.46	0.41
1:B:35:ILE:HG23	1:B:307:MET:HA	2.03	0.41
1:B:167:LEU:HD21	1:B:196:ARG:CZ	2.50	0.41
1:B:202:ASN:O	1:B:206:ASN:N	2.54	0.41
1:A:96:THR:HB	1:A:140:HIS:CD2	2.56	0.41
1:A:70:SER:HB2	1:A:74:GLU:OE1	2.19	0.41
1:B:31:GLU:N	1:B:31:GLU:OE1	2.53	0.41
1:A:198:LYS:HG2	2:A:331:HOH:O	2.19	0.41
1:B:264:ALA:HA	1:B:267:ARG:NH1	2.35	0.41
1:B:131:LYS:HB3	1:B:132:SER:H	1.69	0.41
1:A:274:GLU:HB2	2:A:322:HOH:O	2.19	0.41
1:A:292:LEU:O	1:A:296:ILE:HG13	2.21	0.41
1:A:67:LYS:HE2	1:A:69:LEU:HG	2.01	0.41
1:B:61:LEU:HD23	1:B:62:LEU:CD2	2.49	0.41
1:A:157:ARG:NH2	1:A:240:LEU:HD21	2.35	0.41
1:A:71:ASN:HB3	1:A:74:GLU:OE1	2.20	0.41
1:B:149:LEU:O	1:B:153:VAL:HG22	2.20	0.41
1:A:226:ASP:HB3	1:A:228:LYS:HZ1	1.84	0.41
1:B:223:GLY:HA3	1:B:230:LEU:HD21	2.03	0.41
1:B:22:THR:O	1:B:22:THR:HG22	2.21	0.41
1:B:49:ILE:O	1:B:52:ALA:HB3	2.21	0.41
1:A:255:ILE:O	1:A:257:LYS:HD3	2.21	0.41
1:A:118:LEU:O	1:A:119:LEU:C	2.58	0.41
1:A:132:SER:HG	1:A:135:GLU:HB3	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:ARG:CZ	2:A:398:HOH:O	2.68	0.41
1:A:303:ASP:HA	1:A:306:LYS:HB2	2.01	0.41
1:A:305:GLU:O	1:A:309:VAL:HG22	2.20	0.41
1:B:277:LEU:O	1:B:280:ILE:HB	2.20	0.41
1:A:42:SER:C	1:A:46:ARG:NH1	2.74	0.41
1:B:248:VAL:HG22	1:B:284:TYR:HB2	2.02	0.41
1:B:230:LEU:HG	1:B:234:ARG:CD	2.51	0.41
1:A:138:ALA:O	1:A:139:HIS:HB2	2.20	0.41
1:B:244:GLU:OE1	1:B:244:GLU:N	2.38	0.41
1:A:298:LYS:HE2	1:A:298:LYS:HB3	1.79	0.41
1:A:43:ALA:C	1:A:45:GLN:H	2.23	0.41
1:B:76:ALA:HA	1:B:266:THR:HG21	2.02	0.41
1:B:205:PHE:CE1	1:B:216:ILE:HG12	2.56	0.41
1:B:12:ALA:O	1:B:15:ASP:HB2	2.20	0.41
1:B:179:ILE:HD12	1:B:184:TYR:CD1	2.55	0.41
1:A:193:LEU:HA	1:A:201:ILE:HD13	2.02	0.41
1:A:293:GLU:HG2	1:A:294:LYS:N	2.35	0.41
1:A:186:ASP:O	1:A:189:VAL:HB	2.20	0.41
1:A:297:THR:HB	1:A:301:ARG:CD	2.50	0.41
1:B:104:GLN:NE2	1:B:235:SER:OG	2.54	0.41
1:B:145:PHE:HZ	1:B:228:LYS:HB2	1.84	0.41
1:A:107:MET:HB3	1:A:107:MET:HE2	1.89	0.41
1:A:72:ASP:HB3	1:A:304:TYR:CE1	2.55	0.41
1:A:69:LEU:H	1:A:69:LEU:CD1	2.34	0.41
1:A:286:ARG:CB	1:A:286:ARG:HH11	2.34	0.41
1:B:209:GLN:O	1:B:213:GLY:N	2.52	0.41
1:A:1:SER:HB2	1:A:275:ILE:O	2.21	0.41
1:A:220:LEU:C	1:A:234:ARG:HH21	2.22	0.41
1:B:196:ARG:NH1	1:B:196:ARG:HG2	2.33	0.41
1:A:256:ASN:O	1:A:257:LYS:HG2	2.20	0.41
1:B:232:LEU:C	1:B:232:LEU:HD23	2.41	0.41
1:B:54:HIS:O	1:B:58:GLY:N	2.54	0.41
1:A:215:GLU:HG2	1:A:216:ILE:N	2.36	0.41
1:B:238:GLN:HG3	1:B:238:GLN:O	2.20	0.41
1:A:135:GLU:CG	1:B:196:ARG:HH11	2.34	0.41
1:A:79:LEU:O	1:A:87:ARG:NE	2.53	0.41
1:B:273:ALA:HA	1:B:277:LEU:CD2	2.50	0.41
1:A:154:THR:O	1:B:122:ARG:NH2	2.54	0.41
1:B:220:LEU:HD22	1:B:230:LEU:CD1	2.50	0.41
1:A:179:ILE:HD13	2:A:405:HOH:O	2.21	0.41
2:A:323:HOH:O	1:B:132:SER:HB3	2.21	0.41
1:A:1:SER:C	1:A:278:LYS:HB3	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:VAL:HG22	1:A:267:ARG:HH21	1.85	0.41
1:B:36:SER:HA	1:B:40:HIS:ND1	2.36	0.41
1:A:148:LEU:HD23	1:A:232:LEU:HD23	2.03	0.41
1:A:69:LEU:N	1:A:69:LEU:HD12	2.36	0.41
1:A:126:HIS:HA	1:A:131:LYS:O	2.20	0.41
1:B:287:ARG:HG3	1:B:287:ARG:O	2.21	0.41
1:B:88:ASP:O	1:B:91:LEU:N	2.53	0.41
1:A:303:ASP:HA	1:A:306:LYS:HD3	2.02	0.41
1:A:277:LEU:O	1:A:281:GLY:N	2.53	0.41
1:A:135:GLU:HB3	1:B:195:THR:HB	2.03	0.41
1:A:268:ILE:O	1:A:268:ILE:HG22	2.21	0.41
1:B:65:LEU:HD13	1:B:77:ILE:CG2	2.51	0.41
1:B:290:ILE:HD11	1:B:294:LYS:O	2.21	0.41
1:A:128:ARG:HD3	1:A:129:TYR:CE2	2.56	0.41
1:A:298:LYS:HD2	2:A:409:HOH:O	2.21	0.41
1:A:105:VAL:CG2	1:A:267:ARG:NH2	2.84	0.41
1:A:161:ASP:O	1:A:163:VAL:HG23	2.20	0.41
1:A:35:ILE:HD12	1:A:307:MET:HA	2.03	0.41
1:B:44:GLU:N	1:B:44:GLU:CD	2.73	0.41
1:A:256:ASN:O	1:A:257:LYS:HB2	2.21	0.41
1:B:267:ARG:CG	1:B:267:ARG:HH11	2.28	0.41
1:A:122:ARG:HH21	1:B:156:TYR:CB	2.33	0.41
1:A:248:VAL:CG2	1:A:283:GLU:HB3	2.44	0.41
1:B:143:GLY:C	1:B:145:PHE:N	2.73	0.41
1:A:65:LEU:O	1:A:78:LEU:HD13	2.21	0.41
1:A:185:ASN:ND2	1:A:185:ASN:C	2.75	0.41
1:A:128:ARG:HG2	1:A:129:TYR:CE1	2.56	0.41
1:B:212:HIS:O	1:B:213:GLY:C	2.60	0.41
1:A:97:LYS:O	1:A:98:ARG:HG2	2.21	0.41
1:B:145:PHE:O	1:B:149:LEU:HG	2.21	0.41
1:B:71:ASN:HB3	1:B:74:GLU:OE1	2.21	0.41
1:B:116:THR:O	1:B:117:GLN:C	2.59	0.41
1:B:197:SER:O	1:B:198:LYS:C	2.58	0.41
1:B:293:GLU:HB2	1:B:317:ALA:CB	2.51	0.41
1:A:145:PHE:O	1:A:149:LEU:HG	2.21	0.41
1:A:233:LEU:O	1:A:237:ILE:HG13	2.20	0.41
1:B:216:ILE:O	1:B:220:LEU:HG	2.21	0.41
1:A:107:MET:HE1	1:A:108:GLU:HA	2.03	0.41
1:B:293:GLU:N	1:B:293:GLU:OE1	2.53	0.41
1:B:170:GLN:O	1:B:174:LEU:HB2	2.20	0.41
1:A:275:ILE:HD12	2:A:333:HOH:O	2.21	0.41
1:A:175:VAL:HG12	1:A:179:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:ARG:HD3	1:A:129:TYR:CZ	2.56	0.41
1:A:88:ASP:O	1:A:92:ALA:HB2	2.21	0.41
1:A:130:LYS:HB3	1:B:158:TYR:OH	2.21	0.41
1:B:180:LYS:HD3	1:B:180:LYS:C	2.42	0.41
1:B:82:LEU:HD22	1:B:87:ARG:CA	2.51	0.41
1:B:215:GLU:O	1:B:219:SER:N	2.51	0.41
1:A:161:ASP:CA	1:A:199:ALA:HB2	2.50	0.41
1:B:254:ALA:HB2	2:B:367:HOH:O	2.20	0.41
1:B:271:THR:O	1:B:272:ARG:HD2	2.20	0.41
1:A:78:LEU:O	1:A:79:LEU:C	2.58	0.41
1:B:62:LEU:HD23	1:B:65:LEU:HD12	2.03	0.41
1:B:151:SER:HB3	1:B:194:SER:HB2	2.03	0.41
1:B:252:ARG:CA	1:B:284:TYR:HE1	2.34	0.41
1:A:98:ARG:CA	1:A:98:ARG:NE	2.83	0.41
1:B:71:ASN:HB3	1:B:74:GLU:OE1	2.20	0.41
1:A:107:MET:HB2	1:A:149:LEU:HD21	2.03	0.41
1:A:7:SER:C	1:A:9:SER:H	2.24	0.41
1:B:65:LEU:HD22	1:B:74:GLU:CG	2.51	0.41
1:A:186:ASP:O	1:A:187:GLU:C	2.59	0.41
1:A:298:LYS:HB3	1:A:298:LYS:HE2	1.84	0.41
1:B:175:VAL:O	1:B:179:ILE:HG13	2.21	0.41
1:A:164:ASN:O	1:A:167:LEU:HB2	2.21	0.41
1:A:256:ASN:C	1:A:257:LYS:HG2	2.41	0.41
1:B:137:VAL:HG13	1:B:141:THR:HG21	2.03	0.41
1:A:166:THR:O	1:A:170:GLN:HG3	2.20	0.41
1:B:121:ALA:O	1:B:122:ARG:C	2.59	0.41
1:A:185:ASN:ND2	1:A:185:ASN:C	2.74	0.41
1:B:287:ARG:O	1:B:287:ARG:HG3	2.21	0.41
1:B:241:THR:HG22	1:B:242:ARG:HG3	2.03	0.41
1:A:288:ASN:O	1:A:289:SER:CB	2.69	0.41
1:B:40:HIS:O	1:B:41:ARG:HG2	2.21	0.41
1:A:35:ILE:HD11	1:A:307:MET:HB2	2.02	0.41
1:A:125:TYR:O	1:A:128:ARG:N	2.50	0.41
1:A:161:ASP:O	1:A:162:GLU:C	2.59	0.40
1:B:3:THR:OG1	1:B:278:LYS:N	2.54	0.40
1:B:132:SER:H	1:B:135:GLU:HG2	1.87	0.40
1:B:173:LYS:C	1:B:175:VAL:N	2.74	0.40
1:A:186:ASP:O	1:A:189:VAL:HB	2.21	0.40
1:A:3:THR:OG1	1:A:312:LEU:HA	2.21	0.40
1:A:126:HIS:NE2	1:B:156:TYR:CD2	2.89	0.40
1:B:286:ARG:NH1	1:B:286:ARG:HG2	2.36	0.40
1:A:255:ILE:C	1:A:257:LYS:N	2.74	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:281:GLY:O	1:B:283:GLU:N	2.51	0.40
1:A:67:LYS:CD	1:A:70:SER:HB3	2.51	0.40
1:B:137:VAL:O	1:B:141:THR:HG23	2.20	0.40
1:A:217:LEU:HD11	1:A:238:GLN:HG2	2.02	0.40
1:A:20:LEU:O	1:A:21:ARG:C	2.60	0.40
1:A:132:SER:O	1:A:135:GLU:HG2	2.22	0.40
1:B:252:ARG:NE	1:B:288:ASN:OD1	2.53	0.40
1:A:167:LEU:HD21	1:A:196:ARG:CZ	2.52	0.40
1:B:73:PHE:HD1	1:B:304:TYR:HA	1.87	0.40
1:A:207:ARG:NE	2:A:398:HOH:O	2.53	0.40
1:B:184:TYR:C	1:B:186:ASP:H	2.25	0.40
1:B:164:ASN:HB3	1:B:167:LEU:HB3	2.03	0.40
1:A:179:ILE:HD12	1:A:220:LEU:CD2	2.44	0.40
1:A:4:LEU:HD13	1:A:80:TRP:CH2	2.57	0.40
1:B:60:ASP:HB3	2:B:347:HOH:O	2.21	0.40
1:B:3:THR:HB	1:B:312:LEU:C	2.42	0.40
1:A:234:ARG:NE	2:A:432:HOH:O	2.52	0.40
1:A:251:LEU:HD22	1:A:284:TYR:CD1	2.57	0.40
1:A:165:MET:HG3	2:A:396:HOH:O	2.21	0.40
1:B:150:VAL:HA	1:B:153:VAL:HG22	2.04	0.40
1:A:220:LEU:C	1:A:222:GLU:N	2.75	0.40
1:B:123:GLN:C	1:B:125:TYR:N	2.75	0.40
1:A:217:LEU:O	1:A:221:GLU:HG3	2.21	0.40
1:A:209:GLN:HA	1:A:214:GLU:O	2.21	0.40
1:B:10:VAL:HG13	1:B:11:PRO:HD2	2.04	0.40
1:A:67:LYS:O	1:A:67:LYS:HG2	2.20	0.40
1:A:147:LYS:HD3	2:A:473:HOH:O	2.20	0.40
1:A:264:ALA:C	1:A:266:THR:N	2.74	0.40
1:A:193:LEU:HD11	1:A:233:LEU:HD12	2.03	0.40
1:A:108:GLU:HB2	1:A:246:TYR:OH	2.22	0.40
1:B:255:ILE:O	1:B:257:LYS:N	2.54	0.40
1:A:230:LEU:O	1:A:234:ARG:HG3	2.21	0.40
1:B:114:THR:H	1:B:117:GLN:NE2	2.19	0.40
1:B:302:GLY:N	1:B:305:GLU:OE1	2.54	0.40
1:A:277:LEU:HA	1:A:280:ILE:HD12	2.03	0.40
1:B:170:GLN:O	1:B:174:LEU:HB2	2.21	0.40
1:A:109:VAL:O	1:A:113:ARG:HD3	2.21	0.40
1:A:133:LEU:CD2	1:A:153:VAL:HB	2.51	0.40
1:A:292:LEU:HG	1:A:296:ILE:HD11	2.04	0.40
1:B:165:MET:HE3	1:B:207:ARG:HD3	2.03	0.40
1:B:84:PRO:HG2	2:B:406:HOH:O	2.21	0.40
1:A:193:LEU:HD11	1:A:233:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:242:ARG:CB	1:B:245:LEU:HD12	2.51	0.40
1:A:220:LEU:HB3	1:A:230:LEU:HD11	2.02	0.40
1:A:91:LEU:C	1:A:93:ASN:H	2.25	0.40
1:B:292:LEU:CD2	1:B:312:LEU:HD22	2.51	0.40
1:B:3:THR:HG23	1:B:278:LYS:N	2.36	0.40
1:A:132:SER:O	1:A:134:GLU:N	2.54	0.40
1:A:185:ASN:C	1:A:185:ASN:ND2	2.74	0.40
1:B:290:ILE:O	1:B:290:ILE:HG23	2.22	0.40
1:A:179:ILE:HD13	2:A:407:HOH:O	2.21	0.40
1:A:191:ARG:HH12	1:A:196:ARG:HH21	1.70	0.40
1:B:75:ARG:NH1	1:B:78:LEU:HD23	2.36	0.40
1:A:215:GLU:HA	2:A:360:HOH:O	2.21	0.40
1:A:193:LEU:CD1	1:A:233:LEU:HD12	2.52	0.40
1:B:197:SER:HB2	2:B:328:HOH:O	2.21	0.40
1:B:82:LEU:HD22	1:B:86:GLU:OE2	2.21	0.40
1:B:176:HIS:C	1:B:178:LYS:H	2.24	0.40
1:A:19:GLN:HA	2:A:453:HOH:O	2.21	0.40
1:A:158:TYR:C	1:A:160:GLY:N	2.75	0.40
1:A:193:LEU:HA	1:A:201:ILE:CD1	2.52	0.40
1:B:175:VAL:HG22	1:B:189:VAL:HG22	2.02	0.40
1:B:4:LEU:HG	1:B:6:VAL:HG23	2.03	0.40
1:B:73:PHE:C	1:B:75:ARG:N	2.74	0.40
1:A:188:ASP:HA	1:A:191:ARG:HB3	2.02	0.40
1:A:44:GLU:O	1:A:44:GLU:OE1	2.39	0.40
1:A:105:VAL:O	1:A:105:VAL:HG12	2.21	0.40
1:A:293:GLU:HG2	1:A:294:LYS:N	2.37	0.40
1:A:261:ASP:O	1:A:262:GLU:O	2.40	0.40
1:B:252:ARG:HH22	1:B:287:ARG:CZ	2.34	0.40
1:A:132:SER:O	1:A:135:GLU:HG2	2.21	0.40
1:A:298:LYS:HB3	1:A:298:LYS:HE2	1.81	0.40
1:A:296:ILE:HG21	1:A:308:LEU:HD12	2.04	0.40
1:B:298:LYS:HB3	1:B:298:LYS:HE2	1.83	0.40
1:A:293:GLU:HG2	1:A:294:LYS:HD3	2.03	0.40
1:A:106:LEU:HD22	1:A:133:LEU:HD11	2.02	0.40
1:A:97:LYS:C	1:A:98:ARG:HG2	2.42	0.40
1:A:16:ASP:O	1:A:20:LEU:HG	2.22	0.40
1:B:39:ALA:HA	1:B:311:LEU:HD21	2.04	0.40
1:A:148:LEU:HD21	1:A:236:THR:OG1	2.22	0.40
1:B:294:LYS:HA	1:B:297:THR:HG22	2.03	0.40
1:A:31:GLU:HG2	1:A:303:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	308/317 (97%)	268 (87%)	35 (11%)	5 (2%)	14	23
1	1-B	301/317 (95%)	249 (83%)	42 (14%)	10 (3%)	6	7
1	2-A	308/317 (97%)	266 (86%)	38 (12%)	4 (1%)	18	29
1	2-B	301/317 (95%)	248 (82%)	46 (15%)	7 (2%)	10	14
1	3-A	308/317 (97%)	267 (87%)	32 (10%)	9 (3%)	7	9
1	3-B	301/317 (95%)	241 (80%)	48 (16%)	12 (4%)	5	5
1	4-A	308/317 (97%)	254 (82%)	40 (13%)	14 (4%)	4	4
1	4-B	301/317 (95%)	258 (86%)	40 (13%)	3 (1%)	22	38
1	5-A	308/317 (97%)	262 (85%)	40 (13%)	6 (2%)	12	19
1	5-B	301/317 (95%)	253 (84%)	38 (13%)	10 (3%)	6	7
1	6-A	308/317 (97%)	271 (88%)	30 (10%)	7 (2%)	10	14
1	6-B	301/317 (95%)	266 (88%)	29 (10%)	6 (2%)	11	17
1	7-A	308/317 (97%)	256 (83%)	46 (15%)	6 (2%)	12	19
1	7-B	301/317 (95%)	257 (85%)	39 (13%)	5 (2%)	14	22
1	8-A	308/317 (97%)	263 (85%)	36 (12%)	9 (3%)	7	9
1	8-B	301/317 (95%)	249 (83%)	39 (13%)	13 (4%)	4	4
All	All	4872/5072 (96%)	4128 (85%)	618 (13%)	126 (3%)	8	11

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	298	LYS
1	1-B	88	ASP
1	1-B	108	GLU
1	2-A	13	PRO
1	2-B	97	LYS
1	2-B	187	GLU
1	3-A	79	LEU
1	3-A	157	ARG

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Mol	Chain	Res	Type
1	4-A	37	ILE
1	4-A	262	GLU
1	6-A	298	LYS
1	7-A	130	LYS
1	7-B	298	LYS
1	8-B	186	ASP
1	1-A	59	GLU
1	1-A	68	GLU
1	1-B	198	LYS
1	2-B	55	GLU
1	2-B	157	ARG
1	2-B	213	GLY
1	3-A	24	PHE
1	3-A	78	LEU
1	3-A	81	THR
1	3-B	143	GLY
1	3-B	160	GLY
1	3-B	261	ASP
1	4-A	24	PHE
1	4-A	298	LYS
1	4-B	161	ASP
1	5-A	209	GLN
1	5-B	143	GLY
1	5-B	260	THR
1	6-A	130	LYS
1	6-A	162	GLU
1	6-A	214	GLU
1	6-B	185	ASN
1	6-B	213	GLY
1	6-B	214	GLU
1	7-A	42	SER
1	7-A	159	GLU
1	7-A	162	GLU
1	8-A	139	HIS
1	8-A	289	SER
1	8-B	56	THR
1	8-B	134	GLU
1	8-B	135	GLU
1	8-B	299	ASP
1	1-B	243	PRO
1	1-B	257	LYS
1	2-B	214	GLU

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Mol	Chain	Res	Type
1	3-A	101	SER
1	3-A	197	SER
1	4-A	42	SER
1	4-A	160	GLY
1	5-A	286	ARG
1	5-B	9	SER
1	5-B	139	HIS
1	5-B	197	SER
1	5-B	199	ALA
1	6-A	213	GLY
1	7-A	24	PHE
1	7-B	8	ASP
1	7-B	299	ASP
1	8-A	143	GLY
1	8-A	257	LYS
1	8-A	277	LEU
1	8-B	131	LYS
1	8-B	282	GLU
1	8-B	298	LYS
1	8-B	301	ARG
1	1-A	193	LEU
1	1-A	253	SER
1	1-B	99	TRP
1	2-A	32	ASP
1	2-B	91	LEU
1	3-A	80	TRP
1	3-B	72	ASP
1	3-B	185	ASN
1	3-B	257	LYS
1	4-A	187	GLU
1	4-A	189	VAL
1	4-A	213	GLY
1	5-A	81	THR
1	5-A	257	LYS
1	5-A	262	GLU
1	5-B	157	ARG
1	5-B	245	LEU
1	5-B	256	ASN
1	6-A	8	ASP
1	7-B	157	ARG
1	8-A	160	GLY
1	8-A	276	ASP

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Mol	Chain	Res	Type
1	8-B	217	LEU
1	1-B	39	ALA
1	1-B	244	GLU
1	2-A	221	GLU
1	3-A	42	SER
1	3-B	105	VAL
1	3-B	126	HIS
1	3-B	301	ARG
1	4-A	133	LEU
1	4-A	143	GLY
1	4-A	214	GLU
1	4-A	216	ILE
1	4-B	221	GLU
1	7-A	160	GLY
1	7-B	185	ASN
1	8-B	149	LEU
1	8-B	150	VAL
1	1-B	4	LEU
1	5-A	315	ASP
1	6-A	143	GLY
1	6-B	79	LEU
1	6-B	191	ARG
1	8-B	112	THR
1	3-B	223	GLY
1	8-A	275	ILE
1	6-B	84	PRO
1	1-B	275	ILE
1	2-A	11	PRO
1	3-B	13	PRO
1	4-A	243	PRO
1	8-A	13	PRO
1	3-B	275	ILE
1	4-B	37	ILE
1	5-B	37	ILE

### 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	274/277 (99%)	265 (97%)	9 (3%)	50	76
1	1-B	269/277 (97%)	264 (98%)	5 (2%)	69	90
1	2-A	274/277 (99%)	267 (97%)	7 (3%)	59	84
1	2-B	269/277 (97%)	265 (98%)	4 (2%)	76	93
1	3-A	274/277 (99%)	264 (96%)	10 (4%)	47	73
1	3-B	269/277 (97%)	265 (98%)	4 (2%)	76	93
1	4-A	274/277 (99%)	263 (96%)	11 (4%)	42	68
1	4-B	269/277 (97%)	261 (97%)	8 (3%)	53	80
1	5-A	274/277 (99%)	264 (96%)	10 (4%)	47	73
1	5-B	269/277 (97%)	266 (99%)	3 (1%)	84	96
1	6-A	274/277 (99%)	264 (96%)	10 (4%)	47	73
1	6-B	269/277 (97%)	263 (98%)	6 (2%)	64	88
1	7-A	274/277 (99%)	269 (98%)	5 (2%)	71	91
1	7-B	269/277 (97%)	267 (99%)	2 (1%)	91	98
1	8-A	274/277 (99%)	266 (97%)	8 (3%)	55	81
1	8-B	269/277 (97%)	259 (96%)	10 (4%)	45	72
All	All	4344/4432 (98%)	4232 (97%)	112 (3%)	59	84

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	71	ASN
1	1-A	185	ASN
1	1-A	244	GLU
1	1-A	246	TYR
1	1-A	249	ASP
1	1-A	267	ARG
1	1-A	285	GLN
1	1-A	293	GLU
1	1-A	301	ARG
1	1-B	31	GLU
1	1-B	72	ASP
1	1-B	107	MET
1	1-B	197	SER
1	1-B	257	LYS
1	2-A	67	LYS
1	2-A	88	ASP

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Mol	Chain	Res	Type
1	2-A	102	SER
1	2-A	185	ASN
1	2-A	267	ARG
1	2-A	285	GLN
1	2-A	286	ARG
1	2-B	53	TYR
1	2-B	72	ASP
1	2-B	134	GLU
1	2-B	189	VAL
1	3-A	14	SER
1	3-A	24	PHE
1	3-A	78	LEU
1	3-A	103	ASN
1	3-A	134	GLU
1	3-A	136	ASP
1	3-A	185	ASN
1	3-A	197	SER
1	3-A	272	ARG
1	3-A	285	GLN
1	3-B	88	ASP
1	3-B	136	ASP
1	3-B	267	ARG
1	3-B	303	ASP
1	4-A	63	LYS
1	4-A	68	GLU
1	4-A	96	THR
1	4-A	98	ARG
1	4-A	107	MET
1	4-A	120	HIS
1	4-A	154	THR
1	4-A	185	ASN
1	4-A	222	GLU
1	4-A	252	ARG
1	4-A	285	GLN
1	4-B	16	ASP
1	4-B	31	GLU
1	4-B	32	ASP
1	4-B	107	MET
1	4-B	134	GLU
1	4-B	136	ASP
1	4-B	183	HIS
1	4-B	293	GLU

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Mol	Chain	Res	Type
1	5-A	69	LEU
1	5-A	83	GLU
1	5-A	120	HIS
1	5-A	134	GLU
1	5-A	136	ASP
1	5-A	185	ASN
1	5-A	200	GLN
1	5-A	210	ASP
1	5-A	211	ASP
1	5-A	285	GLN
1	5-B	72	ASP
1	5-B	162	GLU
1	5-B	261	ASP
1	6-A	16	ASP
1	6-A	69	LEU
1	6-A	78	LEU
1	6-A	93	ASN
1	6-A	107	MET
1	6-A	120	HIS
1	6-A	139	HIS
1	6-A	185	ASN
1	6-A	285	GLN
1	6-A	299	ASP
1	6-B	31	GLU
1	6-B	41	ARG
1	6-B	134	GLU
1	6-B	157	ARG
1	6-B	257	LYS
1	6-B	267	ARG
1	7-A	69	LEU
1	7-A	72	ASP
1	7-A	147	LYS
1	7-A	185	ASN
1	7-A	285	GLN
1	7-B	32	ASP
1	7-B	283	GLU
1	8-A	69	LEU
1	8-A	120	HIS
1	8-A	126	HIS
1	8-A	146	ARG
1	8-A	162	GLU
1	8-A	185	ASN

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Mol	Chain	Res	Type
1	8-A	257	LYS
1	8-A	285	GLN
1	8-B	31	GLU
1	8-B	32	ASP
1	8-B	72	ASP
1	8-B	117	GLN
1	8-B	198	LYS
1	8-B	221	GLU
1	8-B	224	ASP
1	8-B	244	GLU
1	8-B	252	ARG
1	8-B	297	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	51	GLN
1	1-A	71	ASN
1	1-A	140	HIS
1	1-A	170	GLN
1	1-A	185	ASN
1	1-A	202	ASN
1	1-A	209	GLN
1	1-A	285	GLN
1	1-B	104	GLN
1	1-B	120	HIS
1	1-B	170	GLN
1	1-B	202	ASN
1	1-B	238	GLN
1	2-A	40	HIS
1	2-A	71	ASN
1	2-A	170	GLN
1	2-A	185	ASN
1	2-A	209	GLN
1	2-A	238	GLN
1	2-A	285	GLN
1	2-A	288	ASN
1	2-B	202	ASN
1	2-B	256	ASN
1	3-A	54	HIS
1	3-A	103	ASN
1	3-A	170	GLN

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Mol	Chain	Res	Type
1	3-A	185	ASN
1	3-A	202	ASN
1	3-A	209	GLN
1	3-A	238	GLN
1	3-B	93	ASN
1	3-B	139	HIS
1	3-B	170	GLN
1	3-B	238	GLN
1	4-A	40	HIS
1	4-A	51	GLN
1	4-A	104	GLN
1	4-A	170	GLN
1	4-A	185	ASN
1	4-A	200	GLN
1	4-A	202	ASN
1	4-A	212	HIS
1	4-A	285	GLN
1	4-A	288	ASN
1	4-B	45	GLN
1	4-B	139	HIS
1	4-B	170	GLN
1	4-B	176	HIS
1	5-A	93	ASN
1	5-A	170	GLN
1	5-A	185	ASN
1	5-A	200	GLN
1	5-A	206	ASN
1	5-A	285	GLN
1	5-B	19	GLN
1	5-B	71	ASN
1	5-B	117	GLN
1	5-B	170	GLN
1	5-B	176	HIS
1	5-B	209	GLN
1	6-A	51	GLN
1	6-A	93	ASN
1	6-A	170	GLN
1	6-A	176	HIS
1	6-A	183	HIS
1	6-A	185	ASN
1	6-A	285	GLN
1	6-B	93	ASN

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Mol	Chain	Res	Type
1	6-B	176	HIS
1	6-B	212	HIS
1	7-A	71	ASN
1	7-A	120	HIS
1	7-A	170	GLN
1	7-A	176	HIS
1	7-A	185	ASN
1	7-A	209	GLN
1	7-A	212	HIS
1	7-A	238	GLN
1	7-A	285	GLN
1	7-B	202	ASN
1	8-A	104	GLN
1	8-A	140	HIS
1	8-A	170	GLN
1	8-A	183	HIS
1	8-A	185	ASN
1	8-A	206	ASN
1	8-A	285	GLN
1	8-B	19	GLN
1	8-B	51	GLN
1	8-B	104	GLN
1	8-B	170	GLN
1	8-B	202	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 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	312/317 (98%)	-0.32	4 (1%) 74 76	11, 35, 68, 92	312 (100%)
1	1-B	307/317 (96%)	-0.11	19 (6%) 20 20	11, 42, 76, 92	307 (100%)
1	2-A	312/317 (98%)	-0.32	4 (1%) 74 76	11, 35, 68, 92	312 (100%)
1	2-B	307/317 (96%)	-0.11	19 (6%) 20 20	11, 42, 76, 92	307 (100%)
1	3-A	312/317 (98%)	-0.32	4 (1%) 74 76	11, 35, 68, 92	312 (100%)
1	3-B	307/317 (96%)	-0.11	19 (6%) 20 20	11, 42, 76, 92	307 (100%)
1	4-A	312/317 (98%)	-0.32	4 (1%) 74 76	11, 35, 68, 92	312 (100%)
1	4-B	307/317 (96%)	-0.11	19 (6%) 20 20	11, 42, 76, 92	307 (100%)
1	5-A	312/317 (98%)	-0.32	4 (1%) 74 76	11, 35, 68, 92	312 (100%)
1	5-B	307/317 (96%)	-0.11	19 (6%) 20 20	11, 42, 76, 92	307 (100%)
1	6-A	312/317 (98%)	-0.32	4 (1%) 74 76	11, 35, 68, 92	312 (100%)
1	6-B	307/317 (96%)	-0.11	19 (6%) 20 20	11, 42, 76, 92	307 (100%)
1	7-A	312/317 (98%)	-0.32	4 (1%) 74 76	11, 35, 68, 92	312 (100%)
1	7-B	307/317 (96%)	-0.11	19 (6%) 20 20	11, 42, 76, 92	307 (100%)
1	8-A	312/317 (98%)	-0.32	4 (1%) 74 76	11, 35, 68, 92	312 (100%)
1	8-B	307/317 (96%)	-0.11	19 (6%) 20 20	11, 42, 76, 92	307 (100%)
All	All	4952/5072 (97%)	-0.22	184 (3%) 45 41	11, 37, 75, 92	4952 (100%)

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	222	GLU	4.9
1	2-B	222	GLU	4.9
1	3-B	222	GLU	4.9
1	4-B	222	GLU	4.9
1	5-B	222	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	6-B	222	GLU	4.9
1	7-B	222	GLU	4.9
1	8-B	222	GLU	4.9
1	1-B	64	THR	4.7
1	2-B	64	THR	4.7
1	3-B	64	THR	4.7
1	4-B	64	THR	4.7
1	5-B	64	THR	4.7
1	6-B	64	THR	4.7
1	7-B	64	THR	4.7
1	8-B	64	THR	4.7
1	1-B	9	SER	4.1
1	2-B	9	SER	4.1
1	3-B	9	SER	4.1
1	4-B	9	SER	4.1
1	5-B	9	SER	4.1
1	6-B	9	SER	4.1
1	7-B	9	SER	4.1
1	8-B	9	SER	4.1
1	1-B	258	THR	3.7
1	2-B	258	THR	3.7
1	3-B	258	THR	3.7
1	4-B	258	THR	3.7
1	5-B	258	THR	3.7
1	6-B	258	THR	3.7
1	7-B	258	THR	3.7
1	8-B	258	THR	3.7
1	1-B	316	ASP	3.2
1	2-B	316	ASP	3.2
1	3-B	316	ASP	3.2
1	4-B	316	ASP	3.2
1	5-B	316	ASP	3.2
1	6-B	316	ASP	3.2
1	7-B	316	ASP	3.2
1	8-B	316	ASP	3.2
1	1-B	221	GLU	3.1
1	2-B	221	GLU	3.1
1	3-B	221	GLU	3.1
1	4-B	221	GLU	3.1
1	5-B	221	GLU	3.1
1	6-B	221	GLU	3.1
1	7-B	221	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	8-B	221	GLU	3.1
1	1-B	12	ALA	3.0
1	2-B	12	ALA	3.0
1	3-B	12	ALA	3.0
1	4-B	12	ALA	3.0
1	5-B	12	ALA	3.0
1	6-B	12	ALA	3.0
1	7-B	12	ALA	3.0
1	8-B	12	ALA	3.0
1	1-A	290	ILE	3.0
1	2-A	290	ILE	3.0
1	3-A	290	ILE	3.0
1	4-A	290	ILE	3.0
1	5-A	290	ILE	3.0
1	6-A	290	ILE	3.0
1	7-A	290	ILE	3.0
1	8-A	290	ILE	3.0
1	1-B	10	VAL	2.9
1	2-B	10	VAL	2.9
1	3-B	10	VAL	2.9
1	4-B	10	VAL	2.9
1	5-B	10	VAL	2.9
1	6-B	10	VAL	2.9
1	7-B	10	VAL	2.9
1	8-B	10	VAL	2.9
1	1-A	259	GLY	2.8
1	2-A	259	GLY	2.8
1	3-A	259	GLY	2.8
1	4-A	259	GLY	2.8
1	5-A	259	GLY	2.8
1	6-A	259	GLY	2.8
1	7-A	259	GLY	2.8
1	8-A	259	GLY	2.8
1	1-A	98	ARG	2.8
1	2-A	98	ARG	2.8
1	3-A	98	ARG	2.8
1	4-A	98	ARG	2.8
1	5-A	98	ARG	2.8
1	6-A	98	ARG	2.8
1	7-A	98	ARG	2.8
1	8-A	98	ARG	2.8
1	1-B	52	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	2-B	52	ALA	2.7
1	3-B	52	ALA	2.7
1	4-B	52	ALA	2.7
1	5-B	52	ALA	2.7
1	6-B	52	ALA	2.7
1	7-B	52	ALA	2.7
1	8-B	52	ALA	2.7
1	1-B	257	LYS	2.7
1	2-B	257	LYS	2.7
1	3-B	257	LYS	2.7
1	4-B	257	LYS	2.7
1	5-B	257	LYS	2.7
1	6-B	257	LYS	2.7
1	7-B	257	LYS	2.7
1	8-B	257	LYS	2.7
1	1-B	314	GLU	2.6
1	2-B	314	GLU	2.6
1	3-B	314	GLU	2.6
1	4-B	314	GLU	2.6
1	5-B	314	GLU	2.6
1	6-B	314	GLU	2.6
1	7-B	314	GLU	2.6
1	8-B	314	GLU	2.6
1	1-B	289	SER	2.6
1	2-B	289	SER	2.6
1	3-B	289	SER	2.6
1	4-B	289	SER	2.6
1	5-B	289	SER	2.6
1	6-B	289	SER	2.6
1	7-B	289	SER	2.6
1	8-B	289	SER	2.6
1	1-B	256	ASN	2.5
1	2-B	256	ASN	2.5
1	3-B	256	ASN	2.5
1	4-B	256	ASN	2.5
1	5-B	256	ASN	2.5
1	6-B	256	ASN	2.5
1	7-B	256	ASN	2.5
1	8-B	256	ASN	2.5
1	1-B	290	ILE	2.2
1	2-B	290	ILE	2.2
1	3-B	290	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	4-B	290	ILE	2.2
1	5-B	290	ILE	2.2
1	6-B	290	ILE	2.2
1	7-B	290	ILE	2.2
1	8-B	290	ILE	2.2
1	1-B	14	SER	2.1
1	2-B	14	SER	2.1
1	3-B	14	SER	2.1
1	4-B	14	SER	2.1
1	5-B	14	SER	2.1
1	6-B	14	SER	2.1
1	7-B	14	SER	2.1
1	8-B	14	SER	2.1
1	1-B	65	LEU	2.1
1	2-B	65	LEU	2.1
1	3-B	65	LEU	2.1
1	4-B	65	LEU	2.1
1	5-B	65	LEU	2.1
1	6-B	65	LEU	2.1
1	7-B	65	LEU	2.1
1	8-B	65	LEU	2.1
1	1-A	260	THR	2.1
1	2-A	260	THR	2.1
1	3-A	260	THR	2.1
1	4-A	260	THR	2.1
1	5-A	260	THR	2.1
1	6-A	260	THR	2.1
1	7-A	260	THR	2.1
1	8-A	260	THR	2.1
1	1-B	224	ASP	2.1
1	2-B	224	ASP	2.1
1	3-B	224	ASP	2.1
1	4-B	224	ASP	2.1
1	5-B	224	ASP	2.1
1	6-B	224	ASP	2.1
1	7-B	224	ASP	2.1
1	8-B	224	ASP	2.1
1	1-B	317	ALA	2.1
1	2-B	317	ALA	2.1
1	3-B	317	ALA	2.1
1	4-B	317	ALA	2.1
1	5-B	317	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	6-B	317	ALA	2.1
1	7-B	317	ALA	2.1
1	8-B	317	ALA	2.1
1	1-B	56	THR	2.1
1	2-B	56	THR	2.1
1	3-B	56	THR	2.1
1	4-B	56	THR	2.1
1	5-B	56	THR	2.1
1	6-B	56	THR	2.1
1	7-B	56	THR	2.1
1	8-B	56	THR	2.1

## 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 ⓘ

There are no such residues in this entry.