



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:57 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

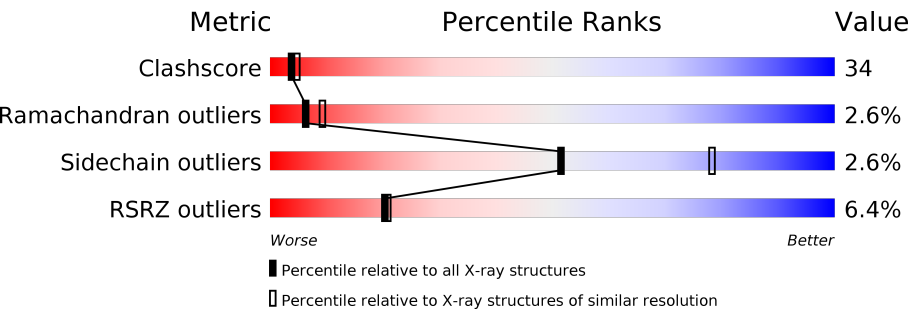
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	317	<div><div>4%</div><div>47%</div><div>48%</div><div>..</div></div>
1	1-B	317	<div><div>10%</div><div>41%</div><div>53%</div><div>..</div></div>
1	2-A	317	<div><div>4%</div><div>44%</div><div>52%</div><div>..</div></div>
1	2-B	317	<div><div>10%</div><div>49%</div><div>47%</div><div>..</div></div>
1	3-A	317	<div><div>4%</div><div>41%</div><div>53%</div><div>...</div></div>
1	3-B	317	<div><div>10%</div><div>42%</div><div>52%</div><div>..</div></div>
1	4-A	317	<div><div>4%</div><div>43%</div><div>50%</div><div>6% .</div></div>

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Mol	Chain	Length	Quality of chain
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	
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 hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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	2-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	3-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	4-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	5-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	6-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	7-A	312	Total	C	N	O	S	0	0	0
			2508	1557	442	504	5			
1	8-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-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	3-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	4-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	5-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	6-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	5			
1	7-B	307	Total	C	N	O	S	0	0	0
			2462	1526	436	495	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

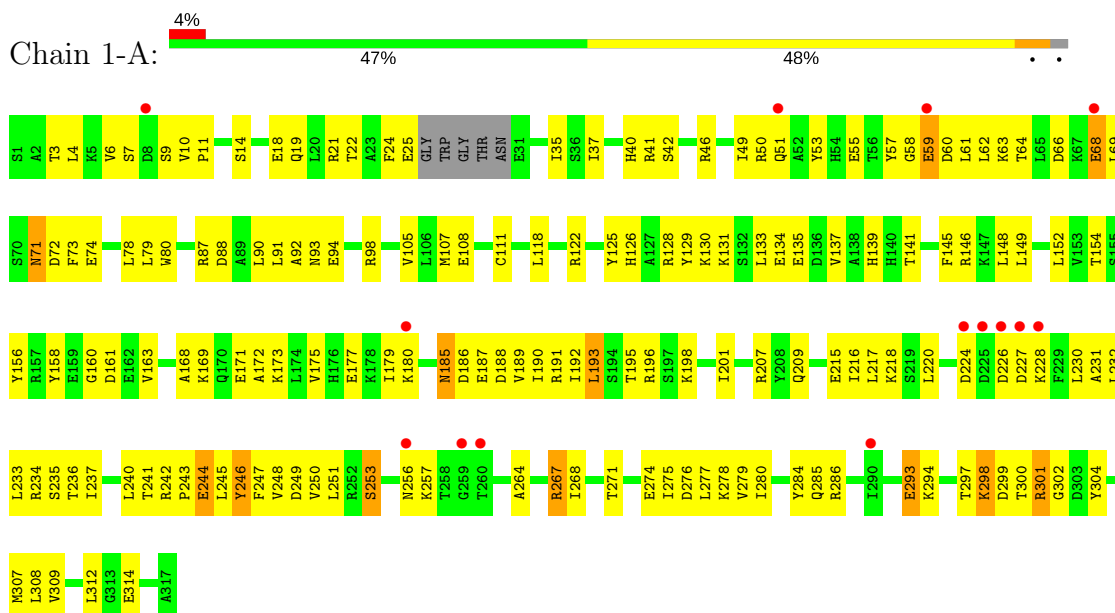
- Molecule 2 is water.

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

3 Residue-property plots

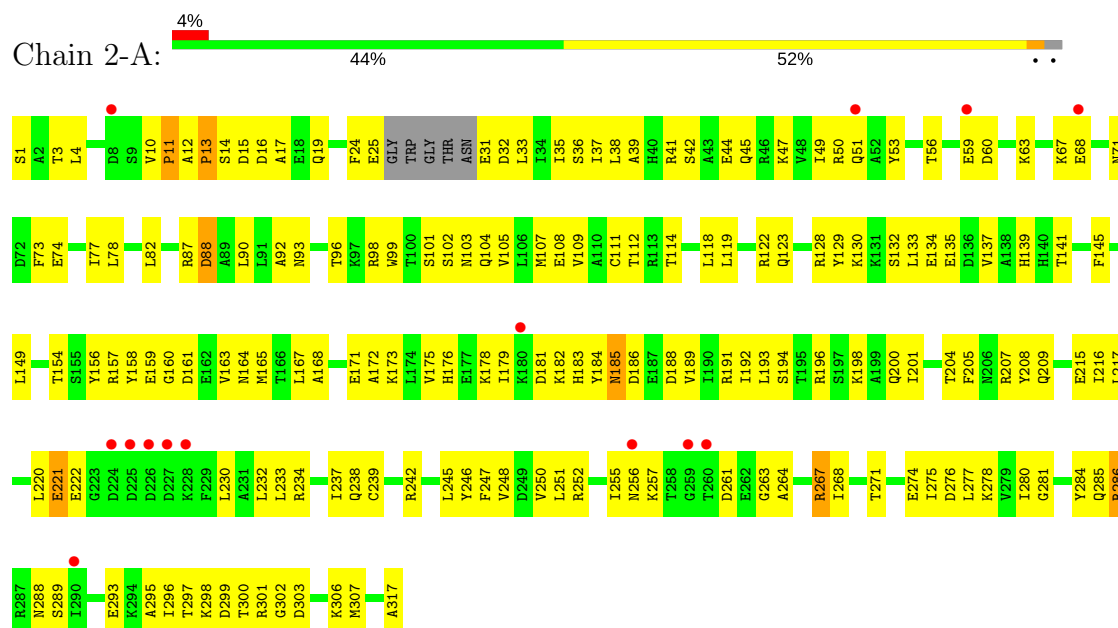
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



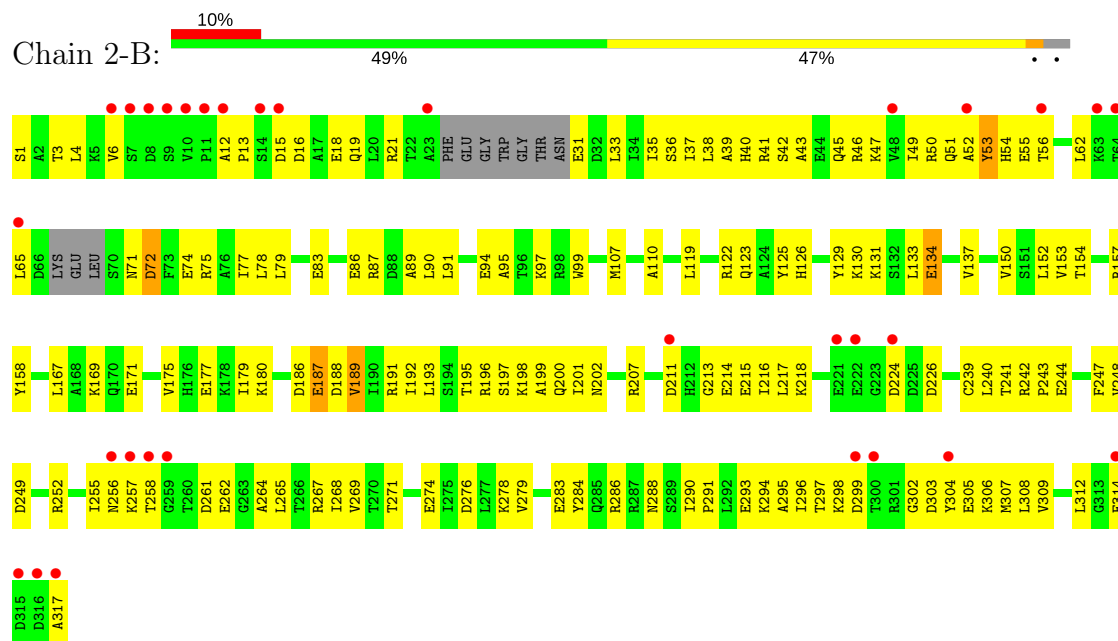
- Molecule 1: Annexin D1

Chain 2-A:



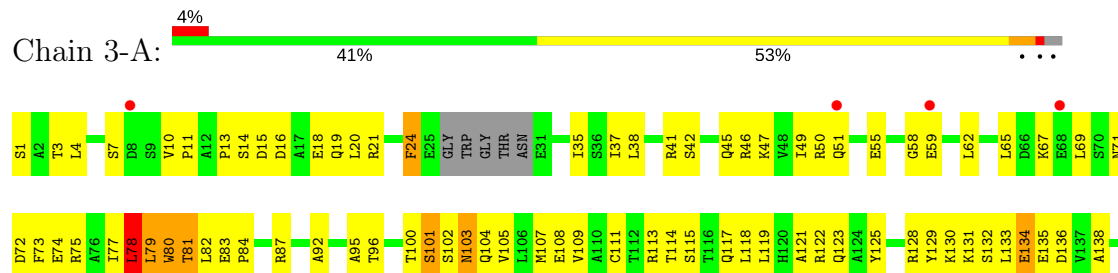
- Molecule 1: Annexin D1

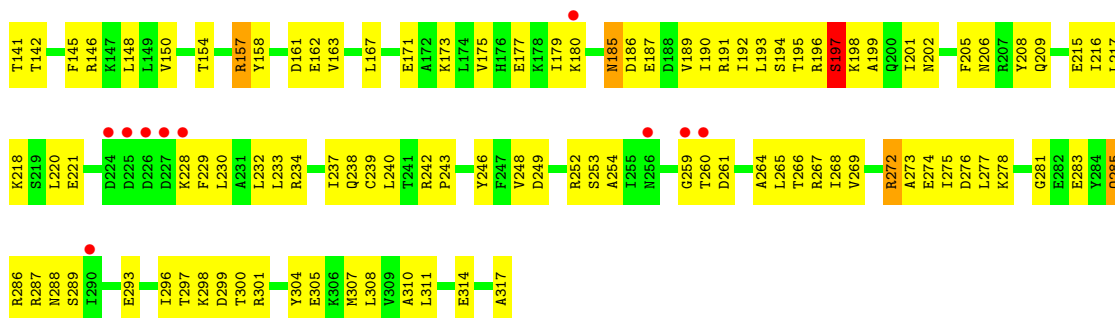
Chain 2-B:



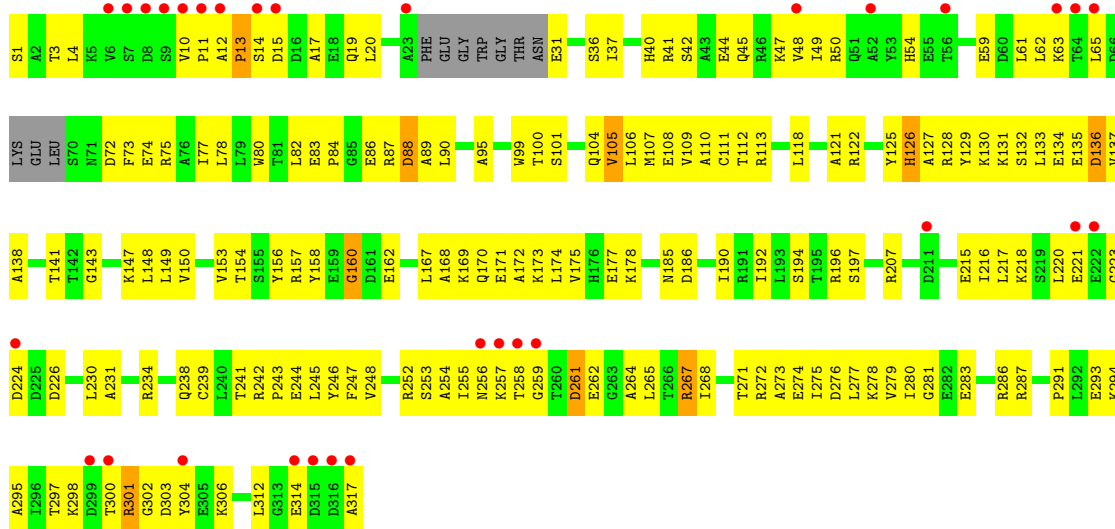
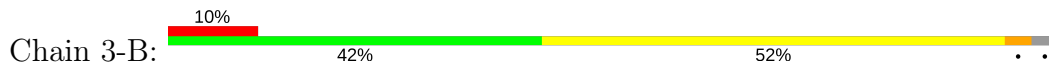
- Molecule 1: Annexin D1

Chain 3-A:

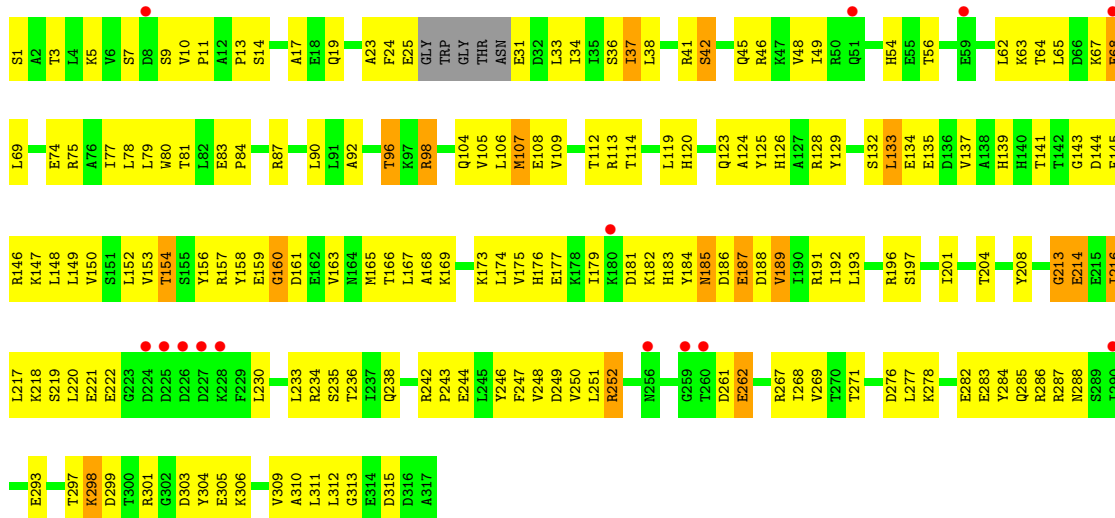
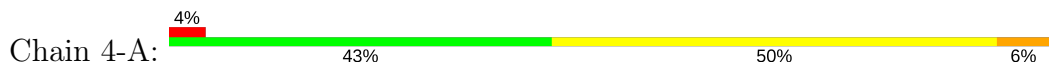




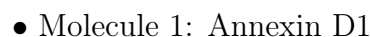
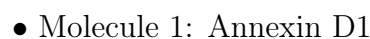
• Molecule 1: Annexin D1

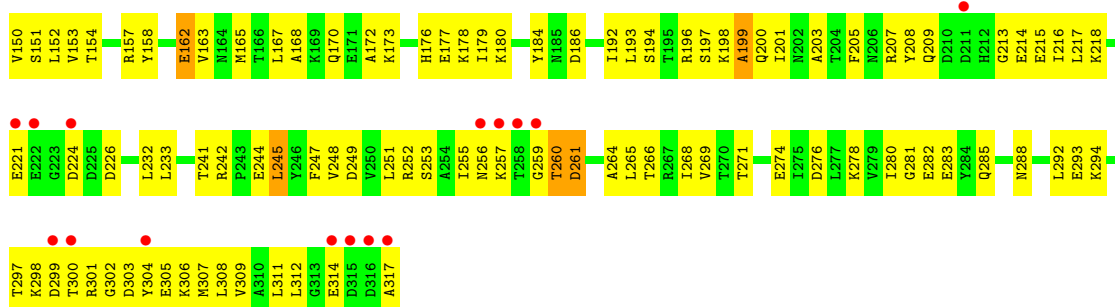


• Molecule 1: Annexin D1

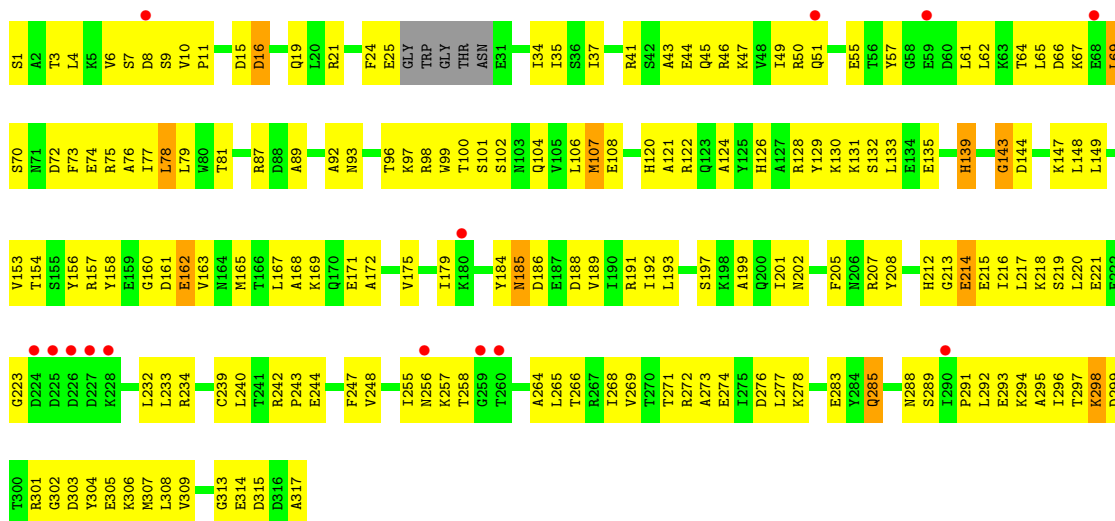


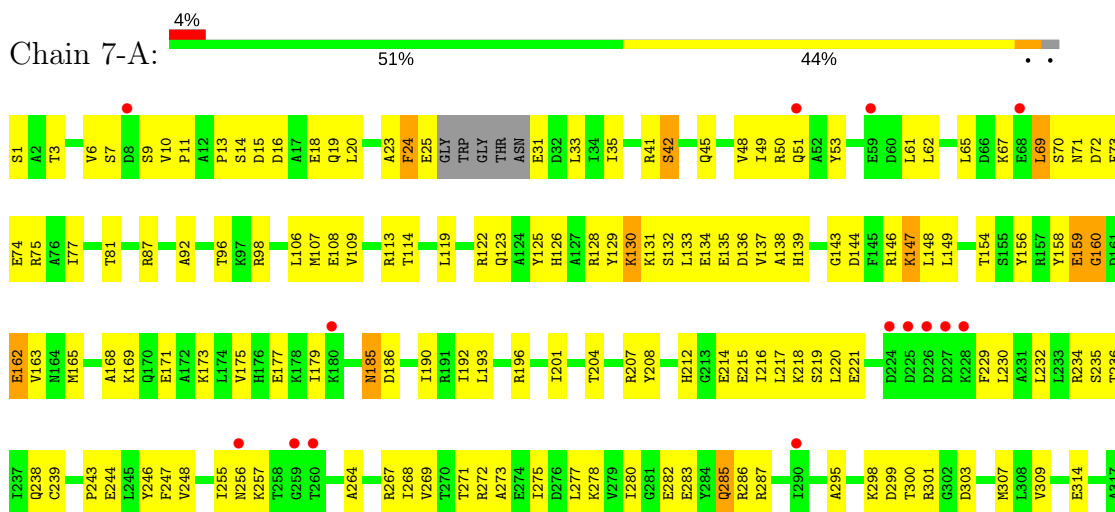
• Molecule 1: Annexin D1



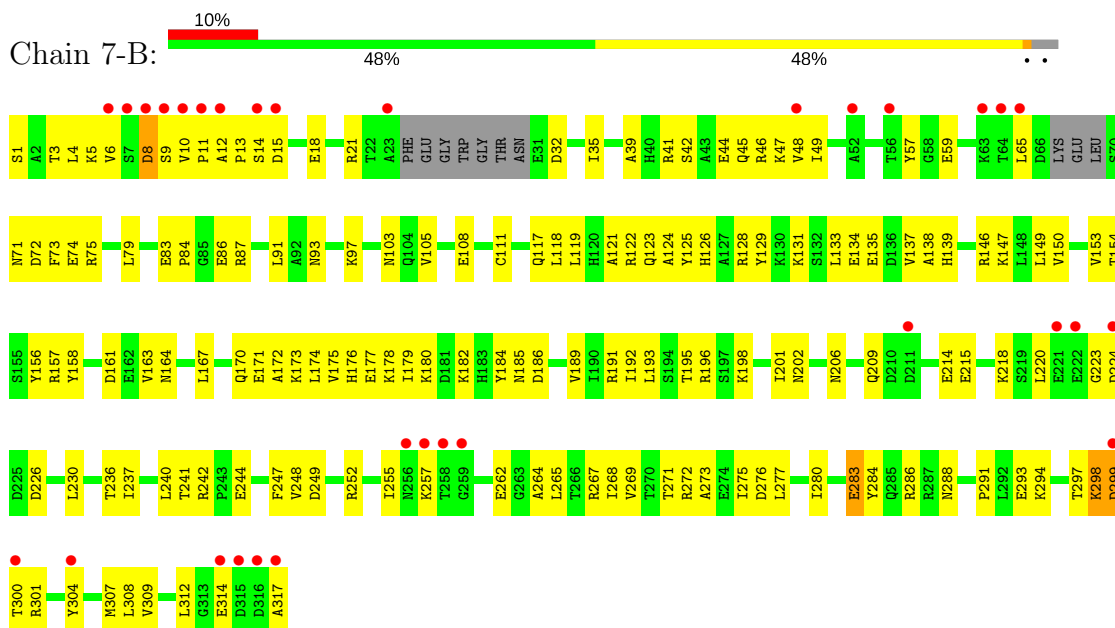


• Molecule 1: Annexin D1

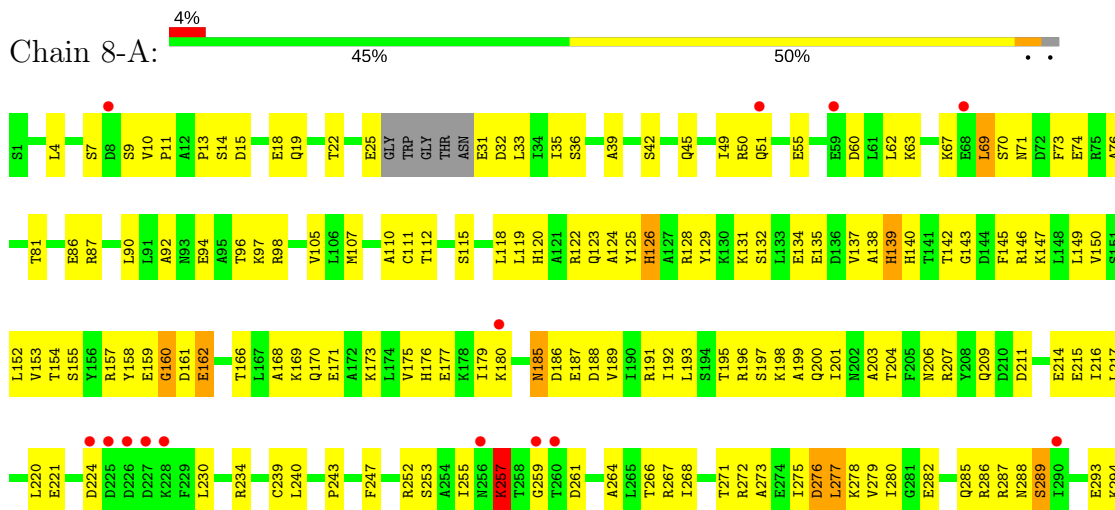


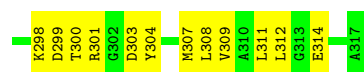


- Molecule 1: Annexin D1

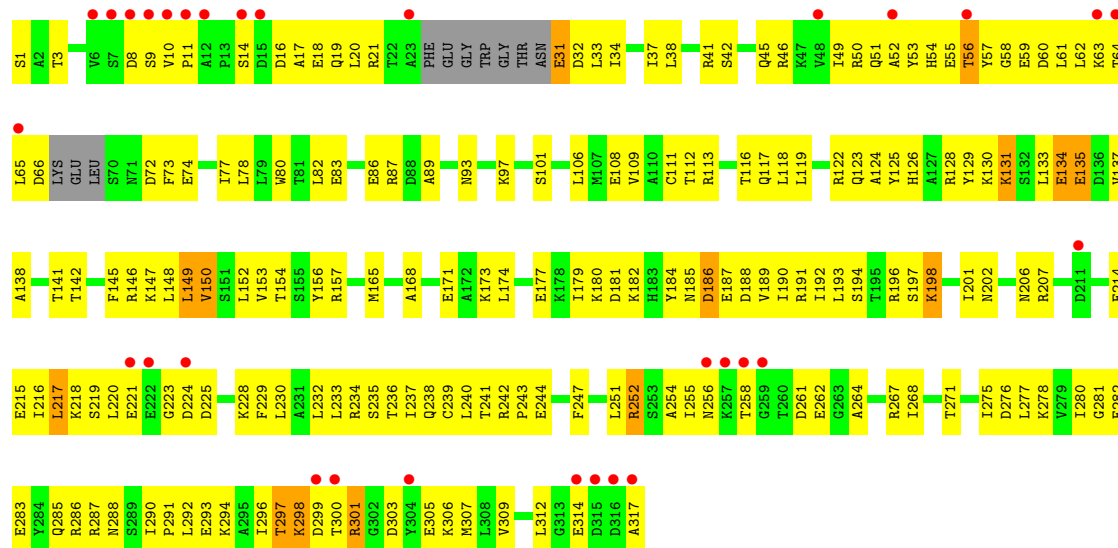


- Molecule 1: Annexin D1





● Molecule 1: Annexin D1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.177 , 0.243 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	42008	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1-A	0.32	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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (2690) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLU:HG2	1:A:154:THR:HG22	1.33	1.09
1:A:272:ARG:HH11	1:A:272:ARG:HA	1.14	1.08
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:B:191:ARG:HH12	1:B:196:ARG:NH2	1.67	0.92
1:A:59:GLU:HG3	1:A:63:LYS:HG3	1.50	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:NH1	1:A:272:ARG:HA	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:A:69:LEU:HD23	1:A:69:LEU:H	1.35	0.87
1:B:303:ASP:HA	1:B:306:LYS:HD3	1.56	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:B:215:GLU:H	1:B:218:LYS:HD2	1.37	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: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:A:1:SER:HB3	1:A:276:ASP:HA	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ASP:HA	1:B:234:ARG:HH12	1.39	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
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:169:LYS:HD2	1:A:207:ARG:HH21	1.42	0.84
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: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:B:247:PHE:HD1	1:B:268:ILE:HD12	1.43	0.84
1:A:169:LYS:HD2	1:A:207:ARG:HH21	1.42	0.84
1:A:144:ASP:HA	1:A:147:LYS:HD3	1.59	0.83
1:A:1:SER:HB3	1:A:276:ASP:HA	1.57	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:191:ARG:HH12	1:B:196:ARG:HH21	1.27	0.82
1:B:65:LEU:HD13	1:B:77:ILE:HG21	1.62	0.82
1:A:39:ALA:HB2	1:A:307:MET:SD	2.20	0.82
1:B:309:VAL:HA	1:B:312:LEU:HD12	1.62	0.82
1:A:286:ARG:HB2	1:A:286:ARG:HH11	1.43	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:87:ARG:HD3	1:B:271:THR:HG22	1.61	0.81
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:180:LYS:HA	1:A:180:LYS:HE2	1.63	0.80
1:A:221:GLU:HA	1:A:234:ARG:NH2	1.96	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:B:65:LEU:HD22	1:B:74:GLU:HB3	1.65	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: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:90:LEU:HD13	1:B:128:ARG:NH2	1.95	0.78
1:B:134:GLU:HG2	1:B:154:THR:HG22	1.64	0.78
1:A:78:LEU:O	1:A:80:TRP:N	2.16	0.78
1:B:50:ARG:HH12	1:B:82:LEU:HD23	1.47	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:A:158:TYR:CE2	1:A:160:GLY:HA3	2.19	0.78
1:A:216:ILE:HA	1:A:219:SER:HB3	1.65	0.78
1:B:291:PRO:HD2	1:B:294:LYS:HD3	1.65	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:B:133:LEU:HD23	1:B:153:VAL:HB	1.66	0.77
1:B:165:MET:HE1	1:B:207:ARG:HD3	1.65	0.77
1:A:114:THR:HG22	2:A:344:HOH:O	1.84	0.77
1:A:191:ARG:HH12	1:A:196:ARG:NH2	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:285:GLN:HG2	1:A:291:PRO:HG3	1.67	0.76
1:A:255:ILE:HG21	1:A:295:ALA:HB1	1.66	0.76
1:B:39:ALA:HB2	1:B:307:MET:SD	2.25	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:B:247:PHE:CD1	1:B:268:ILE:HD12	2.21	0.76
1:A:179:ILE:HD12	1:A:220:LEU:HD21	1.66	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:264:ALA:HA	1:B:267:ARG:NH1	2.01	0.75
1:B:267:ARG:HB3	1:B:267:ARG:NH1	1.96	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:A:135:GLU:HB3	1:B:195:THR:HB	1.68	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:B:65:LEU:HD22	1:B:77:ILE:HB	1.69	0.75
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.52	0.75
1:B:179:ILE:HD11	1:B:220:LEU:HD21	1.69	0.74
1:A:35:ILE:CD1	1:A:307:MET:HB2	2.16	0.74
1:A:14:SER:HA	1:A:17:ALA:HB3	1.70	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: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:202:ASN:HD21	1:B:206:ASN:HD21	1.34	0.74
1:B:53:TYR:O	1:B:57:TYR:HB2	1.87	0.74
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.52	0.74
1:B:251:LEU:HD11	1:B:268:ILE:HG21	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:MET:HE1	1:A:207:ARG:HD3	1.70	0.73
1:A:83:GLU:HG2	1:A:84:PRO:HD2	1.69	0.73
1:A:173:LYS:O	1:A:177:GLU:HG3	1.88	0.73
1:B:303:ASP:HA	1:B:306:LYS:HD3	1.71	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
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:134:GLU:HG3	1:A:154:THR:CG2	2.18	0.73
1:A:1:SER:OG	1:A:278:LYS:HB3	1.89	0.73
1:A:51:GLN:HG2	2:A:472:HOH:O	1.88	0.73
1:B:167:LEU:O	1:B:171:GLU:HG2	1.88	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: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:A:87:ARG:HD3	1:A:271:THR:HG22	1.70	0.72
1:B:277:LEU:HD21	1:B:312:LEU:HD23	1.69	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:A:179:ILE:HD12	1:A:220:LEU:HD21	1.71	0.72
1:B:97:LYS:HA	1:B:97:LYS:HE2	1.70	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:14:SER:O	1:B:18:GLU:HG3	1.89	0.71
1:B:171:GLU:HG3	2:B:332:HOH:O	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:188:ASP:HA	1:A:191:ARG:HB3	1.72	0.70
1:A:34:ILE:HD12	1:A:34:ILE:N	2.06	0.70
1:A:293:GLU:HB3	1:A:312:LEU:HD13	1.73	0.70
1:A:169:LYS:HD2	2:A:396:HOH:O	1.90	0.70
1:A:104:GLN:HG2	1:A:232:LEU:HD13	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:HG22	1:B:267:ARG:NH2	2.06	0.70
1:B:157:ARG:HD3	1:B:196:ARG:O	1.91	0.70
1:A:147:LYS:H	1:A:147:LYS:HD2	1.57	0.70
1:B:277:LEU:HD21	1:B:312:LEU:HD23	1.74	0.70
1:B:42:SER:OG	1:B:45:GLN:HG3	1.92	0.70
1:A:87:ARG:HD3	1:A:271:THR:HG22	1.74	0.70
1:B:177:GLU:HA	1:B:180:LYS:HE2	1.73	0.70
1:A:272:ARG:CA	1:A:272:ARG:HH11	1.99	0.70
1:B:109:VAL:O	1:B:113:ARG:HB2	1.91	0.69
1:B:134:GLU:CG	1:B:154:THR:HG22	2.21	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:A:1:SER:CB	1:A:276:ASP:HA	2.22	0.69
1:B:215:GLU:H	1:B:218:LYS:HD2	1.56	0.69
1:B:301:ARG:NH2	1:B:317:ALA:HB3	2.07	0.69
1:A:224:ASP:O	1:A:230:LEU:HD23	1.91	0.69
1:B:300:THR:HG22	1:B:301:ARG:H	1.57	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:A:175:VAL:O	1:A:179:ILE:HG12	1.93	0.69
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.74	0.69
1:A:90:LEU:O	1:A:94:GLU:HG3	1.92	0.69
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.27	0.69
1:A:22:THR:O	1:A:25:GLU:HG2	1.93	0.69
1:B:1:SER:HB3	1:B:276:ASP:HA	1.73	0.69
1:A:303:ASP:HA	1:A:306:LYS:HD3	1.74	0.69
1:B:38:LEU:HD13	1:B:77:ILE:HD12	1.74	0.69
1:A:156:TYR:HB3	2:B:323:HOH:O	1.93	0.69
1:B:169:LYS:HD2	1:B:207:ARG:HH21	1.56	0.69
1:A:209:GLN:NE2	1:A:215:GLU:HB2	2.08	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:186:ASP:HB3	1:A:189:VAL:HG23	1.74	0.69
1:A:252:ARG:NE	1:A:288:ASN:HD21	1.91	0.69
1:B:71:ASN:HD22	1:B:74:GLU:HG3	1.58	0.69
1:B:97:LYS:HE2	1:B:97:LYS:HA	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:SER:HB3	1:B:259:GLY:H	1.57	0.68
1:A:119:LEU:O	1:A:123:GLN:HG3	1.92	0.68
1:B:147:LYS:HE3	2:B:422:HOH:O	1.91	0.68
1:A:169:LYS:HD2	1:A:207:ARG:NH2	2.07	0.68
1:B:248:VAL:HG21	1:B:283:GLU:HB2	1.75	0.68
1:A:277:LEU:HA	1:A:280:ILE:HD12	1.76	0.68
1:A:67:LYS:HB2	1:A:69:LEU:HD13	1.75	0.68
1:A:93:ASN:OD1	1:A:97:LYS:HE2	1.94	0.68
1:A:220:LEU:HD22	1:A:230:LEU:HD11	1.75	0.68
1:B:198:LYS:HE2	1:B:240:LEU:HD23	1.74	0.68
1:A:1:SER:HB3	1:A:276:ASP:HA	1.74	0.68
1:A:157:ARG:HH22	1:A:194:SER:HA	1.59	0.68
1:A:129:TYR:O	1:A:131:LYS:HG3	1.93	0.68
1:B:71:ASN:HB3	1:B:74:GLU:HG3	1.76	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:B:1:SER:N	1:B:279:VAL:H	1.92	0.67
1:A:65:LEU:HD22	1:A:74:GLU:O	1.93	0.67
1:B:118:LEU:O	1:B:122:ARG:HG3	1.93	0.67
1:A:135:GLU:O	1:A:139:HIS:HB2	1.93	0.67
1:A:248:VAL:HG21	1:A:283:GLU:HB3	1.77	0.67
1:B:314:GLU:HB3	1:B:317:ALA:HB2	1.76	0.67
1:B:296:ILE:HD12	1:B:312:LEU:HD11	1.76	0.67
1:B:235:SER:HA	1:B:238:GLN:HE21	1.59	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:A:6:VAL:HG12	1:A:7:SER:N	2.09	0.67
1:B:171:GLU:HB3	1:B:192:ILE:HD13	1.77	0.67
1:A:98:ARG:HE	1:A:98:ARG:HA	1.58	0.67
1:A:314:GLU:HB3	1:A:317:ALA:HB3	1.75	0.67
1:B:247:PHE:CD1	1:B:268:ILE:HG23	2.29	0.67
1:A:51:GLN:HG2	2:A:473:HOH:O	1.95	0.67
1:A:71:ASN:HD22	1:A:74:GLU:HG3	1.60	0.67
1:B:264:ALA:HA	1:B:267:ARG:HH12	1.58	0.67
1:B:134:GLU:HG3	1:B:154:THR:CG2	2.24	0.67
1:A:252:ARG:HH22	1:A:287:ARG:NH1	1.93	0.67
1:B:202:ASN:HB3	2:B:374:HOH:O	1.95	0.67
1:B:39:ALA:HB2	1:B:307:MET:SD	2.35	0.67
1:A:215:GLU:OE1	1:A:218:LYS:HE3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HG23	1:A:217:LEU:N	2.10	0.67
1:B:10:VAL:HG22	1:B:41:ARG:NH1	2.10	0.67
1:A:221:GLU:HA	1:A:234:ARG:HH21	1.59	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:A:35:ILE:HD11	1:A:73:PHE:HE1	1.60	0.67
1:B:192:ILE:O	1:B:196:ARG:HB2	1.93	0.67
1:A:158:TYR:CE2	1:A:160:GLY:HA3	2.29	0.67
1:A:252:ARG:HG2	1:A:288:ASN:ND2	2.07	0.67
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:230:LEU:HG	1:B:234:ARG:HD2	1.76	0.66
1:B:253:SER:HB3	1:B:259:GLY:N	2.10	0.66
1:A:90:LEU:HA	1:A:129:TYR:OH	1.94	0.66
1:A:196:ARG:CD	1:A:200:GLN:HE21	2.08	0.66
1:B:216:ILE:HG23	1:B:217:LEU:N	2.09	0.66
1:A:14:SER:O	1:A:18:GLU:HG3	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: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:98:ARG:HA	1:A:98:ARG:NE	2.10	0.66
1:B:239:CYS:O	1:B:243:PRO:HG3	1.95	0.66
1:B:169:LYS:HE3	1:B:211:ASP:OD1	1.96	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:B:188:ASP:O	1:B:192:ILE:HG13	1.94	0.66
1:B:89:ALA:HB1	1:B:125:TYR:HB2	1.75	0.66
1:B:214:GLU:OE1	1:B:219:SER:HA	1.95	0.66
1:B:12:ALA:HB3	1:B:15:ASP:OD2	1.96	0.66
1:B:171:GLU:HB3	1:B:192:ILE:HD13	1.76	0.66
1:B:173:LYS:O	1:B:177:GLU:HG3	1.96	0.66
1:B:147:LYS:HD3	2:B:404:HOH:O	1.96	0.66
1:B:216:ILE:HG23	1:B:217:LEU:H	1.60	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:A:67:LYS:HD2	1:A:69:LEU:HB2	1.76	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:42:SER:OG	1:A:45:GLN:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLU:CD	1:B:134:GLU:H	1.96	0.66
1:A:148:LEU:HD12	1:A:190:ILE:HG12	1.78	0.66
1:A:205:PHE:HA	1:A:208:TYR:HB3	1.77	0.66
1:A:269:VAL:HG12	1:A:311:LEU:HD12	1.78	0.66
1:B:65:LEU:CD1	1:B:77:ILE:HG21	2.26	0.66
1:B:13:PRO:HB3	1:B:48:VAL:HG12	1.78	0.65
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:A:288:ASN:O	1:A:289:SER:HB2	1.96	0.65
1:B:38:LEU:CD1	1:B:77:ILE:HD12	2.26	0.65
1:A:107:MET:HE2	1:A:107:MET:C	2.17	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:244:GLU:HA	1:A:280:ILE:HG12	1.77	0.65
1:A:175:VAL:O	1:A:179:ILE:HG12	1.97	0.65
1:B:105:VAL:O	1:B:108:GLU:N	2.29	0.65
1:A:169:LYS:HD2	1:A:207:ARG:NH2	2.10	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: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:223:GLY:HA3	1:B:230:LEU:HD21	1.77	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:65:LEU:HD22	1:B:74:GLU:HB3	1.77	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:61:LEU:HD23	1:B:62:LEU:HD23	1.79	0.65
1:A:69:LEU:H	1:A:69:LEU:HD23	1.62	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:B:198:LYS:C	1:B:200:GLN:H	2.00	0.65
1:B:42:SER:OG	1:B:45:GLN:HG3	1.96	0.65
1:A:209:GLN:HG3	1:A:215:GLU:N	2.12	0.65
1:B:261:ASP:HB3	1:B:264:ALA:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:HA	1:B:41:ARG:NH1	2.12	0.65
1:B:105:VAL:HG22	1:B:267:ARG:NH2	2.12	0.65
1:B:10:VAL:HG21	1:B:45:GLN:HE22	1.61	0.65
1:B:178:LYS:HG3	1:B:186:ASP:OD2	1.97	0.65
1:B:167:LEU:HA	1:B:170:GLN:NE2	2.11	0.65
1:B:300:THR:HG22	1:B:301:ARG:N	2.12	0.65
1:B:41:ARG:HD2	1:B:49:ILE:HD11	1.79	0.65
1:A:205:PHE:O	1:A:208:TYR:HB3	1.97	0.65
1:A:134:GLU:HG2	1:A:154:THR:HG22	1.79	0.64
1:A:273:ALA:HA	1:A:277:LEU:HB2	1.79	0.64
2:A:361:HOH:O	1:B:126:HIS:HD2	1.80	0.64
1:B:300:THR:HG22	1:B:301:ARG:H	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
1:A:215:GLU:H	1:A:218:LYS:HD2	1.61	0.64
1:B:1:SER:HB3	1:B:276:ASP:HA	1.77	0.64
1:B:177:GLU:HA	1:B:180:LYS:HE3	1.77	0.64
1:B:87:ARG:HD2	2:B:321:HOH:O	1.97	0.64
1:A:216:ILE:HG23	1:A:217:LEU:N	2.13	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:B:99:TRP:CZ3	1:B:141:THR:HA	2.32	0.64
1:A:197:SER:O	1:A:201:ILE:HG13	1.97	0.64
1:A:264:ALA:O	1:A:268:ILE:HG12	1.97	0.64
1:A:197:SER:O	1:A:201:ILE:HG13	1.97	0.64
1:A:272:ARG:HH12	1:A:275:ILE:HB	1.63	0.64
1:A:51:GLN:O	1:A:55:GLU:HG3	1.98	0.64
1:A:92:ALA:O	1:A:96:THR:HG23	1.97	0.64
1:B:169:LYS:HE3	1:B:211:ASP:OD1	1.97	0.64
1:A:141:THR:O	1:A:146:ARG:HD3	1.98	0.64
1:A:218:LYS:HA	1:A:221:GLU:OE2	1.98	0.64
1:A:37:ILE:HG23	1:A:41:ARG:CZ	2.27	0.64
1:B:297:THR:HG21	1:B:317:ALA:OXT	1.98	0.64
1:A:234:ARG:HD3	2:A:430:HOH:O	1.98	0.64
1:B:152:LEU:HD23	1:B:194:SER:CB	2.28	0.64
1:A:104:GLN:O	1:A:107:MET:HB3	1.98	0.64
1:A:244:GLU:HA	1:A:280:ILE:HG12	1.80	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:1:SER:HB3	1:A:275:ILE:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:NZ	1:B:173:LYS:HB2	2.13	0.63
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: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:A:161:ASP:HA	1:A:199:ALA:CB	2.28	0.63
1:B:217:LEU:HD21	1:B:237:ILE:HB	1.79	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:A:6:VAL:HG21	1:A:42:SER:HB3	1.81	0.63
1:B:293:GLU:OE2	1:B:314:GLU:HG3	1.98	0.63
1:B:142:THR:O	1:B:145:PHE:HB2	1.98	0.63
1:A:261:ASP:HB3	1:A:264:ALA:HB2	1.80	0.63
1:A:130:LYS:HD2	1:B:158:TYR:OH	1.98	0.63
1:A:298:LYS:HE3	1:A:299:ASP:OD2	1.97	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:B:169:LYS:HG2	1:B:173:LYS:NZ	2.14	0.63
1:B:73:PHE:O	1:B:77:ILE:HG12	1.99	0.63
1:B:134:GLU:HG3	1:B:154:THR:HG22	1.81	0.63
1:A:92:ALA:HB1	1:A:106:LEU:HD21	1.80	0.63
1:A:129:TYR:O	1:A:131:LYS:N	2.32	0.63
1:B:247:PHE:HD1	1:B:268:ILE:HD12	1.63	0.63
1:A:111:CYS:SG	1:A:152:LEU:HD22	2.39	0.63
1:A:90:LEU:O	1:A:94:GLU:HG3	1.99	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:B:215:GLU:HG3	2:B:366:HOH:O	1.99	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:127:ALA:HA	1:B:130:LYS:NZ	2.13	0.62
1:B:37:ILE:O	1:B:41:ARG:HG2	1.98	0.62
1:B:198:LYS:HE2	1:B:240:LEU:HD23	1.81	0.62
1:B:10:VAL:HG22	1:B:45:GLN:NE2	2.15	0.62
1:B:4:LEU:HD22	1:B:274:GLU:HG2	1.81	0.62
1:A:216:ILE:HG23	1:A:217:LEU:N	2.14	0.62
1:B:135:GLU:O	1:B:139:HIS:HB2	2.00	0.62
1:B:44:GLU:O	1:B:48:VAL:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HE3	1:A:299:ASP:OD2	1.99	0.62
1:B:87:ARG:HD2	2:B:322:HOH:O	1.98	0.62
1:A:216:ILE:HG23	1:A:217:LEU:H	1.64	0.62
1:B:1:SER:H3	1:B:279:VAL:HG23	1.64	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:A:50:ARG:O	1:A:53:TYR:HB3	1.98	0.62
1:A:86:GLU:OE2	1:A:128:ARG:NH1	2.32	0.62
1:A:135:GLU:O	1:A:139:HIS:HB2	1.99	0.62
1:B:39:ALA:HB2	1:B:307:MET:SD	2.40	0.62
1:A:273:ALA:HA	1:A:277:LEU:HD22	1.82	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
1:A:193:LEU:HD12	1:A:233:LEU:HD11	1.81	0.62
1:A:3:THR:HB	1:A:312:LEU:O	1.98	0.62
1:A:309:VAL:HA	1:A:312:LEU:HD12	1.82	0.62
1:B:186:ASP:O	1:B:188:ASP:N	2.33	0.62
1:A:46:ARG:HH11	1:A:46:ARG:HG3	1.64	0.62
1:A:60:ASP:HB3	1:A:63:LYS:HG2	1.82	0.62
1:B:209:GLN:HA	1:B:214:GLU:O	1.99	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:A:31:GLU:HG2	1:A:303:ASP:OD1	2.00	0.62
1:B:11:PRO:HG2	1:B:16:ASP:OD2	1.98	0.62
1:B:134:GLU:CG	1:B:154:THR:HG22	2.30	0.62
1:B:173:LYS:HZ2	1:B:173:LYS:HB2	1.65	0.61
1:A:124:ALA:O	1:A:128:ARG:HB2	2.00	0.61
1:B:44:GLU:O	1:B:48:VAL:HG23	2.00	0.61
1:A:98:ARG:HA	1:A:98:ARG:NE	2.14	0.61
1:B:238:GLN:HG2	1:B:246:TYR:HB2	1.81	0.61
1:A:186:ASP:HB3	1:A:189:VAL:HG23	1.81	0.61
1:A:23:ALA:HB1	1:A:34:ILE:CD1	2.29	0.61
1:B:215:GLU:OE1	1:B:218:LYS:HE3	2.00	0.61
1:B:50:ARG:NH1	1:B:82:LEU:HD23	2.14	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:A:19:GLN:HG2	2:A:392:HOH:O	2.00	0.61
1:A:220:LEU:HB2	1:A:234:ARG:NH1	2.15	0.61
1:B:277:LEU:HD21	1:B:312:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:O	1:B:123:GLN:HG3	2.00	0.61
1:A:119:LEU:O	1:A:123:GLN:HG3	1.99	0.61
1:A:293:GLU:OE2	1:A:314:GLU:HG3	1.99	0.61
1:B:149:LEU:O	1:B:152:LEU:N	2.34	0.61
1:B:220:LEU:HD22	1:B:230:LEU:HD11	1.82	0.61
1:A:186:ASP:O	1:A:190:ILE:HG13	2.01	0.61
1:A:107:MET:HE1	1:A:235:SER:HB3	1.83	0.61
1:A:51:GLN:O	1:A:55:GLU:HG3	2.00	0.61
1:B:64:THR:O	1:B:65:LEU:HG	2.01	0.61
1:B:42:SER:HB2	2:B:344:HOH:O	1.99	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:A:162:GLU:O	1:A:163:VAL:HG23	2.01	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
1:A:15:ASP:O	1:A:19:GLN:HG3	2.01	0.61
1:B:300:THR:HG22	1:B:301:ARG:N	2.15	0.61
1:B:255:ILE:C	1:B:257:LYS:H	2.04	0.61
1:B:133:LEU:CD2	1:B:153:VAL:HB	2.31	0.61
1:A:209:GLN:HE21	1:A:215:GLU:CA	2.14	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:A:134:GLU:CG	1:A:154:THR:HG22	2.28	0.61
1:A:264:ALA:O	1:A:268:ILE:HG12	2.01	0.61
1:B:290:ILE:HD11	1:B:294:LYS:O	2.00	0.61
1:B:133:LEU:HD12	1:B:137:VAL:HG23	1.83	0.60
1:A:207:ARG:HB3	1:A:211:ASP:OD2	2.00	0.60
1:B:73:PHE:HB2	1:B:303:ASP:O	2.01	0.60
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: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:A:234:ARG:HD3	2:A:431:HOH:O	2.02	0.60
1:A:73:PHE:O	1:A:77:ILE:HG13	2.02	0.60
1:B:130:LYS:HA	1:B:130:LYS:HE2	1.83	0.60
1:B:125:TYR:O	1:B:129:TYR:HB2	2.01	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:A:35:ILE:CD1	1:A:35:ILE:H	2.13	0.60
1:A:161:ASP:O	1:A:163:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HD12	1:A:290:ILE:N	2.15	0.60
1:B:78:LEU:O	1:B:82:LEU:HB2	2.02	0.60
1:A:13:PRO:HB3	1:A:48:VAL:HG12	1.83	0.60
1:A:309:VAL:HA	1:A:312:LEU:HD12	1.83	0.60
1:B:179:ILE:HD13	1:B:220:LEU:HD21	1.81	0.60
1:A:165:MET:SD	1:A:207:ARG:HD3	2.42	0.60
1:A:184:TYR:HB3	1:A:233:LEU:HD22	1.82	0.60
1:A:201:ILE:O	1:A:204:THR:N	2.35	0.60
1:A:271:THR:O	1:A:272:ARG:HD2	2.01	0.60
1:A:78:LEU:O	1:A:82:LEU:HG	2.01	0.60
1:B:12:ALA:HB3	1:B:15:ASP:OD2	2.02	0.60
1:A:297:THR:HG23	1:A:309:VAL:HG11	1.82	0.60
1:A:122:ARG:O	1:A:126:HIS:HB2	2.02	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:B:12:ALA:HB3	1:B:15:ASP:OD2	2.01	0.60
1:B:304:TYR:CZ	1:B:308:LEU:HD11	2.37	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:186:ASP:O	1:A:190:ILE:HG13	2.02	0.60
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.66	0.60
1:B:60:ASP:OD2	1:B:62:LEU:HB2	2.01	0.60
1:A:168:ALA:HB3	1:A:207:ARG:HG3	1.83	0.60
1:A:68:GLU:OE1	1:A:68:GLU:HA	2.01	0.60
1:A:22:THR:O	1:A:25:GLU:HG2	2.02	0.60
1:B:217:LEU:HD13	1:B:238:GLN:HG2	1.84	0.60
1:A:98:ARG:HA	1:A:98:ARG:HE	1.67	0.60
1:A:165:MET:O	1:A:168:ALA:HB3	2.01	0.60
1:A:75:ARG:HE	1:A:79:LEU:HD11	1.67	0.60
1:A:135:GLU:O	1:A:139:HIS:HB2	2.01	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: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:B:264:ALA:O	1:B:268:ILE:HG12	2.01	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:239:CYS:O	1:B:243:PRO:HG3	2.02	0.59
1:A:216:ILE:HG23	1:A:217:LEU:H	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:145:PHE:HD1	1:A:232:LEU:HD22	1.67	0.59
1:A:171:GLU:HB3	1:A:192:ILE:CD1	2.32	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:37:ILE:O	1:A:41:ARG:HG2	2.02	0.59
1:B:173:LYS:O	1:B:177:GLU:HG3	2.02	0.59
1:B:171:GLU:HB3	1:B:192:ILE:HD13	1.84	0.59
1:A:185:ASN:HD22	1:A:185:ASN:H	1.49	0.59
1:B:264:ALA:O	1:B:268:ILE:HG12	2.02	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:253:SER:HB3	1:A:259:GLY:N	2.17	0.59
1:A:64:THR:O	1:A:65:LEU:HD23	2.02	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
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:158:TYR:HA	2:A:366:HOH:O	2.01	0.59
1:A:77:ILE:O	1:A:80:TRP:HB3	2.03	0.59
1:B:54:HIS:HA	1:B:59:GLU:O	2.01	0.59
1:B:264:ALA:O	1:B:268:ILE:HG12	2.02	0.59
1:A:119:LEU:O	1:A:123:GLN:HG3	2.03	0.59
1:A:173:LYS:O	1:A:177:GLU:HG3	2.02	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: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: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:175:VAL:O	1:A:179:ILE:HG12	2.02	0.59
1:B:178:LYS:HG3	1:B:186:ASP:OD2	2.03	0.59
1:A:111:CYS:HB3	1:A:240:LEU:HG	1.83	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:244:GLU:HA	1:B:280:ILE:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:273:ALA:HA	1:B:277:LEU:HB2	1.85	0.58
1:A:215:GLU:CD	1:A:217:LEU:HD12	2.22	0.58
1:A:91:LEU:HD22	1:A:267:ARG:HD3	1.85	0.58
1:B:18:GLU:HA	1:B:57:TYR:OH	2.03	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:158:TYR:CE2	1:B:160:GLY:HA3	2.38	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:A:186:ASP:HB3	1:A:189:VAL:CG2	2.32	0.58
1:A:264:ALA:O	1:A:268:ILE:HG12	2.02	0.58
1:B:36:SER:HA	1:B:40:HIS:ND1	2.19	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: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:175:VAL:HG13	1:A:189:VAL:HG22	1.85	0.58
1:A:286:ARG:HB2	1:A:286:ARG:NH1	2.19	0.58
1:B:296:ILE:HD12	1:B:312:LEU:HD11	1.85	0.58
1:B:304:TYR:OH	1:B:308:LEU:HD11	2.03	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:3:THR:HB	1:A:312:LEU:HA	1.84	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:74:GLU:HA	1:A:77:ILE:HD12	1.86	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:149:LEU:O	1:B:153:VAL:HG22	2.04	0.58
1:A:272:ARG:HB3	1:A:276:ASP:OD1	2.03	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:B:231:ALA:HA	1:B:234:ARG:HE	1.67	0.58
1:B:71:ASN:HB3	1:B:74:GLU:CG	2.33	0.58
1:B:73:PHE:O	1:B:77:ILE:HG12	2.03	0.58
1:A:255:ILE:C	1:A:257:LYS:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ASN:O	1:B:258:THR:HG23	2.03	0.58
1:B:42:SER:OG	1:B:45:GLN:HG3	2.04	0.58
1:B:65:LEU:HD22	1:B:74:GLU:CD	2.24	0.58
1:B:239:CYS:O	1:B:243:PRO:HG3	2.04	0.58
1:B:303:ASP:HA	1:B:306:LYS:CD	2.33	0.58
1:B:89:ALA:HB1	1:B:125:TYR:CD2	2.39	0.58
1:B:135:GLU:O	1:B:139:HIS:HB2	2.03	0.58
1:B:193:LEU:HA	1:B:201:ILE:HD13	1.86	0.58
1:A:129:TYR:O	1:A:131:LYS:HG3	2.03	0.58
1:A:197:SER:O	1:A:201:ILE:HG13	2.03	0.58
1:B:302:GLY:O	1:B:306:LYS:HD3	2.04	0.58
1:B:64:THR:O	1:B:65:LEU:HD23	2.04	0.58
1:A:171:GLU:HB3	1:A:192:ILE:CD1	2.34	0.58
1:A:129:TYR:O	1:A:131:LYS:HG3	2.04	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:A:35:ILE:HD11	1:A:73:PHE:HE1	1.67	0.58
1:A:125:TYR:CD2	1:A:133:LEU:HD13	2.39	0.58
1:A:198:LYS:HB2	2:A:330:HOH:O	2.04	0.58
1:A:78:LEU:C	1:A:80:TRP:N	2.57	0.58
1:A:71:ASN:ND2	1:A:73:PHE:HB3	2.13	0.58
1:A:195:THR:OG1	1:B:135:GLU:HB3	2.04	0.58
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:90:LEU:HD13	1:A:128:ARG:NH2	2.19	0.57
1:B:79:LEU:CB	1:B:270:THR:HG21	2.33	0.57
1:B:129:TYR:O	1:B:131:LYS:HG3	2.03	0.57
1:A:247:PHE:CD1	1:A:268:ILE:HD12	2.39	0.57
1:A:139:HIS:HD2	2:B:335:HOH:O	1.85	0.57
1:A:77:ILE:HG12	1:A:307:MET:CE	2.34	0.57
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.05	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:A:169:LYS:HD2	1:A:207:ARG:HH21	1.69	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:B:110:ALA:HB1	1:B:152:LEU:O	2.04	0.57
1:A:122:ARG:HH21	1:B:156:TYR:HB3	1.68	0.57
1:A:298:LYS:HE3	1:A:299:ASP:OD2	2.03	0.57
1:A:45:GLN:O	1:A:49:ILE:HG13	2.04	0.57
1:A:107:MET:HE2	1:A:107:MET:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:HG3	1:B:253:SER:H	1.69	0.57
1:B:35:ILE:HG22	1:B:35:ILE:O	2.03	0.57
1:B:216:ILE:HG23	1:B:217:LEU:N	2.19	0.57
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.85	0.57
1:A:276:ASP:OD2	1:A:280:ILE:HD11	2.05	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: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:B:6:VAL:HG13	1:B:41:ARG:HA	1.86	0.57
1:B:143:GLY:HA3	2:B:355:HOH:O	2.05	0.57
1:B:216:ILE:HG23	1:B:217:LEU:H	1.68	0.57
1:A:234:ARG:HD3	2:A:428:HOH:O	2.05	0.57
1:B:281:GLY:C	1:B:283:GLU:H	2.07	0.57
1:B:61:LEU:O	1:B:64:THR:HG22	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:45:GLN:O	1:B:49:ILE:HG13	2.04	0.57
1:B:202:ASN:ND2	1:B:206:ASN:ND2	2.52	0.57
1:A:122:ARG:HH21	1:B:156:TYR:HB3	1.69	0.57
1:B:21:ARG:HG2	1:B:57:TYR:CZ	2.40	0.57
1:B:106:LEU:O	1:B:106:LEU:HD23	2.05	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:202:ASN:ND2	1:B:206:ASN:HD21	2.01	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:A:239:CYS:O	1:A:243:PRO:HG3	2.05	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:242:ARG:HB2	1:A:245:LEU:HD12	1.87	0.57
1:A:92:ALA:O	1:A:96:THR:HG23	2.05	0.57
1:A:99:TRP:CZ3	1:A:141:THR:HA	2.40	0.57
1:A:75:ARG:O	1:A:78:LEU:HB3	2.05	0.57
1:A:132:SER:N	1:A:135:GLU:OE2	2.30	0.57
1:B:19:GLN:CD	1:B:37:ILE:HD11	2.25	0.57
1:A:175:VAL:O	1:A:179:ILE:HG12	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:HB	2:A:372:HOH:O	2.05	0.57
1:A:156:TYR:HB3	1:B:122:ARG:NH2	2.20	0.57
1:B:65:LEU:HD22	1:B:74:GLU:CB	2.35	0.57
1:B:113:ARG:HG3	2:B:376:HOH:O	2.05	0.57
1:B:3:THR:HG23	1:B:278:LYS:N	2.19	0.57
1:A:171:GLU:O	1:A:175:VAL:HG23	2.04	0.57
1:B:84:PRO:HG2	2:B:405:HOH:O	2.04	0.56
1:A:148:LEU:HD23	1:A:232:LEU:HG	1.86	0.56
1:A:125:TYR:O	1:A:129:TYR:HB2	2.05	0.56
1:A:60:ASP:HB3	1:A:63:LYS:HG2	1.86	0.56
1:B:260:THR:O	1:B:260:THR:HG22	2.05	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:A:119:LEU:HD21	1:B:119:LEU:HD21	1.87	0.56
1:A:165:MET:HB3	2:A:397:HOH:O	2.04	0.56
1:A:168:ALA:O	1:A:172:ALA:HB2	2.04	0.56
1:A:242:ARG:HD3	2:A:386:HOH:O	2.05	0.56
1:A:301:ARG:CZ	2:A:368:HOH:O	2.52	0.56
1:A:79:LEU:HD12	1:A:266:THR:HG22	1.87	0.56
1:B:3:THR:OG1	1:B:277:LEU:HB3	2.05	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:132:SER:N	1:A:135:GLU:OE2	2.30	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:165:MET:CE	1:A:207:ARG:HD3	2.34	0.56
1:A:122:ARG:HG2	1:A:133:LEU:HB3	1.88	0.56
1:A:154:THR:HB	1:B:154:THR:OG1	2.04	0.56
1:B:202:ASN:HD21	1:B:206:ASN:HD21	1.53	0.56
1:B:34:ILE:HG22	1:B:38:LEU:HD12	1.86	0.56
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.06	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:B:44:GLU:H	1:B:44:GLU:CD	2.07	0.56
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.86	0.56
1:A:14:SER:O	1:A:18:GLU:HG3	2.04	0.56
1:A:66:ASP:HA	1:A:78:LEU:HD22	1.88	0.56
1:A:103:ASN:O	1:A:104:GLN:HG3	2.05	0.56
1:B:169:LYS:CE	1:B:207:ARG:HH21	2.18	0.56
1:B:146:ARG:HG3	1:B:150:VAL:HG21	1.88	0.56
1:B:71:ASN:HB3	1:B:74:GLU:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LYS:O	1:B:201:ILE:N	2.39	0.56
1:B:84:PRO:HG2	2:B:402:HOH:O	2.06	0.56
1:B:82:LEU:HD22	1:B:87:ARG:N	2.21	0.56
1:A:101:SER:HB2	1:A:145:PHE:CZ	2.40	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:A:104:GLN:NE2	1:A:246:TYR:HE1	2.04	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: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:B:255:ILE:HD12	1:B:284:TYR:OH	2.05	0.56
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.87	0.56
1:A:177:GLU:O	1:A:180:LYS:HB2	2.06	0.56
1:A:92:ALA:O	1:A:96:THR:HG22	2.06	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:171:GLU:O	1:A:175:VAL:HG23	2.06	0.56
1:B:191:ARG:HD3	2:B:320:HOH:O	2.04	0.56
1:B:225:ASP:HA	1:B:234:ARG:NH1	2.17	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:220:LEU:HD11	1:B:237:ILE:HD12	1.87	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:B:78:LEU:O	1:B:82:LEU:HG	2.06	0.56
1:A:107:MET:SD	1:A:236:THR:HA	2.46	0.56
1:A:134:GLU:HB3	1:B:195:THR:HG22	1.88	0.56
1:A:158:TYR:CZ	1:A:160:GLY:HA3	2.40	0.56
1:A:186:ASP:OD2	1:A:188:ASP:HB2	2.05	0.56
1:B:71:ASN:HB3	1:B:74:GLU:HB2	1.87	0.56
1:A:19:GLN:HB3	1:A:33:LEU:HD21	1.86	0.56
1:B:175:VAL:HG23	1:B:192:ILE:CD1	2.36	0.56
1:A:171:GLU:O	1:A:175:VAL:HG23	2.06	0.56
1:A:275:ILE:HD12	2:A:333:HOH:O	2.05	0.56
1:B:272:ARG:O	1:B:277:LEU:HB2	2.06	0.56
1:B:125:TYR:O	1:B:129:TYR:HB2	2.06	0.56
1:B:309:VAL:CG2	1:B:315:ASP: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:CB	1:A:312:LEU:HA	2.36	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:A:125:TYR:CE2	1:A:133:LEU:HD13	2.41	0.56
1:A:158:TYR:HD1	1:B:126:HIS:HB3	1.71	0.56
1:A:122:ARG:CZ	1:A:154:THR:HA	2.36	0.56
1:A:119:LEU:O	1:A:123:GLN:HG3	2.06	0.56
1:B:268:ILE:O	1:B:272:ARG:HG2	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:B:241:THR:HG22	1:B:242:ARG:HG3	1.88	0.56
1:B:119:LEU:O	1:B:123:GLN:HG3	2.07	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:A:158:TYR:CZ	1:A:160:GLY:HA3	2.41	0.55
1:A:165:MET:CE	1:A:207:ARG:HD3	2.32	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:239:CYS:O	1:B:243:PRO:HG3	2.06	0.55
1:A:62:LEU:HD21	1:A:81:THR:CB	2.33	0.55
1:B:254:ALA:HB1	1:B:265:LEU:HB2	1.89	0.55
1:B:248:VAL:HG21	1:B:283:GLU:HB3	1.88	0.55
1:B:96:THR:HG21	1:B:136:ASP:O	2.06	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:B:309:VAL:HA	1:B:312:LEU:HD12	1.88	0.55
1:A:161:ASP:O	1:A:163:VAL:HG23	2.06	0.55
1:B:148:LEU:HA	1:B:190:ILE:CG2	2.36	0.55
1:B:220:LEU:HD12	1:B:234:ARG:HG2	1.87	0.55
1:B:145:PHE:HZ	1:B:228:LYS:HB2	1.71	0.55
1:A:35:ILE:HD12	1:A:307:MET:HA	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:67:LYS:HD3	1:A:70:SER:HB3	1.88	0.55
1:B:73:PHE:CE1	1:B:77:ILE:HD11	2.42	0.55
1:A:293:GLU:O	1:A:297:THR:HG23	2.06	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:B:158:TYR:O	1:B:197:SER:OG	2.23	0.55
1:A:6:VAL:HG12	1:A:7:SER:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASP:OD1	1:B:264:ALA:HB2	2.06	0.55
1:A:179:ILE:HD12	1:A:220:LEU:CD2	2.36	0.55
1:A:89:ALA:HB2	1:A:121:ALA:O	2.07	0.55
1:B:273:ALA:HA	1:B:277:LEU:HB2	1.89	0.55
1:A:173:LYS:O	1:A:177:GLU:HG3	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:109:VAL:HG12	1:B:109:VAL:O	2.07	0.55
1:A:166:THR:HB	2:A:350:HOH:O	2.05	0.55
1:A:235:SER:HA	1:A:238:GLN:OE1	2.07	0.55
1:B:43:ALA:HB2	1:B:274:GLU:OE2	2.07	0.55
1:B:74:GLU:O	1:B:77:ILE:HB	2.06	0.55
1:A:168:ALA:HA	2:A:327:HOH:O	2.06	0.55
1:A:4:LEU:HD12	1:A:311:LEU:HA	1.89	0.55
1:B:75:ARG:NH1	1:B:90:LEU:HD21	2.19	0.55
1:A:135:GLU:C	1:A:137:VAL:H	2.11	0.55
1:A:184:TYR:OH	1:A:223:GLY:HA3	2.07	0.55
1:B:205:PHE:O	1:B:208:TYR:HB3	2.07	0.55
1:A:137:VAL:HG13	1:A:141:THR:HG21	1.89	0.55
1:B:128:ARG:HD3	1:B:129:TYR:CZ	2.41	0.55
1:B:1:SER:OG	1:B:279:VAL:HG23	2.06	0.55
1:B:255:ILE:C	1:B:257:LYS:H	2.08	0.55
1:B:132:SER:OG	1:B:135:GLU:HB3	2.06	0.55
1:A:154:THR:HB	1:B:154:THR:O	2.06	0.55
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:A:208:TYR:HA	1:A:212:HIS:HD2	1.71	0.55
1:B:173:LYS:HE2	2:B:413:HOH:O	2.07	0.55
1:A:162:GLU:HG2	1:B:130:LYS:HB3	1.89	0.55
1:A:300:THR:HG22	1:A:301:ARG:N	2.22	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:1:SER:OG	1:A:276:ASP:HA	2.07	0.54
1:A:50:ARG:CZ	1:A:62:LEU:HD12	2.37	0.54
1:A:47:LYS:HG3	1:A:83:GLU:OE2	2.07	0.54
1:B:127:ALA:HA	1:B:130:LYS:CE	2.36	0.54
1:A:191:ARG:NH1	1:A:191:ARG:HG2	2.22	0.54
1:A:203:ALA:HA	1:A:206:ASN:ND2	2.22	0.54
2:A:364:HOH:O	1:B:126:HIS:HD2	1.88	0.54
1:B:11:PRO:HD2	1:B:41:ARG:HH21	1.72	0.54
1:B:249:ASP:O	1:B:252:ARG:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:92:ALA:O	1:A:125:TYR:HE2	1.88	0.54
1:A:241:THR:HG22	1:A:242:ARG:HG3	1.88	0.54
1:A:58:GLY:O	1:A:59:GLU:HB2	2.08	0.54
1:B:278:LYS:O	1:B:282:GLU:HG3	2.07	0.54
1:B:202:ASN:HD21	1:B:206:ASN:ND2	2.05	0.54
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.42	0.54
1:A:107:MET:HE2	1:A:107:MET:C	2.28	0.54
1:B:192:ILE:O	1:B:201:ILE:HD11	2.07	0.54
1:B:157:ARG:HH22	1:B:194:SER:HA	1.72	0.54
1:A:122:ARG:NH2	1:B:156:TYR:HB2	2.22	0.54
1:A:234:ARG:HD3	2:A:433:HOH:O	2.07	0.54
1:B:209:GLN:HA	1:B:214:GLU:O	2.07	0.54
1:B:176:HIS:O	1:B:180:LYS:HG2	2.07	0.54
1:A:134:GLU:HG3	1:A:154:THR:HG22	1.89	0.54
1:B:241:THR:HG22	1:B:242:ARG:N	2.22	0.54
1:B:230:LEU:HG	1:B:234:ARG:CD	2.37	0.54
1:A:104:GLN:NE2	1:A:246:TYR:CE1	2.76	0.54
1:B:87:ARG:HH11	1:B:271:THR:HG22	1.70	0.54
1:B:73:PHE:CZ	1:B:77:ILE:HD11	2.42	0.54
1:A:118:LEU:O	1:A:122:ARG:HG3	2.06	0.54
1:A:139:HIS:CD2	1:B:196:ARG:HH22	2.25	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:A:271:THR:O	1:A:272:ARG:HD2	2.08	0.54
1:A:43:ALA:HA	1:A:46:ARG:CZ	2.38	0.54
1:A:62:LEU:CD1	1:A:82:LEU:HD23	2.38	0.54
1:A:87:ARG:HD3	1:A:271:THR:HG22	1.90	0.54
1:B:178:LYS:HG3	1:B:186:ASP:OD2	2.07	0.54
1:A:13:PRO:CB	1:A:48:VAL:HG12	2.37	0.54
1:B:248:VAL:HG23	1:B:280:ILE:HG23	1.89	0.54
1:B:86:GLU:HA	1:B:124:ALA:HB1	1.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLN:O	1:B:49:ILE:HG13	2.08	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:B:291:PRO:HB2	1:B:294:LYS:HG3	1.90	0.54
1:A:134:GLU:OE1	1:A:134:GLU:N	2.41	0.54
1:B:259:GLY:O	1:B:261:ASP:N	2.39	0.54
1:B:156:TYR:HD1	2:B:354:HOH:O	1.90	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:A:107:MET:HE2	1:A:107:MET:O	2.06	0.54
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.90	0.54
1:A:132:SER:N	1:A:135:GLU:OE2	2.39	0.54
1:B:134:GLU:CG	1:B:154:THR:HG22	2.19	0.54
1:A:99:TRP:CD1	1:A:103:ASN:HB3	2.43	0.54
1:B:75:ARG:CZ	1:B:79:LEU:HD11	2.38	0.54
1:A:11:PRO:HG2	1:A:16:ASP:OD2	2.08	0.54
1:B:131:LYS:HE3	2:B:325:HOH:O	2.07	0.54
1:A:150:VAL:HA	1:A:153:VAL:CG2	2.37	0.54
1:A:310:ALA:O	1:A:313:GLY:N	2.39	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:B:269:VAL:O	1:B:273:ALA:HB2	2.08	0.54
1:B:293:GLU:OE2	1:B:314:GLU:HG3	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:A:19:GLN:HG2	2:A:392:HOH:O	2.07	0.54
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.08	0.54
1:B:248:VAL:HG21	1:B:283:GLU:HB3	1.89	0.54
1:A:16:ASP:O	1:A:20:LEU:HG	2.08	0.54
1:B:173:LYS:HG2	1:B:173:LYS:O	2.08	0.54
1:A:46:ARG:O	1:A:49:ILE:HB	2.09	0.54
1:A:122:ARG:NH2	1:B:156:TYR:HB3	2.23	0.54
1:B:116:THR:O	1:B:119:LEU:N	2.41	0.54
1:A:108:GLU:OE2	1:A:267:ARG:NH1	2.40	0.54
1:A:115:SER:OG	1:A:159:GLU:HG3	2.08	0.54
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:B:191:ARG:NH1	1:B:196:ARG:NH2	2.48	0.53
1:A:265:LEU:HG	1:A:308:LEU:HD13	1.90	0.53
1:B:113:ARG:HG3	1:B:117:GLN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:SER:HB2	1:B:278:LYS:HD3	1.89	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: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:B:45:GLN:O	1:B:49:ILE:HG13	2.08	0.53
1:B:72:ASP:HB3	1:B:304:TYR:CG	2.43	0.53
1:A:286:ARG:HH11	1:A:286:ARG:CB	2.21	0.53
1:A:167:LEU:HD23	1:A:200:GLN:HE22	1.73	0.53
1:A:109:VAL:HG12	1:A:109:VAL:O	2.07	0.53
1:A:4:LEU:HD22	1:A:274:GLU:HG2	1.89	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:A:33:LEU:O	1:A:37:ILE:HG12	2.08	0.53
1:B:252:ARG:NE	1:B:288:ASN:OD1	2.41	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:242:ARG:HB3	1:B:244:GLU:OE2	2.09	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:131:LYS:HD2	1:A:136:ASP:OD1	2.08	0.53
1:A:239:CYS:O	1:A:243:PRO:HG3	2.09	0.53
1:A:83:GLU:HB3	1:A:84:PRO:HD2	1.89	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: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:107:MET:HG2	1:A:111:CYS:SG	2.48	0.53
1:A:207:ARG:CZ	2:A:397:HOH:O	2.57	0.53
1:B:261:ASP:OD2	1:B:264:ALA:HB2	2.09	0.53
1:A:139:HIS:ND1	2:A:433:HOH:O	2.34	0.53
1:B:14:SER:O	1:B:18:GLU:HG3	2.09	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:A:87:ARG:HD2	1:A:271:THR:HG22	1.90	0.53
1:B:264:ALA:O	1:B:268:ILE:HG12	2.08	0.53
1:A:162:GLU:N	2:A:321:HOH:O	2.40	0.53
1:A:302:GLY:O	1:A:306:LYS:HG3	2.07	0.53
1:A:171:GLU:HB3	1:A:192:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:SER:HB2	1:A:275:ILE:O	2.08	0.53
1:A:169:LYS:HD2	2:A:396:HOH:O	2.08	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:119:LEU:O	1:A:123:GLN:HG3	2.09	0.53
1:B:125:TYR:CD2	1:B:133:LEU:HB2	2.44	0.53
1:B:45:GLN:O	1:B:49:ILE:HG13	2.09	0.53
1:A:224:ASP:HB3	1:A:227:ASP:HB2	1.91	0.53
1:B:101:SER:HB2	1:B:145:PHE:CZ	2.44	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: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: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:192:ILE:O	1:A:201:ILE:HD11	2.09	0.52
1:A:77:ILE:HG12	1:A:307:MET:HE2	1.91	0.52
1:B:83:GLU:HB2	1:B:86:GLU:HG3	1.91	0.52
1:A:154:THR:HB	1:B:154:THR:HB	1.90	0.52
1:A:215:GLU:N	1:A:218:LYS:HD2	2.24	0.52
1:A:215:GLU:O	1:A:219:SER:N	2.40	0.52
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: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: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:247:PHE:CD1	1:A:268:ILE:HD12	2.44	0.52
1:A:297:THR:HG22	1:A:301:ARG:HE	1.74	0.52
1:A:71:ASN:OD1	1:A:74:GLU:HG3	2.08	0.52
1:B:148:LEU:O	1:B:152:LEU:HG	2.10	0.52
1:A:247:PHE:CD1	1:A:268:ILE:HD12	2.44	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:51:GLN:O	1:A:55:GLU:HG3	2.09	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:A:92:ALA:HB1	1:A:106:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:LYS:CD	1:A:207:ARG:HH21	2.18	0.52
1:B:73:PHE:C	1:B:75:ARG:H	2.12	0.52
1:B:244:GLU:O	1:B:248:VAL:HG23	2.09	0.52
1:B:184:TYR:HB3	1:B:233:LEU:CD2	2.36	0.52
1:B:114:THR:HG23	1:B:117:GLN:NE2	2.24	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: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:B:83:GLU:HG2	2:B:396:HOH:O	2.10	0.52
1:A:105:VAL:O	1:A:109:VAL:HG23	2.10	0.52
1:B:214:GLU:HB2	1:B:218:LYS:HD2	1.92	0.52
1:A:111:CYS:SG	1:A:152:LEU:HD22	2.50	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:185:ASN:C	1:A:185:ASN:HD22	2.13	0.52
1:B:281:GLY:HA3	2:B:410:HOH:O	2.09	0.52
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.74	0.52
1:A:107:MET:SD	1:A:107:MET:C	2.88	0.52
1:A:186:ASP:OD2	1:A:188:ASP:HB2	2.08	0.52
1:A:111:CYS:HB3	1:A:239:CYS:CB	2.38	0.52
1:B:179:ILE:HD12	1:B:184:TYR:HD1	1.74	0.52
1:A:67:LYS:HD3	2:A:355:HOH:O	2.09	0.52
1:B:99:TRP:CE3	1:B:141:THR:HA	2.44	0.52
1:B:198:LYS:HA	1:B:201:ILE:HD12	1.92	0.52
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.92	0.52
1:B:181:ASP:O	1:B:182:LYS:HB2	2.07	0.52
1:A:189:VAL:O	1:A:193:LEU:HG	2.10	0.52
1:B:305:GLU:O	1:B:309:VAL:HG22	2.09	0.52
1:B:38:LEU:HD13	1:B:77:ILE:HG23	1.91	0.52
1:B:1:SER:HB3	1:B:276:ASP:HA	1.92	0.52
1:A:15:ASP:O	1:A:19:GLN:HG3	2.09	0.52
1:A:261:ASP:CB	1:A:264:ALA:HB2	2.40	0.52
1:B:306:LYS:HA	1:B:309:VAL:HG22	1.91	0.52
1:B:46:ARG:O	1:B:50:ARG:HG3	2.10	0.52
1:B:276:ASP:O	1:B:280:ILE:HG13	2.07	0.52
1:A:35:ILE:HD11	1:A:73:PHE:HE1	1.75	0.52
1:A:107:MET:O	1:A:111:CYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:65:LEU:O	1:B:78:LEU:HD22	2.09	0.52
1:B:269:VAL:HG21	1:B:308:LEU:HD22	1.90	0.52
1:A:234:ARG:HD3	2:A:399:HOH:O	2.10	0.52
1:B:157:ARG:HH22	1:B:194:SER:HA	1.75	0.52
1:A:1:SER:CB	1:A:276:ASP:HA	2.36	0.52
1:A:171:GLU:HB3	1:A:192:ILE:CD1	2.40	0.52
1:A:247:PHE:CE1	1:A:268:ILE:HD12	2.45	0.52
1:B:50:ARG:CZ	1:B:62:LEU:HD12	2.40	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:19:GLN:HG2	2:A:393:HOH:O	2.10	0.52
1:B:62:LEU:HD13	1:B:78:LEU:HD12	1.92	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:168:ALA:HB1	1:A:204:THR:HA	1.92	0.52
1:B:230:LEU:O	1:B:234:ARG:HG3	2.09	0.52
1:A:31:GLU:C	1:A:33:LEU:H	2.13	0.52
1:B:199:ALA:O	1:B:202:ASN:HB2	2.10	0.52
1:A:133:LEU:O	1:A:137:VAL:HG23	2.10	0.51
1:B:114:THR:H	1:B:117:GLN:HE21	1.58	0.51
1:A:108:GLU:OE2	2:A:318:HOH:O	2.19	0.51
1:B:133:LEU:O	1:B:137:VAL:HG23	2.10	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:A:65:LEU:HD22	1:A:74:GLU:HG2	1.92	0.51
1:B:114:THR:HG23	1:B:117:GLN:OE1	2.10	0.51
1:B:20:LEU:HD13	1:B:61:LEU:HD13	1.92	0.51
1:B:171:GLU:O	1:B:175:VAL:HG23	2.10	0.51
1:A:252:ARG:NH2	1:A:287:ARG:HG3	2.25	0.51
1:A:248:VAL:HA	1:A:251:LEU:HD12	1.92	0.51
1:B:253:SER:HB3	1:B:259:GLY:CA	2.40	0.51
1:A:60:ASP:HB3	1:A:63:LYS:HG2	1.92	0.51
1:B:150:VAL:HA	1:B:153:VAL:CG2	2.40	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:B:158:TYR:HA	2:B:347:HOH: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HE3	1:A:313:GLY:HA3	1.93	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:293:GLU:OE2	1:A:314:GLU:HG3	2.09	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:154:THR:OG1	1:B:154:THR:HB	2.10	0.51
1:B:31:GLU:N	1:B:31:GLU:OE1	2.44	0.51
1:A:166:THR:CB	2:A:350:HOH:O	2.57	0.51
1:B:169:LYS:CE	1:B:207:ARG:HH21	2.23	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:B:187:GLU:H	1:B:187:GLU:CD	2.12	0.51
1:B:175:VAL:HG22	1:B:189:VAL:HG22	1.91	0.51
1:B:71:ASN:HB3	1:B:74:GLU:HG3	1.91	0.51
1:A:218:LYS:HA	1:A:221:GLU:OE2	2.10	0.51
1:A:128:ARG:O	1:A:128:ARG:HG2	2.11	0.51
1:A:238:GLN:O	1:A:242:ARG:N	2.44	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: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: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:B:21:ARG:HG2	1:B:57:TYR:CZ	2.45	0.51
1:A:145:PHE:O	1:A:149:LEU:HG	2.11	0.51
1:A:35:ILE:HD13	1:A:307:MET:SD	2.51	0.51
1:A:122:ARG:NH1	1:A:154:THR:HA	2.25	0.51
1:B:261:ASP:CB	1:B:264:ALA:HB2	2.39	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:220:LEU:C	1:A:234:ARG:HH21	2.12	0.51
1:A:297:THR:HG21	1:A:317:ALA:OXT	2.11	0.51
1:A:107:MET:SD	1:A:236:THR:HA	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASN:OD1	1:B:105:VAL:HG23	2.10	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:168:ALA:O	1:B:172:ALA:HB2	2.11	0.51
1:A:244:GLU:O	1:A:248:VAL:HG23	2.11	0.51
1:B:77:ILE:HD13	1:B:307:MET:CE	2.41	0.51
1:A:135:GLU:CA	1:B:195:THR:HB	2.40	0.51
1:A:167:LEU:HB3	2:A:326:HOH:O	2.11	0.51
1:A:255:ILE:C	1:A:257:LYS:H	2.13	0.51
1:B:286:ARG:HH11	1:B:286:ARG:HG2	1.76	0.51
1:A:1:SER:HG	1:A:278:LYS:HB3	1.75	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:38:LEU:O	1:B:80:TRP:NE1	2.44	0.51
1:B:1:SER:HB2	1:B:275:ILE:O	2.11	0.51
1:B:197:SER:HB2	2:B:329:HOH:O	2.10	0.51
1:A:46:ARG:HE	1:A:81:THR:HA	1.76	0.51
1:A:36:SER:HB2	2:A:471:HOH:O	2.11	0.51
1:A:69:LEU:N	1:A:69:LEU:HD12	2.26	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:A:129:TYR:C	1:A:131:LYS:H	2.13	0.51
1:B:117:GLN:HE22	1:B:275:ILE:HD11	1.76	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:A:107:MET:HE1	1:A:235:SER:HB3	1.94	0.50
1:B:300:THR:HG22	1:B:301:ARG:H	1.76	0.50
1:A:158:TYR:O	1:A:197:SER:HB2	2.11	0.50
1:B:146:ARG:HG3	1:B:150:VAL:HG23	1.92	0.50
1:B:150:VAL:HA	1:B:153:VAL:HG22	1.93	0.50
1:A:158:TYR:OH	1:A:160:GLY:HA3	2.11	0.50
1:A:157:ARG:CG	1:A:197:SER:HA	2.41	0.50
1:B:215:GLU:HA	2:B:365:HOH:O	2.10	0.50
1:B:83:GLU:HB2	1:B:86:GLU:HG3	1.92	0.50
1:B:171:GLU:HB3	1:B:192:ILE:CD1	2.40	0.50
1:A:205:PHE:CE2	1:A:237:ILE:HG23	2.46	0.50
1:A:145:PHE:O	1:A:149:LEU:HG	2.10	0.50
1:A:115:SER:HB2	1:A:159:GLU:CD	2.31	0.50
1:A:300:THR:HG22	1:A:301:ARG:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:HA	1:A:18:GLU:OE1	2.11	0.50
1:B:198:LYS:NZ	2:B:336:HOH:O	2.44	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:7:SER:O	1:A:10:VAL:HG23	2.11	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:118:LEU:O	1:A:121:ALA:N	2.45	0.50
1:B:196:ARG:O	1:B:201:ILE:HD11	2.12	0.50
1:B:251:LEU:HD21	1:B:268:ILE:HB	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:B:150:VAL:HA	1:B:153:VAL:HG22	1.94	0.50
1:A:260:THR:O	1:A:260:THR:HG22	2.12	0.50
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.92	0.50
1:B:231:ALA:CB	1:B:234:ARG:HH21	2.24	0.50
1:B:253:SER:HB3	1:B:259:GLY:HA3	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:B:162:GLU:OE1	1:B:162:GLU:N	2.44	0.50
1:A:1:SER:HB2	1:A:276:ASP:HA	1.94	0.50
1:B:297:THR:HB	1:B:305:GLU:HG2	1.92	0.50
1:A:238:GLN:OE1	1:A:246:TYR:HA	2.11	0.50
1:A:15:ASP:O	1:A:19:GLN:HG3	2.12	0.50
1:A:49:ILE:HG22	1:A:50:ARG:N	2.26	0.50
1:A:69:LEU:HD12	1:A:69:LEU:H	1.76	0.50
1:B:288:ASN:O	1:B:290:ILE:HG22	2.11	0.50
1:A:161:ASP:O	1:A:163:VAL:HG23	2.10	0.50
1:B:62:LEU:HD21	1:B:81:THR:HB	1.94	0.50
1:A:95:ALA:HB1	1:A:103:ASN:HD21	1.76	0.50
1:A:11:PRO:HG2	1:A:16:ASP:OD1	2.12	0.50
1:B:107:MET:HG2	1:B:111:CYS:SG	2.52	0.50
1:B:20:LEU:HD13	1:B:61:LEU:CD1	2.42	0.50
1:A:34:ILE:HD12	1:A:34:ILE:H	1.77	0.50
1:A:35:ILE:HD12	1:A:307:MET:SD	2.52	0.50
1:B:200:GLN:O	1:B:203:ALA:HB3	2.12	0.50
1:B:146:ARG:HG3	1:B:150:VAL:CG2	2.42	0.50
1:A:277:LEU:HA	1:A:280:ILE:HB	1.94	0.50
1:A:50:ARG:O	1:A:53:TYR:HB3	2.12	0.50
1:A:71:ASN:ND2	1:A:74:GLU:HG3	2.25	0.50
1:B:267:ARG:HD2	1:B:267:ARG:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ALA:HB1	1:B:118:LEU:HD22	1.94	0.50
1:B:245:LEU:HD23	1:B:283:GLU:HG3	1.94	0.50
1:B:93:ASN:O	1:B:97:LYS:HG2	2.12	0.50
1:A:128:ARG:O	1:A:128:ARG:HG2	2.12	0.50
1:A:139:HIS:CD2	1:B:196:ARG:HH22	2.30	0.50
1:B:37:ILE:O	1:B:41:ARG:HG2	2.11	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:232:LEU:O	1:B:236:THR:OG1	2.24	0.50
1:A:90:LEU:HD13	1:A:128:ARG:NH2	2.27	0.50
1:A:242:ARG:HB2	1:A:245:LEU:HD12	1.93	0.50
1:B:31:GLU:N	1:B:31:GLU:OE1	2.45	0.50
1:B:8:ASP:O	1:B:9:SER:HB3	2.12	0.50
1:B:186:ASP:HB3	1:B:189:VAL:HG23	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:B:314:GLU:HB3	1:B:317:ALA:HB2	1.94	0.50
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:243:PRO:HG3	2:A:415:HOH:O	2.12	0.49
1:A:7:SER:C	1:A:9:SER:H	2.15	0.49
1:B:105:VAL:HG22	1:B:267:ARG:NH1	2.26	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:13:PRO:HA	1:A:16:ASP:OD2	2.11	0.49
1:B:193:LEU:HD13	1:B:236:THR:HG21	1.94	0.49
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.76	0.49
1:A:246:TYR:CZ	1:A:250:VAL:HG21	2.46	0.49
1:A:7:SER:C	1:A:9:SER:N	2.65	0.49
1:B:157:ARG:NH2	1:B:194:SER:HA	2.27	0.49
1:B:1:SER:HB2	1:B:276:ASP:HA	1.93	0.49
1:B:118:LEU:HD12	1:B:121:ALA: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:A:191:ARG:HH22	1:A:192:ILE:HD11	1.77	0.49
1:A:230:LEU:O	1:A:234:ARG:HG3	2.11	0.49
1:B:277:LEU:CD2	1:B:312:LEU:HD23	2.41	0.49
1:A:248:VAL:HG13	1:A:284:TYR:HD1	1.77	0.49
1:A:38:LEU:C	1:A:40:HIS:H	2.15	0.49
1:B:293:GLU:O	1:B:297:THR:HG22	2.12	0.49
1:B:142:THR:O	1:B:145:PHE:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD23	1:B:188:ASP:HB3	1.95	0.49
1:B:261:ASP:CG	1:B:267:ARG:HH22	2.15	0.49
1:B:172:ALA:C	1:B:174:LEU:H	2.15	0.49
1:B:192:ILE:HG23	1:B:196:ARG:CG	2.43	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:A:135:GLU:OE1	1:B:196:ARG:HD2	2.12	0.49
1:A:50:ARG:NH2	1:A:62:LEU:HD12	2.27	0.49
1:A:126:HIS:HB3	2:A:468:HOH:O	2.12	0.49
1:A:105:VAL:O	1:A:109:VAL:HG23	2.12	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: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: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: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:14:SER:O	1:A:18:GLU:HG3	2.11	0.49
1:A:107:MET:SD	1:A:239:CYS:SG	3.11	0.49
1:B:119:LEU:O	1:B:123:GLN:HG3	2.11	0.49
1:B:82:LEU:HD23	1:B:83:GLU:N	2.28	0.49
1:A:132:SER:HB3	1:B:157:ARG:HA	1.94	0.49
1:B:110:ALA:CB	1:B:118:LEU:HD22	2.42	0.49
1:A:301:ARG:HD2	2:A:370:HOH:O	2.13	0.49
1:A:38:LEU:O	1:A:80:TRP:NE1	2.39	0.49
1:A:286:ARG:HH11	1:A:286:ARG:HB2	1.76	0.49
1:B:148:LEU:O	1:B:152:LEU:HG	2.11	0.49
1:B:243:PRO:O	1:B:246:TYR:N	2.41	0.49
1:A:123:GLN:HA	1:A:126:HIS:HB2	1.95	0.49
1:A:122:ARG:NH2	1:A:154:THR:HA	2.26	0.49
1:A:279:VAL:O	1:A:279:VAL:HG12	2.13	0.49
1:A:172:ALA:HB1	1:A:208:TYR:CB	2.41	0.49
1:A:148:LEU:HD23	1:A:232:LEU:CD2	2.42	0.49
1:A:75:ARG:NE	1:A:79:LEU:HD11	2.27	0.49
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:294:LYS:HE3	1:B:317:ALA:OXT	2.12	0.49
1:A:13:PRO:HA	1:A:16:ASP:OD2	2.13	0.49
1:B:303:ASP:CG	1:B:306:LYS:HZ1	2.16	0.49
1:A:175:VAL:O	1:A:179:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASP:O	1:A:230:LEU:HD23	2.13	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:B:133:LEU:CD1	1:B:137:VAL:HG23	2.43	0.49
1:A:4:LEU:HD22	1:A:274:GLU:HG2	1.94	0.49
1:B:76:ALA:HA	1:B:266:THR:CG2	2.43	0.49
1:B:62:LEU:HD11	1:B:81:THR:HB	1.95	0.49
1:A:185:ASN:HD22	1:A:185:ASN:C	2.17	0.49
1:A:105:VAL:HG22	1:A:267:ARG:HD3	1.95	0.49
1:A:252:ARG:HH22	1:A:287:ARG:CZ	2.25	0.49
1:B:11:PRO:HB2	1:B:15:ASP:CB	2.42	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:220:LEU:HD13	1:A:234:ARG:HG2	1.94	0.49
1:A:302:GLY:HA3	2:A:382:HOH:O	2.12	0.49
1:A:69:LEU:H	1:A:69:LEU:HD12	1.78	0.49
1:B:42:SER:OG	1:B:45:GLN:HG3	2.12	0.49
1:A:220:LEU:HD11	1:A:237:ILE:HD12	1.94	0.49
1:A:227:ASP:HB3	1:A:230:LEU:HB3	1.94	0.49
1:B:255:ILE:C	1:B:257:LYS:N	2.61	0.49
1:A:264:ALA:HA	1:A:267:ARG:HD2	1.95	0.49
1:B:189:VAL:HA	1:B:192:ILE:HD12	1.95	0.49
1:A:297:THR:O	1:A:298:LYS:C	2.50	0.49
1:A:130:LYS:HB3	1:B:162:GLU:HG2	1.94	0.49
1:B:218:LYS:HA	1:B:221:GLU:OE2	2.12	0.49
1:A:104:GLN:HE22	1:A:235:SER:CB	2.24	0.49
1:B:231:ALA:CA	1:B:234:ARG:HH21	2.25	0.49
1:A:6:VAL:CG1	1:A:7:SER:H	2.26	0.49
1:A:69:LEU:HD12	1:A:69:LEU:N	2.27	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:62:LEU:HD21	1:A:81:THR:HB	1.94	0.48
1:A:51:GLN:O	1:A:55:GLU:HG3	2.13	0.48
1:A:161:ASP:O	1:A:163:VAL:HG23	2.12	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: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:B:251:LEU:HD21	1:B:268:ILE:CG2	2.39	0.48
1:A:216:ILE:HG23	1:A:217:LEU:N	2.28	0.48
1:B:244:GLU:HG2	1:B:245:LEU:N	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD11	2:B:350:HOH:O	2.12	0.48
1:B:126:HIS:CE1	1:B:132:SER:HA	2.46	0.48
1:A:114:THR:OG1	1:A:117:GLN:HG3	2.13	0.48
1:B:128:ARG:O	1:B:129:TYR:CG	2.65	0.48
1:A:98:ARG:HH11	1:A:98:ARG:HG2	1.77	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: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:A:119:LEU:HD21	1:B:119:LEU:HD21	1.95	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: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:158:TYR:O	1:A:197:SER:HB2	2.13	0.48
1:A:191:ARG:HG2	2:A:342:HOH:O	2.13	0.48
1:A:195:THR:HB	1:B:135:GLU:N	2.27	0.48
1:A:297:THR:HB	1:A:301:ARG:HD2	1.93	0.48
1:A:125:TYR:HD1	1:A:131:LYS:O	1.97	0.48
1:A:4:LEU:HD22	1:A:274:GLU:HG2	1.94	0.48
1:B:43:ALA:HB2	1:B:274:GLU:OE2	2.13	0.48
1:A:220:LEU:HD22	1:A:230:LEU:CD1	2.43	0.48
1:A:61:LEU:O	1:A:61:LEU:HD23	2.14	0.48
1:A:100:THR:HG22	1:A:102:SER:H	1.78	0.48
1:B:37:ILE:O	1:B:41:ARG:HG2	2.12	0.48
1:A:185:ASN:HD22	1:A:185:ASN:C	2.16	0.48
1:A:157:ARG:CD	1:A:197:SER:HA	2.44	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:35:ILE:HD11	1:A:307:MET:HB2	1.96	0.48
1:B:133:LEU:O	1:B:137:VAL:HG23	2.13	0.48
1:B:179:ILE:CD1	1:B:216:ILE:HD11	2.43	0.48
1:B:198:LYS:O	1:B:200:GLN:N	2.46	0.48
1:B:50:ARG:NH2	1:B:62:LEU:HD12	2.29	0.48
1:B:167:LEU:HD21	1:B:196:ARG:NH2	2.28	0.48
1:B:265:LEU:HG	1:B:308:LEU:HD13	1.96	0.48
1:A:212:HIS:O	1:A:214:GLU:HG2	2.13	0.48
1:A:76:ALA:HA	1:A:266:THR:CG2	2.42	0.48
1:B:247:PHE:HD1	1:B:268:ILE:HG23	1.78	0.48
1:A:261:ASP:CG	1:A:264:ALA:HB2	2.34	0.48
1:A:132:SER:C	1:A:134:GLU:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:HA	2:B:319:HOH:O	2.13	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:B:71:ASN:HB3	1:B:74:GLU:CG	2.43	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:A:67:LYS:CG	1:A:70:SER:HB3	2.43	0.48
1:B:148:LEU:HB2	1:B:190:ILE:CD1	2.43	0.48
1:A:263:GLY:O	1:A:267:ARG:HB3	2.12	0.48
1:B:297:THR:HB	1:B:309:VAL:HG11	1.96	0.48
1:B:293:GLU:HG3	1:B:294:LYS:N	2.28	0.48
1:A:122:ARG:HB3	2:A:323:HOH:O	2.13	0.48
1:A:253:SER:HB3	1:A:259:GLY:H	1.77	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: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:82:LEU:HB3	1:B:86:GLU:HB2	1.96	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:130:LYS:O	1:B:131:LYS:HG3	2.14	0.48
1:B:271:THR:O	1:B:272:ARG:HD2	2.14	0.48
1:B:231:ALA:O	1:B:234:ARG:HB2	2.13	0.48
1:A:173:LYS:O	1:A:177:GLU:HG3	2.13	0.48
1:A:181:ASP:O	1:A:182:LYS:HB2	2.12	0.48
1:A:92:ALA:O	1:A:96:THR:HG23	2.14	0.48
1:B:46:ARG:O	1:B:50:ARG:HG3	2.14	0.48
1:A:87:ARG:NH1	1:A:271:THR:HA	2.29	0.48
1:A:141:THR:O	1:A:146:ARG:HD3	2.14	0.48
1:A:148:LEU:HD23	1:A:232:LEU:CD2	2.43	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:A:158:TYR:CZ	1:A:160:GLY:HA3	2.48	0.48
1:A:175:VAL:O	1:A:179:ILE:HG12	2.13	0.48
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:A:45:GLN:O	1:A:49:ILE:HG13	2.14	0.48
1:B:7:SER:H	1:B:41:ARG:HH22	1.60	0.48
1:B:54:HIS:HA	1:B:59:GLU:O	2.14	0.48
1:A:281:GLY:O	1:A:285:GLN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:VAL:HA	1:B:113:ARG:CZ	2.42	0.48
2:A:320:HOH:O	1:B:156:TYR:HB3	2.13	0.48
1:B:197:SER:O	1:B:200:GLN:N	2.46	0.48
1:B:209:GLN:O	1:B:213:GLY:N	2.47	0.48
1:A:134:GLU:CD	2:A:320:HOH:O	2.53	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:149:LEU:O	1:B:150:VAL:C	2.52	0.48
1:B:252:ARG:CD	1:B:256:ASN:HD21	2.27	0.48
1:B:6:VAL:HG21	1:B:42:SER:HB3	1.96	0.48
1:A:295:ALA:O	1:A:298:LYS:HD3	2.14	0.48
1:B:109:VAL:O	1:B:109:VAL:CG1	2.61	0.48
1:B:293:GLU:O	1:B:297:THR:HG22	2.14	0.48
1:B:40:HIS:O	1:B:41:ARG:HD3	2.13	0.48
1:B:258:THR:O	1:B:258:THR:HG22	2.13	0.48
1:B:42:SER:OG	1:B:45:GLN:HB2	2.14	0.48
1:B:261:ASP:OD2	1:B:264:ALA:HB2	2.14	0.48
1:A:130:LYS:HD2	1:B:158:TYR:OH	2.14	0.48
1:A:247:PHE:CE1	1:A:268:ILE:HD12	2.49	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:185:ASN:HD22	1:A:185:ASN:C	2.16	0.47
1:B:247:PHE:HD1	1:B:268:ILE:HD12	1.79	0.47
1:A:66:ASP:HA	1:A:78:LEU:HD11	1.96	0.47
1:B:163:VAL:HG22	1:B:199:ALA:O	2.13	0.47
1:B:205:PHE:HA	1:B:208:TYR:HB3	1.96	0.47
1:B:259:GLY:HA3	2:B:364:HOH:O	2.13	0.47
1:A:278:LYS:HG2	1:A:282:GLU:OE2	2.14	0.47
1:A:114:THR:HB	1:A:159:GLU:OE2	2.13	0.47
1:A:33:LEU:HD12	1:A:36:SER:OG	2.14	0.47
1:B:187:GLU:HG3	2:B:370:HOH:O	2.12	0.47
1:B:247:PHE:CE1	1:B:268:ILE:HD12	2.49	0.47
1:A:269:VAL:O	1:A:273:ALA:HB2	2.14	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:168:ALA:HA	2:A:328:HOH:O	2.13	0.47
1:A:6:VAL:HA	1:A:40:HIS:O	2.14	0.47
1:A:87:ARG:NH2	2:A:333:HOH:O	2.47	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:B:189:VAL:HG11	1:B:233:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:HD2	2:A:476:HOH:O	2.15	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: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:199:ALA:O	1:A:202:ASN:HB3	2.14	0.47
1:B:174:LEU:HD12	1:B:177:GLU:OE1	2.12	0.47
1:B:238:GLN:NE2	1:B:245:LEU:HD12	2.29	0.47
1:A:37:ILE:O	1:A:41:ARG:HG2	2.14	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: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:B:305:GLU:O	1:B:309:VAL:HG22	2.14	0.47
1:A:307:MET:O	1:A:311:LEU:HG	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:300:THR:HG22	1:A:301:ARG:N	2.30	0.47
1:A:307:MET:O	1:A:311:LEU:HG	2.15	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:126:HIS:O	1:A:130:LYS:N	2.47	0.47
1:A:134:GLU:N	1:A:134:GLU:OE1	2.44	0.47
1:B:10:VAL:HG13	1:B:11:PRO:HD2	1.95	0.47
1:B:169:LYS:HG3	1:B:211:ASP:OD2	2.14	0.47
1:B:255:ILE:O	1:B:257:LYS:HD3	2.14	0.47
1:A:184:TYR:HB3	1:A:233:LEU:HD22	1.96	0.47
1:B:173:LYS:HE3	2:B:413:HOH:O	2.14	0.47
1:B:225:ASP:OD1	1:B:234:ARG:NH2	2.48	0.47
1:A:87:ARG:HD3	1:A:271:THR:HG22	1.96	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: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:A:128:ARG:HD3	1:A:129:TYR:CE2	2.49	0.47
1:B:272:ARG:O	1:B:277:LEU:HB2	2.14	0.47
1:A:250:VAL:CG1	1:A:268:ILE:HD11	2.45	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
1:B:109:VAL:HG13	1:B:113:ARG:NE	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:O	1:A:25:GLU:HB3	2.15	0.47
1:A:74:GLU:HA	1:A:77:ILE:HD12	1.95	0.47
1:A:107:MET:HB2	1:A:149:LEU:HD21	1.95	0.47
1:A:101:SER:O	1:A:228:LYS:HB3	2.15	0.47
1:B:116:THR:O	1:B:118:LEU:N	2.47	0.47
1:A:62:LEU:HD21	1:A:81:THR:CG2	2.44	0.47
1:A:247:PHE:HE2	1:A:272:ARG:NH2	2.12	0.47
1:A:293:GLU:HG2	1:A:294:LYS:N	2.30	0.47
1:B:291:PRO:CD	1:B:294:LYS:HD3	2.40	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:216:ILE:CG2	1:A:217:LEU:N	2.77	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:B:165:MET:HA	1:B:168:ALA:HB3	1.96	0.47
1:B:78:LEU:C	1:B:80:TRP:H	2.18	0.47
1:A:138:ALA:HB2	1:A:150:VAL:HG21	1.97	0.47
1:A:221:GLU:HA	1:A:234:ARG:HH21	1.80	0.47
1:A:246:TYR:CZ	1:A:250:VAL:HG21	2.50	0.47
1:A:105:VAL:HG22	1:A:267:ARG:CZ	2.44	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:156:TYR:HB3	2:B:323:HOH:O	2.13	0.47
1:A:293:GLU:OE2	1:A:314:GLU:HG3	2.15	0.47
1:B:267:ARG:O	1:B:271:THR:HG23	2.14	0.47
1:A:251:LEU:HD21	1:A:268:ILE:HB	1.97	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:B:17:ALA:HB2	1:B:52:ALA:HB3	1.95	0.47
1:A:256:ASN:ND2	2:A:345:HOH:O	2.48	0.47
1:B:169:LYS:HG3	1:B:211:ASP:OD2	2.15	0.47
1:B:265:LEU:O	1:B:269:VAL:HG23	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:101:SER:HB2	1:B:145:PHE:CZ	2.50	0.47
1:A:310:ALA:O	2:A:352:HOH:O	2.20	0.47
1:B:262:GLU:HB3	2:B:383:HOH:O	2.14	0.47
1:A:247:PHE:CE1	1:A:268:ILE:HD12	2.50	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:B:106:LEU:HD22	1:B:149:LEU:CD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD21	1:A:81:THR:HB	1.96	0.47
1:A:288:ASN:O	1:A:289:SER:HB2	2.15	0.47
1:B:137:VAL:O	1:B:141:THR:HG23	2.15	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:144:ASP:O	1:A:147:LYS:HB2	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:171:GLU:O	1:A:175:VAL:HG23	2.14	0.47
1:A:105:VAL:HG22	1:A:267:ARG:NH2	2.30	0.47
1:A:296:ILE:HG22	1:A:296:ILE:O	2.13	0.47
1:A:70:SER:HB3	1:A:74:GLU:HB2	1.97	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: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: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: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:B:252:ARG:HG3	1:B:253:SER:N	2.30	0.47
1:B:59:GLU:OE2	1:B:63:LYS:HD3	2.14	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: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:158:TYR:CZ	1:A:160:GLY:HA3	2.50	0.47
1:A:244:GLU:HA	1:A:280:ILE:CG1	2.44	0.46
1:B:10:VAL:HA	1:B:41:ARG:NH2	2.30	0.46
1:A:122:ARG:NH2	1:B:156:TYR:HB3	2.30	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:B:277:LEU:HG	1:B:312:LEU:HD21	1.97	0.46
1:A:267:ARG:HB3	1:A:267:ARG:NH1	2.29	0.46
1:B:297:THR:CB	1:B:305:GLU:HG2	2.44	0.46
1:A:195:THR:O	2:A:324:HOH:O	2.20	0.46
1:A:261:ASP:CG	1:A:264:ALA:HB2	2.36	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:130:LYS:HA	1:B:158:TYR:CE1	2.49	0.46
1:A:216:ILE:CG2	1:A:217:LEU:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:O	1:A:25:GLU:C	2.52	0.46
1:B:10:VAL:HG13	1:B:41:ARG:CZ	2.46	0.46
1:B:224:ASP:OD2	1:B:226:ASP:HB2	2.14	0.46
1:A:19:GLN:HA	2:A:449:HOH:O	2.15	0.46
1:B:71:ASN:OD1	1:B:73:PHE:N	2.47	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:112:THR:HB	1:B:272:ARG:HH12	1.80	0.46
1:B:17:ALA:HB1	1:B:53:TYR:HB2	1.98	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:111:CYS:SG	1:B:152:LEU:HD22	2.55	0.46
1:B:198:LYS:C	1:B:200:GLN:N	2.67	0.46
1:B:244:GLU:HG2	1:B:245:LEU:N	2.30	0.46
1:B:44:GLU:O	1:B:48:VAL:HG23	2.14	0.46
1:B:185:ASN:HA	1:B:229:PHE:CE2	2.50	0.46
1:B:157:ARG:NH1	1:B:193:LEU:O	2.45	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: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:188:ASP:HA	1:A:191:ARG:NE	2.30	0.46
1:A:243:PRO:HB2	1:A:247:PHE:HE2	1.81	0.46
1:A:256:ASN:O	1:A:257:LYS:HB2	2.15	0.46
1:A:87:ARG:NH1	1:A:271:THR:HG22	2.30	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: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:135:GLU:HB2	1:B:196:ARG:HH11	1.79	0.46
1:B:82:LEU:CD2	1:B:86:GLU:HB3	2.46	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:12:ALA:O	1:B:15:ASP:HB2	2.14	0.46
1:A:35:ILE:CD1	1:A:307:MET:HB2	2.46	0.46
1:A:3:THR:HG23	1:A:277:LEU:HB3	1.96	0.46
1:A:92:ALA:O	1:A:96:THR:HG23	2.15	0.46
1:B:88:ASP:HB3	1:B:121:ALA:HB2	1.97	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:245:LEU:HD11	2:A:389:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:O	1:A:126:HIS:C	2.53	0.46
1:B:148:LEU:HD23	1:B:232:LEU:CD2	2.46	0.46
1:B:111:CYS:C	1:B:113:ARG:H	2.19	0.46
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.97	0.46
1:A:39:ALA:HB2	1:A:307:MET:HE1	1.98	0.46
1:A:23:ALA:HB2	1:A:33:LEU:HD23	1.96	0.46
1:B:149:LEU:O	1:B:153:VAL:HG22	2.16	0.46
1:B:184:TYR:CZ	1:B:230:LEU:HD13	2.49	0.46
1:B:241:THR:HG22	1:B:242:ARG:HG3	1.98	0.46
1:B:105:VAL:O	1:B:105:VAL:HG12	2.15	0.46
1:A:195:THR:CB	1:B:135:GLU:HB3	2.45	0.46
1:A:178:LYS:O	1:A:183:HIS:N	2.44	0.46
1:A:209:GLN:NE2	1:A:215:GLU:HG3	2.31	0.46
1:B:18:GLU:O	1:B:21:ARG:HB3	2.15	0.46
1:A:80:TRP:CH2	1:A:311:LEU:HD22	2.51	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:88:ASP:OD1	1:B:109:VAL:HG13	2.14	0.46
1:B:1:SER:N	1:B:279:VAL:HG23	2.30	0.46
1:B:54:HIS:HA	1:B:59:GLU:O	2.15	0.46
1:A:181:ASP:O	1:A:182:LYS:HB2	2.15	0.46
1:A:139:HIS:CD2	1:B:196:ARG:HH22	2.33	0.46
1:A:300:THR:O	1:A:301:ARG:HG3	2.16	0.46
1:B:182:LYS:HD2	1:B:184:TYR:OH	2.14	0.46
1:B:104:GLN:HG3	1:B:232:LEU:CD1	2.45	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: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:B:21:ARG:HG2	1:B:57:TYR:CE1	2.50	0.46
1:B:198:LYS:NZ	2:B:335:HOH:O	2.47	0.46
1:B:72:ASP:HA	1:B:75:ARG:HB3	1.97	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
1:A:44:GLU:O	1:A:47:LYS:HB3	2.15	0.46
1:B:166:THR:O	1:B:170:GLN:HG3	2.16	0.46
1:B:150:VAL:O	1:B:153:VAL:HG22	2.15	0.46
1:A:231:ALA:HA	1:A:234:ARG:HD2	1.98	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:261:ASP:HB3	1:A:264:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:N	2:B:319:HOH:O	2.48	0.46
1:A:184:TYR:CE2	1:A:230:LEU:HD22	2.50	0.46
1:B:293:GLU:OE1	1:B:293:GLU:N	2.38	0.46
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:104:GLN:O	1:A:108:GLU:HB2	2.15	0.46
1:B:149:LEU:O	1:B:153:VAL:HG13	2.16	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:A:185:ASN:HD22	1:A:185:ASN:C	2.19	0.46
1:A:275:ILE:HG22	1:A:276:ASP:N	2.31	0.46
1:A:72:ASP:HB3	1:A:304:TYR:CD1	2.51	0.46
1:B:192:ILE:O	1:B:196:ARG:HB2	2.16	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:A:203:ALA:HA	1:A:206:ASN:HD22	1.81	0.46
1:A:173:LYS:O	1:A:176:HIS:HB3	2.16	0.46
1:B:12:ALA:HB1	1:B:13:PRO:HD2	1.96	0.46
1:B:138:ALA:O	1:B:146:ARG:HD3	2.16	0.46
1:B:4:LEU:HG	1:B:6:VAL:HG23	1.98	0.46
1:A:21:ARG:HD3	1:A:57:TYR:CD2	2.50	0.46
1:A:79:LEU:O	1:A:87:ARG:NE	2.49	0.46
1:B:151:SER:HB3	1:B:194:SER:OG	2.16	0.46
1:A:104:GLN:OE1	1:A:246:TYR:HE1	1.99	0.46
1:A:37:ILE:HA	1:A:41:ARG:NH1	2.27	0.46
1:B:84:PRO:O	1:B:88:ASP:HB2	2.16	0.46
1:A:109:VAL:O	1:A:113:ARG:HD3	2.16	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:B:296:ILE:CD1	1:B:312:LEU:HD11	2.43	0.46
1:A:247:PHE:HD1	1:A:268:ILE:HD12	1.80	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:A:155:SER:OG	1:A:157:ARG:HG3	2.16	0.46
1:A:168:ALA:O	1:A:204:THR:HG23	2.15	0.46
1:B:184:TYR:O	1:B:233:LEU:HD22	2.16	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:B:261:ASP:CG	1:B:264:ALA:HB2	2.36	0.46
1:A:134:GLU:CD	1:A:134:GLU:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ALA:HA	1:B:277:LEU:CB	2.45	0.46
1:A:193:LEU:HD12	1:A:233:LEU:CD1	2.45	0.46
1:B:113:ARG:N	1:B:113:ARG:HD2	2.30	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: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
1:A:192:ILE:HG23	1:A:196:ARG:HG3	1.98	0.45
1:A:87:ARG:CD	1:A:271:THR:HG22	2.44	0.45
1:B:248:VAL:HG13	1:B:284:TYR:HA	1.98	0.45
1:A:303:ASP:HA	1:A:306:LYS:HD3	1.97	0.45
1:A:171:GLU:HB3	1:A:192:ILE:HD13	1.98	0.45
1:A:173:LYS:O	1:A:177:GLU:HB2	2.15	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: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:109:VAL:HA	1:B:113:ARG:HE	1.82	0.45
1:B:293:GLU:HG2	1:B:294:LYS:H	1.81	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:304:TYR:O	1:A:308:LEU:HG	2.16	0.45
1:B:19:GLN:OE1	1:B:37:ILE:HD11	2.16	0.45
1:A:278:LYS:HE3	2:A:401:HOH:O	2.15	0.45
1:B:220:LEU:HB3	1:B:230:LEU:HD11	1.98	0.45
1:B:112:THR:HG22	1:B:243:PRO:CG	2.46	0.45
1:B:87:ARG:HD3	1:B:271:THR:HG22	1.99	0.45
1:A:139:HIS:HD2	2:B:334:HOH:O	1.99	0.45
1:A:188:ASP:O	1:A:192:ILE:HG13	2.15	0.45
1:B:71:ASN:OD1	1:B:73:PHE:N	2.46	0.45
1:A:187:GLU:HA	1:A:190:ILE:HD12	1.98	0.45
1:B:73:PHE:CZ	1:B:77:ILE:HD11	2.50	0.45
1:A:35:ILE:HD11	1:A:73:PHE:CE1	2.51	0.45
1:B:216:ILE:CG2	1:B:217:LEU:N	2.78	0.45
1:B:265:LEU:O	1:B:269:VAL:HG23	2.17	0.45
1:A:132:SER:OG	1:A:135:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:HA	2:A:452:HOH:O	2.15	0.45
1:A:165:MET:HE3	1:A:207:ARG:HD3	1.97	0.45
1:B:75:ARG:HE	1:B:79:LEU:CD1	2.26	0.45
1:A:14:SER:O	1:A:18:GLU:HG3	2.16	0.45
1:B:86:GLU:O	1:B:89:ALA:HB3	2.17	0.45
1:A:267:ARG:HD3	1:A:268:ILE:HD13	1.98	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: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:267:ARG:HB3	1:A:267:ARG:CZ	2.46	0.45
1:A:146:ARG:HG3	1:A:150:VAL:HG23	1.98	0.45
1:A:7:SER:C	1:A:9:SER:H	2.19	0.45
1:A:38:LEU:HD13	1:A:81:THR:OG1	2.17	0.45
1:B:106:LEU:CD2	1:B:149:LEU:HB3	2.45	0.45
1:A:158:TYR:CZ	1:A:160:GLY:HA3	2.51	0.45
1:A:19:GLN:HA	2:A:448:HOH:O	2.14	0.45
1:B:93:ASN:O	1:B:97:LYS:HG2	2.17	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:A:69:LEU:H	1:A:69:LEU:CD2	2.15	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:B:215:GLU:HB3	1:B:218:LYS:HG3	1.99	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:195:THR:HG22	1:B:134:GLU:HB3	1.97	0.45
1:A:267:ARG:HG3	1:A:271:THR:CG2	2.46	0.45
1:A:287:ARG:O	1:A:287:ARG:NH1	2.46	0.45
1:B:247:PHE:HD1	1:B:268:ILE:HD12	1.77	0.45
1:A:142:THR:O	1:A:145:PHE:HB2	2.17	0.45
1:B:111:CYS:HB3	1:B:240:LEU:HG	1.99	0.45
1:A:202:ASN:HD21	1:A:206:ASN:HD21	1.65	0.45
1:A:75:ARG:CZ	1:A:79:LEU:HD21	2.46	0.45
1:B:100:THR:OG1	1:B:101:SER:N	2.50	0.45
1:A:248:VAL:HG12	1:A:249:ASP:N	2.31	0.45
1:B:179:ILE:CD1	1:B:216:ILE:HD11	2.45	0.45
1:A:87:ARG:NH1	1:A:88:ASP:OD1	2.49	0.45
1:B:116:THR:C	1:B:118:LEU:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:HE	1:B:288:ASN:ND2	2.15	0.45
1:B:47:LYS:HE2	1:B:83:GLU:OE1	2.16	0.45
1:A:128:ARG:HB2	2:A:445:HOH:O	2.15	0.45
1:A:257:LYS:N	1:A:257:LYS:HD3	2.32	0.45
1:B:97:LYS:HE2	1:B:97:LYS:CA	2.45	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: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:50:ARG:HD2	1:A:81:THR:HG22	1.97	0.45
1:A:158:TYR:CZ	1:B:130:LYS:HA	2.52	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:B:264:ALA:O	1:B:268:ILE:HG12	2.16	0.45
1:B:290:ILE:HG23	1:B:290:ILE:O	2.15	0.45
1:B:62:LEU:HD21	1:B:81:THR:CG2	2.45	0.45
1:B:21:ARG:CZ	2:B:342:HOH:O	2.63	0.45
1:A:103:ASN:HB2	2:A:400:HOH:O	2.15	0.45
1:A:129:TYR:C	1:A:131:LYS:N	2.69	0.45
1:A:150:VAL:O	1:A:154:THR:OG1	2.16	0.45
1:A:239:CYS:O	1:A:243:PRO:HG3	2.16	0.45
1:A:276:ASP:O	1:A:278:LYS:N	2.49	0.45
1:A:76:ALA:HA	1:A:266:THR:CG2	2.47	0.45
1:B:1:SER:HB2	1:B:275:ILE:O	2.16	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:47:LYS:HE2	1:B:83:GLU:OE2	2.15	0.45
1:B:86:GLU:O	1:B:89:ALA:HB3	2.17	0.45
1:A:119:LEU:O	1:A:123:GLN:HG3	2.17	0.45
1:B:237:ILE:O	1:B:237:ILE:HG22	2.15	0.45
1:A:10:VAL:CG1	1:A:11:PRO:HD2	2.45	0.45
1:A:112:THR:HG21	1:A:247:PHE:CE2	2.51	0.45
1:A:79:LEU:HD23	1:A:79:LEU:N	2.32	0.45
1:B:262:GLU:HB3	2:B:379:HOH:O	2.17	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:B:184:TYR:HB3	1:B:233:LEU:HD22	1.99	0.45
1:A:134:GLU:HG3	1:A:154:THR:CG2	2.47	0.45
1:A:282:GLU:O	1:A:285:GLN:HB2	2.17	0.45
1:A:35:ILE:HD11	1:A:307:MET:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:THR:HG22	1:B:239:CYS:HB3	1.98	0.45
1:A:7:SER:O	1:A:10:VAL:HG23	2.16	0.45
1:A:3:THR:OG1	1:A:277:LEU:HD23	2.16	0.45
1:A:37:ILE:O	1:A:41:ARG:HG2	2.16	0.45
1:B:293:GLU:CB	1:B:314:GLU:HG3	2.47	0.45
1:A:298:LYS:HG2	1:A:299:ASP:N	2.32	0.45
1:A:7:SER:C	1:A:9:SER:N	2.70	0.45
1:B:76:ALA:HA	1:B:266:THR:CG2	2.47	0.45
1:B:87:ARG:HH12	1:B:271:THR:HA	1.76	0.45
1:B:71:ASN:OD1	1:B:73:PHE:N	2.49	0.45
1:B:95:ALA:O	1:B:99:TRP:HB2	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:B:14:SER:O	1:B:18:GLU:HG3	2.16	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:B:18:GLU:HA	1:B:57:TYR:CE2	2.51	0.45
1:B:41:ARG:HD2	1:B:49:ILE:CD1	2.47	0.45
1:A:112:THR:HG22	1:A:239:CYS:O	2.16	0.45
1:A:12:ALA:HB3	1:A:15:ASP:OD2	2.17	0.45
1:B:125:TYR:CG	1:B:133:LEU:HB2	2.51	0.45
2:A:327:HOH:O	1:B:196:ARG:HB3	2.17	0.45
1:A:134:GLU:HB3	1:B:195:THR:HG22	1.98	0.45
1:B:192:ILE:HG23	1:B:196:ARG:HG3	1.99	0.45
1:B:36:SER:HA	1:B:40:HIS:CE1	2.52	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: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:142:THR:O	1:B:145:PHE:HB2	2.17	0.45
1:B:141:THR:OG1	1:B:146:ARG:HB2	2.17	0.45
1:B:216:ILE:CG2	1:B:217:LEU:N	2.80	0.45
1:B:285:GLN:HG3	1:B:290:ILE:N	2.32	0.45
1:A:25:GLU:HB3	2:A:441:HOH:O	2.16	0.44
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.82	0.44
1:B:72:ASP:HB3	1:B:304:TYR:CD1	2.53	0.44
1:A:89:ALA:HB2	1:A:124:ALA:HB3	1.99	0.44
1:A:304:TYR:CE1	1:A:308:LEU:HD11	2.51	0.44
1:B:261:ASP:OD2	1:B:264:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ALA:O	1:B:99:TRP:HB2	2.17	0.44
1:A:144:ASP:HA	1:A:147:LYS:CG	2.48	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
1:B:71:ASN:ND2	1:B:73:PHE:HB3	2.25	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:66:ASP:HA	1:B:78:LEU:HD13	1.98	0.44
1:A:93:ASN:HB2	1:A:129:TYR:CE2	2.52	0.44
1:B:256:ASN:C	1:B:258:THR:H	2.21	0.44
1:A:217:LEU:HD11	1:A:238:GLN:HG2	1.99	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: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:157:ARG:CB	2:B:319:HOH:O	2.65	0.44
1:B:261:ASP:CG	1:B:267:ARG:HH22	2.20	0.44
1:A:233:LEU:O	1:A:237:ILE:HG13	2.17	0.44
1:B:128:ARG:HG2	1:B:128:ARG:O	2.17	0.44
1:A:118:LEU:O	1:A:118:LEU:HD12	2.17	0.44
1:B:10:VAL:HG21	1:B:45:GLN:NE2	2.30	0.44
1:A:191:ARG:HH12	1:A:196:ARG:NH2	2.15	0.44
1:A:227:ASP:OD1	1:A:230:LEU:HB2	2.17	0.44
1:A:92:ALA:CB	1:A:106:LEU:HD23	2.48	0.44
1:B:165:MET:CE	1:B:207:ARG:HD3	2.47	0.44
1:B:109:VAL:HG13	1:B:113:ARG:HE	1.81	0.44
1:B:236:THR:O	1:B:240:LEU:HG	2.18	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: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:244:GLU:O	1:B:248:VAL:HG23	2.18	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:A:293:GLU:HB2	1:A:317:ALA:OXT	2.17	0.44
1:A:302:GLY:HA3	2:A:378:HOH:O	2.15	0.44
1:B:71:ASN:OD1	1:B:72:ASP:N	2.51	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:B:150:VAL:O	1:B:153:VAL:N	2.50	0.44
1:B:169:LYS:HD2	1:B:207:ARG:HH21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HG3	1:A:299:ASP:OD1	2.17	0.44
1:A:176:HIS:NE2	1:A:180:LYS:HE2	2.32	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:B:261:ASP:OD1	1:B:267:ARG:NH2	2.50	0.44
1:B:158:TYR:O	1:B:197:SER:HB2	2.18	0.44
1:B:16:ASP:OD1	1:B:37:ILE:HD13	2.18	0.44
1:A:10:VAL:HG13	1:A:11:PRO:HD2	2.00	0.44
1:A:271:THR:O	1:A:272:ARG:HD2	2.17	0.44
1:A:51:GLN:C	1:A:53:TYR:N	2.69	0.44
1:A:154:THR:HB	1:B:154:THR:O	2.18	0.44
1:B:107:MET:SD	1:B:107:MET:C	2.96	0.44
1:B:165:MET:CE	1:B:207:ARG:HD3	2.47	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:144:ASP:O	1:A:147:LYS:HB2	2.17	0.44
1:B:51:GLN:HE21	1:B:55:GLU:HG3	1.82	0.44
1:A:168:ALA:CB	1:A:207:ARG:HG3	2.45	0.44
1:A:10:VAL:HG13	1:A:41:ARG:NE	2.32	0.44
1:A:130:LYS:HD2	1:B:158:TYR:OH	2.17	0.44
1:A:291:PRO:HB2	1:A:293:GLU:CD	2.38	0.44
1:A:15:ASP:OD1	1:A:18:GLU:OE1	2.35	0.44
1:B:73:PHE:CZ	1:B:77:ILE:HD11	2.53	0.44
1:A:218:LYS:HG2	1:A:221:GLU:OE2	2.18	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:171:GLU:HB3	1:A:192:ILE:HD11	2.00	0.44
1:B:198:LYS:O	1:B:201:ILE:HB	2.17	0.44
1:A:117:GLN:HE22	1:A:275:ILE:HD11	1.81	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:A:108:GLU:HB2	1:A:246:TYR:OH	2.16	0.44
1:B:44:GLU:O	1:B:48:VAL:HG23	2.17	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: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:41:ARG:O	1:A:46:ARG:HG3	2.17	0.44
1:B:35:ILE:HG12	1:B:307:MET:HB2	1.99	0.44
1:A:207:ARG:NE	2:A:397:HOH:O	2.51	0.44
1:B:103:ASN:HB2	2:B:368:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:SER:O	1:B:118:LEU:HB3	2.18	0.44
1:B:128:ARG:HD3	1:B:129:TYR:CE2	2.52	0.44
1:B:158:TYR:CZ	1:B:160:GLY:HA3	2.52	0.44
1:B:167:LEU:HA	1:B:170:GLN:NE2	2.33	0.44
1:B:261:ASP:CG	1:B:267:ARG:HH22	2.20	0.44
1:A:109:VAL:O	1:A:113:ARG:HD3	2.17	0.44
1:A:191:ARG:HH12	1:A:196:ARG:HH21	1.66	0.44
1:A:298:LYS:HG3	2:A:415:HOH:O	2.17	0.44
1:B:248:VAL:HG21	1:B:283:GLU:CB	2.45	0.44
1:B:65:LEU:HD23	1:B:74:GLU:HB3	1.99	0.44
1:B:36:SER:O	1:B:40:HIS:ND1	2.51	0.44
1:A:106:LEU:HB2	1:A:149:LEU:HD13	1.98	0.44
1:A:70:SER:OG	1:A:75:ARG:HB2	2.17	0.44
1:B:256:ASN:C	1:B:257:LYS:HD3	2.38	0.44
1:B:298:LYS:HG2	1:B:299:ASP:CG	2.38	0.44
1:A:286:ARG:NH2	2:A:363:HOH:O	2.46	0.44
1:B:129:TYR:O	1:B:131:LYS:HG3	2.18	0.44
1:B:178:LYS:HG3	1:B:186:ASP:CG	2.38	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:B:182:LYS:O	1:B:184:TYR:N	2.45	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:A:186:ASP:O	1:A:190:ILE:HG13	2.18	0.44
1:A:214:GLU:HG3	1:A:219:SER:HB2	1.99	0.44
1:A:278:LYS:HE3	1:A:282:GLU:OE2	2.18	0.44
1:B:247:PHE:CD1	1:B:268:ILE:HG23	2.53	0.44
1:A:242:ARG:HG3	1:A:244:GLU:CD	2.37	0.44
1:A:34:ILE:HG21	1:A:77:ILE:HD13	2.00	0.44
1:B:126:HIS:ND1	1:B:131:LYS:O	2.51	0.44
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.82	0.44
1:B:238:GLN:HE22	1:B:245:LEU:HD12	1.82	0.44
1:B:304:TYR:CZ	1:B:308:LEU:HD11	2.53	0.44
1:B:31:GLU:N	1:B:31:GLU:OE1	2.51	0.44
1:B:166:THR:O	1:B:170:GLN:HG3	2.17	0.44
1:B:298:LYS:O	1:B:300:THR:N	2.51	0.44
1:B:65:LEU:O	1:B:78:LEU:HB2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:O	1:A:126:HIS:C	2.56	0.44
1:A:192:ILE:O	1:A:196:ARG:HB2	2.18	0.44
1:A:300:THR:O	1:A:305:GLU:HG2	2.18	0.44
1:A:3:THR:HG23	1:A:277:LEU:HB3	1.99	0.44
1:A:304:TYR:O	1:A:308:LEU:HG	2.18	0.44
1:A:50:ARG:CZ	1:A:62:LEU:HD12	2.48	0.44
1:A:98:ARG:HE	1:A:98:ARG:HA	1.82	0.44
1:B:134:GLU:CG	1:B:154:THR:HG22	2.48	0.44
1:B:165:MET:HE2	1:B:165:MET:HB3	1.78	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:A:158:TYR:CA	2:A:366:HOH:O	2.63	0.43
1:A:144:ASP:HA	1:A:147:LYS:HZ1	1.81	0.43
1:B:301:ARG:HG2	2:B:404:HOH:O	2.18	0.43
1:B:218:LYS:HA	1:B:221:GLU:HG3	2.00	0.43
1:B:47:LYS:HE2	1:B:83:GLU:OE1	2.18	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:215:GLU:HG3	1:B:217:LEU:H	1.83	0.43
1:B:244:GLU:N	1:B:244:GLU:OE1	2.51	0.43
1:B:33:LEU:O	1:B:33:LEU:HG	2.18	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:62:LEU:O	1:B:66:ASP:HB2	2.17	0.43
1:A:38:LEU:HD12	1:A:77:ILE:HD12	1.99	0.43
1:B:75:ARG:CZ	1:B:79:LEU:HD11	2.48	0.43
1:A:98:ARG:CA	1:A:98:ARG:HE	2.28	0.43
1:A:11:PRO:CG	1:A:41:ARG:HH21	2.31	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:193:LEU:HD22	1:A:240:LEU:HD12	2.00	0.43
1:A:195:THR:OG1	1:B:135:GLU:HB3	2.18	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: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:B:233:LEU:O	1:B:236:THR:HB	2.18	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:A:114:THR:HB	1:A:159:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASP:OD1	1:A:185:ASN:HB2	2.18	0.43
1:B:117:GLN:NE2	2:B:377:HOH:O	2.51	0.43
1:B:202:ASN:HD21	1:B:206:ASN:HD21	1.65	0.43
1:B:252:ARG:HA	1:B:284:TYR:HE1	1.83	0.43
1:A:99:TRP:CZ2	1:A:101:SER:HA	2.53	0.43
1:A:158:TYR:CE1	1:B:130:LYS:HA	2.53	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: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:248:VAL:HG21	1:A:283:GLU:CB	2.48	0.43
1:A:72:ASP:HB3	1:A:304:TYR:CG	2.53	0.43
1:B:294:LYS:HB3	1:B:294:LYS:HE2	1.89	0.43
1:B:86:GLU:HA	1:B:124:ALA:HB1	1.99	0.43
1:A:107:MET:HG2	1:A:111:CYS:SG	2.58	0.43
1:B:146:ARG:HG3	1:B:150:VAL:HG21	1.99	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:A:287:ARG:O	1:A:287:ARG:NH1	2.41	0.43
1:B:161:ASP:O	1:B:163:VAL:HG23	2.17	0.43
1:B:71:ASN:OD1	1:B:73:PHE:N	2.51	0.43
1:A:70:SER:HB2	1:A:74:GLU:HB2	2.00	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:18:GLU:O	1:B:21:ARG:HB3	2.19	0.43
1:B:255:ILE:C	1:B:257:LYS:N	2.71	0.43
1:A:107:MET:SD	1:A:107:MET:C	2.96	0.43
1:A:184:TYR:CE2	1:A:230:LEU:HD13	2.54	0.43
1:A:264:ALA:O	1:A:268:ILE:HG12	2.17	0.43
1:B:130:LYS:O	1:B:131:LYS:HB3	2.19	0.43
1:B:277:LEU:CD2	1:B:312:LEU:HD23	2.45	0.43
1:B:65:LEU:HD23	1:B:74:GLU:CB	2.48	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:51:GLN:N	1:B:51:GLN:CD	2.71	0.43
1:B:75:ARG:NH1	1:B:79:LEU:HD11	2.33	0.43
1:A:107:MET:HB2	1:A:232:LEU:HD11	2.00	0.43
1:B:267:ARG:HH11	1:B:268:ILE:HD11	1.84	0.43
1:A:143:GLY:HA2	2:A:319:HOH:O	2.19	0.43
1:A:43:ALA:N	1:A:46:ARG:NH1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HB2	1:A:46:ARG:HG2	2.01	0.43
1:A:50:ARG:NH2	1:A:62:LEU:HD12	2.33	0.43
1:A:64:THR:HG23	1:A:65:LEU:HG	2.01	0.43
1:B:13:PRO:HG3	1:B:48:VAL:HG12	1.99	0.43
1:A:4:LEU:HD22	1:A:274:GLU:HG2	2.00	0.43
1:B:73:PHE:HD1	1:B:304:TYR:HA	1.84	0.43
1:B:298:LYS:HB3	1:B:298:LYS:HE2	1.80	0.43
1:B:77:ILE:HD13	1:B:307:MET:HG2	2.00	0.43
1:B:169:LYS:HG2	1:B:173:LYS:HZ3	1.83	0.43
1:A:200:GLN:O	1:A:200:GLN:HG3	2.18	0.43
1:B:215:GLU:HB3	1:B:218:LYS:CG	2.42	0.43
1:B:244:GLU:HG2	1:B:245:LEU:H	1.84	0.43
1:B:303:ASP:N	1:B:306:LYS:HZ3	2.17	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: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:B:87:ARG:HD2	2:B:322:HOH:O	2.18	0.43
1:B:20:LEU:HD13	1:B:61:LEU:CD1	2.48	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:132:SER:CA	2:B:318:HOH:O	2.66	0.43
1:A:108:GLU:OE1	1:A:246:TYR:OH	2.35	0.43
1:B:17:ALA:HB1	1:B:53:TYR:HB2	2.00	0.43
1:B:284:TYR:CD2	1:B:292:LEU:HB2	2.53	0.43
1:A:130:LYS:HA	1:B:158:TYR:CE1	2.53	0.43
1:A:290:ILE:H	1:A:290:ILE:CD1	2.30	0.43
1:B:34:ILE:HG22	1:B:38:LEU:HD12	1.99	0.43
1:B:51:GLN:HG3	1:B:55:GLU:OE2	2.19	0.43
1:B:247:PHE:CD1	1:B:268:ILE:HD12	2.53	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:67:LYS:HB2	1:A:69:LEU:CD2	2.49	0.43
1:A:100:THR:C	1:A:102:SER:H	2.21	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:B:297:THR:HG21	1:B:317:ALA:OXT	2.18	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:101:SER:HB3	1:B:145:PHE:CZ	2.53	0.43
1:A:220:LEU:C	1:A:222:GLU:H	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:265:LEU:HD21	1:B:296:ILE:HD13	2.00	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:B:298:LYS:HG2	1:B:299:ASP:N	2.34	0.43
1:A:129:TYR:O	1:A:131:LYS:N	2.51	0.43
1:A:216:ILE:CG2	1:A:217:LEU:N	2.81	0.43
1:A:288:ASN:O	1:A:289:SER:HB2	2.19	0.43
1:A:111:CYS:SG	1:A:240:LEU:HD21	2.59	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: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
1:A:105:VAL:HG22	1:A:267:ARG:NH2	2.33	0.43
1:B:246:TYR:O	1:B:250:VAL:HG23	2.19	0.43
1:B:278:LYS:O	1:B:282:GLU:HG3	2.18	0.43
1:B:298:LYS:HG2	1:B:299:ASP:OD1	2.18	0.43
1:A:209:GLN:HG3	1:A:215:GLU:CA	2.49	0.43
1:A:278:LYS:C	1:A:280:ILE:N	2.72	0.43
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:122:ARG:NH1	1:A:154:THR:HA	2.34	0.43
1:A:41:ARG:HA	1:A:45:GLN:OE1	2.19	0.43
1:A:71:ASN:HD22	1:A:74:GLU:HG3	1.83	0.43
1:A:288:ASN:O	1:A:289:SER:CB	2.66	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:216:ILE:HG23	1:A:217:LEU:H	1.82	0.43
1:A:297:THR:O	1:A:299:ASP:N	2.51	0.43
1:A:107:MET:HB2	1:A:232:LEU:HD11	2.00	0.43
1:A:205:PHE:CE1	1:A:216:ILE:HD13	2.54	0.43
1:A:67:LYS:HB2	1:A:69:LEU:CD2	2.49	0.43
1:A:62:LEU:HD21	1:A:81:THR:HG21	2.00	0.43
1:B:150:VAL:O	1:B:154:THR:OG1	2.21	0.43
1:B:179:ILE:CD1	1:B:216:ILE:HD11	2.49	0.43
1:B:275:ILE:HG22	1:B:276:ASP:N	2.34	0.43
1:A:50:ARG:HE	1:A:60:ASP:CG	2.20	0.43
1:A:7:SER:C	1:A:9:SER:N	2.72	0.43
1:B:223:GLY:HA3	1:B:230:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ALA:O	1:A:202:ASN:HB3	2.19	0.43
1:B:175:VAL:O	1:B:179:ILE:HG13	2.19	0.43
1:A:248:VAL:CG2	1:A:283:GLU:HB3	2.48	0.43
1:B:293:GLU:CG	1:B:314:GLU:HG3	2.48	0.43
1:A:135:GLU:O	1:A:139:HIS:CB	2.65	0.43
1:A:14:SER:O	1:A:17:ALA:HB3	2.19	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:B:34:ILE:CG2	1:B:38:LEU:HD12	2.48	0.43
1:A:200:GLN:O	1:A:203:ALA:N	2.52	0.43
1:B:129:TYR:O	1:B:131:LYS:HG3	2.19	0.43
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: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
1:A:24:PHE:CZ	1:A:61:LEU:HD11	2.54	0.42
1:B:131:LYS:HD3	1:B:136:ASP:OD1	2.18	0.42
1:B:82:LEU:HD11	1:B:90:LEU:HD22	2.01	0.42
1:A:157:ARG:HG2	1:A:197:SER:HA	2.00	0.42
1:A:176:HIS:HB2	1:A:208:TYR:CE2	2.54	0.42
1:B:99:TRP:CG	1:B:100:THR:N	2.86	0.42
1:B:139:HIS:HB3	1:B:140:HIS:CE1	2.54	0.42
1:B:162:GLU:N	1:B:162:GLU:OE1	2.52	0.42
1:A:24:PHE:CE2	1:A:61:LEU:HD11	2.54	0.42
1:A:215:GLU:OE2	1:A:217:LEU:HD12	2.19	0.42
1:A:247:PHE:CD1	1:A:268:ILE:HG23	2.55	0.42
1:A:229:PHE:O	1:A:232:LEU:HB3	2.18	0.42
1:B:178:LYS:HG3	1:B:186:ASP:CG	2.39	0.42
1:A:19:GLN:HG2	2:A:390:HOH:O	2.18	0.42
1:B:11:PRO:HG3	1:B:41:ARG:HH21	1.84	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:236:THR:HG22	1:A:236:THR: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:B:53:TYR:C	1:B:53:TYR:CD1	2.92	0.42
1:A:128:ARG:HD3	1:A:129:TYR:CE2	2.55	0.42
1:A:164:ASN:N	1:A:200:GLN:OE1	2.50	0.42
1:A:44:GLU:O	1:A:47:LYS:HB3	2.19	0.42
1:B:286:ARG:NH1	1:B:286:ARG:HG2	2.34	0.42
1:A:265:LEU:CD2	1:A:308:LEU:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ARG:CG	1:B:117:GLN:HB3	2.50	0.42
1:A:37:ILE:HG23	1:A:41:ARG:NH1	2.33	0.42
1:A:261:ASP:O	1:A:262:GLU:C	2.57	0.42
1:B:18:GLU:HA	1:B:57:TYR:OH	2.19	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:33:LEU:O	1:B:37:ILE:HG13	2.19	0.42
1:A:21:ARG:HG2	1:A:57:TYR:CZ	2.54	0.42
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:33:LEU:O	1:B:37:ILE:HG13	2.19	0.42
1:A:105:VAL:HG22	1:A:267:ARG:HH12	1.84	0.42
1:B:157:ARG:CA	2:B:361:HOH:O	2.60	0.42
1:B:230:LEU:HG	1:B:234:ARG:HD2	2.01	0.42
1:B:108:GLU:OE2	1:B:267:ARG:HD2	2.19	0.42
1:A:246:TYR:O	1:A:250:VAL:HG23	2.19	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: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:284:TYR:O	1:B:288:ASN:HB2	2.19	0.42
1:A:293:GLU:HA	1:A:296:ILE:HD12	2.01	0.42
1:A:35:ILE:HD12	1:A:307:MET:SD	2.59	0.42
1:B:132:SER:OG	1:B:135:GLU:N	2.51	0.42
1:A:72:ASP:HB3	1:A:304:TYR:CD1	2.54	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:3:THR:HB	1:B:312:LEU:O	2.20	0.42
1:B:65:LEU:HD22	1:B:74:GLU:CG	2.50	0.42
1:A:246:TYR:C	1:A:248:VAL:H	2.22	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:130:LYS:HB3	1:B:162:GLU:OE2	2.19	0.42
1:A:185:ASN:C	1:A:185:ASN:ND2	2.73	0.42
1:A:71:ASN:OD1	1:A:74:GLU:HG3	2.18	0.42
1:B:218:LYS:O	1:B:221:GLU:HB2	2.18	0.42
1:A:161:ASP:OD1	1:A:199:ALA:HB2	2.19	0.42
1:A:186:ASP:HB3	1:A:189:VAL:CG2	2.48	0.42
1:A:22:THR:O	1:A:25:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:OD1	1:A:276:ASP:N	2.51	0.42
1:A:35:ILE:HG23	1:A:307:MET:HA	2.02	0.42
1:B:18:GLU:O	1:B:21:ARG:HB3	2.20	0.42
1:B:54:HIS:O	1:B:56:THR:N	2.50	0.42
1:A:298:LYS:HE2	1:A:298:LYS:HB3	1.80	0.42
1:A:61:LEU:O	1:A:64:THR:HG22	2.20	0.42
1:B:119:LEU:O	1:B:122:ARG:N	2.52	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: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: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:B:304:TYR:CZ	1:B:308:LEU:HD11	2.54	0.42
1:B:75:ARG:HH11	1:B:75:ARG:HG2	1.84	0.42
1:A:105:VAL:HG22	1:A:267:ARG:NH1	2.34	0.42
1:A:118:LEU:O	1:A:122:ARG:HB2	2.20	0.42
1:A:286:ARG:NH2	2:A:366:HOH:O	2.53	0.42
1:B:235:SER:O	1:B:238:GLN:HB2	2.19	0.42
1:B:300:THR:CG2	1:B:301:ARG:H	2.29	0.42
1:B:56:THR:O	1:B:57:TYR:CG	2.72	0.42
1:A:154:THR:HB	1:B:154:THR:HB	2.00	0.42
1:A:204:THR:HG22	1:A:204:THR:O	2.19	0.42
1:B:134:GLU:HG3	1:B:154:THR:HG22	2.01	0.42
1:B:150:VAL:O	1:B:154:THR:HG23	2.19	0.42
1:A:122:ARG:HD2	1:A:153:VAL:O	2.19	0.42
1:A:148:LEU:HD13	1:A:229:PHE:CE1	2.55	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:168:ALA:HB1	1:A:204:THR:HA	2.00	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: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: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:B:216:ILE:HG23	1:B:217:LEU:N	2.34	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:A:157:ARG:HH12	1:A:194:SER:HA	1.84	0.42
1:A:303:ASP:CA	1:A:306:LYS:HD3	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:NH2	1:B:156:TYR:CB	2.82	0.42
1:A:72:ASP:HB3	1:A:304:TYR:CE1	2.54	0.42
1:A:122:ARG:O	1:A:123:GLN:C	2.58	0.42
1:A:158:TYR:OH	1:B:130:LYS:NZ	2.52	0.42
1:A:191:ARG:HD2	1:B:138:ALA:HB1	2.02	0.42
1:A:112:THR:HG21	1:A:247:PHE:CZ	2.54	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:168:ALA:O	1:A:172:ALA:HB2	2.19	0.42
1:A:218:LYS:HA	1:A:221:GLU:OE2	2.20	0.42
1:A:250:VAL:HG11	1:A:268:ILE:HD11	2.00	0.42
1:A:307:MET:O	1:A:311:LEU:HG	2.19	0.42
1:A:215:GLU:HG3	2:A:363:HOH:O	2.19	0.42
1:A:304:TYR:CZ	1:A:308:LEU:HD11	2.55	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:133:LEU:O	1:A:137:VAL:HG23	2.20	0.42
1:A:98:ARG:CA	1:A:98:ARG:HE	2.31	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:B:272:ARG:HH21	1:B:276:ASP:CG	2.23	0.42
1:A:72:ASP:HB3	1:A:304:TYR:CD1	2.55	0.42
1:B:216:ILE:CG2	1:B:217:LEU:N	2.82	0.42
1:B:251:LEU:O	1:B:255:ILE:HG13	2.20	0.42
1:B:91:LEU:O	1:B:94:GLU:HG2	2.19	0.42
1:A:46:ARG:O	1:A:50:ARG:HG3	2.20	0.42
1:B:245:LEU:O	1:B:248:VAL:N	2.52	0.42
1:A:33:LEU:C	1:A:33:LEU:HD23	2.40	0.42
1:B:131:LYS:HZ1	1:B:135:GLU:CD	2.23	0.42
1:B:178:LYS:O	1:B:180:LYS:N	2.52	0.42
1:A:126:HIS:HE1	1:A:132:SER:HB3	1.85	0.42
1:A:7:SER:O	1:A:9:SER:N	2.53	0.42
1:B:16:ASP:OD1	1:B:37:ILE:HD13	2.20	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:B:294:LYS:HA	1:B:297:THR:HG22	2.02	0.42
1:B:302:GLY:O	1:B:306:LYS:HG3	2.19	0.42
1:A:264:ALA:O	1:A:268:ILE:HG12	2.19	0.42
1:A:35:ILE:HG13	1:A:73:PHE:CE1	2.54	0.42
2:A:362:HOH:O	1:B:126:HIS:CD2	2.72	0.42
1:A:244:GLU:OE1	1:A:245:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LYS:HB3	1:B:135:GLU:CD	2.40	0.42
1:B:301:ARG:HG2	1:B:301:ARG:O	2.20	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:B:304:TYR:CZ	1:B:308:LEU:HD11	2.54	0.42
1:B:13:PRO:HB2	1:B:52:ALA:HB2	2.02	0.42
1:A:132:SER:O	1:A:133:LEU:C	2.58	0.42
1:A:65:LEU:HD13	1:A:77:ILE:HB	2.01	0.42
1:B:196:ARG:HB2	1:B:201:ILE:HG13	2.02	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:38:LEU:O	1:B:46:ARG:HD3	2.20	0.42
1:A:148:LEU:C	1:A:148:LEU:HD23	2.40	0.42
1:B:287:ARG:O	1:B:287:ARG:HG3	2.19	0.42
1:B:281:GLY:O	1:B:285:GLN:N	2.49	0.42
1:B:294:LYS:HE2	1:B:294:LYS:HB3	1.90	0.42
1:B:298:LYS:HB3	1:B:298:LYS:HE2	1.84	0.42
1:A:200:GLN:OE1	2:A:327:HOH:O	2.21	0.42
1:B:150:VAL:O	1:B:154:THR:HG23	2.19	0.42
1:A:188:ASP:O	1:A:192:ILE:HG13	2.20	0.42
1:B:125:TYR:HD1	1:B:131:LYS:O	2.03	0.41
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: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: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: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: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:71:ASN:HD22	1:B:74:GLU:CG	2.28	0.41
1:A:167:LEU:O	1:A:171:GLU:HB2	2.19	0.41
1:B:108:GLU:OE1	1:B:267:ARG:NH1	2.53	0.41
1:B:72:ASP:CG	1:B:72:ASP:O	2.57	0.41
1:A:115:SER:O	1:A:118:LEU:HB3	2.20	0.41
1:A:135:GLU:HB2	1:B:196:ARG:HD3	2.02	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:213:GLY:O	1:A:214:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:LEU:O	1:A:64:THR:N	2.52	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:103:ASN:HA	2:A:442:HOH:O	2.21	0.41
1:A:252:ARG:HH21	1:A:287:ARG:HG3	1.84	0.41
1:B:87:ARG:NH1	2:B:322:HOH:O	2.28	0.41
1:A:87:ARG:CD	1:A:271:THR:HG22	2.50	0.41
1:A:301:ARG:HD2	2:A:371:HOH:O	2.20	0.41
1:B:186:ASP:O	1:B:187:GLU:C	2.58	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: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:126:HIS:HA	1:A:131:LYS:O	2.20	0.41
1:A:171:GLU:O	1:A:175:VAL:HG23	2.20	0.41
1:A:1:SER:HA	1:A:278:LYS:HB3	2.02	0.41
1:A:205:PHE:HA	1:A:208:TYR:HB3	2.02	0.41
1:A:107:MET:HE3	1:A:239:CYS:HB2	2.02	0.41
1:A:65:LEU:O	1:A:78:LEU:HD13	2.21	0.41
1:B:251:LEU:O	1:B:254:ALA:HB3	2.20	0.41
1:A:3:THR:HG23	1:A:278:LYS:N	2.35	0.41
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:87:ARG:CD	1:B:271:THR:HG22	2.47	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: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:67:LYS:HE2	1:A:69:LEU:HG	2.01	0.41
1:B:192:ILE:C	1:B:201:ILE:HD11	2.41	0.41
1:A:274:GLU:HB2	2:A:322:HOH:O	2.19	0.41
1:B:131:LYS:HB3	1:B:132:SER:H	1.69	0.41
1:B:264:ALA:HA	1:B:267:ARG:NH1	2.35	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:A:242:ARG:HB3	1:A:244:GLU:OE1	2.20	0.41
1:B:104:GLN:C	1:B:106:LEU:N	2.73	0.41
1:B:242:ARG:HD3	1:B:245:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:C	1:B:40:HIS:H	2.23	0.41
1:A:292:LEU:O	1:A:296:ILE:HG13	2.21	0.41
1:A:198:LYS:HG2	2:A:331:HOH:O	2.19	0.41
1:A:70:SER:HB2	1:A:74:GLU:OE1	2.19	0.41
1:A:96:THR:HB	1:A:140:HIS:CD2	2.56	0.41
1:B:202:ASN:O	1:B:206:ASN:N	2.54	0.41
1:B:31:GLU:N	1:B:31:GLU:OE1	2.53	0.41
1:B:167:LEU:HD21	1:B:196:ARG:CZ	2.50	0.41
1:B:35:ILE:HG23	1:B:307:MET:HA	2.03	0.41
1:A:157:ARG:NH2	1:A:240:LEU:HD21	2.35	0.41
1:B:61:LEU:HD23	1:B:62:LEU:CD2	2.49	0.41
1:A:118:LEU:O	1:A:119:LEU:C	2.58	0.41
1:B:22:THR:O	1:B:22:THR:HG22	2.21	0.41
1:A:226:ASP:HB3	1:A:228:LYS:HZ1	1.84	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:B:223:GLY:HA3	1:B:230:LEU:HD21	2.03	0.41
1:A:132:SER:HG	1:A:135:GLU:HB3	1.84	0.41
1:A:207:ARG:CZ	2:A:398:HOH:O	2.68	0.41
1:A:255:ILE:O	1:A:257:LYS:HD3	2.21	0.41
1:B:49:ILE:O	1:B:52:ALA:HB3	2.21	0.41
1:A:193:LEU:HA	1:A:201:ILE:HD13	2.02	0.41
1:B:179:ILE:HD12	1:B:184:TYR:CD1	2.55	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:A:298:LYS:HE2	1:A:298:LYS:HB3	1.79	0.41
1:B:244:GLU:N	1:B:244:GLU:OE1	2.38	0.41
1:A:42:SER:C	1:A:46:ARG:NH1	2.74	0.41
1:B:277:LEU:O	1:B:280:ILE:HB	2.20	0.41
1:B:248:VAL:HG22	1:B:284:TYR:HB2	2.02	0.41
1:A:43:ALA:C	1:A:45:GLN:H	2.23	0.41
1:B:12:ALA:O	1:B:15:ASP:HB2	2.20	0.41
1:B:205:PHE:CE1	1:B:216:ILE:HG12	2.56	0.41
1:B:76:ALA:HA	1:B:266:THR:HG21	2.02	0.41
1:A:138:ALA:O	1:A:139:HIS:HB2	2.20	0.41
1:B:230:LEU:HG	1:B:234:ARG:CD	2.51	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:B:273:ALA:HA	1:B:277:LEU:CD2	2.50	0.41
1:A:186:ASP:O	1:A:189:VAL:HB	2.20	0.41
1:A:293:GLU:HG2	1:A:294:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:CG	1:B:196:ARG:HH11	2.34	0.41
1:B:238:GLN:HG3	1:B:238:GLN:O	2.20	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:107:MET:HB3	1:A:107:MET:HE2	1.89	0.41
1:A:297:THR:HB	1:A:301:ARG:CD	2.50	0.41
1:A:69:LEU:CD1	1:A:69:LEU:H	2.34	0.41
1:A:72:ASP:HB3	1:A:304:TYR:CE1	2.55	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:79:LEU:O	1:A:87:ARG:NE	2.53	0.41
1:A:215:GLU:HG2	1:A:216:ILE:N	2.36	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: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:A:256:ASN:O	1:A:257:LYS:HG2	2.20	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:HB2	2.21	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:179:ILE:HD13	2:A:405:HOH:O	2.21	0.41
1:A:1:SER:C	1:A:278:LYS:HB3	2.41	0.41
2:A:323:HOH:O	1:B:132:SER:HB3	2.21	0.41
1:A:298:LYS:HD2	2:A:409:HOH:O	2.21	0.41
1:A:303:ASP:HA	1:A:306:LYS:HD3	2.02	0.41
1:A:105:VAL:HG22	1:A:267:ARG:HH21	1.85	0.41
1:A:126:HIS:HA	1:A:131:LYS:O	2.20	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:B:287:ARG:HG3	1:B:287:ARG:O	2.21	0.41
1:B:36:SER:HA	1:B:40:HIS:ND1	2.36	0.41
1:B:88:ASP:O	1:B:91:LEU:N	2.53	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:128:ARG:HD3	1:A:129:TYR:CE2	2.56	0.41
1:B:290:ILE:HD11	1:B:294:LYS:O	2.21	0.41
1:B:65:LEU:HD13	1:B:77:ILE:CG2	2.51	0.41
1:A:268:ILE:O	1:A:268:ILE:HG22	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:MET:HB2	1:A:149:LEU:HD21	2.03	0.41
1:B:252:ARG:CA	1:B:284:TYR:HE1	2.34	0.41
1:B:71:ASN:HB3	1:B:74:GLU:OE1	2.20	0.41
1:A:7:SER:C	1:A:9:SER:H	2.24	0.41
1:A:98:ARG:CA	1:A:98:ARG:NE	2.83	0.41
1:A:248:VAL:CG2	1:A:283:GLU:HB3	2.44	0.41
1:A:97:LYS:O	1:A:98:ARG:HG2	2.21	0.41
1:B:143:GLY:C	1:B:145:PHE:N	2.73	0.41
1:B:212:HIS:O	1:B:213:GLY:C	2.60	0.41
1:A:122:ARG:HH21	1:B:156:TYR:CB	2.33	0.41
1:A:128:ARG:HG2	1:A:129:TYR:CE1	2.56	0.41
1:A:185:ASN:ND2	1:A:185:ASN:C	2.75	0.41
1:A:65:LEU:O	1:A:78:LEU:HD13	2.21	0.41
1:B:267:ARG:CG	1:B:267:ARG:HH11	2.28	0.41
1:A:78:LEU:O	1:A:79:LEU:C	2.58	0.41
1:B:271:THR:O	1:B:272:ARG:HD2	2.20	0.41
1:A:107:MET:HE1	1:A:108:GLU:HA	2.03	0.41
1:B:170:GLN:O	1:B:174:LEU:HB2	2.20	0.41
1:B:293:GLU:N	1:B:293:GLU:OE1	2.53	0.41
1:B:216:ILE:O	1:B:220:LEU:HG	2.21	0.41
1:A:145:PHE:O	1:A:149:LEU:HG	2.21	0.41
1:B:116:THR:O	1:B:117:GLN:C	2.59	0.41
1:B:145:PHE:O	1:B:149:LEU:HG	2.21	0.41
1:B:197:SER:O	1:B:198:LYS:C	2.58	0.41
1:B:71:ASN:HB3	1:B:74:GLU:OE1	2.21	0.41
1:A:233:LEU:O	1:A:237:ILE:HG13	2.20	0.41
1:B:293:GLU:HB2	1:B:317:ALA:CB	2.51	0.41
1:B:151:SER:HB3	1:B:194:SER:HB2	2.03	0.41
1:B:62:LEU:HD23	1:B:65:LEU:HD12	2.03	0.41
1:A:161:ASP:CA	1:A:199:ALA:HB2	2.50	0.41
1:B:215:GLU:O	1:B:219:SER:N	2.51	0.41
1:B:254:ALA:HB2	2:B:367:HOH:O	2.20	0.41
1:B:82:LEU:HD22	1:B:87:ARG:CA	2.51	0.41
1:A:128:ARG:HD3	1:A:129:TYR:CZ	2.56	0.41
1:A:175:VAL:HG12	1:A:179:ILE:HG12	2.03	0.41
1:A:275:ILE:HD12	2:A:333:HOH:O	2.21	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:A:125:TYR:O	1:A:128:ARG:N	2.50	0.41
1:A:35:ILE:HD11	1:A:307:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:ND2	1:A:185:ASN:C	2.74	0.41
1:B:121:ALA:O	1:B:122:ARG:C	2.59	0.41
1:B:241:THR:HG22	1:B:242:ARG:HG3	2.03	0.41
1:B:287:ARG:O	1:B:287:ARG:HG3	2.21	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:65:LEU:HD22	1:B:74:GLU:CG	2.51	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:166:THR:O	1:A:170:GLN:HG3	2.20	0.41
1:B:137:VAL:HG13	1:B:141:THR:HG21	2.03	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:175:VAL:O	1:B:179:ILE:HG13	2.21	0.41
1:A:161:ASP:O	1:A:162:GLU:C	2.59	0.40
1:A:20:LEU:O	1:A:21:ARG:C	2.60	0.40
1:A:217:LEU:HD11	1:A:238:GLN:HG2	2.02	0.40
1:A:126:HIS:NE2	1:B:156:TYR:CD2	2.89	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: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:B:3:THR:OG1	1:B:278:LYS:N	2.54	0.40
1:A:132:SER:O	1:A:135:GLU:HG2	2.22	0.40
1:A:255:ILE:C	1:A:257:LYS:N	2.74	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:B:281:GLY:O	1:B:283:GLU:N	2.51	0.40
1:B:286:ARG:NH1	1:B:286:ARG:HG2	2.36	0.40
1:B:164:ASN:HB3	1:B:167:LEU:HB3	2.03	0.40
1:B:184:TYR:C	1:B:186:ASP:H	2.25	0.40
1:A:167:LEU:HD21	1:A:196:ARG:CZ	2.52	0.40
1:A:207:ARG:NE	2:A:398:HOH:O	2.53	0.40
1:B:73:PHE:HD1	1:B:304:TYR:HA	1.87	0.40
1:B:252:ARG:NE	1:B:288:ASN:OD1	2.53	0.40
1:A:109:VAL:O	1:A:113:ARG:HD3	2.21	0.40
1:B:170:GLN:O	1:B:174:LEU:HB2	2.21	0.40
1:A:179:ILE:HD12	1:A:220:LEU:CD2	2.44	0.40
1:A:193:LEU:HD11	1:A:233:LEU:HD12	2.03	0.40
1:A:264:ALA:C	1:A:266:THR:N	2.74	0.40
1:A:165:MET:HG3	2:A:396:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:150:VAL:HA	1:B:153:VAL:HG22	2.04	0.40
1:B:3:THR:HB	1:B:312:LEU:C	2.42	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:A:230:LEU:O	1:A:234:ARG:HG3	2.21	0.40
1:A:108:GLU:HB2	1:A:246:TYR:OH	2.22	0.40
1:A:277:LEU:HA	1:A:280:ILE:HD12	2.03	0.40
1:B:114:THR:H	1:B:117:GLN:NE2	2.19	0.40
1:B:255:ILE:O	1:B:257:LYS:N	2.54	0.40
1:B:302:GLY:N	1:B:305:GLU:OE1	2.54	0.40
1:A:147:LYS:HD3	2:A:473:HOH:O	2.20	0.40
1:A:209:GLN:HA	1:A:214:GLU:O	2.21	0.40
1:A:217:LEU:O	1:A:221:GLU:HG3	2.21	0.40
1:A:67:LYS:O	1:A:67:LYS:HG2	2.20	0.40
1:B:10:VAL:HG13	1:B:11:PRO:HD2	2.04	0.40
1:B:123:GLN:C	1:B:125:TYR:N	2.75	0.40
1:A:220:LEU:C	1:A:222:GLU:N	2.75	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:A:133:LEU:CD2	1:A:153:VAL:HB	2.51	0.40
1:A:193:LEU:HD11	1:A:233:LEU:CD1	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: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:75:ARG:NH1	1:B:78:LEU:HD23	2.36	0.40
1:A:132:SER:O	1:A:134:GLU:N	2.54	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: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:242:ARG:CB	1:B:245:LEU:HD12	2.51	0.40
1:A:19:GLN:HA	2:A:453:HOH:O	2.21	0.40
1:B:176:HIS:C	1:B:178:LYS:H	2.24	0.40
1:B:82:LEU:HD22	1:B:86:GLU:OE2	2.21	0.40
1:A:179:ILE:HD13	2:A:407:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:HH12	1:A:196:ARG:HH21	1.70	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:31:GLU:HG2	1:A:303:ASP:OD2	2.22	0.40
1:B:294:LYS:HA	1:B:297:THR:HG22	2.03	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: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: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: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:105:VAL:HG12	1:A:105:VAL:O	2.21	0.40
1:A:293:GLU:HG2	1:A:294:LYS:N	2.37	0.40
1:A:106:LEU:HD22	1:A:133:LEU:HD11	2.02	0.40
1:A:148:LEU:HD21	1:A:236:THR:OG1	2.22	0.40
1:A:16:ASP:O	1:A:20:LEU:HG	2.22	0.40
1:A:293:GLU:HG2	1:A:294:LYS:HD3	2.03	0.40
1:A:97:LYS:C	1:A:98:ARG:HG2	2.42	0.40
1:B:39:ALA:HA	1:B:311:LEU:HD21	2.04	0.40
1:A:298:LYS:HE2	1:A:298:LYS:HB3	1.81	0.40
1:A:132:SER:O	1:A:135:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	308/317 (97%)	268 (87%)	35 (11%)	5 (2%)	11	19
1	1-B	301/317 (95%)	249 (83%)	42 (14%)	10 (3%)	4	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-A	308/317 (97%)	266 (86%)	38 (12%)	4 (1%)	14	25
1	2-B	301/317 (95%)	248 (82%)	46 (15%)	7 (2%)	7	11
1	3-A	308/317 (97%)	267 (87%)	32 (10%)	9 (3%)	5	7
1	3-B	301/317 (95%)	241 (80%)	48 (16%)	12 (4%)	3	4
1	4-A	308/317 (97%)	254 (82%)	40 (13%)	14 (4%)	3	3
1	4-B	301/317 (95%)	258 (86%)	40 (13%)	3 (1%)	18	32
1	5-A	308/317 (97%)	262 (85%)	40 (13%)	6 (2%)	9	15
1	5-B	301/317 (95%)	253 (84%)	38 (13%)	10 (3%)	4	6
1	6-A	308/317 (97%)	271 (88%)	30 (10%)	7 (2%)	7	11
1	6-B	301/317 (95%)	266 (88%)	29 (10%)	6 (2%)	9	14
1	7-A	308/317 (97%)	256 (83%)	46 (15%)	6 (2%)	9	15
1	7-B	301/317 (95%)	257 (85%)	39 (13%)	5 (2%)	11	18
1	8-A	308/317 (97%)	263 (85%)	36 (12%)	9 (3%)	5	7
1	8-B	301/317 (95%)	249 (83%)	39 (13%)	13 (4%)	3	3
All	All	4872/5072 (96%)	4128 (85%)	618 (13%)	126 (3%)	6	9

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	43	70
1	1-B	269/277 (97%)	264 (98%)	5 (2%)	62	85
1	2-A	274/277 (99%)	267 (97%)	7 (3%)	51	78
1	2-B	269/277 (97%)	265 (98%)	4 (2%)	70	89
1	3-A	274/277 (99%)	264 (96%)	10 (4%)	40	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-B	269/277 (97%)	265 (98%)	4 (2%)	70	89
1	4-A	274/277 (99%)	263 (96%)	11 (4%)	36	62
1	4-B	269/277 (97%)	261 (97%)	8 (3%)	46	74
1	5-A	274/277 (99%)	264 (96%)	10 (4%)	40	67
1	5-B	269/277 (97%)	266 (99%)	3 (1%)	78	92
1	6-A	274/277 (99%)	264 (96%)	10 (4%)	40	67
1	6-B	269/277 (97%)	263 (98%)	6 (2%)	57	82
1	7-A	274/277 (99%)	269 (98%)	5 (2%)	64	86
1	7-B	269/277 (97%)	267 (99%)	2 (1%)	87	96
1	8-A	274/277 (99%)	266 (97%)	8 (3%)	48	75
1	8-B	269/277 (97%)	259 (96%)	10 (4%)	39	66
All	All	4344/4432 (98%)	4232 (97%)	112 (3%)	51	78

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	1-A	312/317 (98%)	-0.01	14 (4%) 34 36	11, 35, 68, 92	312 (100%)
1	1-B	307/317 (96%)	0.30	31 (10%) 8 7	11, 42, 76, 92	307 (100%)
1	2-A	312/317 (98%)	-0.01	14 (4%) 34 36	11, 35, 68, 92	312 (100%)
1	2-B	307/317 (96%)	0.30	31 (10%) 8 7	11, 42, 76, 92	307 (100%)
1	3-A	312/317 (98%)	-0.01	14 (4%) 34 36	11, 35, 68, 92	312 (100%)
1	3-B	307/317 (96%)	0.30	31 (10%) 8 7	11, 42, 76, 92	307 (100%)
1	4-A	312/317 (98%)	-0.01	14 (4%) 34 36	11, 35, 68, 92	312 (100%)
1	4-B	307/317 (96%)	0.30	31 (10%) 8 7	11, 42, 76, 92	307 (100%)
1	5-A	312/317 (98%)	-0.01	14 (4%) 34 36	11, 35, 68, 92	312 (100%)
1	5-B	307/317 (96%)	0.30	31 (10%) 8 7	11, 42, 76, 92	307 (100%)
1	6-A	312/317 (98%)	-0.01	14 (4%) 34 36	11, 35, 68, 92	312 (100%)
1	6-B	307/317 (96%)	0.30	31 (10%) 8 7	11, 42, 76, 92	307 (100%)
1	7-A	312/317 (98%)	-0.01	14 (4%) 34 36	11, 35, 68, 92	312 (100%)
1	7-B	307/317 (96%)	0.30	31 (10%) 8 7	11, 42, 76, 92	307 (100%)
1	8-A	312/317 (98%)	-0.01	14 (4%) 34 36	11, 35, 68, 92	312 (100%)
1	8-B	307/317 (96%)	0.30	31 (10%) 8 7	11, 42, 76, 92	307 (100%)
All	All	4952/5072 (97%)	0.15	360 (7%) 20 16	11, 37, 75, 92	4952 (100%)

All (360) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	64	THR	6.9
1	2-B	64	THR	6.9
1	3-B	64	THR	6.9
1	4-B	64	THR	6.9
1	5-B	64	THR	6.9

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Mol	Chain	Res	Type	RSRZ
1	6-B	64	THR	6.9
1	7-B	64	THR	6.9
1	8-B	64	THR	6.9
1	1-B	222	GLU	6.6
1	2-B	222	GLU	6.6
1	3-B	222	GLU	6.6
1	4-B	222	GLU	6.6
1	5-B	222	GLU	6.6
1	6-B	222	GLU	6.6
1	7-B	222	GLU	6.6
1	8-B	222	GLU	6.6
1	1-B	52	ALA	6.2
1	2-B	52	ALA	6.2
1	3-B	52	ALA	6.2
1	4-B	52	ALA	6.2
1	5-B	52	ALA	6.2
1	6-B	52	ALA	6.2
1	7-B	52	ALA	6.2
1	8-B	52	ALA	6.2
1	1-B	258	THR	5.1
1	2-B	258	THR	5.1
1	3-B	258	THR	5.1
1	4-B	258	THR	5.1
1	5-B	258	THR	5.1
1	6-B	258	THR	5.1
1	7-B	258	THR	5.1
1	8-B	258	THR	5.1
1	1-B	9	SER	5.0
1	2-B	9	SER	5.0
1	3-B	9	SER	5.0
1	4-B	9	SER	5.0
1	5-B	9	SER	5.0
1	6-B	9	SER	5.0
1	7-B	9	SER	5.0
1	8-B	9	SER	5.0
1	1-B	221	GLU	4.7
1	2-B	221	GLU	4.7
1	3-B	221	GLU	4.7
1	4-B	221	GLU	4.7
1	5-B	221	GLU	4.7
1	6-B	221	GLU	4.7
1	7-B	221	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	8-B	221	GLU	4.7
1	1-B	316	ASP	4.5
1	2-B	316	ASP	4.5
1	3-B	316	ASP	4.5
1	4-B	316	ASP	4.5
1	5-B	316	ASP	4.5
1	6-B	316	ASP	4.5
1	7-B	316	ASP	4.5
1	8-B	316	ASP	4.5
1	1-B	23	ALA	4.3
1	2-B	23	ALA	4.3
1	3-B	23	ALA	4.3
1	4-B	23	ALA	4.3
1	5-B	23	ALA	4.3
1	6-B	23	ALA	4.3
1	7-B	23	ALA	4.3
1	8-B	23	ALA	4.3
1	1-B	14	SER	4.0
1	2-B	14	SER	4.0
1	3-B	14	SER	4.0
1	4-B	14	SER	4.0
1	5-B	14	SER	4.0
1	6-B	14	SER	4.0
1	7-B	14	SER	4.0
1	8-B	14	SER	4.0
1	1-B	12	ALA	3.7
1	2-B	12	ALA	3.7
1	3-B	12	ALA	3.7
1	4-B	12	ALA	3.7
1	5-B	12	ALA	3.7
1	6-B	12	ALA	3.7
1	7-B	12	ALA	3.7
1	8-B	12	ALA	3.7
1	1-B	56	THR	3.7
1	2-B	56	THR	3.7
1	3-B	56	THR	3.7
1	4-B	56	THR	3.7
1	5-B	56	THR	3.7
1	6-B	56	THR	3.7
1	7-B	56	THR	3.7
1	8-B	56	THR	3.7
1	1-B	314	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	2-B	314	GLU	3.4
1	3-B	314	GLU	3.4
1	4-B	314	GLU	3.4
1	5-B	314	GLU	3.4
1	6-B	314	GLU	3.4
1	7-B	314	GLU	3.4
1	8-B	314	GLU	3.4
1	1-B	6	VAL	3.4
1	2-B	6	VAL	3.4
1	3-B	6	VAL	3.4
1	4-B	6	VAL	3.4
1	5-B	6	VAL	3.4
1	6-B	6	VAL	3.4
1	7-B	6	VAL	3.4
1	8-B	6	VAL	3.4
1	1-B	257	LYS	3.3
1	2-B	257	LYS	3.3
1	3-B	257	LYS	3.3
1	4-B	257	LYS	3.3
1	5-B	257	LYS	3.3
1	6-B	257	LYS	3.3
1	7-B	257	LYS	3.3
1	8-B	257	LYS	3.3
1	1-A	259	GLY	3.2
1	2-A	259	GLY	3.2
1	3-A	259	GLY	3.2
1	4-A	259	GLY	3.2
1	5-A	259	GLY	3.2
1	6-A	259	GLY	3.2
1	7-A	259	GLY	3.2
1	8-A	259	GLY	3.2
1	1-B	63	LYS	3.1
1	2-B	63	LYS	3.1
1	3-B	63	LYS	3.1
1	4-B	63	LYS	3.1
1	5-B	63	LYS	3.1
1	6-B	63	LYS	3.1
1	7-B	63	LYS	3.1
1	8-B	63	LYS	3.1
1	1-A	8	ASP	3.0
1	1-B	224	ASP	3.0
1	2-A	8	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	2-B	224	ASP	3.0
1	3-A	8	ASP	3.0
1	3-B	224	ASP	3.0
1	4-A	8	ASP	3.0
1	4-B	224	ASP	3.0
1	5-A	8	ASP	3.0
1	5-B	224	ASP	3.0
1	6-A	8	ASP	3.0
1	6-B	224	ASP	3.0
1	7-A	8	ASP	3.0
1	7-B	224	ASP	3.0
1	8-A	8	ASP	3.0
1	8-B	224	ASP	3.0
1	1-B	256	ASN	3.0
1	2-B	256	ASN	3.0
1	3-B	256	ASN	3.0
1	4-B	256	ASN	3.0
1	5-B	256	ASN	3.0
1	6-B	256	ASN	3.0
1	7-B	256	ASN	3.0
1	8-B	256	ASN	3.0
1	1-B	7	SER	3.0
1	2-B	7	SER	3.0
1	3-B	7	SER	3.0
1	4-B	7	SER	3.0
1	5-B	7	SER	3.0
1	6-B	7	SER	3.0
1	7-B	7	SER	3.0
1	8-B	7	SER	3.0
1	1-B	317	ALA	2.9
1	2-B	317	ALA	2.9
1	3-B	317	ALA	2.9
1	4-B	317	ALA	2.9
1	5-B	317	ALA	2.9
1	6-B	317	ALA	2.9
1	7-B	317	ALA	2.9
1	8-B	317	ALA	2.9
1	1-A	225	ASP	2.8
1	2-A	225	ASP	2.8
1	3-A	225	ASP	2.8
1	4-A	225	ASP	2.8
1	5-A	225	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	6-A	225	ASP	2.8
1	7-A	225	ASP	2.8
1	8-A	225	ASP	2.8
1	1-A	256	ASN	2.7
1	2-A	256	ASN	2.7
1	3-A	256	ASN	2.7
1	4-A	256	ASN	2.7
1	5-A	256	ASN	2.7
1	6-A	256	ASN	2.7
1	7-A	256	ASN	2.7
1	8-A	256	ASN	2.7
1	1-A	68	GLU	2.6
1	2-A	68	GLU	2.6
1	3-A	68	GLU	2.6
1	4-A	68	GLU	2.6
1	5-A	68	GLU	2.6
1	6-A	68	GLU	2.6
1	7-A	68	GLU	2.6
1	8-A	68	GLU	2.6
1	1-B	48	VAL	2.6
1	2-B	48	VAL	2.6
1	3-B	48	VAL	2.6
1	4-B	48	VAL	2.6
1	5-B	48	VAL	2.6
1	6-B	48	VAL	2.6
1	7-B	48	VAL	2.6
1	8-B	48	VAL	2.6
1	1-A	290	ILE	2.6
1	2-A	290	ILE	2.6
1	3-A	290	ILE	2.6
1	4-A	290	ILE	2.6
1	5-A	290	ILE	2.6
1	6-A	290	ILE	2.6
1	7-A	290	ILE	2.6
1	8-A	290	ILE	2.6
1	1-B	65	LEU	2.6
1	2-B	65	LEU	2.6
1	3-B	65	LEU	2.6
1	4-B	65	LEU	2.6
1	5-B	65	LEU	2.6
1	6-B	65	LEU	2.6
1	7-B	65	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	8-B	65	LEU	2.6
1	1-A	226	ASP	2.5
1	2-A	226	ASP	2.5
1	3-A	226	ASP	2.5
1	4-A	226	ASP	2.5
1	5-A	226	ASP	2.5
1	6-A	226	ASP	2.5
1	7-A	226	ASP	2.5
1	8-A	226	ASP	2.5
1	1-B	10	VAL	2.5
1	2-B	10	VAL	2.5
1	3-B	10	VAL	2.5
1	4-B	10	VAL	2.5
1	5-B	10	VAL	2.5
1	6-B	10	VAL	2.5
1	7-B	10	VAL	2.5
1	8-B	10	VAL	2.5
1	1-A	227	ASP	2.5
1	2-A	227	ASP	2.5
1	3-A	227	ASP	2.5
1	4-A	227	ASP	2.5
1	5-A	227	ASP	2.5
1	6-A	227	ASP	2.5
1	7-A	227	ASP	2.5
1	8-A	227	ASP	2.5
1	1-A	260	THR	2.4
1	2-A	260	THR	2.4
1	3-A	260	THR	2.4
1	4-A	260	THR	2.4
1	5-A	260	THR	2.4
1	6-A	260	THR	2.4
1	7-A	260	THR	2.4
1	8-A	260	THR	2.4
1	1-B	211	ASP	2.4
1	2-B	211	ASP	2.4
1	3-B	211	ASP	2.4
1	4-B	211	ASP	2.4
1	5-B	211	ASP	2.4
1	6-B	211	ASP	2.4
1	7-B	211	ASP	2.4
1	8-B	211	ASP	2.4
1	1-B	8	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	2-B	8	ASP	2.4
1	3-B	8	ASP	2.4
1	4-B	8	ASP	2.4
1	5-B	8	ASP	2.4
1	6-B	8	ASP	2.4
1	7-B	8	ASP	2.4
1	8-B	8	ASP	2.4
1	1-B	299	ASP	2.3
1	2-B	299	ASP	2.3
1	3-B	299	ASP	2.3
1	4-B	299	ASP	2.3
1	5-B	299	ASP	2.3
1	6-B	299	ASP	2.3
1	7-B	299	ASP	2.3
1	8-B	299	ASP	2.3
1	1-B	300	THR	2.2
1	2-B	300	THR	2.2
1	3-B	300	THR	2.2
1	4-B	300	THR	2.2
1	5-B	300	THR	2.2
1	6-B	300	THR	2.2
1	7-B	300	THR	2.2
1	8-B	300	THR	2.2
1	1-B	304	TYR	2.2
1	2-B	304	TYR	2.2
1	3-B	304	TYR	2.2
1	4-B	304	TYR	2.2
1	5-B	304	TYR	2.2
1	6-B	304	TYR	2.2
1	7-B	304	TYR	2.2
1	8-B	304	TYR	2.2
1	1-B	315	ASP	2.2
1	2-B	315	ASP	2.2
1	3-B	315	ASP	2.2
1	4-B	315	ASP	2.2
1	5-B	315	ASP	2.2
1	6-B	315	ASP	2.2
1	7-B	315	ASP	2.2
1	8-B	315	ASP	2.2
1	1-A	59	GLU	2.2
1	2-A	59	GLU	2.2
1	3-A	59	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	4-A	59	GLU	2.2
1	5-A	59	GLU	2.2
1	6-A	59	GLU	2.2
1	7-A	59	GLU	2.2
1	8-A	59	GLU	2.2
1	1-B	15	ASP	2.2
1	2-B	15	ASP	2.2
1	3-B	15	ASP	2.2
1	4-B	15	ASP	2.2
1	5-B	15	ASP	2.2
1	6-B	15	ASP	2.2
1	7-B	15	ASP	2.2
1	8-B	15	ASP	2.2
1	1-B	11	PRO	2.1
1	2-B	11	PRO	2.1
1	3-B	11	PRO	2.1
1	4-B	11	PRO	2.1
1	5-B	11	PRO	2.1
1	6-B	11	PRO	2.1
1	7-B	11	PRO	2.1
1	8-B	11	PRO	2.1
1	1-B	259	GLY	2.1
1	2-B	259	GLY	2.1
1	3-B	259	GLY	2.1
1	4-B	259	GLY	2.1
1	5-B	259	GLY	2.1
1	6-B	259	GLY	2.1
1	7-B	259	GLY	2.1
1	8-B	259	GLY	2.1
1	1-A	224	ASP	2.1
1	1-A	228	LYS	2.1
1	2-A	224	ASP	2.1
1	2-A	228	LYS	2.1
1	3-A	224	ASP	2.1
1	3-A	228	LYS	2.1
1	4-A	224	ASP	2.1
1	4-A	228	LYS	2.1
1	5-A	224	ASP	2.1
1	5-A	228	LYS	2.1
1	6-A	224	ASP	2.1
1	6-A	228	LYS	2.1
1	7-A	224	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	7-A	228	LYS	2.1
1	8-A	224	ASP	2.1
1	8-A	228	LYS	2.1
1	1-A	51	GLN	2.1
1	2-A	51	GLN	2.1
1	3-A	51	GLN	2.1
1	4-A	51	GLN	2.1
1	5-A	51	GLN	2.1
1	6-A	51	GLN	2.1
1	7-A	51	GLN	2.1
1	8-A	51	GLN	2.1
1	1-A	180	LYS	2.0
1	2-A	180	LYS	2.0
1	3-A	180	LYS	2.0
1	4-A	180	LYS	2.0
1	5-A	180	LYS	2.0
1	6-A	180	LYS	2.0
1	7-A	180	LYS	2.0
1	8-A	180	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.