



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:04 pm BST

PDB ID : 4BXN
Title : Eg5(WT) complex
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Deposited on : 2013-07-15
Resolution : 2.79 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

<https://www.wwpdb.org/validation/2017/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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

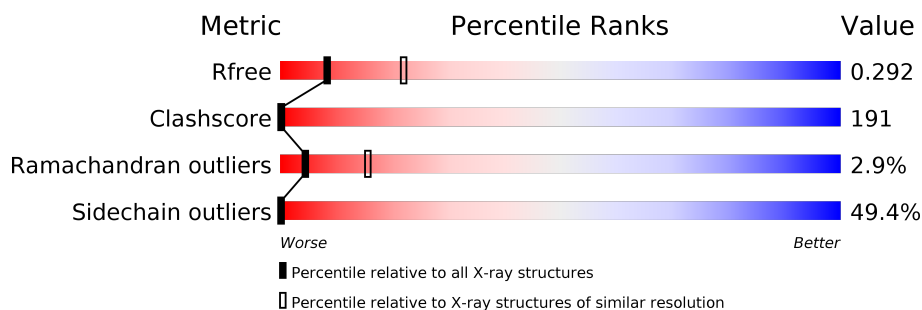
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	B	601	-	-	X	-
3	CD	A	1365	-	-	X	-
3	CD	B	1367	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	1376	-	-	X	-
4	CL	A	1377	-	-	X	-
4	CL	A	1378	-	-	X	-
4	CL	A	1381	-	-	X	-
4	CL	B	1377	-	-	X	-
5	6LX	A	1375	-	-	X	-

2 Entry composition [i](#)

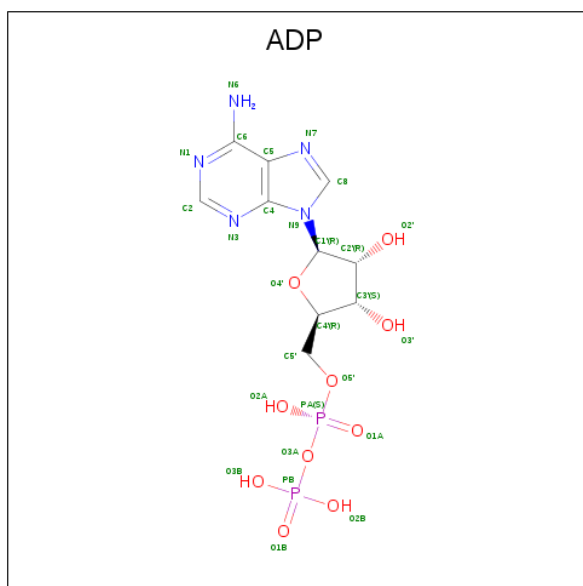
There are 6 unique types of molecules in this entry. The entry contains 5521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	2	0	0
			2663	1669	460	524	10			
1	B	345	Total	C	N	O	S	1	0	0
			2642	1657	455	520	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

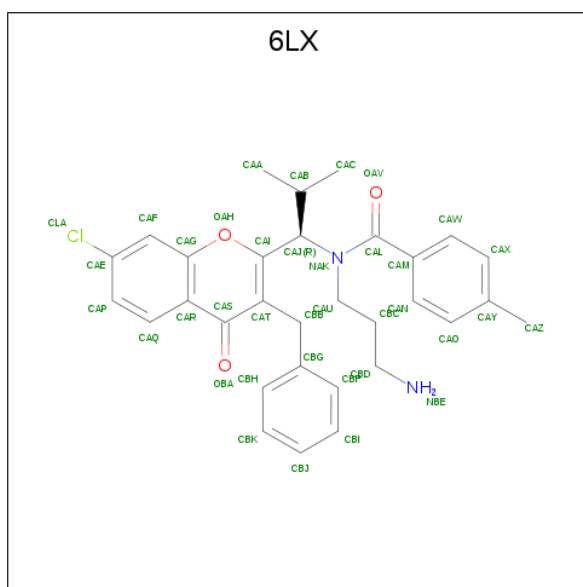
- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	13	Total Cd 13 13	0	0
3	A	9	Total Cd 9 9	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total Cl 3 3	0	0
4	A	5	Total Cl 5 5	0	0

- Molecule 5 is N-(3-aminopropyl)-N-[(1R)-1-(3-benzyl-7-chloro-4-oxo-4H-chromen-2-yl)-2-methylpropyl]-4-methylbenzamide (three-letter code: 6LX) (formula: $C_{31}H_{33}ClN_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 37	C 31	Cl 1	N 2	O 3	0	0
5	B	1	Total 37	C 31	Cl 1	N 2	O 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	32	Total O 32 32	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	26	Total	O	0	0
			26	26		

H308	Y309	P310	Y311	R312	E313	S314	R315	L316	T317	R318	I319	L320	Q321	D322	S323	L324	T328	R329	T330	S331	I332	I333	A334	T335	I336	S337	P338	A339	S340	L341	N342	L343	E344	E345	T346	L347	S348	T349	L350	E351	Y352	A353	H354	R355	A356	K357	N358	I359	L360	N361	K362	P363	E364	VAL	ASN	GLN	LYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	81.43Å 81.43Å 115.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.93 – 2.79 27.94 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.1 (27.93-2.79) 97.1 (27.94-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.230 , 0.274 0.280 , 0.292	Depositor DCC
R_{free} test set	1059 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l 0.075 for h,-h-k,-l 0.070 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 20599 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5521	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6LX, CL, ADP, CD

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	A	0.31	0/2702	0.46	0/3658
1	B	0.31	0/2680	0.58	2/3630 (0.1%)
All	All	0.31	0/5382	0.52	2/7288 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASN	C-N-CD	-18.59	79.70	120.60
1	B	309	VAL	C-N-CD	-5.21	109.13	120.60

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	A	2663	0	2620	1036	18
1	B	2642	0	2599	1012	25
2	A	27	0	12	3	0
2	B	27	0	12	21	0
3	A	9	0	0	3	1
3	B	13	0	0	3	2
4	A	5	0	0	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	3	0
5	A	37	0	33	89	0
5	B	37	0	33	9	0
6	A	32	0	0	12	0
6	B	26	0	0	4	0
All	All	5521	0	5309	2061	32

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 191.

All (2061) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PHE:CE2	1:A:81:VAL:HG22	1.21	1.63
1:A:28:PHE:CE1	1:A:339:ALA:CB	1.80	1.63
1:A:28:PHE:CZ	1:A:339:ALA:CB	1.77	1.62
1:A:211:TYR:CE1	5:A:1375:6LX:HAA1	1.34	1.60
1:B:113:PHE:CE2	1:B:118:GLU:HG3	1.26	1.60
1:B:239:PHE:CE1	1:B:241:VAL:CG1	1.80	1.59
1:A:225:ALA:HA	1:A:231:TYR:CD2	1.13	1.59
1:B:82:TYR:CE1	1:B:86:VAL:CG1	1.79	1.58
1:A:272:ILE:CD1	1:A:355:ARG:NH2	1.69	1.55
1:B:239:PHE:CE1	1:B:241:VAL:HG12	1.34	1.53
1:A:226:THR:C	1:A:228:MET:HB2	1.15	1.52
1:B:174:PRO:HA	1:B:220:LYS:CD	1.06	1.51
1:B:82:TYR:CZ	1:B:86:VAL:HG11	1.46	1.51
1:A:72:PHE:CZ	1:A:81:VAL:HG22	1.47	1.49
1:A:230:ALA:HB1	1:A:234:ARG:CB	1.41	1.49
1:B:25:CYS:SG	3:B:1365:CD:CD	1.18	1.49
1:A:167:GLU:HG3	1:A:181:ARG:CB	1.44	1.47
1:B:127:TRP:CZ2	1:B:208:ASP:HA	1.51	1.45
1:B:174:PRO:CA	1:B:220:LYS:HD2	0.98	1.45
1:A:28:PHE:CE1	1:A:339:ALA:HB2	1.46	1.45
1:B:41:VAL:CA	1:B:52:VAL:HG23	1.44	1.44
1:A:167:GLU:CG	1:A:181:ARG:HB3	1.44	1.43
1:A:272:ILE:HD11	1:A:355:ARG:CZ	1.48	1.43
1:B:22:VAL:CG2	1:B:333:ILE:HG22	1.47	1.43
1:A:102:PHE:CZ	1:A:332:ILE:HG23	1.54	1.43
1:A:160:LEU:CD1	1:A:171:LEU:HD23	1.48	1.43
1:B:239:PHE:CZ	1:B:241:VAL:HG12	1.54	1.43
1:A:105:GLY:CA	1:A:269:SER:OG	1.64	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:CG2	1:B:147:LEU:HD21	1.49	1.42
1:B:211:TYR:CE1	1:B:215:GLU:OE1	1.71	1.41
1:B:300:THR:CG2	1:B:356:ALA:HA	1.48	1.41
1:B:24:ARG:NH2	1:B:114:THR:HG23	1.36	1.41
1:B:118:GLU:CB	1:B:132:LEU:HD13	1.27	1.41
1:B:82:TYR:CD1	1:B:86:VAL:HB	1.55	1.41
1:A:160:LEU:HD12	1:A:171:LEU:CD2	1.52	1.40
1:A:252:GLY:CA	1:A:253:GLU:HB3	1.49	1.40
1:A:226:THR:C	1:A:228:MET:CB	1.91	1.39
1:B:142:GLN:O	1:B:146:LYS:CG	1.68	1.39
1:A:279:ASP:CB	1:A:283:ARG:HG2	1.50	1.39
1:B:300:THR:HG22	1:B:356:ALA:CA	1.52	1.38
1:A:211:TYR:HE1	5:A:1375:6LX:CAA	1.36	1.37
1:B:163:ILE:HB	1:B:236:HIS:CD2	1.58	1.37
1:A:117:GLY:C	5:A:1375:6LX:HAN	1.42	1.36
1:B:252:GLY:CA	1:B:253:GLU:HB3	1.48	1.36
1:A:72:PHE:CE2	1:A:81:VAL:CG2	2.06	1.36
1:A:272:ILE:CD1	1:A:355:ARG:CZ	2.02	1.35
1:B:113:PHE:CE2	1:B:118:GLU:CG	2.09	1.35
1:A:225:ALA:CA	1:A:231:TYR:CD2	2.05	1.34
1:B:24:ARG:HH21	1:B:114:THR:CG2	1.39	1.34
1:A:152:THR:HG22	1:A:247:GLU:CG	1.54	1.34
1:B:249:THR:OG1	1:B:252:GLY:N	1.57	1.34
1:B:172:LEU:CB	1:B:200:GLU:OE2	1.75	1.34
1:A:280:LYS:O	1:A:284:GLU:CG	1.76	1.33
1:B:197:LYS:HD2	1:B:198:GLY:N	1.42	1.33
1:B:81:VAL:O	1:B:85:VAL:HG23	1.22	1.33
1:B:161:LEU:HD22	1:B:162:GLU:N	1.41	1.33
1:A:224:ALA:O	1:A:228:MET:HG2	1.27	1.32
1:A:28:PHE:CE1	1:A:339:ALA:HB3	1.49	1.32
1:A:294:THR:O	1:A:298:VAL:HG23	1.22	1.32
1:B:344:GLU:O	1:B:347:LEU:CD1	1.77	1.31
1:B:351:GLU:OE1	1:B:355:ARG:NH2	1.60	1.31
1:B:143:ILE:CG2	1:B:147:LEU:CD2	2.08	1.30
1:A:225:ALA:CA	1:A:231:TYR:HD2	1.38	1.30
1:B:211:TYR:HE1	1:B:215:GLU:CD	1.30	1.30
1:B:142:GLN:O	1:B:146:LYS:HG3	1.21	1.30
1:A:225:ALA:O	1:A:228:MET:HB3	1.18	1.29
1:A:116:GLU:O	5:A:1375:6LX:HBB2	1.32	1.29
1:B:143:ILE:HG22	1:B:147:LEU:CD2	1.61	1.29
1:A:280:LYS:O	1:A:284:GLU:HG3	1.13	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:O	1:B:346:THR:HG23	1.27	1.28
1:A:118:GLU:N	5:A:1375:6LX:CAO	1.95	1.27
1:B:118:GLU:O	1:B:132:LEU:CB	1.80	1.27
1:B:253:GLU:OE2	1:B:255:LEU:HD11	1.29	1.27
1:A:280:LYS:C	1:A:284:GLU:OE2	1.72	1.27
1:B:195:ILE:HD13	1:B:196:ILE:N	1.50	1.26
1:B:252:GLY:HA2	1:B:253:GLU:CB	1.53	1.26
1:B:118:GLU:O	1:B:132:LEU:HB3	1.26	1.26
1:B:173:ASN:O	1:B:175:SER:N	1.66	1.26
1:A:252:GLY:HA2	1:A:253:GLU:CB	1.65	1.25
1:B:171:LEU:HB3	1:B:177:ASP:OD2	1.14	1.25
1:A:207:LYS:O	1:A:210:VAL:HG13	1.36	1.25
1:A:28:PHE:CD1	1:A:339:ALA:HB2	1.71	1.24
1:B:106:GLN:O	1:B:109:THR:CG2	1.84	1.24
1:B:168:LEU:O	1:B:182:LEU:HD21	1.13	1.24
1:B:212:GLN:O	1:B:216:LYS:HG3	1.35	1.23
1:B:344:GLU:O	1:B:347:LEU:HD13	1.08	1.23
1:B:20:GLN:HE21	1:B:329:ARG:NH1	1.33	1.23
1:B:113:PHE:CZ	1:B:118:GLU:HG3	1.72	1.23
1:B:82:TYR:CE1	1:B:86:VAL:HG12	1.49	1.23
1:B:195:ILE:C	1:B:195:ILE:HD13	1.56	1.23
1:A:117:GLY:C	5:A:1375:6LX:CAN	2.06	1.22
1:A:230:ALA:CB	1:A:234:ARG:HB2	1.69	1.22
1:A:147:LEU:CD1	1:A:154:PHE:CD2	2.22	1.22
1:B:352:TYR:CD1	1:B:355:ARG:NH1	2.05	1.22
5:A:1375:6LX:HAJ	5:A:1375:6LX:CBF	1.68	1.22
1:A:88:PRO:O	1:A:91:ASP:OD1	1.55	1.22
1:A:113:PHE:CE1	1:A:114:THR:HG23	1.75	1.22
1:B:239:PHE:CZ	1:B:241:VAL:CG1	2.15	1.22
1:B:32:GLU:OE1	1:B:339:ALA:HB2	1.40	1.22
1:B:118:GLU:HB3	1:B:132:LEU:CD1	1.49	1.21
1:B:281:ARG:CD	1:B:281:ARG:H	1.50	1.21
1:A:272:ILE:HD11	1:A:355:ARG:NH1	1.56	1.21
1:A:54:THR:OG1	1:A:62:SER:HB2	1.39	1.21
1:B:211:TYR:CE1	1:B:215:GLU:CD	2.11	1.21
1:A:226:THR:O	1:A:228:MET:HB2	1.07	1.21
1:B:300:THR:HA	1:B:356:ALA:O	1.35	1.20
1:B:28:PHE:CE1	1:B:39:SER:OG	1.95	1.20
1:A:30:LEU:HD13	1:A:30:LEU:C	1.62	1.20
1:B:143:ILE:O	1:B:147:LEU:CD2	1.88	1.20
1:A:225:ALA:O	1:A:228:MET:CB	1.88	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HG21	1:A:311:TYR:CE2	1.74	1.20
1:A:66:TYR:OH	1:A:350:LEU:O	1.56	1.19
1:A:318:ARG:NH1	4:A:1381:CL:CL	2.13	1.19
1:A:294:THR:O	1:A:298:VAL:CG2	1.89	1.19
1:B:72:PHE:HB3	1:B:76:THR:HG21	1.22	1.19
1:B:22:VAL:HG23	1:B:333:ILE:CA	1.71	1.18
1:B:20:GLN:NE2	1:B:329:ARG:NH1	1.89	1.18
1:A:298:VAL:CG1	1:A:311:TYR:CD1	2.27	1.18
1:B:128:GLU:OE2	1:B:208:ASP:OD1	1.59	1.18
1:B:174:PRO:CA	1:B:220:LYS:CD	1.77	1.18
1:B:73:GLY:O	1:B:75:SER:N	1.75	1.18
1:B:79:ILE:HD11	1:B:83:ARG:NH2	1.57	1.18
1:B:40:ILE:O	1:B:52:VAL:HG22	1.42	1.17
1:A:152:THR:HG22	1:A:247:GLU:CD	1.62	1.17
1:A:78:GLN:NE2	1:A:133:ALA:O	1.78	1.17
1:A:127:TRP:CE3	1:A:128:GLU:OE2	1.97	1.17
1:A:205:HIS:NE2	6:A:2018:HOH:O	1.75	1.17
1:B:43:CYS:SG	3:B:1367:CD:CD	1.53	1.17
1:A:160:LEU:HD22	1:A:239:PHE:HB2	1.22	1.16
1:B:211:TYR:HE1	1:B:215:GLU:OE1	0.84	1.16
1:B:163:ILE:HB	1:B:236:HIS:NE2	1.58	1.16
1:A:298:VAL:HG11	1:A:311:TYR:CD1	1.80	1.16
1:A:298:VAL:HG12	1:A:311:TYR:CE1	1.80	1.16
1:A:27:PRO:CD	1:A:74:ALA:HB1	1.75	1.16
1:B:296:GLY:O	1:B:300:THR:CG2	1.93	1.16
1:A:242:THR:HG23	1:A:260:LYS:CD	1.75	1.16
1:A:284:GLU:O	1:A:289:ASN:CG	1.84	1.16
1:B:93:VAL:HG21	1:B:261:LEU:CD2	1.76	1.16
1:B:22:VAL:HG21	1:B:333:ILE:CG2	1.74	1.15
1:A:69:ASP:O	1:A:70:MET:SD	2.04	1.15
1:B:171:LEU:HB3	1:B:220:LYS:HE3	1.21	1.15
1:B:40:ILE:H	1:B:40:ILE:CD1	1.58	1.15
1:B:127:TRP:NE1	1:B:128:GLU:OE2	1.80	1.14
1:B:40:ILE:C	1:B:52:VAL:HG22	1.68	1.14
1:A:225:ALA:C	1:A:228:MET:HB3	1.67	1.14
1:B:171:LEU:CB	1:B:177:ASP:OD2	1.93	1.14
1:B:105:GLY:HA3	1:B:109:THR:CB	1.70	1.14
1:B:337:SER:OG	1:B:342:ASN:OD1	1.64	1.14
1:A:221:ARG:HH21	5:A:1375:6LX:CAP	1.61	1.13
1:B:20:GLN:NE2	1:B:329:ARG:CZ	2.11	1.13
1:B:302:LEU:N	1:B:302:LEU:HD23	1.56	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG22	1:A:247:GLU:CB	1.77	1.13
1:A:336:ILE:O	1:A:336:ILE:HD12	1.45	1.13
1:B:344:GLU:C	1:B:347:LEU:CD1	2.14	1.13
1:B:344:GLU:HA	1:B:347:LEU:HD11	1.18	1.13
1:A:41:VAL:CG2	1:A:338:PRO:HA	1.78	1.12
1:B:112:THR:HG22	1:B:116:GLU:HG3	1.21	1.12
1:A:118:GLU:O	5:A:1375:6LX:CAY	1.97	1.12
5:A:1375:6LX:HAJ	5:A:1375:6LX:HBFB	1.21	1.12
1:A:294:THR:CB	1:A:314:SER:OG	1.98	1.12
1:B:40:ILE:O	1:B:52:VAL:CG2	1.96	1.12
1:B:127:TRP:CZ2	1:B:208:ASP:CA	2.32	1.12
1:A:296:GLY:O	1:A:300:THR:OG1	1.68	1.11
1:B:172:LEU:HB3	1:B:200:GLU:OE2	1.44	1.11
1:A:133:ALA:HB2	5:A:1375:6LX:CAZ	1.80	1.11
1:A:274:ARG:HA	1:A:351:GLU:HG3	1.19	1.11
1:A:221:ARG:NH2	5:A:1375:6LX:CAQ	2.12	1.11
1:A:294:THR:OG1	1:A:314:SER:OG	1.66	1.11
1:B:171:LEU:CB	1:B:220:LYS:HE3	1.79	1.11
1:B:264:VAL:HG12	1:B:266:LEU:CD2	1.80	1.11
1:B:316:LEU:H	1:B:316:LEU:CD2	1.60	1.11
1:B:40:ILE:C	1:B:52:VAL:CG2	2.19	1.11
1:B:41:VAL:HG13	1:B:52:VAL:HG21	1.11	1.11
1:B:171:LEU:HB2	1:B:220:LYS:HE2	1.33	1.11
1:B:172:LEU:HB2	1:B:200:GLU:OE2	1.39	1.11
1:B:296:GLY:O	1:B:300:THR:HG23	0.96	1.11
1:A:23:VAL:HG21	1:A:68:PHE:CE2	1.86	1.11
1:B:171:LEU:HB2	1:B:220:LYS:CE	1.80	1.11
1:B:311:TYR:OH	1:B:324:LEU:CB	1.99	1.11
1:A:30:LEU:HD13	1:A:30:LEU:O	1.49	1.10
1:B:22:VAL:CG2	1:B:333:ILE:CG2	2.27	1.10
1:A:147:LEU:HD13	1:A:154:PHE:CD2	1.85	1.10
1:A:41:VAL:HG13	1:A:52:VAL:HG21	1.11	1.10
1:A:152:THR:CG2	1:A:247:GLU:HB2	1.81	1.10
1:A:324:LEU:H	1:A:324:LEU:HD23	0.95	1.10
1:A:109:THR:OG1	1:A:335:THR:HB	1.49	1.10
1:B:118:GLU:CB	1:B:132:LEU:CD1	2.15	1.10
1:A:41:VAL:HG13	1:A:52:VAL:CG2	1.80	1.10
1:B:315:LYS:O	1:B:319:ILE:HG13	1.51	1.10
1:B:192:ARG:HB3	1:B:322:ASP:HA	1.15	1.10
1:B:171:LEU:CB	1:B:220:LYS:CE	2.29	1.10
1:B:311:TYR:OH	1:B:324:LEU:HB2	1.51	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:HA	1:A:229:ASN:H	1.11	1.09
1:A:23:VAL:HG21	1:A:68:PHE:HE2	0.96	1.09
1:B:173:ASN:HB2	1:B:176:SER:OG	1.49	1.09
1:B:168:LEU:H	1:B:168:LEU:HD23	1.15	1.09
1:A:115:MET:O	1:A:136:ILE:HG13	1.51	1.09
1:A:105:GLY:O	1:A:268:GLY:HA2	1.52	1.09
1:A:28:PHE:CZ	1:A:339:ALA:HB2	1.62	1.09
1:B:82:TYR:CE1	1:B:86:VAL:CB	2.35	1.09
1:B:112:THR:CG2	1:B:116:GLU:HG3	1.81	1.09
1:A:118:GLU:OE1	1:A:132:LEU:HD12	1.50	1.09
1:A:228:MET:HG3	1:A:231:TYR:CD2	1.86	1.09
1:A:27:PRO:HD3	1:A:74:ALA:CB	1.83	1.09
1:A:293:LEU:HB3	1:A:297:ARG:NH2	1.68	1.09
1:B:230:ALA:HB1	1:B:234:ARG:HE	1.10	1.09
1:A:113:PHE:HE1	1:A:114:THR:HG23	0.94	1.09
1:A:249:THR:O	1:A:252:GLY:O	1.71	1.09
1:B:143:ILE:O	1:B:147:LEU:HD22	1.51	1.09
1:A:324:LEU:N	1:A:324:LEU:HD23	1.58	1.08
1:A:78:GLN:NE2	1:A:132:LEU:O	1.85	1.08
1:B:100:THR:HG23	1:B:262:ASN:OD1	1.50	1.08
1:B:40:ILE:N	1:B:40:ILE:HD12	1.65	1.08
1:B:296:GLY:HA3	1:B:352:TYR:CZ	1.88	1.08
1:B:22:VAL:HG23	1:B:333:ILE:HA	1.11	1.08
1:A:118:GLU:O	5:A:1375:6LX:CAZ	2.02	1.08
1:B:143:ILE:HG22	1:B:147:LEU:HD23	1.18	1.08
1:B:231:TYR:O	1:B:232:SER:HB2	1.48	1.08
1:B:302:LEU:H	1:B:302:LEU:CD2	1.63	1.08
1:B:164:TYR:OH	1:B:230:ALA:HB3	1.50	1.08
1:A:309:VAL:CG2	1:A:311:TYR:CE2	2.36	1.07
1:B:20:GLN:HE22	1:B:329:ARG:CZ	1.67	1.07
1:B:41:VAL:HG13	1:B:52:VAL:CG2	1.82	1.07
1:A:114:THR:O	1:A:134:GLY:HA3	1.54	1.07
1:A:167:GLU:O	1:A:168:LEU:HD12	1.54	1.07
1:B:104:TYR:OH	1:B:349:THR:HB	1.54	1.07
1:A:225:ALA:HB1	1:A:231:TYR:HB2	1.33	1.07
1:A:192:ARG:HH12	1:A:325:GLY:HA3	1.19	1.07
1:B:134:GLY:O	1:B:137:PRO:HG2	1.53	1.07
1:A:133:ALA:HB2	5:A:1375:6LX:HAZ1	1.12	1.07
1:B:77:LYS:NZ	6:B:2006:HOH:O	1.79	1.07
1:A:113:PHE:CD1	1:A:114:THR:N	2.22	1.07
1:A:272:ILE:HD12	1:A:355:ARG:NH2	1.45	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HD22	1:B:341:LEU:H	1.15	1.07
1:B:266:LEU:N	1:B:266:LEU:HD23	1.69	1.07
1:A:160:LEU:CD2	1:A:239:PHE:HB2	1.82	1.07
1:B:250:ILE:HD13	1:B:250:ILE:N	1.69	1.07
1:A:167:GLU:CG	1:A:181:ARG:CB	2.16	1.06
1:A:105:GLY:HA2	1:A:269:SER:OG	0.89	1.06
1:B:82:TYR:CD1	1:B:86:VAL:CB	2.37	1.06
1:A:218:ALA:HB2	5:A:1375:6LX:CAF	1.85	1.06
1:B:344:GLU:CA	1:B:347:LEU:HD11	1.83	1.06
1:B:357:LYS:HB3	1:B:357:LYS:HZ2	1.17	1.06
1:A:236:HIS:O	1:A:265:ASP:O	1.74	1.06
1:B:343:LEU:O	1:B:346:THR:CG2	2.01	1.06
1:A:93:VAL:HG23	1:A:99:CYS:SG	1.96	1.06
1:A:147:LEU:HD12	1:A:154:PHE:CE2	1.90	1.06
1:B:274:ARG:HG3	1:B:274:ARG:HH11	1.16	1.06
1:A:118:GLU:N	5:A:1375:6LX:HAO	1.68	1.06
1:B:157:LYS:HE3	1:B:242:THR:HB	1.37	1.05
1:A:242:THR:HG23	1:A:260:LYS:HD3	1.36	1.05
1:B:347:LEU:H	1:B:347:LEU:HD12	1.15	1.05
1:A:226:THR:O	1:A:228:MET:CB	2.00	1.05
1:A:225:ALA:HB1	1:A:231:TYR:CB	1.85	1.05
1:A:91:ASP:O	1:A:94:ILE:HG22	1.56	1.05
1:A:117:GLY:HA2	1:A:134:GLY:H	1.16	1.05
1:B:41:VAL:CG1	1:B:52:VAL:CG2	2.35	1.05
1:A:28:PHE:CZ	1:A:339:ALA:HB1	1.87	1.05
1:A:167:GLU:HG2	1:A:181:ARG:HB3	1.39	1.05
1:A:47:ARG:O	1:A:48:LYS:HG3	1.56	1.05
1:B:121:PRO:C	1:B:122:ASN:OD1	1.94	1.05
1:A:120:SER:OG	1:A:130:ASP:OD1	1.75	1.05
1:A:133:ALA:CB	5:A:1375:6LX:HAZ1	1.86	1.04
1:A:66:TYR:OH	1:A:354:HIS:HB2	1.54	1.04
1:B:174:PRO:N	1:B:220:LYS:CD	2.19	1.04
1:B:113:PHE:CZ	1:B:118:GLU:CG	2.35	1.04
1:B:142:GLN:O	1:B:146:LYS:HG2	1.51	1.04
1:B:228:MET:SD	1:B:228:MET:N	2.30	1.04
1:B:134:GLY:O	1:B:137:PRO:HD2	1.55	1.04
1:A:28:PHE:CZ	1:A:339:ALA:HB3	1.66	1.04
1:A:49:GLU:OE1	1:A:66:TYR:O	1.74	1.04
1:B:239:PHE:HE1	1:B:241:VAL:HG13	1.22	1.04
1:A:242:THR:CG2	1:A:260:LYS:HG2	1.85	1.04
1:B:134:GLY:O	1:B:137:PRO:CG	2.04	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.38	1.04
1:B:41:VAL:N	1:B:52:VAL:HG23	1.71	1.04
1:A:147:LEU:HD12	1:A:154:PHE:CD2	1.90	1.04
1:A:272:ILE:HD13	1:A:355:ARG:NH2	1.73	1.04
1:A:102:PHE:CZ	1:A:332:ILE:CG2	2.39	1.04
1:A:167:GLU:HG3	1:A:181:ARG:HB2	1.38	1.04
1:A:23:VAL:CG2	1:A:68:PHE:HE2	1.71	1.04
1:B:177:ASP:O	1:B:178:VAL:HG13	1.58	1.04
1:B:82:TYR:CZ	1:B:86:VAL:CG1	2.19	1.04
1:B:17:LYS:O	1:B:19:ILE:O	1.76	1.03
1:A:170:ASP:OD2	1:A:200:GLU:HB2	1.56	1.03
1:A:249:THR:HB	1:A:252:GLY:H	1.21	1.03
1:A:28:PHE:CE2	1:A:32:GLU:HB2	1.92	1.03
1:A:152:THR:CG2	1:A:247:GLU:CD	2.26	1.03
1:B:127:TRP:HZ2	1:B:208:ASP:CA	1.66	1.03
1:B:102:PHE:HZ	1:B:320:LEU:HD11	1.21	1.03
1:B:269:SER:N	1:B:270:GLU:OE2	1.91	1.03
1:A:211:TYR:CE1	5:A:1375:6LX:CAA	2.22	1.02
1:B:344:GLU:HA	1:B:347:LEU:CD1	1.87	1.02
1:B:116:GLU:O	5:B:1375:6LX:HBB1	1.58	1.02
1:A:242:THR:HG23	1:A:260:LYS:CG	1.88	1.02
1:B:143:ILE:O	1:B:147:LEU:HD23	1.59	1.02
1:B:128:GLU:OE2	1:B:208:ASP:CG	1.98	1.02
1:B:22:VAL:HG22	1:B:332:ILE:O	1.59	1.02
1:B:344:GLU:CA	1:B:347:LEU:CD1	2.38	1.02
1:A:215:GLU:O	5:A:1375:6LX:CLA	2.14	1.02
1:A:207:LYS:O	1:A:210:VAL:CG1	2.06	1.02
1:A:86:VAL:C	1:A:88:PRO:HD2	1.80	1.02
1:B:105:GLY:HA3	1:B:109:THR:HB	1.39	1.02
1:B:98:ASN:O	1:B:328:THR:OG1	1.75	1.02
1:A:245:MET:CB	1:A:257:LYS:HD3	1.90	1.02
1:B:134:GLY:O	1:B:137:PRO:CD	2.08	1.02
1:A:274:ARG:HA	1:A:351:GLU:CG	1.90	1.01
1:B:76:THR:O	1:B:77:LYS:HE2	1.57	1.01
1:B:304:GLU:HB2	1:B:306:THR:HG22	1.42	1.01
1:B:127:TRP:NE1	1:B:128:GLU:CD	2.12	1.01
1:B:139:THR:O	1:B:143:ILE:HG13	1.61	1.01
1:B:168:LEU:O	1:B:182:LEU:CD2	2.07	1.01
1:B:93:VAL:HG21	1:B:261:LEU:HD23	1.40	1.01
1:B:249:THR:OG1	1:B:252:GLY:CA	2.08	1.01
1:B:316:LEU:O	1:B:320:LEU:HB2	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:LEU:O	1:B:351:GLU:N	1.93	1.01
1:A:104:TYR:CZ	1:A:269:SER:HB3	1.96	1.01
1:A:125:TYR:HB2	1:A:129:GLU:HB3	1.38	1.01
1:A:309:VAL:HG21	1:A:311:TYR:HE2	1.04	1.01
1:B:344:GLU:C	1:B:347:LEU:HD13	1.77	1.01
1:A:41:VAL:HG21	1:A:338:PRO:HA	1.05	1.01
1:B:131:PRO:HA	1:B:138:ARG:NH2	1.76	1.01
1:B:41:VAL:HA	1:B:52:VAL:HG23	1.06	1.01
1:B:163:ILE:CB	1:B:236:HIS:CD2	2.43	1.01
1:A:21:VAL:HG23	1:A:357:LYS:HG3	1.43	1.00
1:A:280:LYS:O	1:A:284:GLU:CD	1.98	1.00
1:A:152:THR:CG2	1:A:247:GLU:OE1	2.08	1.00
1:A:30:LEU:C	1:A:30:LEU:CD1	2.30	1.00
1:B:225:ALA:HA	1:B:231:TYR:CD1	1.97	1.00
1:B:353:ALA:O	1:B:357:LYS:O	1.79	1.00
1:A:118:GLU:N	5:A:1375:6LX:CAN	2.20	1.00
1:A:156:VAL:CG1	1:A:204:VAL:HB	1.92	1.00
1:A:311:TYR:O	1:A:317:THR:OG1	1.79	1.00
1:B:227:LEU:HD23	1:B:229:ASN:CB	1.92	1.00
1:A:280:LYS:O	1:A:284:GLU:OE2	1.80	1.00
1:A:120:SER:HB2	1:A:124:GLU:CG	1.91	0.99
1:A:49:GLU:OE1	1:A:67:THR:HA	1.61	0.99
1:B:174:PRO:CA	1:B:220:LYS:HD3	1.91	0.99
1:B:239:PHE:HE1	1:B:241:VAL:CG1	1.40	0.99
1:B:352:TYR:O	1:B:356:ALA:N	1.96	0.99
1:A:273:GLY:HA3	1:A:280:LYS:HA	1.43	0.99
1:B:174:PRO:HA	1:B:220:LYS:CG	1.93	0.99
1:B:212:GLN:O	1:B:216:LYS:CG	2.10	0.99
1:B:41:VAL:HA	1:B:52:VAL:CG2	1.92	0.99
1:A:28:PHE:CE2	1:A:339:ALA:HB2	1.98	0.99
1:A:105:GLY:HA2	1:A:269:SER:CB	1.93	0.98
1:B:41:VAL:CA	1:B:52:VAL:CG2	2.40	0.98
1:B:294:THR:O	1:B:298:VAL:HG23	1.63	0.98
1:A:135:ILE:O	1:A:139:THR:N	1.95	0.98
1:A:78:GLN:NE2	1:A:133:ALA:C	2.15	0.98
1:B:163:ILE:HD12	1:B:236:HIS:NE2	1.76	0.98
1:A:279:ASP:CB	1:A:283:ARG:CG	2.41	0.98
1:B:127:TRP:CH2	1:B:207:LYS:HG2	1.98	0.98
1:B:127:TRP:CE2	1:B:208:ASP:HA	1.98	0.98
1:A:73:GLY:H	1:A:76:THR:HG21	1.27	0.98
1:A:41:VAL:HG21	1:A:338:PRO:CA	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:VAL:HG12	1:B:266:LEU:HD21	1.40	0.98
1:A:157:LYS:HA	1:A:203:THR:HA	1.43	0.98
1:A:224:ALA:O	1:A:228:MET:CG	2.11	0.98
1:A:245:MET:HB3	1:A:257:LYS:HD3	1.46	0.98
1:A:320:LEU:O	1:A:324:LEU:CD2	2.12	0.98
1:A:117:GLY:O	5:A:1375:6LX:HAN	1.64	0.98
1:B:110:GLY:HA2	2:B:601:ADP:C8	1.99	0.97
1:B:98:ASN:HD21	1:B:260:LYS:HD2	1.24	0.97
1:A:285:ALA:C	1:A:289:ASN:HD22	1.67	0.97
1:B:126:THR:O	1:B:130:ASP:OD2	1.80	0.97
1:B:171:LEU:CD2	1:B:220:LYS:HG2	1.92	0.97
1:B:227:LEU:HA	1:B:228:MET:C	1.84	0.97
1:A:156:VAL:HG11	1:A:204:VAL:HB	1.43	0.97
1:A:28:PHE:CE2	1:A:339:ALA:CB	2.46	0.97
1:A:23:VAL:CG2	1:A:68:PHE:CE2	2.45	0.97
1:A:156:VAL:HG13	1:A:204:VAL:HG23	1.44	0.97
1:A:249:THR:HB	1:A:252:GLY:N	1.79	0.97
1:B:316:LEU:N	1:B:316:LEU:HD22	1.77	0.97
1:B:123:GLU:OE1	1:B:123:GLU:HA	1.61	0.97
1:A:293:LEU:HB3	1:A:297:ARG:HH21	1.26	0.96
1:B:298:VAL:HG22	1:B:310:PRO:HB2	1.43	0.96
1:A:113:PHE:HD1	1:A:114:THR:N	1.60	0.96
1:A:226:THR:HA	1:A:229:ASN:N	1.80	0.96
1:B:81:VAL:O	1:B:85:VAL:CG2	2.13	0.96
1:B:296:GLY:HA2	1:B:299:ILE:HG22	1.44	0.96
1:B:302:LEU:H	1:B:302:LEU:HD23	0.82	0.96
1:B:40:ILE:H	1:B:40:ILE:HD12	0.80	0.96
1:A:272:ILE:HG22	1:A:348:SER:HB3	1.43	0.96
1:B:239:PHE:CE1	1:B:241:VAL:HG11	1.97	0.96
1:B:109:THR:O	1:B:335:THR:HB	1.64	0.96
1:B:253:GLU:OE2	1:B:255:LEU:CD1	2.13	0.96
1:A:83:ARG:HA	1:A:87:CYS:HB2	1.44	0.96
1:B:20:GLN:HG2	1:B:330:THR:O	1.66	0.96
1:B:102:PHE:CZ	1:B:320:LEU:HD11	2.01	0.95
1:A:160:LEU:HD12	1:A:171:LEU:HD23	0.96	0.95
1:A:314:SER:HB2	1:A:317:THR:HG23	1.48	0.95
1:B:106:GLN:CB	1:B:270:GLU:OE1	2.14	0.95
1:B:296:GLY:HA3	1:B:352:TYR:CE1	2.00	0.95
1:B:352:TYR:HD1	1:B:355:ARG:NH1	1.56	0.95
1:B:168:LEU:HD23	1:B:168:LEU:N	1.82	0.95
1:A:186:ASP:OD1	1:A:318:ARG:NH2	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ALA:HA	5:A:1375:6LX:HAO	1.48	0.95
1:A:324:LEU:CD2	1:A:324:LEU:N	2.30	0.95
1:B:93:VAL:HG21	1:B:261:LEU:HD22	1.48	0.95
1:B:172:LEU:CD1	1:B:173:ASN:ND2	2.30	0.95
1:A:309:VAL:CG2	1:A:311:TYR:CD2	2.49	0.95
5:A:1375:6LX:CAY	5:A:1375:6LX:HBI	1.97	0.94
1:B:300:THR:CA	1:B:356:ALA:O	2.14	0.94
1:A:217:GLY:HA3	5:A:1375:6LX:HAP	1.45	0.94
1:B:131:PRO:HA	1:B:138:ARG:HH22	1.27	0.94
1:B:161:LEU:CD2	1:B:162:GLU:N	2.30	0.94
1:B:357:LYS:HB3	1:B:357:LYS:NZ	1.80	0.94
1:B:127:TRP:HZ2	1:B:208:ASP:HA	1.16	0.94
1:B:41:VAL:CG1	1:B:52:VAL:HG21	1.92	0.94
1:B:53:ARG:O	1:B:54:THR:HG22	1.66	0.94
1:A:118:GLU:OE1	1:A:132:LEU:CD1	2.14	0.94
1:B:143:ILE:HG23	1:B:147:LEU:HD21	0.97	0.94
1:B:239:PHE:CZ	1:B:241:VAL:HG11	2.02	0.94
1:A:118:GLU:H	5:A:1375:6LX:HAO	1.29	0.94
1:B:311:TYR:CD1	1:B:317:THR:O	2.21	0.94
1:B:239:PHE:CE1	1:B:241:VAL:HG13	1.93	0.94
1:A:334:ALA:HB1	1:A:349:THR:HG22	1.50	0.94
1:B:22:VAL:HG23	1:B:333:ILE:CB	1.97	0.94
1:A:324:LEU:CD2	1:A:324:LEU:H	1.76	0.94
1:B:20:GLN:NE2	1:B:329:ARG:NH2	2.14	0.94
1:A:144:PHE:CE1	1:A:207:LYS:HB3	2.04	0.93
1:A:49:GLU:OE1	1:A:67:THR:CA	2.16	0.93
1:A:67:THR:O	1:A:68:PHE:HD1	1.49	0.93
1:B:104:TYR:OH	1:B:349:THR:CB	2.15	0.93
1:B:157:LYS:HG3	1:B:242:THR:O	1.67	0.93
1:B:227:LEU:HA	1:B:229:ASN:N	1.84	0.93
1:A:82:TYR:OH	1:A:142:GLN:OE1	1.86	0.93
1:B:164:TYR:HB3	1:B:169:PHE:CE1	2.02	0.93
1:A:226:THR:CA	1:A:228:MET:HB3	1.97	0.93
1:A:284:GLU:C	1:A:289:ASN:ND2	2.21	0.93
1:A:54:THR:HG1	1:A:62:SER:HB2	1.33	0.93
1:B:164:TYR:HE1	1:B:234:ARG:CD	1.80	0.93
1:A:44:ASP:OD2	1:A:47:ARG:CB	2.17	0.93
1:B:82:TYR:CE1	1:B:86:VAL:HG11	1.67	0.93
1:A:102:PHE:CE2	1:A:332:ILE:HG23	2.03	0.93
3:A:1365:CD:CD	1:B:87:CYS:SG	1.77	0.93
1:A:225:ALA:C	1:A:231:TYR:HD2	1.72	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ASN:OD1	1:B:323:SER:OG	1.83	0.93
1:A:72:PHE:HE2	1:A:81:VAL:HG22	1.23	0.93
1:A:202:ILE:HD13	1:A:202:ILE:H	1.34	0.93
1:B:174:PRO:N	1:B:220:LYS:HD3	1.82	0.93
1:A:144:PHE:CD1	1:A:207:LYS:HB3	2.04	0.92
1:B:316:LEU:HD22	1:B:316:LEU:H	1.30	0.92
1:A:227:LEU:N	1:A:228:MET:C	2.23	0.92
1:B:211:TYR:O	1:B:215:GLU:N	2.01	0.92
3:A:1365:CD:CD	1:B:87:CYS:HG	0.87	0.92
1:A:225:ALA:HA	1:A:231:TYR:CG	2.03	0.92
1:B:262:ASN:ND2	1:B:262:ASN:H	1.66	0.92
1:B:281:ARG:CD	1:B:281:ARG:N	2.30	0.92
1:A:117:GLY:HA2	1:A:134:GLY:N	1.83	0.92
1:A:284:GLU:O	1:A:289:ASN:ND2	2.03	0.92
1:A:298:VAL:HG12	1:A:311:TYR:CD1	2.00	0.92
1:A:102:PHE:HZ	1:A:332:ILE:HG23	1.15	0.92
1:A:272:ILE:HG22	1:A:348:SER:CB	2.00	0.92
1:A:281:ARG:N	1:A:284:GLU:OE2	2.03	0.92
1:A:72:PHE:CZ	1:A:81:VAL:CG2	2.38	0.92
1:A:102:PHE:HZ	1:A:332:ILE:CG2	1.80	0.92
1:A:273:GLY:O	1:A:355:ARG:NH2	2.03	0.92
1:B:239:PHE:CD1	1:B:263:LEU:CD1	2.52	0.92
1:A:118:GLU:HB3	1:A:132:LEU:HB3	1.49	0.92
1:B:195:ILE:C	1:B:195:ILE:CD1	2.30	0.92
1:A:160:LEU:HD22	1:A:239:PHE:CB	2.00	0.91
1:A:167:GLU:C	1:A:168:LEU:CD1	2.38	0.91
1:B:22:VAL:CG2	1:B:333:ILE:HA	1.99	0.91
1:A:28:PHE:CD2	1:A:32:GLU:HG2	2.05	0.91
1:A:90:LEU:O	1:A:94:ILE:N	2.03	0.91
1:B:171:LEU:CB	1:B:220:LYS:HE2	1.99	0.91
1:A:309:VAL:HG23	1:A:311:TYR:HD2	1.35	0.91
1:A:167:GLU:HG3	1:A:181:ARG:HB3	0.94	0.91
1:A:160:LEU:HD13	1:A:161:LEU:N	1.85	0.91
1:B:116:GLU:O	5:B:1375:6LX:CBB	2.18	0.91
1:B:110:GLY:CA	2:B:601:ADP:N7	2.34	0.91
1:B:100:THR:HA	1:B:262:ASN:ND2	1.85	0.91
1:A:242:THR:HG23	1:A:260:LYS:HG2	1.47	0.91
1:A:26:ARG:HA	1:A:74:ALA:HA	1.53	0.91
1:A:217:GLY:N	5:A:1375:6LX:CLA	2.41	0.90
1:B:183:GLN:OE1	1:B:185:PHE:CZ	2.24	0.90
1:A:211:TYR:CZ	5:A:1375:6LX:HAA1	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLY:CA	1:B:109:THR:CB	2.49	0.90
1:B:265:ASP:C	1:B:266:LEU:HD23	1.90	0.90
1:B:164:TYR:HB3	1:B:169:PHE:HE1	1.35	0.90
1:B:187:ASP:HB3	1:B:195:ILE:HG22	1.51	0.90
1:B:112:THR:HG22	1:B:116:GLU:CG	2.00	0.90
1:A:236:HIS:HA	1:A:265:ASP:O	1.72	0.90
1:A:66:TYR:CZ	1:A:354:HIS:HB2	2.06	0.90
1:B:118:GLU:O	1:B:132:LEU:HB2	1.71	0.90
1:A:236:HIS:CA	1:A:265:ASP:O	2.19	0.90
1:B:177:ASP:C	1:B:178:VAL:HG13	1.90	0.90
1:A:160:LEU:CG	1:A:171:LEU:HD23	2.02	0.90
1:B:174:PRO:HB3	1:B:220:LYS:HB2	1.51	0.90
1:B:52:VAL:O	1:B:53:ARG:O	1.88	0.90
1:A:69:ASP:C	1:A:70:MET:SD	2.49	0.90
1:A:67:THR:O	1:A:68:PHE:CD1	2.25	0.90
1:A:157:LYS:HG2	1:A:203:THR:HG22	1.55	0.89
1:A:116:GLU:O	5:A:1375:6LX:CBB	2.18	0.89
1:B:127:TRP:CD1	1:B:128:GLU:OE1	2.25	0.89
1:A:109:THR:HG23	1:A:111:LYS:HG2	1.54	0.89
1:A:230:ALA:CB	1:A:234:ARG:CB	2.35	0.89
1:A:87:CYS:SG	4:A:1377:CL:CL	2.67	0.89
1:B:274:ARG:HG3	1:B:274:ARG:NH1	1.81	0.89
1:A:137:PRO:HB3	5:A:1375:6LX:CBK	2.02	0.89
1:B:106:GLN:O	1:B:109:THR:HG23	0.92	0.89
1:A:309:VAL:CG2	1:A:311:TYR:HE2	1.79	0.89
1:B:100:THR:CG2	1:B:262:ASN:OD1	2.19	0.89
1:B:197:LYS:CD	1:B:198:GLY:H	1.85	0.89
1:A:134:GLY:O	1:A:137:PRO:HG2	1.72	0.89
1:B:197:LYS:HD2	1:B:198:GLY:H	1.02	0.89
1:B:26:ARG:O	1:B:338:PRO:HG3	1.73	0.89
1:B:32:GLU:CD	1:B:339:ALA:CB	2.40	0.89
1:B:72:PHE:HB3	1:B:76:THR:CG2	2.03	0.89
1:A:334:ALA:HB1	1:A:349:THR:CG2	2.03	0.89
1:B:112:THR:O	1:B:116:GLU:N	2.05	0.88
1:B:177:ASP:O	1:B:178:VAL:HG22	1.73	0.88
1:B:296:GLY:HA2	1:B:299:ILE:CG2	2.03	0.88
1:A:221:ARG:NH2	5:A:1375:6LX:CAP	2.34	0.88
1:A:28:PHE:CG	1:A:339:ALA:HB2	2.07	0.88
1:B:113:PHE:CE2	1:B:118:GLU:CB	2.56	0.88
1:B:266:LEU:CD2	1:B:266:LEU:N	2.37	0.88
1:A:242:THR:CG2	1:A:260:LYS:CG	2.48	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:HG23	1:B:147:LEU:CD2	1.88	0.88
1:B:163:ILE:CB	1:B:236:HIS:NE2	2.35	0.88
1:B:24:ARG:CZ	2:B:601:ADP:HN62	1.86	0.88
1:A:117:GLY:CA	1:A:134:GLY:H	1.87	0.88
1:A:226:THR:CA	1:A:228:MET:CB	2.51	0.88
1:B:102:PHE:HZ	1:B:320:LEU:CD1	1.86	0.88
1:B:239:PHE:CD1	1:B:263:LEU:HD11	2.08	0.88
1:A:19:ILE:O	1:A:20:GLN:NE2	2.07	0.88
1:B:144:PHE:O	1:B:148:THR:HB	1.71	0.88
1:B:261:LEU:HD13	1:B:262:ASN:N	1.89	0.88
1:B:342:ASN:O	1:B:345:GLU:N	2.07	0.88
1:A:106:GLN:N	1:A:269:SER:H	1.71	0.88
1:A:228:MET:HG3	1:A:231:TYR:CE2	2.09	0.88
1:A:51:SER:HA	1:A:64:LYS:O	1.73	0.88
1:B:112:THR:O	1:B:116:GLU:HB2	1.72	0.88
1:A:120:SER:HB2	1:A:124:GLU:HG2	1.56	0.88
1:A:213:ILE:HA	1:A:216:LYS:HE2	1.55	0.88
1:A:272:ILE:HD12	1:A:355:ARG:CZ	1.89	0.88
1:A:73:GLY:H	1:A:76:THR:CG2	1.86	0.88
1:A:113:PHE:HD1	1:A:114:THR:H	1.16	0.87
1:B:143:ILE:C	1:B:147:LEU:HD23	1.94	0.87
1:A:124:GLU:OE2	1:A:125:TYR:CE1	2.27	0.87
1:A:135:ILE:O	1:A:139:THR:HB	1.72	0.87
1:A:44:ASP:OD2	1:A:47:ARG:HB3	1.72	0.87
1:B:247:GLU:O	1:B:255:LEU:N	2.06	0.87
1:A:152:THR:HG22	1:A:247:GLU:HB2	1.43	0.87
1:B:311:TYR:O	1:B:317:THR:OG1	1.91	0.87
1:B:316:LEU:N	1:B:316:LEU:CD2	2.30	0.87
1:B:171:LEU:HD22	1:B:220:LYS:HG2	1.55	0.87
1:B:301:ALA:O	1:B:306:THR:HG23	1.75	0.87
1:B:20:GLN:HE21	1:B:329:ARG:HH12	0.90	0.87
1:A:156:VAL:CG1	1:A:204:VAL:CB	2.53	0.86
1:A:309:VAL:HG23	1:A:311:TYR:CD2	2.06	0.86
1:B:81:VAL:HG12	1:B:85:VAL:HG21	1.55	0.86
1:A:242:THR:HG22	1:A:260:LYS:HG2	1.57	0.86
1:A:118:GLU:C	5:A:1375:6LX:CAY	2.43	0.86
1:A:302:LEU:CG	1:A:311:TYR:OH	2.22	0.86
1:B:183:GLN:OE1	1:B:185:PHE:CE2	2.28	0.86
1:B:20:GLN:HE22	1:B:329:ARG:NH2	1.69	0.86
1:A:114:THR:O	1:A:134:GLY:CA	2.23	0.86
1:A:160:LEU:HD13	1:A:161:LEU:H	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:C	1:A:336:ILE:HD12	1.95	0.86
1:B:82:TYR:CE1	1:B:86:VAL:HB	2.03	0.86
1:A:125:TYR:N	1:A:125:TYR:CD1	2.43	0.86
1:A:157:LYS:CG	1:A:203:THR:HG22	2.06	0.86
1:A:49:GLU:OE1	1:A:66:TYR:C	2.14	0.86
1:A:66:TYR:CE1	1:A:354:HIS:HB2	2.10	0.86
1:A:66:TYR:OH	1:A:354:HIS:CB	2.23	0.86
1:A:298:VAL:CG1	1:A:311:TYR:CG	2.58	0.86
1:B:311:TYR:OH	1:B:324:LEU:HB3	1.76	0.86
1:A:152:THR:CB	1:A:247:GLU:HB2	2.05	0.86
1:A:65:THR:OG1	1:A:361:ASN:OD1	1.93	0.85
1:B:127:TRP:CZ2	1:B:207:LYS:HG2	2.10	0.85
1:A:270:GLU:O	1:A:348:SER:OG	1.94	0.85
1:A:315:LYS:H	1:A:315:LYS:CE	1.89	0.85
1:B:166:GLU:OE1	1:B:166:GLU:HA	1.76	0.85
1:B:192:ARG:HB3	1:B:322:ASP:CA	2.04	0.85
1:A:114:THR:O	1:A:135:ILE:N	2.09	0.85
1:A:196:ILE:HG13	1:A:199:LEU:HB2	1.56	0.85
1:A:73:GLY:N	1:A:76:THR:HG21	1.91	0.85
1:B:296:GLY:CA	1:B:299:ILE:HG22	2.05	0.85
1:B:351:GLU:OE1	1:B:355:ARG:CZ	2.24	0.85
1:A:111:LYS:O	1:A:115:MET:HB2	1.75	0.85
1:A:272:ILE:HG22	1:A:348:SER:CA	2.07	0.85
1:B:113:PHE:HE2	1:B:118:GLU:CG	1.68	0.85
1:B:22:VAL:HG21	1:B:333:ILE:HG22	0.85	0.85
1:A:225:ALA:O	1:A:228:MET:CG	2.25	0.85
1:A:27:PRO:HD3	1:A:74:ALA:HB1	0.91	0.85
1:A:120:SER:HB2	1:A:124:GLU:HG3	1.56	0.85
1:A:192:ARG:NH1	1:A:325:GLY:HA3	1.91	0.85
1:A:148:THR:HG22	1:A:149:ASP:OD1	1.77	0.85
1:A:249:THR:OG1	1:A:253:GLU:OE1	1.94	0.85
1:B:161:LEU:HD22	1:B:161:LEU:C	1.92	0.85
1:B:249:THR:CG2	1:B:255:LEU:HD21	2.07	0.85
1:A:167:GLU:C	1:A:168:LEU:HD13	1.97	0.85
1:A:94:ILE:O	1:A:245:MET:HE1	1.76	0.85
1:B:72:PHE:CB	1:B:76:THR:HG21	2.05	0.85
1:B:172:LEU:HG	1:B:173:ASN:N	1.92	0.84
1:A:214:LEU:HD12	5:A:1375:6LX:CAQ	2.07	0.84
1:B:305:ARG:O	1:B:305:ARG:HG3	1.74	0.84
1:A:28:PHE:CE2	1:A:32:GLU:CG	2.60	0.84
1:A:41:VAL:CG1	1:A:52:VAL:CG2	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:VAL:N	1:B:332:ILE:O	2.11	0.84
1:A:54:THR:OG1	1:A:62:SER:CB	2.24	0.84
1:B:117:GLY:CA	1:B:134:GLY:N	2.41	0.84
1:B:250:ILE:H	1:B:250:ILE:HD13	1.36	0.84
1:B:192:ARG:HD3	1:B:322:ASP:OD1	1.78	0.84
1:B:32:GLU:CD	1:B:339:ALA:HB2	1.98	0.84
1:B:135:ILE:O	1:B:139:THR:OG1	1.96	0.84
1:B:32:GLU:OE1	1:B:339:ALA:CB	2.24	0.84
1:A:281:ARG:O	1:A:285:ALA:HB2	1.78	0.84
1:A:41:VAL:HA	1:A:52:VAL:CG2	2.07	0.84
1:A:113:PHE:HE1	1:A:114:THR:CG2	1.87	0.84
1:A:230:ALA:HB1	1:A:234:ARG:HB3	1.59	0.84
1:B:104:TYR:O	1:B:104:TYR:CD1	2.31	0.84
1:B:118:GLU:C	1:B:132:LEU:HB3	1.98	0.84
1:A:156:VAL:O	1:A:204:VAL:N	2.10	0.84
1:A:28:PHE:CE2	1:A:32:GLU:CB	2.60	0.84
1:A:298:VAL:HG12	1:A:311:TYR:CZ	2.12	0.84
1:A:221:ARG:HH21	5:A:1375:6LX:CAQ	1.83	0.84
1:B:227:LEU:CA	1:B:228:MET:C	2.46	0.84
1:A:32:GLU:OE2	1:A:37:ALA:N	2.11	0.83
1:A:230:ALA:O	1:A:234:ARG:N	2.11	0.83
1:A:152:THR:HG21	1:A:247:GLU:OE1	1.77	0.83
1:B:352:TYR:CE1	1:B:355:ARG:NH1	2.45	0.83
1:A:265:ASP:OD1	6:A:2020:HOH:O	1.94	0.83
1:B:164:TYR:CE1	1:B:234:ARG:HD2	2.13	0.83
1:A:47:ARG:C	1:A:48:LYS:HG3	1.96	0.83
1:B:104:TYR:CE1	1:B:334:ALA:HB1	2.12	0.83
1:B:76:THR:C	1:B:77:LYS:HE2	1.97	0.83
1:A:234:ARG:NH2	6:A:2013:HOH:O	2.10	0.83
1:A:91:ASP:OD2	3:A:1367:CD:CD	1.46	0.83
1:B:316:LEU:HD23	1:B:316:LEU:H	1.41	0.83
1:B:230:ALA:HB1	1:B:234:ARG:NE	1.92	0.83
1:B:225:ALA:HA	1:B:231:TYR:CE1	2.14	0.83
1:B:134:GLY:C	1:B:137:PRO:HD2	1.97	0.83
1:A:302:LEU:HG	1:A:311:TYR:OH	1.79	0.82
1:A:67:THR:HG21	1:A:359:ILE:HG22	1.61	0.82
1:B:127:TRP:CH2	1:B:207:LYS:O	2.31	0.82
1:B:164:TYR:CZ	1:B:230:ALA:HB3	2.14	0.82
1:B:264:VAL:HG12	1:B:266:LEU:HD22	1.61	0.82
1:B:342:ASN:C	1:B:346:THR:HG22	1.99	0.82
1:A:143:ILE:O	1:A:147:LEU:HG	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLY:N	2:B:601:ADP:O3A	2.11	0.82
1:A:113:PHE:O	1:A:117:GLY:CA	2.28	0.82
1:A:298:VAL:CG1	1:A:311:TYR:CE1	2.55	0.82
1:A:221:ARG:HH22	5:A:1375:6LX:CAQ	1.88	0.82
1:A:302:LEU:HG	1:A:311:TYR:HH	1.44	0.82
1:A:109:THR:HG21	1:A:335:THR:OG1	1.78	0.82
1:B:120:SER:CB	1:B:125:TYR:HB2	2.08	0.82
1:A:197:LYS:HE3	1:B:250:ILE:HG13	1.62	0.82
1:B:26:ARG:O	6:B:2002:HOH:O	1.96	0.82
1:A:156:VAL:O	1:A:203:THR:CA	2.28	0.82
1:A:273:GLY:H	1:A:284:GLU:HG2	1.44	0.82
1:B:104:TYR:HE1	1:B:334:ALA:HB1	1.43	0.82
1:B:195:ILE:HD13	1:B:196:ILE:CA	2.10	0.82
1:B:22:VAL:CG2	1:B:333:ILE:CA	2.55	0.82
1:B:82:TYR:OH	1:B:90:LEU:HD22	1.79	0.82
1:A:23:VAL:HG22	1:A:334:ALA:HB3	1.61	0.82
1:A:336:ILE:C	1:A:336:ILE:CD1	2.48	0.82
1:B:24:ARG:HH21	1:B:114:THR:HG23	0.93	0.82
1:A:161:LEU:HB3	1:A:238:VAL:HG22	1.60	0.82
1:B:296:GLY:C	1:B:300:THR:HG23	1.98	0.82
1:B:234:ARG:HH11	1:B:288:ILE:HD13	1.45	0.82
1:B:304:GLU:H	1:B:304:GLU:CD	1.84	0.82
1:A:78:GLN:OE1	1:A:113:PHE:CE1	2.33	0.81
1:B:66:TYR:CD2	1:B:350:LEU:HG	2.15	0.81
1:A:160:LEU:CD1	1:A:171:LEU:CD2	2.31	0.81
1:B:314:SER:HB3	1:B:317:THR:HG23	1.60	0.81
1:B:20:GLN:N	1:B:330:THR:O	2.12	0.81
1:A:226:THR:CA	1:A:229:ASN:H	1.91	0.81
1:B:187:ASP:OD2	1:B:193:GLY:O	1.99	0.81
1:B:228:MET:O	1:B:229:ASN:CB	2.29	0.81
1:B:316:LEU:O	1:B:320:LEU:CB	2.28	0.81
1:A:147:LEU:HD13	1:A:154:PHE:CG	2.14	0.81
1:A:105:GLY:C	1:A:269:SER:OG	2.18	0.81
1:B:127:TRP:CE2	1:B:128:GLU:CD	2.54	0.81
1:B:142:GLN:C	1:B:146:LYS:HG3	2.01	0.81
1:A:236:HIS:C	1:A:265:ASP:O	2.19	0.81
1:A:249:THR:HB	1:A:252:GLY:CA	2.10	0.81
1:A:47:ARG:HA	1:A:47:ARG:HE	1.44	0.81
1:A:118:GLU:H	1:A:133:ALA:HA	1.42	0.81
1:A:118:GLU:O	5:A:1375:6LX:HAZ2	1.81	0.81
1:A:41:VAL:CG2	1:A:338:PRO:CA	2.52	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:TYR:OH	1:B:230:ALA:CB	2.29	0.81
1:B:47:ARG:HB2	1:B:49:GLU:OE1	1.81	0.81
1:B:127:TRP:CH2	1:B:207:LYS:CG	2.64	0.81
1:B:143:ILE:C	1:B:147:LEU:CD2	2.47	0.81
1:B:302:LEU:N	1:B:302:LEU:CD2	2.30	0.81
1:B:352:TYR:O	1:B:356:ALA:CB	2.28	0.81
1:A:161:LEU:HD12	1:A:169:PHE:O	1.80	0.81
1:A:228:MET:O	1:A:229:ASN:HB3	1.79	0.81
1:B:164:TYR:CE1	1:B:234:ARG:CD	2.63	0.81
1:B:230:ALA:CB	1:B:234:ARG:HE	1.92	0.80
1:B:195:ILE:CD1	1:B:196:ILE:N	2.40	0.80
1:B:329:ARG:HB3	1:B:329:ARG:HH11	1.44	0.80
1:A:214:LEU:CD1	5:A:1375:6LX:CAQ	2.60	0.80
1:B:143:ILE:CG2	1:B:147:LEU:HD23	1.96	0.80
1:A:296:GLY:C	1:A:300:THR:HG1	1.83	0.80
1:B:53:ARG:O	1:B:54:THR:CG2	2.30	0.80
1:B:211:TYR:CE1	1:B:215:GLU:HB2	2.16	0.80
1:B:164:TYR:HE1	1:B:234:ARG:NE	1.78	0.80
1:A:225:ALA:C	1:A:228:MET:CB	2.39	0.80
1:A:160:LEU:CD1	1:A:161:LEU:N	2.44	0.80
1:A:245:MET:HB2	1:A:257:LYS:HD3	1.62	0.80
1:A:310:PRO:HB2	1:A:313:GLU:OE1	1.83	0.80
1:B:113:PHE:CE2	1:B:118:GLU:HB2	2.16	0.79
1:A:28:PHE:CD2	1:A:339:ALA:HB2	2.17	0.79
1:A:342:ASN:HB2	1:A:345:GLU:CG	2.12	0.79
1:B:117:GLY:HA3	1:B:134:GLY:H	1.47	0.79
1:B:32:GLU:O	1:B:37:ALA:HB2	1.83	0.79
1:A:314:SER:HB2	1:A:317:THR:CG2	2.11	0.79
1:B:127:TRP:HZ2	1:B:208:ASP:N	1.79	0.79
1:B:333:ILE:O	1:B:333:ILE:CG1	2.30	0.79
1:B:177:ASP:O	1:B:178:VAL:CG1	2.31	0.79
1:B:347:LEU:HA	1:B:350:LEU:HB2	1.65	0.79
1:A:118:GLU:C	5:A:1375:6LX:CAO	2.51	0.79
1:A:112:THR:O	1:A:116:GLU:N	2.16	0.79
1:A:225:ALA:CB	1:A:231:TYR:CB	2.59	0.79
1:B:227:LEU:HA	1:B:228:MET:HB2	1.64	0.79
1:B:239:PHE:CD1	1:B:263:LEU:HD12	2.18	0.78
1:B:79:ILE:HD11	1:B:83:ARG:HH21	1.44	0.78
1:B:86:VAL:HG21	1:B:135:ILE:HG23	1.63	0.78
1:A:73:GLY:O	1:A:76:THR:CG2	2.31	0.78
1:A:86:VAL:C	1:A:88:PRO:CD	2.51	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HD2	2:B:601:ADP:C1'	2.13	0.78
1:B:47:ARG:C	1:B:48:LYS:HG3	2.02	0.78
2:A:601:ADP:O1B	6:A:2009:HOH:O	2.01	0.78
1:B:26:ARG:NE	1:B:108:GLY:O	2.15	0.78
1:B:163:ILE:CD1	1:B:236:HIS:NE2	2.46	0.78
1:B:174:PRO:C	1:B:220:LYS:HD2	2.02	0.78
1:B:311:TYR:HH	1:B:324:LEU:CB	1.92	0.78
1:A:165:ASN:HA	6:A:2014:HOH:O	1.83	0.78
1:A:218:ALA:HB2	5:A:1375:6LX:HAF	1.65	0.78
1:B:131:PRO:CA	1:B:138:ARG:NH2	2.46	0.78
1:B:38:HIS:N	1:B:38:HIS:ND1	2.32	0.78
1:A:166:GLU:HB3	6:A:2015:HOH:O	1.84	0.78
1:B:22:VAL:CG2	1:B:333:ILE:CB	2.59	0.78
1:B:53:ARG:C	1:B:54:THR:HG22	2.04	0.78
1:B:172:LEU:HG	1:B:173:ASN:H	1.46	0.78
1:A:218:ALA:CB	5:A:1375:6LX:CAF	2.62	0.78
2:A:601:ADP:O2'	6:A:2029:HOH:O	2.02	0.78
1:B:136:ILE:HG12	1:B:263:LEU:CD1	2.12	0.78
1:A:167:GLU:O	1:A:168:LEU:CD1	2.32	0.78
1:B:83:ARG:O	1:B:87:CYS:HB2	1.84	0.78
1:A:127:TRP:HE3	1:A:128:GLU:OE2	1.61	0.77
1:A:227:LEU:N	1:A:228:MET:HB2	1.98	0.77
1:A:21:VAL:CG2	1:A:357:LYS:HG3	2.13	0.77
1:B:246:LYS:NZ	6:B:2009:HOH:O	2.14	0.77
1:B:311:TYR:HD1	1:B:317:THR:O	1.65	0.77
1:B:41:VAL:CB	1:B:52:VAL:HG23	2.14	0.77
1:B:174:PRO:N	1:B:220:LYS:HD2	1.89	0.77
1:B:144:PHE:CZ	1:B:206:ASN:HA	2.18	0.77
1:B:40:ILE:C	1:B:52:VAL:HG23	1.95	0.77
1:A:123:GLU:O	1:A:124:GLU:OE1	2.03	0.77
1:A:225:ALA:C	1:A:228:MET:CG	2.53	0.77
1:A:67:THR:HG21	1:A:359:ILE:CG2	2.15	0.77
1:B:247:GLU:N	1:B:255:LEU:O	2.15	0.77
1:A:226:THR:N	1:A:228:MET:HB3	1.98	0.77
1:B:249:THR:CG2	1:B:255:LEU:CD2	2.63	0.77
1:B:357:LYS:CB	1:B:357:LYS:HZ2	1.95	0.77
1:B:82:TYR:HE1	1:B:86:VAL:HG12	0.94	0.77
1:A:118:GLU:CA	5:A:1375:6LX:CAO	2.62	0.77
1:A:177:ASP:OD2	1:A:180:GLU:N	2.16	0.77
1:A:96:GLY:HA2	1:A:258:ILE:O	1.84	0.77
1:B:127:TRP:CD1	1:B:128:GLU:CD	2.58	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:CG1	1:B:263:LEU:HD13	2.13	0.77
1:B:47:ARG:HH12	1:B:364:GLU:CB	1.98	0.77
1:A:21:VAL:HG21	1:A:357:LYS:HB2	1.67	0.77
1:B:247:GLU:O	1:B:255:LEU:HB2	1.85	0.77
1:B:40:ILE:N	1:B:40:ILE:CD1	2.30	0.77
1:B:104:TYR:O	1:B:104:TYR:HD1	1.66	0.76
1:B:98:ASN:HD21	1:B:260:LYS:CD	1.98	0.76
1:A:284:GLU:O	1:A:289:ASN:CB	2.33	0.76
1:A:32:GLU:OE2	1:A:37:ALA:O	2.04	0.76
1:B:121:PRO:O	1:B:124:GLU:CG	2.33	0.76
1:B:192:ARG:CB	1:B:322:ASP:HA	2.08	0.76
5:A:1375:6LX:CBF	5:A:1375:6LX:CAJ	2.57	0.76
1:A:65:THR:OG1	1:A:361:ASN:CG	2.24	0.76
1:A:156:VAL:O	1:A:203:THR:HA	1.85	0.76
1:B:168:LEU:CD2	1:B:168:LEU:N	2.49	0.76
1:B:128:GLU:CD	1:B:208:ASP:OD1	2.22	0.76
1:B:262:ASN:ND2	1:B:262:ASN:N	2.30	0.76
1:A:137:PRO:HB3	5:A:1375:6LX:CBJ	2.15	0.76
1:A:167:GLU:C	1:A:168:LEU:HD12	2.00	0.76
1:A:336:ILE:O	1:A:336:ILE:CD1	2.30	0.76
1:B:110:GLY:HA3	2:B:601:ADP:N7	1.99	0.76
1:B:164:TYR:CB	1:B:169:PHE:HE1	1.98	0.76
1:A:173:ASN:ND2	1:A:200:GLU:OE2	2.19	0.76
1:A:105:GLY:C	1:A:269:SER:H	1.89	0.76
1:A:152:THR:HB	1:A:247:GLU:HB2	1.67	0.76
1:B:161:LEU:HD22	1:B:162:GLU:H	1.45	0.76
1:A:197:LYS:CE	1:B:250:ILE:HG13	2.16	0.76
1:B:344:GLU:O	1:B:347:LEU:HD12	1.83	0.76
1:B:165:ASN:H	1:B:288:ILE:CG1	1.99	0.76
1:A:225:ALA:CB	1:A:231:TYR:HB2	2.14	0.75
1:A:106:GLN:CB	1:A:345:GLU:HB3	2.16	0.75
1:B:24:ARG:NH2	1:B:114:THR:CG2	2.13	0.75
1:B:171:LEU:HD23	1:B:220:LYS:HG2	1.67	0.75
1:A:230:ALA:HB1	1:A:234:ARG:HB2	0.79	0.75
1:B:304:GLU:O	1:B:305:ARG:HB3	1.84	0.75
1:B:41:VAL:N	1:B:52:VAL:CG2	2.40	0.75
1:B:66:TYR:CZ	1:B:350:LEU:HB3	2.20	0.75
1:B:96:GLY:HA2	1:B:259:GLY:HA3	1.68	0.75
1:A:201:GLU:O	1:A:201:GLU:HG2	1.84	0.75
1:A:73:GLY:N	1:A:76:THR:CG2	2.48	0.75
1:B:341:LEU:CD2	1:B:341:LEU:H	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:CYS:N	1:A:88:PRO:HD2	2.01	0.75
1:A:117:GLY:CA	5:A:1375:6LX:HAN	2.14	0.75
5:A:1375:6LX:CAX	5:A:1375:6LX:HBI	2.16	0.75
1:B:192:ARG:HH11	1:B:192:ARG:HG3	1.50	0.75
1:B:250:ILE:CD1	1:B:250:ILE:N	2.44	0.75
1:B:128:GLU:CG	1:B:208:ASP:OD1	2.34	0.75
1:A:136:ILE:O	1:A:140:LEU:HB2	1.85	0.75
1:B:127:TRP:CZ2	1:B:208:ASP:OD1	2.39	0.75
1:B:130:ASP:O	1:B:138:ARG:NH2	2.20	0.75
1:B:110:GLY:HA2	2:B:601:ADP:N7	1.98	0.75
1:A:160:LEU:HD12	1:A:171:LEU:HD22	1.63	0.75
1:B:120:SER:OG	1:B:125:TYR:HB2	1.87	0.75
1:A:225:ALA:HA	1:A:231:TYR:CE2	2.12	0.74
1:A:44:ASP:OD2	1:A:47:ARG:HB2	1.85	0.74
1:B:136:ILE:N	1:B:137:PRO:HD2	2.02	0.74
1:A:225:ALA:O	1:A:228:MET:HG3	1.86	0.74
1:A:47:ARG:O	1:A:48:LYS:CG	2.35	0.74
1:B:98:ASN:HB3	1:B:323:SER:HA	1.69	0.74
1:A:227:LEU:N	1:A:228:MET:CB	2.51	0.74
1:A:66:TYR:CE2	1:A:68:PHE:HZ	2.05	0.74
1:B:17:LYS:O	1:B:18:ASN:C	2.25	0.74
1:A:41:VAL:CG1	1:A:52:VAL:HG21	2.04	0.74
1:A:217:GLY:CA	5:A:1375:6LX:HAP	2.17	0.74
1:A:72:PHE:HE2	1:A:81:VAL:CG2	1.80	0.74
1:A:87:CYS:N	1:A:88:PRO:CD	2.50	0.74
1:B:166:GLU:OE1	1:B:166:GLU:CA	2.35	0.74
1:A:135:ILE:O	1:A:139:THR:CB	2.36	0.74
1:A:262:ASN:C	1:A:263:LEU:HD13	2.08	0.74
1:A:285:ALA:O	1:A:289:ASN:ND2	2.20	0.74
1:B:226:THR:O	1:B:228:MET:HG2	1.88	0.74
1:A:214:LEU:O	5:A:1375:6LX:CAE	2.36	0.73
1:A:143:ILE:HD11	1:A:147:LEU:HD11	1.69	0.73
1:A:228:MET:HG3	1:A:231:TYR:HD2	1.50	0.73
1:A:67:THR:CG2	1:A:359:ILE:CG2	2.65	0.73
1:A:72:PHE:HZ	1:A:81:VAL:N	1.85	0.73
1:B:117:GLY:HA3	1:B:134:GLY:N	2.03	0.73
1:B:172:LEU:HG	1:B:173:ASN:HD22	1.52	0.73
1:A:28:PHE:HE2	1:A:32:GLU:CG	2.00	0.73
1:B:227:LEU:HB3	1:B:228:MET:O	1.88	0.73
1:B:311:TYR:HH	1:B:324:LEU:HB3	1.52	0.73
1:B:121:PRO:O	1:B:124:GLU:HG3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:HG21	1:B:135:ILE:CG2	2.18	0.73
1:A:32:GLU:CD	1:A:37:ALA:HB3	2.08	0.73
1:A:72:PHE:CZ	1:A:81:VAL:N	2.56	0.73
1:B:90:LEU:HD12	1:B:90:LEU:O	1.88	0.73
1:B:96:GLY:HA2	1:B:259:GLY:CA	2.18	0.73
1:A:248:THR:HG23	1:A:254:GLU:OE2	1.88	0.73
1:A:41:VAL:HA	1:A:52:VAL:HG23	1.71	0.73
1:A:194:VAL:HG11	1:A:318:ARG:HG3	1.71	0.73
1:A:227:LEU:N	1:A:229:ASN:N	2.36	0.73
1:A:153:GLU:HG3	1:A:246:LYS:O	1.89	0.73
1:A:28:PHE:CD2	1:A:32:GLU:CG	2.72	0.73
1:A:28:PHE:HD2	1:A:32:GLU:HG2	1.52	0.73
1:A:118:GLU:O	5:A:1375:6LX:CAO	2.36	0.73
1:A:272:ILE:HD12	1:A:355:ARG:HH21	1.51	0.73
1:A:281:ARG:O	1:A:285:ALA:N	2.21	0.73
1:A:320:LEU:O	1:A:324:LEU:HD21	1.88	0.73
1:A:73:GLY:O	1:A:76:THR:HG23	1.88	0.73
1:B:110:GLY:CA	2:B:601:ADP:C8	2.71	0.73
1:B:147:LEU:HB3	1:B:154:PHE:CD1	2.24	0.73
1:B:28:PHE:HE1	1:B:39:SER:OG	1.72	0.73
1:B:113:PHE:CZ	1:B:118:GLU:HG2	2.22	0.72
1:B:172:LEU:HD12	1:B:173:ASN:ND2	2.03	0.72
1:A:296:GLY:O	1:A:300:THR:CB	2.37	0.72
1:A:152:THR:HG22	1:A:247:GLU:HG3	1.68	0.72
1:A:43:CYS:SG	1:A:73:GLY:HA2	2.29	0.72
1:B:98:ASN:ND2	1:B:260:LYS:HD2	2.04	0.72
1:B:265:ASP:C	1:B:266:LEU:CD2	2.57	0.72
1:A:249:THR:HB	1:A:252:GLY:HA3	1.69	0.72
1:B:171:LEU:HD12	1:B:171:LEU:H	1.54	0.72
1:B:249:THR:OG1	1:B:252:GLY:HA3	1.86	0.72
1:B:85:VAL:HG11	1:B:333:ILE:HG21	1.72	0.72
1:B:76:THR:O	1:B:77:LYS:CE	2.36	0.72
1:A:49:GLU:CD	1:A:67:THR:HA	2.06	0.72
1:A:202:ILE:HD13	1:A:202:ILE:N	2.04	0.72
1:A:96:GLY:CA	1:A:258:ILE:O	2.37	0.72
1:B:303:VAL:HG21	1:B:357:LYS:HZ2	1.54	0.72
1:B:347:LEU:N	1:B:347:LEU:HD12	2.00	0.72
1:A:114:THR:C	1:A:134:GLY:HA3	2.10	0.71
1:A:116:GLU:C	5:A:1375:6LX:HBB2	2.10	0.71
1:B:295:LEU:O	1:B:299:ILE:N	2.21	0.71
1:B:77:LYS:HE2	1:B:77:LYS:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:H	1:A:229:ASN:N	1.89	0.71
1:A:133:ALA:CA	5:A:1375:6LX:HAZ1	2.19	0.71
1:A:210:VAL:O	1:A:214:LEU:N	2.22	0.71
1:A:25:CYS:HB3	1:A:43:CYS:CB	2.20	0.71
1:B:342:ASN:HD22	1:B:343:LEU:H	1.38	0.71
1:A:32:GLU:OE2	1:A:37:ALA:CA	2.39	0.71
1:A:78:GLN:HE22	1:A:133:ALA:C	1.94	0.71
1:A:136:ILE:N	1:A:137:PRO:HD2	2.06	0.71
1:B:171:LEU:HB3	1:B:220:LYS:CE	2.03	0.71
1:B:211:TYR:CD1	1:B:215:GLU:HB2	2.25	0.71
1:B:279:ASP:O	1:B:283:ARG:N	2.21	0.71
1:B:362:LYS:HG3	1:B:363:PRO:HD2	1.73	0.71
1:B:48:LYS:HD2	1:B:362:LYS:HZ1	1.55	0.71
1:A:315:LYS:H	1:A:315:LYS:HE3	1.53	0.71
1:A:162:GLU:OE1	1:A:171:LEU:HD11	1.91	0.71
1:B:165:ASN:O	1:B:166:GLU:HB2	1.90	0.71
1:B:249:THR:HG22	1:B:255:LEU:CD2	2.21	0.71
1:B:22:VAL:CG2	1:B:332:ILE:O	2.37	0.71
1:B:40:ILE:O	1:B:52:VAL:HA	1.89	0.71
1:A:113:PHE:O	1:A:117:GLY:HA2	1.90	0.71
1:A:117:GLY:C	5:A:1375:6LX:CAO	2.47	0.71
1:B:127:TRP:HH2	1:B:207:LYS:CG	2.03	0.71
1:A:227:LEU:N	1:A:228:MET:CA	2.53	0.71
1:A:25:CYS:HB3	1:A:43:CYS:HB3	1.73	0.70
1:B:352:TYR:O	1:B:356:ALA:HB3	1.89	0.70
1:A:115:MET:O	1:A:136:ILE:CG1	2.35	0.70
1:A:156:VAL:CG1	1:A:204:VAL:HG23	2.21	0.70
1:B:19:ILE:HA	1:B:330:THR:HB	1.73	0.70
1:B:357:LYS:NZ	1:B:357:LYS:CB	2.47	0.70
1:B:40:ILE:O	1:B:52:VAL:CA	2.39	0.70
1:A:125:TYR:HD1	1:A:125:TYR:H	1.36	0.70
1:A:194:VAL:HG11	1:A:318:ARG:CG	2.21	0.70
1:A:225:ALA:HB1	1:A:231:TYR:HB3	1.71	0.70
1:A:294:THR:CG2	1:A:314:SER:OG	2.38	0.70
1:A:42:GLU:O	4:A:1376:CL:CL	2.46	0.70
1:A:66:TYR:OH	1:A:354:HIS:N	2.23	0.70
1:A:206:ASN:HB2	1:A:209:GLU:HB3	1.72	0.70
1:B:245:MET:HG3	1:B:257:LYS:O	1.90	0.70
1:A:156:VAL:CG1	1:A:204:VAL:CG2	2.69	0.70
1:A:156:VAL:HG13	1:A:204:VAL:CG2	2.18	0.70
1:A:302:LEU:CG	1:A:311:TYR:HH	2.02	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LEU:O	1:A:347:LEU:HD23	1.90	0.70
1:A:82:TYR:HE2	1:A:139:THR:HA	1.54	0.70
1:B:112:THR:O	1:B:116:GLU:CB	2.40	0.70
1:B:19:ILE:HD12	1:B:19:ILE:H	1.57	0.70
1:A:35:ALA:HB1	1:A:341:LEU:HG	1.71	0.70
1:B:172:LEU:CD1	1:B:173:ASN:HD21	2.05	0.70
1:B:81:VAL:CG1	1:B:85:VAL:HG21	2.22	0.70
1:A:166:GLU:O	1:A:167:GLU:CD	2.30	0.70
1:A:302:LEU:HD11	1:A:311:TYR:OH	1.90	0.70
1:A:302:LEU:CD1	1:A:311:TYR:OH	2.40	0.70
1:B:144:PHE:CG	1:B:207:LYS:HB3	2.27	0.70
1:B:158:VAL:N	1:B:202:ILE:O	2.19	0.70
1:B:276:GLY:O	1:B:278:VAL:HG12	1.91	0.70
1:A:253:GLU:OE2	1:A:253:GLU:C	2.30	0.70
1:A:129:GLU:CA	1:A:129:GLU:OE1	2.40	0.69
1:A:28:PHE:CD2	1:A:32:GLU:CB	2.74	0.69
1:A:320:LEU:O	1:A:324:LEU:HD23	1.92	0.69
1:B:77:LYS:HE2	1:B:77:LYS:CA	2.22	0.69
1:A:173:ASN:O	1:A:220:LYS:NZ	2.26	0.69
1:A:89:ILE:HD13	1:A:99:CYS:HB3	1.73	0.69
1:A:290:GLN:O	1:A:294:THR:OG1	2.10	0.69
1:A:213:ILE:O	1:A:216:LYS:HG3	1.92	0.69
1:B:53:ARG:O	1:B:54:THR:CB	2.40	0.69
1:A:106:GLN:HA	1:A:268:GLY:CA	2.23	0.69
1:A:66:TYR:CE2	1:A:68:PHE:CZ	2.80	0.69
1:B:172:LEU:CD1	1:B:173:ASN:HD22	2.04	0.69
1:B:20:GLN:NE2	1:B:329:ARG:HH12	1.64	0.69
1:B:24:ARG:HH21	1:B:114:THR:HG21	1.51	0.69
1:A:72:PHE:CE2	1:A:81:VAL:HG21	2.24	0.69
5:A:1375:6LX:HAC2	5:A:1375:6LX:HAW	1.73	0.69
1:B:106:GLN:CA	1:B:270:GLU:OE1	2.40	0.69
1:B:26:ARG:HD2	2:B:601:ADP:O4'	1.92	0.69
1:B:182:LEU:H	1:B:182:LEU:HD23	1.57	0.69
1:A:128:GLU:CD	1:A:128:GLU:H	1.96	0.69
1:A:186:ASP:HB2	1:A:318:ARG:HH12	1.58	0.69
1:B:118:GLU:C	1:B:132:LEU:HD12	2.13	0.69
1:B:158:VAL:HG13	1:B:202:ILE:HG22	1.75	0.69
1:B:177:ASP:O	1:B:178:VAL:CG2	2.41	0.69
1:B:48:LYS:C	1:B:71:VAL:HG21	2.14	0.69
1:A:118:GLU:H	5:A:1375:6LX:CAO	1.90	0.68
1:A:168:LEU:CD1	1:A:168:LEU:N	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:TRP:CZ2	1:B:208:ASP:N	2.58	0.68
1:B:142:GLN:C	1:B:146:LYS:CG	2.59	0.68
1:A:83:ARG:O	1:A:88:PRO:HD3	1.93	0.68
1:B:342:ASN:O	1:B:346:THR:HG22	1.93	0.68
1:B:354:HIS:HA	1:B:357:LYS:O	1.93	0.68
1:A:162:GLU:OE2	1:A:237:SER:HB2	1.92	0.68
1:B:303:VAL:HG21	1:B:357:LYS:NZ	2.08	0.68
1:B:30:LEU:HD13	1:B:30:LEU:O	1.92	0.68
1:A:39:SER:HB3	1:A:338:PRO:C	2.13	0.68
1:B:127:TRP:HH2	1:B:207:LYS:HG2	1.56	0.68
1:B:360:LEU:HD12	1:B:361:ASN:H	1.58	0.68
1:A:65:THR:HG1	1:A:361:ASN:CG	1.97	0.68
1:A:113:PHE:C	1:A:113:PHE:CD1	2.65	0.68
1:A:129:GLU:HA	1:A:129:GLU:OE1	1.92	0.68
1:A:214:LEU:O	5:A:1375:6LX:CAP	2.41	0.68
1:A:227:LEU:H	1:A:228:MET:C	1.96	0.68
1:A:243:ILE:HG13	1:A:259:GLY:O	1.94	0.68
1:A:309:VAL:CB	1:A:311:TYR:CE2	2.77	0.68
1:A:104:TYR:CE2	1:A:352:TYR:CG	2.82	0.68
1:B:105:GLY:HA3	1:B:109:THR:OG1	1.93	0.68
1:B:172:LEU:CG	1:B:173:ASN:HD22	2.07	0.68
1:B:93:VAL:CG2	1:B:261:LEU:HD23	2.20	0.68
1:A:118:GLU:CA	5:A:1375:6LX:CAN	2.72	0.68
1:A:186:ASP:CG	1:A:318:ARG:HH22	1.98	0.68
1:A:32:GLU:OE2	1:A:37:ALA:HB3	1.93	0.68
1:A:81:VAL:O	1:A:85:VAL:HG22	1.93	0.68
1:B:172:LEU:HD12	1:B:173:ASN:HD21	1.56	0.68
1:B:239:PHE:HB3	1:B:263:LEU:HD12	1.74	0.68
1:B:234:ARG:HH11	1:B:288:ILE:CD1	2.07	0.68
5:A:1375:6LX:CAO	5:A:1375:6LX:HBI	2.24	0.68
1:A:210:VAL:O	1:A:214:LEU:HB2	1.93	0.68
1:B:347:LEU:H	1:B:347:LEU:CD1	1.95	0.68
1:A:116:GLU:OE1	5:A:1375:6LX:CAS	2.42	0.68
1:A:133:ALA:HB1	1:A:137:PRO:CG	2.24	0.68
1:A:80:ASP:O	1:A:84:SER:OG	2.11	0.68
1:B:249:THR:O	1:B:252:GLY:N	2.23	0.68
1:B:173:ASN:CB	1:B:176:SER:OG	2.34	0.67
1:A:156:VAL:HG11	1:A:204:VAL:CB	2.20	0.67
1:A:65:THR:OG1	1:A:361:ASN:ND2	2.27	0.67
1:B:117:GLY:CA	1:B:134:GLY:H	2.05	0.67
1:A:170:ASP:C	1:A:170:ASP:OD1	2.32	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:HB	1:A:314:SER:OG	1.93	0.67
1:A:315:LYS:N	1:A:315:LYS:CE	2.57	0.67
1:A:93:VAL:HG23	1:A:99:CYS:HG	1.60	0.67
1:B:197:LYS:C	1:B:197:LYS:HD2	2.04	0.67
1:B:341:LEU:HD22	1:B:341:LEU:N	2.00	0.67
1:B:41:VAL:HG12	1:B:52:VAL:HB	1.77	0.67
1:A:249:THR:O	1:A:252:GLY:C	2.32	0.67
1:A:281:ARG:O	1:A:285:ALA:CB	2.41	0.67
1:A:23:VAL:HG23	1:A:68:PHE:CE2	2.29	0.67
1:A:217:GLY:O	1:A:221:ARG:HG2	1.95	0.67
1:A:245:MET:HB2	1:A:257:LYS:HG2	1.77	0.67
1:A:112:THR:HB	2:A:601:ADP:O2A	1.95	0.67
1:B:288:ILE:HD12	1:B:288:ILE:H	1.59	0.67
1:B:296:GLY:O	1:B:299:ILE:HG22	1.95	0.67
1:B:76:THR:HA	1:B:80:ASP:OD2	1.94	0.67
1:A:272:ILE:HG22	1:A:348:SER:HA	1.75	0.67
1:B:118:GLU:HB3	1:B:132:LEU:CG	2.23	0.67
1:B:172:LEU:HG	1:B:173:ASN:ND2	2.10	0.67
1:B:165:ASN:H	1:B:288:ILE:HG12	1.58	0.67
1:B:165:ASN:HA	1:B:288:ILE:HD11	1.77	0.66
1:A:28:PHE:CE2	1:A:32:GLU:HG2	2.27	0.66
1:A:347:LEU:N	1:A:347:LEU:CD2	2.58	0.66
1:A:174:PRO:O	1:A:177:ASP:O	2.13	0.66
1:A:90:LEU:O	1:A:94:ILE:HB	1.96	0.66
1:B:20:GLN:NE2	1:B:329:ARG:HH22	1.92	0.66
1:A:197:LYS:NZ	1:B:250:ILE:HG13	2.11	0.66
1:A:119:ARG:HB2	5:A:1375:6LX:CAX	2.26	0.66
1:A:218:ALA:CB	5:A:1375:6LX:HAF	2.24	0.66
1:A:284:GLU:HB2	1:A:293:LEU:HD21	1.76	0.66
1:B:177:ASP:C	1:B:178:VAL:CG1	2.63	0.66
1:A:67:THR:HG22	1:A:359:ILE:HB	1.76	0.66
1:B:163:ILE:CG2	1:B:236:HIS:CD2	2.78	0.66
1:A:170:ASP:OD2	1:A:200:GLU:CB	2.38	0.66
1:B:342:ASN:O	1:B:343:LEU:C	2.33	0.66
1:A:25:CYS:HB3	1:A:43:CYS:SG	2.36	0.66
1:A:91:ASP:C	1:A:94:ILE:HG22	2.15	0.66
1:B:311:TYR:CZ	1:B:321:GLN:HA	2.31	0.66
1:A:116:GLU:O	5:A:1375:6LX:HBF	1.96	0.66
1:A:196:ILE:HG13	1:A:199:LEU:CB	2.26	0.66
1:A:125:TYR:HB2	1:A:129:GLU:CB	2.21	0.66
1:A:236:HIS:CD2	1:A:266:LEU:HD23	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:HB2	1:A:345:GLU:HG2	1.78	0.66
1:B:187:ASP:CB	1:B:195:ILE:HG22	2.26	0.66
1:B:226:THR:O	1:B:228:MET:CG	2.44	0.66
1:B:82:TYR:HD1	1:B:82:TYR:O	1.78	0.66
1:A:242:THR:CG2	1:A:260:LYS:CD	2.63	0.65
1:B:174:PRO:HB3	1:B:220:LYS:CB	2.26	0.65
1:B:239:PHE:CG	1:B:263:LEU:HD12	2.31	0.65
1:A:168:LEU:HD13	1:A:168:LEU:N	2.11	0.65
1:A:160:LEU:HD13	1:A:238:VAL:O	1.97	0.65
1:A:249:THR:CB	1:A:252:GLY:HA3	2.26	0.65
1:A:156:VAL:CG1	1:A:204:VAL:H	2.08	0.65
1:A:270:GLU:C	1:A:348:SER:OG	2.34	0.65
1:A:51:SER:CA	1:A:64:LYS:O	2.43	0.65
1:B:333:ILE:HG13	1:B:333:ILE:O	1.96	0.65
1:B:155:SER:HB2	1:B:244:HIS:HB2	1.78	0.65
5:A:1375:6LX:HBF	5:A:1375:6LX:CAN	2.27	0.65
1:A:156:VAL:HG13	1:A:204:VAL:H	1.61	0.65
1:A:315:LYS:N	1:A:315:LYS:HE2	2.12	0.65
1:B:47:ARG:HB2	1:B:49:GLU:CD	2.17	0.65
1:B:172:LEU:HD11	1:B:173:ASN:ND2	2.11	0.65
1:B:296:GLY:HA3	1:B:352:TYR:OH	1.96	0.65
1:B:296:GLY:CA	1:B:352:TYR:CZ	2.75	0.65
1:A:28:PHE:HE1	1:A:339:ALA:HB3	1.49	0.65
1:A:78:GLN:OE1	1:A:113:PHE:CZ	2.50	0.65
1:A:105:GLY:O	1:A:268:GLY:CA	2.38	0.65
1:A:28:PHE:HE2	1:A:32:GLU:CD	2.00	0.65
1:B:77:LYS:HA	1:B:77:LYS:CE	2.26	0.65
1:B:112:THR:CG2	1:B:116:GLU:CG	2.66	0.65
1:B:157:LYS:CG	1:B:242:THR:O	2.44	0.65
1:B:121:PRO:O	1:B:122:ASN:OD1	2.14	0.64
1:B:268:GLY:C	1:B:270:GLU:OE2	2.36	0.64
1:B:73:GLY:C	1:B:75:SER:H	1.94	0.64
1:A:41:VAL:CG2	1:A:338:PRO:O	2.45	0.64
1:A:351:GLU:O	1:A:355:ARG:HG2	1.97	0.64
1:A:47:ARG:C	1:A:48:LYS:CG	2.65	0.64
1:A:82:TYR:HE2	1:A:139:THR:CA	2.10	0.64
1:B:104:TYR:OH	1:B:349:THR:CA	2.45	0.64
1:B:41:VAL:HG21	1:B:338:PRO:HA	1.77	0.64
1:A:82:TYR:CE2	1:A:139:THR:HA	2.32	0.64
1:B:192:ARG:CG	1:B:192:ARG:HH11	2.09	0.64
1:B:113:PHE:HE2	1:B:118:GLU:HG3	0.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ASP:H	1:B:220:LYS:NZ	1.95	0.64
1:B:270:GLU:OE2	1:B:270:GLU:N	2.30	0.64
1:B:26:ARG:NH1	1:B:27:PRO:O	2.29	0.64
1:A:230:ALA:HB1	1:A:234:ARG:CG	2.22	0.64
1:A:234:ARG:NH2	1:A:234:ARG:O	2.30	0.64
1:B:183:GLN:CD	1:B:185:PHE:CZ	2.71	0.64
1:B:253:GLU:HG2	1:B:254:GLU:N	2.12	0.64
1:B:296:GLY:C	1:B:299:ILE:HG22	2.17	0.64
1:A:113:PHE:CE1	1:A:114:THR:CG2	2.67	0.64
1:A:229:ASN:O	1:A:229:ASN:ND2	2.30	0.64
1:A:49:GLU:OE2	6:A:2004:HOH:O	2.15	0.64
1:B:77:LYS:H	1:B:80:ASP:CG	2.01	0.64
1:A:86:VAL:O	1:A:88:PRO:N	2.31	0.64
1:B:227:LEU:HD23	1:B:229:ASN:CA	2.27	0.64
1:A:234:ARG:NE	1:A:234:ARG:O	2.30	0.64
1:A:98:ASN:HB2	1:A:323:SER:HA	1.78	0.64
1:A:347:LEU:N	1:A:347:LEU:HD22	2.13	0.64
1:B:122:ASN:N	1:B:122:ASN:OD1	2.30	0.64
1:B:24:ARG:O	1:B:24:ARG:HG3	1.97	0.64
1:B:26:ARG:HH11	1:B:26:ARG:HG2	1.63	0.64
1:B:49:GLU:N	1:B:49:GLU:OE1	2.30	0.64
1:A:26:ARG:HA	1:A:74:ALA:CA	2.26	0.63
1:A:272:ILE:CG2	1:A:348:SER:HA	2.28	0.63
1:A:298:VAL:HG11	1:A:311:TYR:CG	2.27	0.63
1:A:44:ASP:OD1	1:A:44:ASP:C	2.35	0.63
1:B:225:ALA:CA	1:B:231:TYR:CE1	2.80	0.63
1:B:214:LEU:HB3	5:B:1375:6LX:HAA2	1.80	0.63
1:B:99:CYS:HA	1:B:328:THR:OG1	1.98	0.63
1:A:53:ARG:CG	1:A:60:LYS:O	2.47	0.63
1:B:172:LEU:N	1:B:220:LYS:HE2	2.13	0.63
1:B:26:ARG:HG2	1:B:26:ARG:NH1	2.14	0.63
1:B:225:ALA:HA	1:B:231:TYR:HD1	1.56	0.63
1:A:177:ASP:OD1	1:A:179:SER:N	2.31	0.63
1:A:211:TYR:OH	5:A:1375:6LX:HAC1	1.98	0.63
1:A:105:GLY:C	1:A:269:SER:N	2.52	0.63
1:B:182:LEU:HB2	1:B:197:LYS:O	1.97	0.63
1:B:249:THR:CB	1:B:252:GLY:HA3	2.29	0.63
1:A:296:GLY:O	1:A:300:THR:N	2.30	0.63
1:B:79:ILE:HG13	1:B:80:ASP:N	2.10	0.63
1:B:304:GLU:OE1	1:B:306:THR:HG23	1.93	0.63
1:A:126:THR:O	1:A:129:GLU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:TYR:OH	1:B:86:VAL:HG11	1.97	0.63
1:A:184:MET:HG2	1:A:196:ILE:CG2	2.28	0.62
1:A:294:THR:HG21	1:A:314:SER:OG	1.98	0.62
1:B:163:ILE:CG1	1:B:236:HIS:NE2	2.62	0.62
1:B:344:GLU:C	1:B:347:LEU:HD12	2.15	0.62
1:A:214:LEU:HD11	5:A:1375:6LX:HAQ	1.82	0.62
1:A:187:ASP:O	1:A:190:ASN:O	2.16	0.62
1:A:225:ALA:O	1:A:231:TYR:HD2	1.81	0.62
1:A:25:CYS:O	1:A:73:GLY:C	2.37	0.62
1:B:165:ASN:HA	1:B:288:ILE:CD1	2.29	0.62
1:B:252:GLY:HA2	1:B:253:GLU:HB3	0.70	0.62
1:A:249:THR:CB	1:A:252:GLY:H	2.07	0.62
1:A:139:THR:HG21	1:A:263:LEU:HD21	1.80	0.62
1:B:117:GLY:HA2	1:B:134:GLY:N	2.15	0.62
1:B:95:MET:HB3	1:B:97:TYR:HD1	1.64	0.62
1:A:274:ARG:O	1:A:277:ALA:HB2	1.98	0.62
1:A:28:PHE:CD2	1:A:32:GLU:HB2	2.33	0.62
1:B:170:ASP:OD2	1:B:199:LEU:HA	1.98	0.62
1:A:215:GLU:C	5:A:1375:6LX:CLA	2.74	0.62
1:A:144:PHE:CD2	1:A:207:LYS:HB2	2.34	0.62
1:A:49:GLU:OE1	1:A:67:THR:N	2.32	0.62
1:B:105:GLY:CA	1:B:109:THR:HB	2.23	0.62
1:A:43:CYS:HB3	4:A:1376:CL:CL	2.36	0.62
1:A:245:MET:HE2	1:A:257:LYS:HG2	1.82	0.62
1:A:25:CYS:CB	1:A:43:CYS:HB3	2.29	0.62
1:A:54:THR:O	1:A:55:GLY:C	2.37	0.62
1:B:221:ARG:HB2	1:B:231:TYR:OH	2.00	0.62
1:A:170:ASP:O	1:A:220:LYS:NZ	2.32	0.62
1:B:104:TYR:C	1:B:104:TYR:CD1	2.70	0.62
1:B:143:ILE:CA	1:B:147:LEU:CD2	2.78	0.62
1:B:171:LEU:CA	1:B:177:ASP:OD2	2.47	0.62
1:B:287:ASN:N	1:B:287:ASN:OD1	2.30	0.62
1:A:253:GLU:OE2	1:A:254:GLU:N	2.32	0.62
1:A:265:ASP:N	1:A:265:ASP:OD1	2.32	0.62
1:B:227:LEU:HB3	1:B:228:MET:C	2.19	0.62
1:A:134:GLY:O	1:A:137:PRO:CG	2.44	0.61
1:A:160:LEU:HB3	1:A:171:LEU:HB2	1.82	0.61
1:A:167:GLU:OE2	1:A:181:ARG:HG3	2.00	0.61
1:A:184:MET:HG2	1:A:196:ILE:HG23	1.81	0.61
1:A:245:MET:HB2	1:A:257:LYS:CD	2.28	0.61
1:B:118:GLU:HB3	1:B:132:LEU:HD13	0.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LYS:O	1:B:19:ILE:N	2.33	0.61
1:B:47:ARG:NH2	1:B:363:PRO:O	2.29	0.61
1:A:32:GLU:CD	1:A:32:GLU:O	2.38	0.61
1:B:33:ARG:HH11	1:B:33:ARG:HB2	1.65	0.61
1:B:85:VAL:HG11	1:B:333:ILE:CG2	2.30	0.61
1:A:41:VAL:HA	1:A:52:VAL:HG22	1.79	0.61
1:B:172:LEU:CG	1:B:173:ASN:ND2	2.63	0.61
1:A:225:ALA:O	1:A:231:TYR:CD2	2.53	0.61
1:B:126:THR:C	1:B:130:ASP:OD2	2.39	0.61
1:B:270:GLU:CD	1:B:270:GLU:N	2.50	0.61
1:B:294:THR:O	1:B:298:VAL:N	2.19	0.61
1:B:89:ILE:HD11	1:B:329:ARG:O	1.99	0.61
1:B:93:VAL:HG23	1:B:99:CYS:SG	2.40	0.61
1:B:126:THR:HG22	1:B:129:GLU:HB2	1.82	0.61
1:B:220:LYS:O	1:B:224:ALA:CB	2.49	0.61
1:B:222:THR:O	1:B:225:ALA:HB3	2.01	0.61
1:B:299:ILE:HA	1:B:302:LEU:HG	1.82	0.61
1:B:161:LEU:HD22	1:B:162:GLU:CA	2.29	0.61
1:A:213:ILE:O	1:A:216:LYS:HD2	2.00	0.61
1:A:245:MET:CE	1:A:257:LYS:CG	2.79	0.61
1:B:249:THR:HG21	1:B:255:LEU:HD21	1.83	0.61
1:B:315:LYS:O	1:B:319:ILE:CG1	2.41	0.61
1:B:40:ILE:O	1:B:53:ARG:N	2.34	0.61
1:A:216:LYS:C	5:A:1375:6LX:CLA	2.76	0.61
1:A:225:ALA:C	1:A:228:MET:HG3	2.21	0.61
1:B:110:GLY:H	2:B:601:ADP:PB	2.23	0.61
1:B:41:VAL:HG12	1:B:52:VAL:CG2	2.31	0.61
1:A:91:ASP:HA	1:A:94:ILE:CG2	2.31	0.61
1:B:106:GLN:HA	1:B:270:GLU:OE1	2.01	0.60
1:B:173:ASN:O	1:B:174:PRO:C	2.38	0.60
1:A:145:GLU:OE1	6:A:2012:HOH:O	2.16	0.60
1:A:161:LEU:N	1:A:238:VAL:O	2.25	0.60
1:A:253:GLU:OE2	1:A:254:GLU:CA	2.49	0.60
1:A:28:PHE:HE2	1:A:32:GLU:HB2	1.56	0.60
1:A:271:ASN:HD21	1:A:284:GLU:HA	1.67	0.60
1:A:309:VAL:HB	1:A:311:TYR:CE2	2.36	0.60
1:A:41:VAL:CG1	1:A:52:VAL:HG23	2.30	0.60
1:B:300:THR:HG22	1:B:356:ALA:HA	0.67	0.60
4:A:1376:CL:CL	4:A:1378:CL:CL	2.93	0.60
1:B:357:LYS:HG3	1:B:359:ILE:HD13	1.83	0.60
1:B:164:TYR:CE1	1:B:234:ARG:NE	2.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLY:HA2	2:B:601:ADP:O2A	2.01	0.60
1:A:152:THR:CG2	1:A:247:GLU:CB	2.49	0.60
1:A:264:VAL:HG23	1:A:265:ASP:N	2.16	0.60
1:A:73:GLY:C	1:A:76:THR:HG22	2.22	0.60
1:B:170:ASP:C	1:B:170:ASP:OD1	2.40	0.60
1:B:343:LEU:O	1:B:347:LEU:HD11	2.02	0.60
1:A:25:CYS:SG	4:A:1376:CL:CL	2.97	0.60
1:B:128:GLU:HG2	1:B:208:ASP:OD1	2.01	0.60
1:A:252:GLY:HA2	1:A:253:GLU:HB3	0.68	0.60
1:B:133:ALA:HB1	1:B:137:PRO:CG	2.31	0.60
1:B:221:ARG:CB	1:B:231:TYR:OH	2.49	0.60
1:B:342:ASN:HA	1:B:345:GLU:HB2	1.83	0.60
1:B:126:THR:HG23	1:B:129:GLU:H	1.67	0.60
1:A:263:LEU:HD13	1:A:263:LEU:N	2.16	0.59
1:A:106:GLN:N	1:A:269:SER:OG	2.34	0.59
1:A:284:GLU:O	1:A:289:ASN:HB3	2.01	0.59
1:A:86:VAL:N	1:A:88:PRO:HD2	2.17	0.59
1:B:343:LEU:C	1:B:346:THR:CG2	2.69	0.59
1:B:127:TRP:CH2	1:B:207:LYS:C	2.75	0.59
1:B:117:GLY:HA3	1:B:133:ALA:HA	1.84	0.59
1:B:28:PHE:CZ	1:B:339:ALA:HA	2.36	0.59
1:B:341:LEU:O	1:B:345:GLU:OE1	2.21	0.59
1:B:83:ARG:O	1:B:88:PRO:HD3	2.02	0.59
1:A:294:THR:O	1:A:298:VAL:HG22	1.97	0.59
1:B:231:TYR:O	1:B:232:SER:CB	2.34	0.59
1:B:136:ILE:O	1:B:140:LEU:HG	2.03	0.59
1:B:354:HIS:CA	1:B:357:LYS:O	2.50	0.59
1:B:77:LYS:N	1:B:80:ASP:OD2	2.30	0.59
1:B:183:GLN:O	1:B:197:LYS:N	2.29	0.59
1:B:17:LYS:O	1:B:19:ILE:C	2.41	0.59
1:B:300:THR:CB	1:B:356:ALA:O	2.50	0.59
1:A:133:ALA:HB1	1:A:137:PRO:CB	2.32	0.59
1:A:82:TYR:C	1:A:82:TYR:CD1	2.76	0.59
1:B:128:GLU:N	1:B:128:GLU:OE1	2.30	0.59
1:B:221:ARG:CA	1:B:231:TYR:OH	2.51	0.59
1:A:228:MET:CG	1:A:231:TYR:CE2	2.85	0.59
1:B:239:PHE:HZ	1:B:241:VAL:HG11	1.64	0.59
1:B:113:PHE:CD2	1:B:118:GLU:HB2	2.38	0.59
1:B:127:TRP:CZ2	1:B:207:LYS:C	2.76	0.59
1:B:93:VAL:CG2	1:B:261:LEU:CD2	2.68	0.59
1:B:295:LEU:O	1:B:299:ILE:HB	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:HG2	1:B:335:THR:HG22	1.84	0.59
1:A:28:PHE:CE2	1:A:339:ALA:HB1	2.26	0.58
1:A:264:VAL:CG2	1:A:265:ASP:N	2.66	0.58
1:A:37:ALA:HB1	1:A:341:LEU:H	1.68	0.58
1:B:136:ILE:N	1:B:137:PRO:CD	2.66	0.58
1:A:135:ILE:HG22	1:A:139:THR:OG1	2.03	0.58
1:A:185:PHE:O	1:A:195:ILE:N	2.30	0.58
1:A:29:ASN:OD1	1:A:29:ASN:N	2.33	0.58
1:B:214:LEU:CD1	5:B:1375:6LX:CBK	2.82	0.58
1:A:28:PHE:HE2	1:A:32:GLU:CB	2.09	0.58
1:A:347:LEU:H	1:A:347:LEU:CD2	2.17	0.58
1:B:131:PRO:C	1:B:138:ARG:HH21	2.07	0.58
1:B:353:ALA:O	1:B:357:LYS:N	2.35	0.58
1:A:126:THR:O	1:A:129:GLU:N	2.36	0.58
1:A:114:THR:O	1:A:134:GLY:C	2.42	0.58
1:A:156:VAL:O	1:A:203:THR:HB	2.03	0.58
1:A:104:TYR:CE2	1:A:269:SER:HB3	2.39	0.58
1:A:323:SER:O	1:A:328:THR:HB	2.03	0.58
1:A:67:THR:CG2	1:A:359:ILE:HG21	2.33	0.58
1:B:116:GLU:HB3	5:B:1375:6LX:NBE	2.18	0.58
1:B:210:VAL:HG13	1:B:214:LEU:HG	1.86	0.58
1:B:82:TYR:O	1:B:86:VAL:N	2.34	0.58
1:B:227:LEU:HD23	1:B:229:ASN:HA	1.85	0.58
1:B:274:ARG:CG	1:B:274:ARG:HH11	1.98	0.58
1:A:165:ASN:ND2	1:A:165:ASN:N	2.50	0.58
1:B:43:CYS:HG	3:B:1367:CD:CD	1.37	0.58
1:B:192:ARG:CD	1:B:322:ASP:OD1	2.51	0.58
1:A:213:ILE:O	1:A:216:LYS:CD	2.52	0.57
1:A:162:GLU:HG2	1:A:231:TYR:HE1	1.69	0.57
1:A:281:ARG:CA	1:A:284:GLU:OE2	2.52	0.57
1:A:32:GLU:OE2	1:A:37:ALA:CB	2.52	0.57
1:B:29:ASN:OD1	1:B:31:ALA:N	2.37	0.57
1:A:323:SER:OG	1:A:324:LEU:HD23	2.04	0.57
1:A:109:THR:CB	1:A:335:THR:HB	2.32	0.57
1:A:270:GLU:N	1:A:270:GLU:OE1	2.37	0.57
1:A:320:LEU:O	1:A:324:LEU:CG	2.51	0.57
1:A:320:LEU:O	1:A:324:LEU:HG	2.04	0.57
1:A:39:SER:HB3	1:A:339:ALA:HA	1.85	0.57
1:B:177:ASP:O	1:B:178:VAL:CB	2.52	0.57
1:A:104:TYR:CG	1:A:105:GLY:N	2.72	0.57
1:B:246:LYS:HA	1:B:255:LEU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:CA	1:B:347:LEU:HD13	2.24	0.57
1:A:192:ARG:HH12	1:A:325:GLY:CA	2.06	0.57
1:A:302:LEU:CD2	1:A:311:TYR:OH	2.52	0.57
1:B:311:TYR:HD1	1:B:317:THR:C	2.08	0.57
1:B:67:THR:HG21	1:B:360:LEU:O	2.05	0.57
1:A:116:GLU:HB3	5:A:1375:6LX:HBC1	1.85	0.57
1:A:131:PRO:HA	1:A:138:ARG:NH2	2.19	0.57
1:A:271:ASN:OD1	1:A:283:ARG:O	2.22	0.57
1:A:29:ASN:O	1:A:32:GLU:HB3	2.04	0.57
1:A:272:ILE:CG2	1:A:348:SER:CA	2.82	0.57
1:B:127:TRP:CE2	1:B:128:GLU:OE2	2.53	0.57
5:A:1375:6LX:OAH	5:A:1375:6LX:HAU1	2.03	0.57
1:B:108:GLY:HA2	2:B:601:ADP:H5'1	1.87	0.57
1:A:147:LEU:CD1	1:A:154:PHE:HD2	2.09	0.57
1:A:196:ILE:HG13	1:A:199:LEU:HG	1.87	0.57
1:B:183:GLN:NE2	1:B:185:PHE:HZ	2.02	0.57
1:B:171:LEU:HD22	1:B:220:LYS:CG	2.31	0.57
1:B:32:GLU:OE2	1:B:339:ALA:CB	2.53	0.57
1:B:261:LEU:HD13	1:B:262:ASN:H	1.70	0.57
1:A:133:ALA:HB1	1:A:137:PRO:HB2	1.87	0.57
1:A:164:TYR:HE2	1:A:231:TYR:HH	1.48	0.57
1:A:245:MET:HB2	1:A:257:LYS:CG	2.35	0.57
1:B:220:LYS:O	1:B:224:ALA:N	2.32	0.57
1:B:227:LEU:CA	1:B:229:ASN:N	2.66	0.57
1:B:48:LYS:HD2	1:B:362:LYS:NZ	2.19	0.56
1:B:24:ARG:NE	2:B:601:ADP:HN62	2.02	0.56
1:A:252:GLY:CA	1:A:253:GLU:CB	2.36	0.56
1:B:267:ALA:HB1	4:B:1377:CL:CL	2.41	0.56
1:A:214:LEU:CD1	5:A:1375:6LX:HAQ	2.35	0.56
1:A:302:LEU:HD21	1:A:311:TYR:OH	2.05	0.56
1:A:28:PHE:CD1	1:A:339:ALA:CB	2.51	0.56
1:B:211:TYR:CD1	1:B:215:GLU:OE1	2.51	0.56
1:B:220:LYS:O	1:B:224:ALA:HB2	2.05	0.56
1:B:232:SER:H	1:B:235:SER:HB3	1.69	0.56
1:B:239:PHE:CE1	1:B:263:LEU:HD11	2.39	0.56
1:B:80:ASP:OD1	1:B:80:ASP:N	2.33	0.56
1:B:261:LEU:CD1	1:B:262:ASN:N	2.66	0.56
1:A:214:LEU:HD11	5:A:1375:6LX:CAQ	2.34	0.56
1:A:157:LYS:HG3	1:A:203:THR:HG22	1.86	0.56
1:A:270:GLU:HA	1:A:345:GLU:HA	1.87	0.56
1:A:26:ARG:NH2	1:A:27:PRO:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:N	1:A:342:ASN:OD1	2.38	0.56
1:A:205:HIS:ND1	1:A:205:HIS:N	2.39	0.56
1:A:245:MET:HE2	1:A:257:LYS:CG	2.35	0.56
1:B:118:GLU:C	1:B:132:LEU:CD1	2.74	0.56
1:A:218:ALA:CB	5:A:1375:6LX:CAE	2.80	0.56
1:B:115:MET:O	1:B:136:ILE:HD12	2.05	0.56
1:B:93:VAL:O	1:B:96:GLY:N	2.38	0.56
1:B:249:THR:C	1:B:252:GLY:N	2.59	0.56
1:A:20:GLN:O	1:A:332:ILE:HD12	2.06	0.56
1:A:226:THR:CA	1:A:229:ASN:N	2.59	0.56
1:A:302:LEU:CD2	1:A:311:TYR:HH	2.19	0.56
1:A:86:VAL:CA	1:A:88:PRO:HD2	2.36	0.56
1:B:192:ARG:NH1	1:B:192:ARG:CG	2.69	0.56
1:A:106:GLN:CA	1:A:268:GLY:HA2	2.35	0.56
1:A:165:ASN:ND2	1:A:165:ASN:H	2.03	0.56
1:A:321:GLN:O	1:A:325:GLY:N	2.31	0.56
1:B:219:ALA:O	1:B:223:THR:N	2.28	0.56
1:A:116:GLU:O	5:A:1375:6LX:CBF	2.53	0.56
1:B:93:VAL:HG11	1:B:261:LEU:HB2	1.87	0.56
1:A:271:ASN:ND2	1:A:284:GLU:HA	2.21	0.55
1:A:51:SER:CB	1:A:64:LYS:O	2.54	0.55
1:B:163:ILE:CG2	1:B:236:HIS:HD2	2.18	0.55
1:A:196:ILE:HG13	1:A:199:LEU:CG	2.37	0.55
1:A:308:HIS:CE1	1:B:87:CYS:HB3	2.41	0.55
1:A:82:TYR:HE2	1:A:139:THR:N	2.04	0.55
1:B:111:LYS:HE2	1:B:266:LEU:O	2.06	0.55
1:B:264:VAL:CG1	1:B:266:LEU:HD21	2.25	0.55
1:A:234:ARG:NH1	1:A:288:ILE:HB	2.19	0.55
1:B:316:LEU:O	1:B:320:LEU:N	2.39	0.55
1:B:66:TYR:CE2	1:B:350:LEU:HB3	2.41	0.55
1:A:137:PRO:HB3	5:A:1375:6LX:CBH	2.36	0.55
1:A:214:LEU:HD12	5:A:1375:6LX:CAP	2.36	0.55
1:A:228:MET:N	1:A:228:MET:SD	2.79	0.55
1:A:354:HIS:O	1:A:357:LYS:O	2.24	0.55
1:A:98:ASN:CB	1:A:323:SER:HA	2.36	0.55
1:B:261:LEU:CD1	1:B:261:LEU:C	2.74	0.55
1:B:300:THR:HG22	1:B:356:ALA:C	2.25	0.55
1:A:245:MET:CE	1:A:257:LYS:HG2	2.36	0.55
1:B:96:GLY:O	1:B:259:GLY:HA2	2.06	0.55
1:A:163:ILE:CG2	1:A:163:ILE:O	2.53	0.55
1:A:160:LEU:HG	1:A:171:LEU:HD23	1.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PRO:O	1:B:124:GLU:HG2	2.04	0.55
1:B:211:TYR:O	1:B:215:GLU:CB	2.55	0.55
1:B:89:ILE:HG21	1:B:101:ILE:HD11	1.88	0.55
1:A:149:ASP:OD1	1:A:149:ASP:N	2.40	0.55
1:A:73:GLY:CA	1:A:76:THR:HG22	2.37	0.55
1:B:352:TYR:O	1:B:356:ALA:CA	2.55	0.55
1:B:77:LYS:HE2	1:B:77:LYS:N	2.22	0.55
1:A:177:ASP:OD1	1:A:177:ASP:C	2.45	0.55
1:A:72:PHE:CE2	1:A:76:THR:OG1	2.59	0.55
1:B:112:THR:HG23	1:B:116:GLU:HG3	1.86	0.55
1:A:144:PHE:CE2	1:A:207:LYS:HB2	2.42	0.55
1:A:272:ILE:HG21	1:A:348:SER:O	2.07	0.55
1:A:41:VAL:HG23	1:A:338:PRO:CA	2.35	0.55
1:B:41:VAL:CG1	1:B:52:VAL:HG23	2.14	0.55
1:B:118:GLU:CA	1:B:132:LEU:HB3	2.37	0.54
1:B:174:PRO:CB	1:B:220:LYS:CD	2.76	0.54
1:B:225:ALA:HB2	1:B:231:TYR:HE1	1.72	0.54
1:B:311:TYR:CE1	1:B:317:THR:O	2.60	0.54
1:B:41:VAL:CG2	1:B:338:PRO:HA	2.37	0.54
1:A:117:GLY:HA3	1:A:137:PRO:HG3	1.89	0.54
1:A:253:GLU:CD	1:A:253:GLU:C	2.65	0.54
1:B:234:ARG:O	1:B:267:ALA:CB	2.56	0.54
1:B:62:SER:O	1:B:63:ARG:CB	2.55	0.54
1:A:104:TYR:CD1	1:A:105:GLY:N	2.74	0.54
1:A:274:ARG:CD	1:A:347:LEU:HD12	2.36	0.54
1:A:160:LEU:C	1:A:160:LEU:CD1	2.75	0.54
1:B:227:LEU:C	1:B:228:MET:SD	2.86	0.54
1:B:232:SER:H	1:B:235:SER:CB	2.21	0.54
1:B:239:PHE:HZ	1:B:241:VAL:CG1	2.06	0.54
1:A:192:ARG:NH2	1:A:322:ASP:HA	2.23	0.54
1:A:218:ALA:HB2	5:A:1375:6LX:CAE	2.33	0.54
1:A:285:ALA:C	1:A:289:ASN:ND2	2.50	0.54
1:A:67:THR:C	1:A:68:PHE:CD1	2.80	0.54
1:B:165:ASN:N	1:B:288:ILE:CG1	2.67	0.54
1:B:247:GLU:O	1:B:255:LEU:CB	2.53	0.54
1:B:53:ARG:O	1:B:54:THR:HB	2.07	0.54
1:B:188:PRO:HG2	1:B:189:ARG:HD2	1.90	0.54
1:B:353:ALA:O	1:B:357:LYS:CG	2.55	0.54
1:B:47:ARG:O	1:B:48:LYS:HG3	2.06	0.54
1:A:162:GLU:HG2	1:A:231:TYR:CE1	2.42	0.54
1:A:72:PHE:HZ	1:A:81:VAL:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLN:O	1:B:109:THR:CB	2.53	0.54
1:B:157:LYS:HE3	1:B:242:THR:CB	2.24	0.54
1:B:100:THR:CG2	1:B:262:ASN:CG	2.75	0.54
1:B:239:PHE:CB	1:B:263:LEU:HD12	2.37	0.54
1:A:245:MET:HE3	1:A:257:LYS:CG	2.37	0.54
1:A:35:ALA:HB1	1:A:341:LEU:CG	2.36	0.54
1:B:127:TRP:CE2	1:B:128:GLU:HG3	2.43	0.54
1:B:211:TYR:CE1	1:B:215:GLU:CB	2.88	0.54
1:B:213:ILE:HG22	1:B:214:LEU:N	2.22	0.54
1:B:245:MET:O	1:B:256:VAL:HA	2.08	0.54
1:A:134:GLY:C	1:A:137:PRO:HD2	2.28	0.54
1:B:143:ILE:C	1:B:147:LEU:HD22	2.24	0.54
1:B:163:ILE:HG12	1:B:168:LEU:HB3	1.91	0.54
1:B:227:LEU:CB	1:B:228:MET:C	2.75	0.54
1:B:26:ARG:HD2	2:B:601:ADP:N9	2.23	0.54
1:B:304:GLU:HB2	1:B:306:THR:CG2	2.27	0.54
1:A:143:ILE:CD1	1:A:147:LEU:HD11	2.36	0.53
1:A:156:VAL:O	1:A:203:THR:CB	2.55	0.53
1:A:351:GLU:HB3	1:A:355:ARG:HH21	1.72	0.53
1:A:72:PHE:CZ	1:A:76:THR:OG1	2.61	0.53
1:B:221:ARG:HB2	1:B:231:TYR:HH	1.72	0.53
1:B:343:LEU:O	1:B:347:LEU:CD1	2.56	0.53
1:A:134:GLY:O	1:A:137:PRO:HD2	2.08	0.53
1:B:113:PHE:HB2	2:B:601:ADP:N7	2.24	0.53
1:A:136:ILE:N	1:A:137:PRO:CD	2.71	0.53
1:A:181:ARG:H	1:A:181:ARG:CD	2.20	0.53
1:A:78:GLN:NE2	1:A:132:LEU:C	2.58	0.53
1:B:221:ARG:O	1:B:225:ALA:N	2.41	0.53
1:A:144:PHE:CZ	1:A:207:LYS:CB	2.91	0.53
1:A:22:VAL:HB	1:A:333:ILE:HG13	1.91	0.53
1:A:299:ILE:CG2	1:A:300:THR:N	2.71	0.53
1:B:116:GLU:C	5:B:1375:6LX:HBB1	2.28	0.53
1:B:78:GLN:HG3	1:B:132:LEU:O	2.08	0.53
1:A:118:GLU:OE1	1:A:132:LEU:HD13	2.06	0.53
1:A:148:THR:HG22	1:A:149:ASP:N	2.24	0.53
1:A:304:GLU:O	1:A:305:ARG:CB	2.56	0.53
1:B:234:ARG:O	1:B:267:ALA:HB2	2.09	0.53
1:B:300:THR:HG21	1:B:356:ALA:HA	1.75	0.53
1:A:160:LEU:HD22	1:A:239:PHE:CA	2.39	0.53
1:A:66:TYR:CD2	1:A:68:PHE:CZ	2.97	0.53
1:B:103:ALA:O	1:B:266:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:TYR:HB3	1:B:169:PHE:CZ	2.42	0.53
1:B:195:ILE:O	1:B:195:ILE:HD13	2.03	0.53
1:B:226:THR:O	1:B:228:MET:HB2	2.09	0.53
1:B:26:ARG:O	1:B:338:PRO:CG	2.53	0.53
1:B:32:GLU:O	1:B:37:ALA:CB	2.53	0.53
1:A:119:ARG:HB2	5:A:1375:6LX:CAW	2.38	0.53
1:A:169:PHE:CE1	1:A:181:ARG:HA	2.44	0.53
1:A:144:PHE:CZ	1:A:207:LYS:HB3	2.42	0.53
1:A:143:ILE:HD13	1:A:243:ILE:HD13	1.90	0.53
1:B:173:ASN:O	1:B:175:SER:CA	2.54	0.53
1:B:291:SER:HB3	1:B:314:SER:OG	2.08	0.53
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.91	0.53
1:A:242:THR:HG21	1:A:260:LYS:HE2	1.91	0.53
1:A:91:ASP:HA	1:A:94:ILE:HG22	1.90	0.53
1:B:261:LEU:C	1:B:261:LEU:HD13	2.30	0.53
1:B:333:ILE:HG12	1:B:333:ILE:O	2.08	0.53
1:B:342:ASN:H	1:B:342:ASN:ND2	2.06	0.53
1:B:41:VAL:HG12	1:B:52:VAL:CB	2.39	0.53
1:A:239:PHE:C	1:A:239:PHE:CD1	2.82	0.53
1:A:270:GLU:CA	1:A:345:GLU:HA	2.39	0.53
1:A:347:LEU:O	1:A:351:GLU:OE2	2.27	0.53
1:A:66:TYR:HE1	1:A:354:HIS:HB2	1.68	0.53
1:A:50:VAL:HG12	1:A:71:VAL:HG11	1.91	0.53
1:B:20:GLN:O	1:B:332:ILE:N	2.38	0.53
1:B:82:TYR:C	1:B:82:TYR:HD1	2.12	0.53
1:A:153:GLU:N	1:A:246:LYS:O	2.42	0.53
1:A:306:THR:HG22	1:A:307:PRO:HD2	1.89	0.53
1:B:227:LEU:HA	1:B:228:MET:CB	2.19	0.53
1:A:184:MET:C	1:A:184:MET:SD	2.87	0.52
1:A:323:SER:OG	1:A:324:LEU:CD2	2.57	0.52
1:A:86:VAL:C	1:A:88:PRO:N	2.63	0.52
1:B:183:GLN:NE2	1:B:185:PHE:CZ	2.78	0.52
1:B:98:ASN:OD1	1:B:323:SER:CB	2.57	0.52
1:A:104:TYR:HE2	1:A:352:TYR:CG	2.28	0.52
1:A:231:TYR:O	1:A:232:SER:OG	2.27	0.52
1:A:234:ARG:CA	1:A:234:ARG:HE	2.23	0.52
1:B:25:CYS:O	1:B:25:CYS:SG	2.67	0.52
1:A:109:THR:OG1	1:A:335:THR:CB	2.40	0.52
1:A:70:MET:SD	1:A:70:MET:N	2.80	0.52
1:B:106:GLN:O	1:B:109:THR:N	2.43	0.52
1:B:265:ASP:CA	1:B:266:LEU:HD23	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:TYR:CE2	1:B:350:LEU:HG	2.44	0.52
1:B:82:TYR:C	1:B:82:TYR:CD1	2.83	0.52
1:A:113:PHE:O	1:A:117:GLY:N	2.42	0.52
1:A:105:GLY:C	1:A:268:GLY:HA2	2.26	0.52
1:B:127:TRP:CZ2	1:B:207:LYS:O	2.62	0.52
1:B:252:GLY:CA	1:B:253:GLU:CB	2.32	0.52
1:B:106:GLN:HA	1:B:270:GLU:CD	2.30	0.52
1:A:104:TYR:CE1	1:A:292:LEU:HD13	2.45	0.52
1:B:161:LEU:CD2	1:B:162:GLU:H	2.09	0.52
1:B:23:VAL:HG13	1:B:23:VAL:O	2.09	0.52
1:A:184:MET:SD	1:A:185:PHE:N	2.83	0.52
1:A:245:MET:CE	1:A:257:LYS:HG3	2.39	0.52
1:A:114:THR:HA	1:A:134:GLY:CA	2.40	0.52
1:B:40:ILE:HG13	1:B:340:SER:HA	1.90	0.52
1:B:51:SER:HB3	1:B:63:ARG:CG	2.40	0.52
1:B:82:TYR:OH	1:B:86:VAL:CG1	2.57	0.52
1:A:154:PHE:CD1	1:A:154:PHE:N	2.78	0.52
1:A:230:ALA:CA	1:A:234:ARG:HB2	2.37	0.52
1:A:352:TYR:HA	1:A:355:ARG:HG2	1.91	0.52
1:B:204:VAL:CG2	1:B:204:VAL:O	2.58	0.52
1:B:172:LEU:H	1:B:220:LYS:HE2	1.71	0.52
1:B:82:TYR:HH	1:B:90:LEU:HD22	1.72	0.52
1:A:213:ILE:O	1:A:216:LYS:CG	2.57	0.51
1:A:347:LEU:H	1:A:347:LEU:HD23	1.74	0.51
1:B:127:TRP:CE2	1:B:128:GLU:CG	2.93	0.51
1:B:301:ALA:O	1:B:306:THR:CG2	2.53	0.51
1:B:304:GLU:N	1:B:304:GLU:CD	2.58	0.51
1:B:32:GLU:OE2	1:B:339:ALA:HB3	2.09	0.51
1:A:268:GLY:O	1:A:270:GLU:OE1	2.27	0.51
1:B:134:GLY:N	1:B:137:PRO:HG3	2.24	0.51
1:B:127:TRP:CE2	1:B:208:ASP:OD1	2.64	0.51
5:A:1375:6LX:CBI	5:A:1375:6LX:CAO	2.89	0.51
1:A:106:GLN:HA	1:A:268:GLY:HA3	1.92	0.51
1:A:23:VAL:HA	1:A:334:ALA:O	2.11	0.51
1:B:211:TYR:CZ	1:B:215:GLU:CD	2.79	0.51
1:B:211:TYR:OH	1:B:215:GLU:OE2	2.23	0.51
1:B:164:TYR:CB	1:B:169:PHE:CE1	2.80	0.51
1:A:106:GLN:CB	1:A:345:GLU:CB	2.88	0.51
1:A:234:ARG:CZ	1:A:234:ARG:O	2.58	0.51
1:A:274:ARG:HG3	1:A:351:GLU:HG2	1.91	0.51
1:B:329:ARG:HB3	1:B:329:ARG:NH1	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:CG	1:B:54:THR:H	2.22	0.51
1:B:79:ILE:CD1	1:B:83:ARG:NH2	2.50	0.51
1:A:165:ASN:HD22	1:A:165:ASN:N	2.07	0.51
1:A:144:PHE:CG	1:A:207:LYS:HB3	2.44	0.51
1:A:73:GLY:O	1:A:76:THR:HG22	2.11	0.51
1:B:92:GLU:HG3	1:B:97:TYR:HB2	1.92	0.51
1:A:72:PHE:CZ	1:A:81:VAL:CB	2.94	0.51
1:B:100:THR:CA	1:B:262:ASN:ND2	2.64	0.51
1:A:110:GLY:O	1:A:113:PHE:HD1	1.93	0.51
1:A:134:GLY:O	1:A:137:PRO:CD	2.59	0.51
2:B:601:ADP:H8	2:B:601:ADP:O5'	1.93	0.51
1:A:160:LEU:HD12	1:A:161:LEU:N	2.25	0.51
1:A:168:LEU:C	1:A:169:PHE:CD1	2.85	0.51
1:A:236:HIS:CD2	1:A:266:LEU:CD2	2.94	0.51
1:A:274:ARG:HG3	1:A:351:GLU:CG	2.40	0.51
1:A:35:ALA:HB1	1:A:341:LEU:CD1	2.41	0.51
1:B:207:LYS:HG2	1:B:208:ASP:N	2.23	0.51
1:A:109:THR:HG21	1:A:335:THR:CB	2.41	0.50
1:A:194:VAL:HG11	1:A:318:ARG:HG2	1.93	0.50
1:B:143:ILE:HA	1:B:146:LYS:HG3	1.93	0.50
1:A:316:LEU:O	1:A:320:LEU:HG	2.10	0.50
1:B:28:PHE:CD1	1:B:39:SER:OG	2.57	0.50
1:B:81:VAL:HG12	1:B:85:VAL:CG2	2.35	0.50
1:A:111:LYS:O	1:A:115:MET:N	2.33	0.50
1:A:175:SER:C	1:A:177:ASP:H	2.15	0.50
1:A:40:ILE:H	1:A:40:ILE:HD12	1.75	0.50
1:B:147:LEU:H	1:B:147:LEU:HD22	1.76	0.50
1:A:105:GLY:O	1:A:111:LYS:NZ	2.44	0.50
1:A:135:ILE:O	1:A:139:THR:CA	2.60	0.50
1:B:165:ASN:CA	1:B:288:ILE:HD11	2.41	0.50
1:B:296:GLY:HA2	1:B:299:ILE:HG21	1.91	0.50
1:A:156:VAL:O	1:A:203:THR:C	2.50	0.50
1:A:26:ARG:HA	1:A:74:ALA:CB	2.42	0.50
1:B:121:PRO:HB2	1:B:122:ASN:OD1	2.11	0.50
1:B:127:TRP:CH2	1:B:207:LYS:HG3	2.45	0.50
1:A:148:THR:CG2	1:A:149:ASP:N	2.75	0.50
1:A:89:ILE:CD1	1:A:99:CYS:HB3	2.41	0.50
1:B:173:ASN:C	1:B:175:SER:N	2.52	0.50
1:B:178:VAL:HG23	1:B:178:VAL:O	2.12	0.50
1:B:314:SER:HB3	1:B:317:THR:CG2	2.39	0.50
1:A:105:GLY:O	1:A:106:GLN:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:HG2	1:A:208:ASP:N	2.27	0.50
1:A:226:THR:N	1:A:228:MET:CB	2.64	0.50
1:A:106:GLN:CA	1:A:268:GLY:CA	2.90	0.50
1:B:78:GLN:OE1	1:B:132:LEU:O	2.30	0.50
1:B:187:ASP:OD1	1:B:187:ASP:O	2.30	0.50
1:A:284:GLU:OE1	1:A:293:LEU:HD11	2.12	0.50
1:A:32:GLU:OE1	1:A:32:GLU:O	2.30	0.50
1:A:91:ASP:CA	1:A:94:ILE:HG22	2.41	0.50
1:A:97:TYR:N	1:A:97:TYR:CD1	2.80	0.50
1:B:164:TYR:O	1:B:167:GLU:HG2	2.12	0.50
1:B:249:THR:CA	1:B:252:GLY:HA3	2.42	0.50
1:A:126:THR:OG1	1:A:129:GLU:HB2	2.12	0.50
1:B:144:PHE:O	1:B:148:THR:CB	2.53	0.50
1:A:170:ASP:O	1:A:170:ASP:OD1	2.30	0.49
1:A:197:LYS:HZ1	1:B:250:ILE:HG13	1.77	0.49
1:A:164:TYR:CZ	1:A:228:MET:SD	3.05	0.49
1:A:35:ALA:O	1:A:36:SER:CB	2.59	0.49
1:B:183:GLN:HE22	1:B:185:PHE:HZ	1.60	0.49
1:B:22:VAL:HG22	1:B:332:ILE:C	2.28	0.49
1:A:117:GLY:CA	5:A:1375:6LX:CAN	2.81	0.49
1:A:28:PHE:CE2	1:A:32:GLU:CD	2.83	0.49
1:A:32:GLU:OE2	1:A:37:ALA:C	2.49	0.49
1:B:141:HIS:HA	1:B:207:LYS:HE3	1.93	0.49
1:B:160:LEU:HD12	1:B:161:LEU:N	2.26	0.49
1:B:274:ARG:NH1	1:B:347:LEU:HD22	2.27	0.49
1:A:104:TYR:HE1	1:A:292:LEU:HD13	1.77	0.49
1:B:145:GLU:O	1:B:149:ASP:HB2	2.12	0.49
1:B:296:GLY:CA	1:B:352:TYR:OH	2.60	0.49
1:B:301:ALA:C	1:B:306:THR:HG23	2.30	0.49
1:A:204:VAL:HG12	1:A:206:ASN:O	2.12	0.49
1:A:162:GLU:CG	1:A:231:TYR:HE1	2.26	0.49
1:B:100:THR:HA	1:B:262:ASN:CG	2.32	0.49
1:A:126:THR:O	1:A:129:GLU:CB	2.60	0.49
1:B:127:TRP:CZ2	1:B:128:GLU:HG3	2.47	0.49
1:B:249:THR:CG2	1:B:255:LEU:HD22	2.42	0.49
1:B:252:GLY:HA3	1:B:253:GLU:HB3	1.74	0.49
1:A:250:ILE:HA	6:A:2019:HOH:O	2.13	0.49
1:A:262:ASN:C	1:A:263:LEU:CD1	2.78	0.49
1:B:214:LEU:CB	5:B:1375:6LX:HAA2	2.43	0.49
1:B:157:LYS:O	1:B:241:VAL:HA	2.12	0.49
1:A:126:THR:O	1:A:130:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PHE:HE2	1:A:32:GLU:OE1	1.96	0.49
1:B:293:LEU:O	1:B:352:TYR:OH	2.31	0.49
1:A:192:ARG:HH22	1:A:325:GLY:HA3	1.77	0.49
1:A:109:THR:CG2	1:A:335:THR:OG1	2.57	0.49
1:B:120:SER:HB3	1:B:125:TYR:HB2	1.93	0.49
1:B:82:TYR:OH	1:B:139:THR:HG23	2.13	0.49
1:B:354:HIS:O	1:B:357:LYS:O	2.31	0.49
1:B:73:GLY:C	1:B:75:SER:N	2.55	0.49
1:A:166:GLU:O	1:A:167:GLU:OE1	2.30	0.49
1:A:185:PHE:O	1:A:195:ILE:HG13	2.13	0.49
1:A:72:PHE:CZ	1:A:81:VAL:CA	2.96	0.49
1:B:264:VAL:CG1	1:B:266:LEU:HD22	2.38	0.49
1:B:35:ALA:O	1:B:36:SER:C	2.49	0.49
1:A:104:TYR:HE2	1:A:352:TYR:CB	2.26	0.48
1:A:156:VAL:HG12	1:A:204:VAL:HB	1.88	0.48
1:A:274:ARG:HA	1:A:351:GLU:HG2	1.90	0.48
1:A:294:THR:HG21	1:A:314:SER:CB	2.43	0.48
1:B:227:LEU:H	1:B:227:LEU:HD12	1.78	0.48
1:B:274:ARG:O	1:B:277:ALA:N	2.46	0.48
1:B:299:ILE:HG23	1:B:300:THR:N	2.27	0.48
1:B:40:ILE:CD1	1:B:338:PRO:O	2.61	0.48
1:A:144:PHE:CE2	1:A:207:LYS:CB	2.96	0.48
1:A:27:PRO:CD	1:A:74:ALA:CB	2.65	0.48
1:A:161:LEU:O	1:A:238:VAL:N	2.43	0.48
1:A:184:MET:SD	1:A:194:VAL:HB	2.54	0.48
1:A:192:ARG:CZ	1:A:325:GLY:HA3	2.43	0.48
1:A:32:GLU:OE1	1:A:37:ALA:HB3	2.13	0.48
1:A:78:GLN:O	1:A:81:VAL:HG23	2.13	0.48
1:A:19:ILE:C	1:A:20:GLN:HE21	2.11	0.48
1:A:304:GLU:O	1:A:305:ARG:HB2	2.14	0.48
1:B:342:ASN:ND2	1:B:342:ASN:N	2.61	0.48
1:A:120:SER:OG	1:A:130:ASP:CG	2.50	0.48
1:A:160:LEU:H	1:A:172:LEU:CD2	2.27	0.48
1:B:131:PRO:CA	1:B:138:ARG:HH22	2.09	0.48
1:B:295:LEU:O	1:B:299:ILE:CB	2.60	0.48
1:A:104:TYR:CE2	1:A:352:TYR:CD2	3.01	0.48
1:A:134:GLY:O	1:A:138:ARG:HG3	2.13	0.48
1:A:156:VAL:CG1	1:A:204:VAL:N	2.76	0.48
1:A:225:ALA:CB	1:A:231:TYR:HB3	2.39	0.48
1:A:281:ARG:HA	1:A:284:GLU:OE2	2.12	0.48
1:B:187:ASP:OD1	1:B:190:ASN:N	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:TYR:C	1:B:231:TYR:CD1	2.87	0.48
1:B:343:LEU:N	1:B:346:THR:HG22	2.28	0.48
1:A:236:HIS:O	1:A:265:ASP:C	2.50	0.48
1:A:152:THR:CG2	1:A:247:GLU:CG	2.51	0.48
1:A:73:GLY:N	1:A:76:THR:HG22	2.28	0.48
1:B:110:GLY:HA2	2:B:601:ADP:H8	1.74	0.48
1:B:204:VAL:HG23	1:B:204:VAL:O	2.12	0.48
1:A:136:ILE:O	1:A:140:LEU:HD23	2.13	0.48
1:A:164:TYR:CE2	1:A:231:TYR:OH	2.58	0.48
1:A:232:SER:HB3	6:A:2009:HOH:O	2.14	0.48
1:B:157:LYS:CE	1:B:242:THR:HB	2.27	0.48
1:B:361:ASN:OD1	1:B:361:ASN:N	2.46	0.48
1:A:109:THR:HG21	1:A:335:THR:HG1	1.77	0.47
1:A:125:TYR:N	1:A:125:TYR:HD1	1.96	0.47
1:A:308:HIS:ND1	1:B:88:PRO:HG3	2.29	0.47
1:B:227:LEU:CA	1:B:228:MET:HB2	2.41	0.47
1:B:22:VAL:HG22	1:B:333:ILE:HG22	1.75	0.47
1:B:353:ALA:O	1:B:357:LYS:HG3	2.14	0.47
1:A:295:LEU:O	1:A:299:ILE:HB	2.14	0.47
1:B:171:LEU:HA	1:B:177:ASP:OD2	2.13	0.47
1:B:236:HIS:ND1	1:B:236:HIS:C	2.67	0.47
1:B:82:TYR:CD1	1:B:82:TYR:O	2.62	0.47
5:A:1375:6LX:CAW	5:A:1375:6LX:HAC2	2.44	0.47
1:A:135:ILE:CG2	1:A:139:THR:OG1	2.63	0.47
1:A:30:LEU:CD1	1:A:31:ALA:N	2.77	0.47
1:B:113:PHE:HZ	1:B:118:GLU:CG	2.18	0.47
1:B:197:LYS:CD	1:B:198:GLY:N	2.39	0.47
1:B:30:LEU:HD13	1:B:30:LEU:C	2.35	0.47
1:A:66:TYR:CZ	1:A:350:LEU:O	2.60	0.47
1:B:95:MET:HB3	1:B:97:TYR:CD1	2.47	0.47
1:B:98:ASN:HD21	1:B:260:LYS:CG	2.27	0.47
1:A:129:GLU:N	1:A:129:GLU:OE1	2.48	0.47
1:A:242:THR:CG2	1:A:260:LYS:HE2	2.45	0.47
1:B:122:ASN:HB2	1:B:123:GLU:H	1.51	0.47
1:A:112:THR:HG23	1:A:116:GLU:HG3	1.97	0.47
1:A:121:PRO:O	1:A:122:ASN:HB2	2.14	0.47
1:A:202:ILE:HG12	1:A:202:ILE:O	2.13	0.47
1:A:283:ARG:NH2	1:A:344:GLU:OE2	2.48	0.47
1:B:53:ARG:C	1:B:54:THR:CG2	2.74	0.47
1:B:79:ILE:CD1	1:B:83:ARG:HH21	2.20	0.47
1:A:117:GLY:O	5:A:1375:6LX:CAN	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:HB2	1:A:197:LYS:HE2	1.51	0.47
1:A:85:VAL:O	1:A:88:PRO:HG2	2.14	0.47
1:B:121:PRO:CB	1:B:122:ASN:OD1	2.63	0.47
1:B:250:ILE:CD1	1:B:250:ILE:H	2.08	0.47
1:A:114:THR:CA	1:A:134:GLY:HA3	2.44	0.47
1:A:137:PRO:CB	5:A:1375:6LX:CBK	2.85	0.47
1:A:174:PRO:HB3	1:A:220:LYS:HD2	1.97	0.47
1:A:283:ARG:HA	1:A:283:ARG:HD2	1.64	0.47
1:A:290:GLN:HE21	1:A:290:GLN:HB3	1.54	0.47
1:B:142:GLN:HG3	1:B:146:LYS:HD2	1.97	0.47
1:B:232:SER:HB3	1:B:233:SER:H	1.54	0.47
1:B:250:ILE:O	6:B:2017:HOH:O	2.21	0.47
1:B:254:GLU:C	1:B:255:LEU:HD13	2.35	0.47
1:A:37:ALA:HB2	1:A:341:LEU:HB2	1.97	0.47
1:A:263:LEU:CD1	1:A:263:LEU:N	2.76	0.47
1:B:227:LEU:CD2	1:B:229:ASN:HA	2.45	0.47
1:B:299:ILE:CG2	1:B:300:THR:N	2.77	0.47
1:B:30:LEU:HA	1:B:33:ARG:HB3	1.97	0.47
1:A:167:GLU:CD	1:A:181:ARG:HG3	2.35	0.47
1:A:47:ARG:O	1:A:48:LYS:CB	2.62	0.47
1:B:264:VAL:CG1	1:B:266:LEU:CD2	2.73	0.47
1:A:42:GLU:C	4:A:1378:CL:CL	2.91	0.46
1:A:236:HIS:ND1	1:A:236:HIS:N	2.63	0.46
1:A:285:ALA:N	1:A:289:ASN:ND2	2.64	0.46
1:A:73:GLY:C	1:A:76:THR:CG2	2.83	0.46
1:A:83:ARG:HA	1:A:87:CYS:CB	2.31	0.46
1:B:134:GLY:C	1:B:137:PRO:CD	2.72	0.46
1:B:221:ARG:O	1:B:231:TYR:CE1	2.67	0.46
1:B:30:LEU:O	1:B:34:LYS:N	2.45	0.46
1:B:353:ALA:O	1:B:357:LYS:C	2.48	0.46
1:B:113:PHE:HB2	2:B:601:ADP:C8	2.50	0.46
5:A:1375:6LX:CBF	5:A:1375:6LX:CAN	2.93	0.46
1:A:229:ASN:C	1:A:229:ASN:ND2	2.69	0.46
1:B:127:TRP:HZ2	1:B:208:ASP:OD1	1.94	0.46
1:B:104:TYR:CZ	1:B:349:THR:HB	2.47	0.46
1:A:114:THR:HA	1:A:134:GLY:HA2	1.97	0.46
1:A:167:GLU:CG	1:A:181:ARG:CG	2.89	0.46
1:B:224:ALA:O	1:B:228:MET:HG2	2.16	0.46
1:B:295:LEU:HD13	1:B:295:LEU:HA	1.78	0.46
1:B:308:HIS:ND1	1:B:309:VAL:N	2.63	0.46
1:A:284:GLU:CB	1:A:293:LEU:HD21	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:OH	1:A:354:HIS:CA	2.63	0.46
1:B:169:PHE:CD1	1:B:169:PHE:N	2.84	0.46
1:B:166:GLU:OE2	1:B:287:ASN:O	2.34	0.46
1:A:119:ARG:HB2	5:A:1375:6LX:HAX	1.97	0.46
1:A:178:VAL:O	1:A:179:SER:HB2	2.15	0.46
1:A:272:ILE:HD11	1:A:355:ARG:HH12	1.66	0.46
1:A:39:SER:HB3	1:A:339:ALA:N	2.30	0.46
1:A:51:SER:HB3	1:A:64:LYS:O	2.16	0.46
1:A:81:VAL:O	1:A:85:VAL:CG2	2.59	0.46
1:B:194:VAL:O	1:B:194:VAL:HG23	2.15	0.46
1:B:211:TYR:CD1	1:B:211:TYR:C	2.88	0.46
1:B:234:ARG:HD3	1:B:288:ILE:HD13	1.98	0.46
1:B:280:LYS:O	1:B:284:GLU:O	2.34	0.46
1:B:346:THR:O	1:B:349:THR:OG1	2.25	0.46
1:A:209:GLU:CD	1:A:213:ILE:CD1	2.84	0.46
1:A:308:HIS:HE1	1:B:87:CYS:HB3	1.79	0.46
1:B:195:ILE:HD13	1:B:196:ILE:C	2.36	0.46
1:A:144:PHE:CG	1:A:207:LYS:CB	2.98	0.46
1:A:196:ILE:CG1	1:A:199:LEU:HG	2.46	0.46
1:A:283:ARG:HH21	1:A:344:GLU:CD	2.19	0.46
1:A:126:THR:N	1:A:129:GLU:HB2	2.31	0.46
1:A:274:ARG:O	1:A:280:LYS:HG3	2.16	0.46
1:B:299:ILE:CA	1:B:302:LEU:HG	2.44	0.46
1:B:354:HIS:C	1:B:357:LYS:O	2.54	0.46
1:A:167:GLU:CD	1:A:181:ARG:CB	2.80	0.46
1:B:170:ASP:OD1	1:B:171:LEU:N	2.49	0.46
1:B:40:ILE:HD13	1:B:41:VAL:N	2.30	0.46
1:B:47:ARG:CB	1:B:49:GLU:OE1	2.60	0.46
1:A:163:ILE:HG22	1:A:163:ILE:O	2.16	0.46
1:B:165:ASN:N	1:B:288:ILE:HG13	2.32	0.46
1:A:113:PHE:O	1:A:117:GLY:C	2.55	0.45
1:A:164:TYR:HE2	1:A:231:TYR:OH	1.97	0.45
1:B:242:THR:HG23	1:B:260:LYS:HG2	1.98	0.45
1:B:93:VAL:C	1:B:96:GLY:H	2.19	0.45
1:A:42:GLU:C	4:A:1376:CL:CL	2.92	0.45
1:A:187:ASP:HB2	1:A:195:ILE:HG12	1.98	0.45
1:A:324:LEU:HA	1:A:328:THR:HG21	1.97	0.45
1:B:157:LYS:HA	1:B:202:ILE:O	2.16	0.45
1:B:195:ILE:CD1	1:B:196:ILE:C	2.84	0.45
1:A:24:ARG:HG3	1:A:72:PHE:HB3	1.98	0.45
1:B:112:THR:O	1:B:116:GLU:CA	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLY:N	4:B:1377:CL:CL	2.86	0.45
1:B:40:ILE:HG12	1:B:343:LEU:CB	2.46	0.45
1:A:78:GLN:OE1	1:A:114:THR:HG22	2.17	0.45
1:A:196:ILE:CD1	1:A:199:LEU:HG	2.47	0.45
1:A:38:HIS:O	1:A:340:SER:CB	2.65	0.45
1:B:87:CYS:CB	1:B:88:PRO:HD3	2.47	0.45
1:A:234:ARG:C	1:A:234:ARG:HE	2.19	0.45
1:A:233:SER:O	1:A:267:ALA:HA	2.17	0.45
1:B:164:TYR:HH	1:B:230:ALA:HB3	1.73	0.45
1:A:41:VAL:CA	1:A:52:VAL:CG2	2.89	0.45
1:B:145:GLU:O	1:B:149:ASP:N	2.38	0.45
1:B:211:TYR:CE1	1:B:215:GLU:CG	2.96	0.45
1:A:226:THR:HA	1:A:228:MET:HB3	1.90	0.45
1:A:154:PHE:HA	1:A:244:HIS:O	2.15	0.45
1:A:153:GLU:CG	1:A:246:LYS:O	2.63	0.45
1:A:248:THR:HA	1:A:253:GLU:O	2.17	0.45
1:A:294:THR:CB	1:A:314:SER:HG	2.13	0.45
1:A:320:LEU:HB3	1:A:324:LEU:HD21	1.99	0.45
1:A:90:LEU:O	1:A:94:ILE:CB	2.63	0.45
1:B:145:GLU:O	1:B:149:ASP:CB	2.65	0.45
1:B:171:LEU:HD22	1:B:220:LYS:HB3	1.98	0.45
1:A:19:ILE:H	1:A:19:ILE:HG12	1.35	0.45
1:A:351:GLU:CB	1:A:355:ARG:HH21	2.30	0.45
1:A:41:VAL:CG2	1:A:338:PRO:C	2.86	0.45
1:B:256:VAL:C	1:B:257:LYS:HD2	2.37	0.45
1:A:153:GLU:O	1:A:246:LYS:N	2.34	0.45
1:B:157:LYS:O	1:B:242:THR:N	2.47	0.45
1:B:225:ALA:CB	1:B:231:TYR:HE1	2.30	0.45
1:B:26:ARG:CG	1:B:26:ARG:HH11	2.27	0.45
1:B:28:PHE:CE1	1:B:39:SER:CB	2.97	0.45
1:A:144:PHE:CD2	1:A:207:LYS:CB	2.99	0.45
1:A:161:LEU:CB	1:A:238:VAL:HG22	2.40	0.45
1:A:250:ILE:HG13	1:A:250:ILE:H	1.42	0.45
1:A:236:HIS:HA	1:A:266:LEU:HA	1.99	0.45
1:A:294:THR:HG21	1:A:314:SER:N	2.31	0.45
1:A:192:ARG:HG2	1:A:321:GLN:NE2	2.32	0.45
1:B:135:ILE:O	1:B:139:THR:N	2.35	0.45
1:B:173:ASN:HA	1:B:174:PRO:HD2	1.49	0.45
1:B:173:ASN:O	1:B:176:SER:N	2.46	0.45
1:B:93:VAL:CG2	1:B:261:LEU:HD22	2.32	0.45
1:A:117:GLY:CA	5:A:1375:6LX:HAO	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:CG1	1:A:156:VAL:O	2.65	0.44
1:A:157:LYS:CA	1:A:203:THR:HA	2.32	0.44
1:A:264:VAL:C	1:A:265:ASP:OD1	2.56	0.44
1:B:115:MET:SD	1:B:135:ILE:HD12	2.57	0.44
1:B:158:VAL:O	1:B:202:ILE:HB	2.16	0.44
1:B:182:LEU:HD23	1:B:182:LEU:N	2.29	0.44
1:B:258:ILE:HD11	1:B:260:LYS:HE2	2.00	0.44
1:B:342:ASN:O	1:B:346:THR:N	2.42	0.44
1:B:48:LYS:C	1:B:71:VAL:CG2	2.84	0.44
1:B:226:THR:O	1:B:228:MET:CB	2.64	0.44
1:B:78:GLN:CG	1:B:132:LEU:O	2.65	0.44
1:A:154:PHE:HD1	1:A:154:PHE:N	2.15	0.44
1:B:96:GLY:O	1:B:258:ILE:O	2.36	0.44
1:A:178:VAL:O	1:A:179:SER:CB	2.64	0.44
1:A:88:PRO:C	1:A:91:ASP:OD1	2.46	0.44
1:B:128:GLU:O	1:B:141:HIS:CD2	2.70	0.44
1:B:239:PHE:C	1:B:239:PHE:CD1	2.91	0.44
1:B:41:VAL:HA	1:B:52:VAL:CB	2.45	0.44
1:A:192:ARG:NH2	1:A:325:GLY:HA3	2.31	0.44
1:A:39:SER:HB3	1:A:339:ALA:CA	2.47	0.44
1:A:342:ASN:HB3	1:A:345:GLU:OE2	2.18	0.44
1:A:362:LYS:HA	1:A:362:LYS:HD2	1.44	0.44
1:B:110:GLY:N	2:B:601:ADP:PB	2.89	0.44
1:B:78:GLN:CD	1:B:132:LEU:O	2.56	0.44
1:A:121:PRO:O	1:A:122:ASN:CB	2.64	0.44
1:A:178:VAL:HG11	6:A:2031:HOH:O	2.18	0.44
1:A:228:MET:HB3	1:A:229:ASN:H	1.62	0.44
1:A:238:VAL:CG2	1:A:238:VAL:O	2.62	0.44
1:A:23:VAL:CG2	1:A:68:PHE:CD2	2.99	0.44
1:A:106:GLN:CA	1:A:269:SER:H	2.28	0.44
1:B:143:ILE:CA	1:B:146:LYS:HG3	2.47	0.44
1:B:158:VAL:HG22	1:B:158:VAL:O	2.17	0.44
1:B:297:ARG:HG3	1:B:298:VAL:N	2.31	0.44
1:B:320:LEU:HA	1:B:320:LEU:HD23	1.82	0.44
1:B:337:SER:CB	1:B:342:ASN:OD1	2.62	0.44
1:A:234:ARG:CA	1:A:234:ARG:NE	2.80	0.44
1:A:241:VAL:HG12	1:A:241:VAL:O	2.18	0.44
1:B:207:LYS:O	1:B:210:VAL:HB	2.18	0.44
1:B:318:ARG:O	1:B:321:GLN:CG	2.65	0.44
1:A:114:THR:HA	1:A:134:GLY:HA3	2.00	0.44
1:A:230:ALA:CB	1:A:234:ARG:HB3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:MET:HE3	1:A:257:LYS:HG3	2.00	0.44
1:B:160:LEU:HD12	1:B:161:LEU:H	1.83	0.44
1:B:19:ILE:HG21	1:B:299:ILE:HD11	1.99	0.44
1:B:296:GLY:N	1:B:352:TYR:OH	2.51	0.44
1:B:62:SER:O	1:B:63:ARG:HB2	2.17	0.44
1:A:355:ARG:HG3	1:A:356:ALA:N	2.33	0.44
1:B:359:ILE:H	1:B:359:ILE:HG12	1.73	0.44
1:A:117:GLY:CA	5:A:1375:6LX:CAO	2.96	0.43
1:A:156:VAL:HG12	1:A:204:VAL:N	2.33	0.43
1:A:156:VAL:HG12	1:A:204:VAL:H	1.82	0.43
1:A:315:LYS:CA	1:A:315:LYS:HE2	2.46	0.43
1:A:295:LEU:HB3	1:A:352:TYR:OH	2.18	0.43
1:B:300:THR:CG2	1:B:356:ALA:CA	2.42	0.43
1:A:309:VAL:HG21	1:A:311:TYR:CD2	2.26	0.43
1:B:133:ALA:HB1	1:B:137:PRO:HG3	2.00	0.43
1:B:202:ILE:O	1:B:202:ILE:HG22	2.18	0.43
1:B:40:ILE:O	1:B:52:VAL:CB	2.61	0.43
1:B:94:ILE:HD12	1:B:245:MET:CE	2.48	0.43
5:A:1375:6LX:CBI	5:A:1375:6LX:HAB	2.48	0.43
1:A:131:PRO:C	1:A:138:ARG:HH21	2.21	0.43
1:A:231:TYR:C	1:A:232:SER:OG	2.54	0.43
1:A:272:ILE:HD13	1:A:273:GLY:O	2.18	0.43
1:A:351:GLU:N	1:A:351:GLU:CD	2.72	0.43
1:B:225:ALA:CA	1:B:231:TYR:HE1	2.30	0.43
1:B:270:GLU:CD	1:B:270:GLU:H	2.13	0.43
1:A:225:ALA:CA	1:A:231:TYR:CG	2.79	0.43
1:A:241:VAL:O	1:A:241:VAL:CG1	2.66	0.43
1:A:230:ALA:O	1:A:234:ARG:HB2	2.18	0.43
1:A:323:SER:O	1:A:328:THR:CB	2.65	0.43
1:A:47:ARG:HE	1:A:47:ARG:CA	2.21	0.43
1:B:114:THR:O	1:B:134:GLY:HA2	2.18	0.43
1:B:296:GLY:O	1:B:300:THR:N	2.41	0.43
1:A:131:PRO:HA	1:A:138:ARG:HH22	1.82	0.43
1:A:227:LEU:CA	1:A:228:MET:C	2.87	0.43
1:A:284:GLU:H	1:A:284:GLU:HG3	1.47	0.43
1:A:293:LEU:HA	1:A:293:LEU:HD13	1.80	0.43
1:A:68:PHE:HB2	1:A:71:VAL:HG22	2.00	0.43
1:B:240:SER:O	1:B:240:SER:OG	2.30	0.43
1:B:249:THR:H	1:B:252:GLY:HA3	1.84	0.43
1:B:98:ASN:CB	1:B:323:SER:HA	2.45	0.43
1:B:52:VAL:O	1:B:52:VAL:CG1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LYS:HA	1:A:255:LEU:O	2.18	0.43
1:A:352:TYR:CA	1:A:355:ARG:HG2	2.49	0.43
1:B:137:PRO:HB3	5:B:1375:6LX:CBJ	2.49	0.43
1:B:18:ASN:O	1:B:20:GLN:CD	2.57	0.43
1:B:100:THR:HG23	1:B:262:ASN:CG	2.29	0.43
1:B:40:ILE:HG12	1:B:343:LEU:HA	2.00	0.43
1:A:152:THR:HG22	1:A:247:GLU:OE1	1.85	0.43
1:A:168:LEU:C	1:A:169:PHE:HD1	2.21	0.43
1:A:270:GLU:CB	1:A:345:GLU:HA	2.49	0.43
1:A:272:ILE:CG2	1:A:348:SER:O	2.67	0.43
1:A:110:GLY:O	1:A:113:PHE:CD1	2.71	0.43
1:A:196:ILE:HD11	1:A:199:LEU:HG	2.01	0.43
1:A:279:ASP:CB	1:A:283:ARG:CB	2.95	0.43
1:A:294:THR:C	1:A:298:VAL:HG23	2.21	0.43
1:B:221:ARG:HH21	1:B:232:SER:HA	1.84	0.43
1:B:234:ARG:HA	4:B:1377:CL:CL	2.56	0.42
1:B:168:LEU:HD11	1:B:184:MET:HE2	2.01	0.42
1:B:221:ARG:HA	1:B:231:TYR:OH	2.19	0.42
1:B:111:LYS:N	2:B:601:ADP:O1B	2.52	0.42
1:A:157:LYS:HG3	1:A:203:THR:CG2	2.49	0.42
1:A:271:ASN:ND2	1:A:271:ASN:C	2.72	0.42
1:A:274:ARG:O	1:A:277:ALA:CB	2.67	0.42
1:A:306:THR:CG2	1:A:307:PRO:HD2	2.48	0.42
1:A:95:MET:HB3	1:A:97:TYR:CE1	2.54	0.42
1:B:248:THR:HA	1:B:253:GLU:O	2.19	0.42
1:B:301:ALA:HA	1:B:304:GLU:HG2	1.78	0.42
1:B:342:ASN:HD22	1:B:343:LEU:N	2.10	0.42
5:A:1375:6LX:HAB	5:A:1375:6LX:CBF	2.48	0.42
1:A:144:PHE:CZ	1:A:207:LYS:HA	2.54	0.42
1:A:253:GLU:O	1:A:253:GLU:OE2	2.37	0.42
1:B:214:LEU:HD13	5:B:1375:6LX:CBH	2.50	0.42
1:B:239:PHE:CG	1:B:263:LEU:CD1	2.93	0.42
1:B:317:THR:HG1	1:B:318:ARG:N	2.17	0.42
1:A:21:VAL:HG21	1:A:357:LYS:CB	2.45	0.42
1:B:110:GLY:HA2	2:B:601:ADP:PA	2.58	0.42
1:B:299:ILE:CG2	1:B:356:ALA:HB1	2.49	0.42
1:B:89:ILE:HG22	1:B:90:LEU:N	2.33	0.42
1:A:102:PHE:C	1:A:102:PHE:CD1	2.93	0.42
1:A:117:GLY:HA2	1:A:134:GLY:CA	2.48	0.42
1:A:126:THR:O	1:A:129:GLU:CA	2.67	0.42
1:A:186:ASP:HB2	4:A:1381:CL:CL	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:HA2	1:A:299:ILE:HG22	2.01	0.42
1:A:306:THR:HA	1:A:307:PRO:HD3	1.87	0.42
1:A:194:VAL:HG21	1:A:319:ILE:HG13	2.01	0.42
1:A:21:VAL:HA	1:A:332:ILE:O	2.19	0.42
1:A:140:LEU:O	1:A:143:ILE:HG22	2.20	0.42
1:A:50:VAL:O	1:A:50:VAL:HG22	2.18	0.42
1:B:59:ASP:HB3	1:B:60:LYS:H	1.58	0.42
1:A:133:ALA:N	5:A:1375:6LX:HAZ1	2.33	0.42
1:A:223:THR:CG2	1:A:224:ALA:N	2.83	0.42
1:A:226:THR:C	1:A:229:ASN:N	2.72	0.42
1:A:82:TYR:O	1:A:86:VAL:HB	2.20	0.42
1:B:174:PRO:CA	1:B:177:ASP:OD1	2.68	0.42
1:B:227:LEU:CG	1:B:229:ASN:HA	2.49	0.42
1:B:247:GLU:O	1:B:255:LEU:CA	2.67	0.42
1:B:300:THR:HG22	1:B:356:ALA:CB	2.39	0.42
1:B:72:PHE:CE2	1:B:81:VAL:HG13	2.55	0.42
1:B:86:VAL:HG21	1:B:135:ILE:HG21	2.01	0.42
1:A:277:ALA:HB3	1:A:279:ASP:O	2.20	0.42
1:A:281:ARG:O	1:A:285:ALA:CA	2.68	0.42
1:B:120:SER:OG	1:B:125:TYR:CB	2.65	0.42
1:B:276:GLY:O	1:B:278:VAL:N	2.53	0.42
1:A:25:CYS:O	1:A:73:GLY:O	2.38	0.42
1:B:101:ILE:HB	1:B:263:LEU:HA	2.02	0.42
1:B:118:GLU:H	1:B:132:LEU:C	2.23	0.42
1:B:348:SER:O	1:B:351:GLU:HB3	2.20	0.42
1:B:69:ASP:OD1	1:B:69:ASP:N	2.52	0.42
1:A:242:THR:CG2	1:A:260:LYS:CE	2.98	0.41
1:B:234:ARG:NH1	1:B:288:ILE:CD1	2.79	0.41
1:A:118:GLU:CD	1:A:132:LEU:HD13	2.39	0.41
1:B:133:ALA:HB1	1:B:137:PRO:CB	2.50	0.41
1:B:21:VAL:HA	1:B:332:ILE:HB	2.01	0.41
1:B:221:ARG:CG	1:B:222:THR:N	2.83	0.41
5:A:1375:6LX:CBF	5:A:1375:6LX:CAB	2.98	0.41
1:A:225:ALA:CA	1:A:231:TYR:HB2	2.50	0.41
1:A:242:THR:HG23	1:A:260:LYS:CE	2.45	0.41
1:A:48:LYS:HB3	1:A:48:LYS:HE3	1.75	0.41
1:A:27:PRO:N	1:A:74:ALA:HB1	2.31	0.41
1:B:210:VAL:CG1	1:B:214:LEU:CD1	2.98	0.41
1:A:42:GLU:CA	4:A:1378:CL:CL	3.05	0.41
1:A:217:GLY:CA	5:A:1375:6LX:CAP	2.95	0.41
1:A:109:THR:CG2	1:A:335:THR:CB	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ARG:O	1:B:321:GLN:HG2	2.20	0.41
1:B:344:GLU:HG3	1:B:345:GLU:N	2.35	0.41
1:B:90:LEU:HD12	1:B:90:LEU:C	2.40	0.41
1:A:112:THR:HG22	1:A:116:GLU:HB2	2.02	0.41
1:A:93:VAL:HA	1:A:97:TYR:O	2.20	0.41
1:B:104:TYR:CE1	1:B:334:ALA:CB	2.94	0.41
1:B:138:ARG:O	1:B:142:GLN:HB2	2.21	0.41
1:B:161:LEU:HD21	1:B:168:LEU:HB2	2.03	0.41
1:A:134:GLY:N	1:A:137:PRO:CG	2.83	0.41
1:A:315:LYS:HB3	1:A:315:LYS:HE2	1.89	0.41
1:A:49:GLU:OE1	1:A:67:THR:CB	2.65	0.41
1:B:135:ILE:C	1:B:137:PRO:HD2	2.41	0.41
1:B:22:VAL:HG12	1:B:70:MET:CB	2.50	0.41
1:B:22:VAL:O	1:B:333:ILE:HA	2.21	0.41
1:B:253:GLU:CG	1:B:254:GLU:N	2.83	0.41
1:B:304:GLU:CB	1:B:306:THR:HG22	2.30	0.41
1:A:113:PHE:CD1	1:A:114:THR:HG23	2.43	0.41
1:A:213:ILE:CA	1:A:216:LYS:HE2	2.38	0.41
1:A:106:GLN:C	1:A:268:GLY:HA2	2.41	0.41
1:B:162:GLU:O	1:B:169:PHE:N	2.47	0.41
1:B:258:ILE:O	1:B:258:ILE:HG13	2.11	0.41
1:B:111:LYS:CE	1:B:266:LEU:O	2.69	0.41
1:B:316:LEU:O	1:B:320:LEU:CG	2.69	0.41
1:B:104:TYR:CZ	1:B:349:THR:HG22	2.55	0.41
1:A:298:VAL:HG12	1:A:311:TYR:CE2	2.55	0.41
1:A:37:ALA:CB	1:A:341:LEU:H	2.34	0.41
1:A:360:LEU:HD13	1:A:360:LEU:HA	1.86	0.41
1:A:41:VAL:HG21	1:A:338:PRO:C	2.40	0.41
1:A:94:ILE:O	1:A:245:MET:CE	2.57	0.41
1:B:177:ASP:N	1:B:220:LYS:NZ	2.66	0.41
1:B:294:THR:HG22	1:B:298:VAL:CG2	2.51	0.41
1:B:53:ARG:CG	1:B:54:THR:N	2.84	0.41
1:A:72:PHE:CE1	1:A:81:VAL:HG13	2.56	0.41
1:A:72:PHE:CZ	1:A:80:ASP:HB3	2.56	0.41
1:B:195:ILE:CD1	1:B:195:ILE:O	2.66	0.41
1:B:19:ILE:N	1:B:19:ILE:HD12	2.29	0.41
1:B:212:GLN:C	1:B:216:LYS:HG3	2.26	0.41
1:A:21:VAL:CG2	1:A:357:LYS:CG	2.94	0.41
1:A:225:ALA:CB	1:A:231:TYR:CG	3.03	0.41
1:A:262:ASN:O	1:A:263:LEU:CD1	2.69	0.41
1:A:22:VAL:O	1:A:333:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:CD	1:A:67:THR:CA	2.77	0.41
1:B:221:ARG:HA	1:B:224:ALA:HB3	2.03	0.41
1:B:161:LEU:O	1:B:237:SER:HA	2.21	0.41
1:B:317:THR:HA	1:B:320:LEU:HB2	2.02	0.41
1:A:175:SER:O	1:A:177:ASP:N	2.54	0.40
1:A:192:ARG:HH22	1:A:325:GLY:CA	2.35	0.40
1:A:104:TYR:OH	1:A:269:SER:HB3	2.20	0.40
1:B:190:ASN:OD1	1:B:192:ARG:HB2	2.21	0.40
1:B:299:ILE:HG23	1:B:356:ALA:HB1	2.02	0.40
1:B:353:ALA:HB1	1:B:359:ILE:HD11	2.03	0.40
5:A:1375:6LX:CAM	5:A:1375:6LX:HBF	2.51	0.40
1:A:66:TYR:HD1	1:A:66:TYR:HA	1.76	0.40
1:B:23:VAL:HG23	1:B:336:ILE:HD11	2.03	0.40
1:B:164:TYR:O	1:B:167:GLU:CG	2.69	0.40
1:B:186:ASP:HA	1:B:194:VAL:HG12	2.02	0.40
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.89	0.40
1:B:360:LEU:HD13	1:B:360:LEU:HA	1.80	0.40
1:A:192:ARG:HG2	1:A:321:GLN:HE21	1.87	0.40
1:A:270:GLU:HB3	1:A:345:GLU:HA	2.03	0.40
1:B:164:TYR:CD1	1:B:234:ARG:HD2	2.56	0.40
1:A:136:ILE:O	1:A:140:LEU:CB	2.64	0.40
1:A:147:LEU:CD1	1:A:154:PHE:CE2	2.67	0.40
1:B:222:THR:HG22	1:B:223:THR:N	2.36	0.40
1:B:93:VAL:O	1:B:96:GLY:CA	2.69	0.40

All (32) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH2	1:B:253:GLU:CD[3_565]	0.48	1.72
1:A:59:ASP:OD2	1:A:287:ASN:ND2[3_565]	0.80	1.40
1:B:33:ARG:CZ	1:B:253:GLU:OE1[3_565]	0.90	1.30
1:A:344:GLU:OE2	3:B:1369:CD:CD[3_565]	1.04	1.16
1:B:33:ARG:NH2	1:B:253:GLU:CG[3_565]	1.07	1.13
1:A:209:GLU:N	1:B:344:GLU:OE2[1_545]	1.18	1.02
1:A:278:VAL:CG1	1:B:154:PHE:O[3_565]	1.23	0.97
1:A:251:ASP:OD2	1:B:189:ARG:NH1[3_455]	1.40	0.80
1:B:33:ARG:NH2	1:B:253:GLU:OE1[3_565]	1.41	0.79
1:B:54:THR:O	3:A:1366:CD:CD[1_565]	1.43	0.77
1:A:208:ASP:C	1:B:344:GLU:OE2[1_545]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:CZ	1:B:253:GLU:CD[3_565]	1.45	0.75
1:A:203:THR:OG1	1:B:283:ARG:CG[1_545]	1.47	0.73
1:B:33:ARG:NE	1:B:253:GLU:OE1[3_565]	1.51	0.69
1:A:87:CYS:SG	3:B:1368:CD:CD[3_455]	1.60	0.60
1:B:33:ARG:NH2	1:B:253:GLU:OE2[3_565]	1.64	0.56
1:B:60:LYS:O	1:B:287:ASN:ND2[3_465]	1.72	0.48
1:A:208:ASP:CA	1:B:344:GLU:OE2[1_545]	1.77	0.43
1:A:206:ASN:CB	1:B:344:GLU:OE1[1_545]	1.81	0.39
1:A:59:ASP:CG	1:A:287:ASN:ND2[3_565]	1.82	0.38
1:A:123:GLU:OE2	1:A:189:ARG:NH1[3_555]	1.83	0.37
1:A:206:ASN:OD1	1:B:274:ARG:CD[1_545]	1.84	0.36
1:B:33:ARG:NH1	1:B:253:GLU:OE1[3_565]	1.85	0.35
1:A:212:GLN:NE2	1:B:345:GLU:OE1[1_545]	1.96	0.24
1:B:33:ARG:CZ	1:B:253:GLU:CG[3_565]	1.98	0.22
1:B:297:ARG:NH2	4:A:1377:CL:CL[2_564]	1.98	0.22
1:B:60:LYS:CB	1:B:287:ASN:CB[3_465]	2.07	0.13
1:A:59:ASP:OD2	1:A:287:ASN:CG[3_565]	2.12	0.08
1:B:33:ARG:NH2	1:B:253:GLU:CB[3_565]	2.12	0.08
1:A:208:ASP:N	1:B:344:GLU:OE2[1_545]	2.14	0.06
1:A:27:PRO:CB	1:A:253:GLU:N[3_555]	2.18	0.02
1:A:208:ASP:CB	1:B:344:GLU:OE2[1_545]	2.18	0.02

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	A	343/368 (93%)	325 (95%)	9 (3%)	9 (3%)	5	18
1	B	341/368 (93%)	318 (93%)	12 (4%)	11 (3%)	4	13
All	All	684/736 (93%)	643 (94%)	21 (3%)	20 (3%)	4	15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	179	SER
1	B	18	ASN
1	B	53	ARG
1	B	74	ALA
1	B	174	PRO
1	B	178	VAL
1	B	229	ASN
1	B	232	SER
1	B	277	ALA
1	B	343	LEU
1	A	88	PRO
1	A	87	CYS
1	A	237	SER
1	A	363	PRO
1	B	63	ARG
1	A	122	ASN
1	A	253	GLU
1	B	253	GLU
1	A	176	SER

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	A	290/322 (90%)	141 (49%)	149 (51%)	0	0
1	B	287/322 (89%)	151 (53%)	136 (47%)	0	0
All	All	577/644 (90%)	292 (51%)	285 (49%)	0	0

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	26	ARG
1	A	29	ASN
1	A	30	LEU

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Mol	Chain	Res	Type
1	A	36	SER
1	A	38	HIS
1	A	39	SER
1	A	40	ILE
1	A	41	VAL
1	A	42	GLU
1	A	44	ASP
1	A	46	VAL
1	A	47	ARG
1	A	48	LYS
1	A	54	THR
1	A	59	ASP
1	A	65	THR
1	A	66	TYR
1	A	67	THR
1	A	69	ASP
1	A	70	MET
1	A	71	VAL
1	A	72	PHE
1	A	76	THR
1	A	81	VAL
1	A	82	TYR
1	A	83	ARG
1	A	84	SER
1	A	85	VAL
1	A	89	ILE
1	A	91	ASP
1	A	92	GLU
1	A	93	VAL
1	A	95	MET
1	A	97	TYR
1	A	98	ASN
1	A	107	THR
1	A	109	THR
1	A	111	LYS
1	A	113	PHE
1	A	114	THR
1	A	115	MET
1	A	118	GLU
1	A	123	GLU
1	A	124	GLU
1	A	125	TYR

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Mol	Chain	Res	Type
1	A	127	TRP
1	A	128	GLU
1	A	129	GLU
1	A	143	ILE
1	A	148	THR
1	A	149	ASP
1	A	154	PHE
1	A	155	SER
1	A	156	VAL
1	A	157	LYS
1	A	160	LEU
1	A	162	GLU
1	A	163	ILE
1	A	165	ASN
1	A	166	GLU
1	A	167	GLU
1	A	168	LEU
1	A	170	ASP
1	A	171	LEU
1	A	177	ASP
1	A	178	VAL
1	A	181	ARG
1	A	182	LEU
1	A	183	GLN
1	A	190	ASN
1	A	194	VAL
1	A	196	ILE
1	A	197	LYS
1	A	202	ILE
1	A	205	HIS
1	A	207	LYS
1	A	208	ASP
1	A	209	GLU
1	A	211	TYR
1	A	213	ILE
1	A	214	LEU
1	A	216	LYS
1	A	222	THR
1	A	223	THR
1	A	227	LEU
1	A	228	MET
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	231	TYR
1	A	232	SER
1	A	234	ARG
1	A	235	SER
1	A	236	HIS
1	A	237	SER
1	A	239	PHE
1	A	241	VAL
1	A	242	THR
1	A	243	ILE
1	A	244	HIS
1	A	245	MET
1	A	248	THR
1	A	249	THR
1	A	250	ILE
1	A	251	ASP
1	A	253	GLU
1	A	254	GLU
1	A	257	LYS
1	A	260	LYS
1	A	263	LEU
1	A	264	VAL
1	A	265	ASP
1	A	266	LEU
1	A	269	SER
1	A	270	GLU
1	A	271	ASN
1	A	272	ILE
1	A	275	SER
1	A	278	VAL
1	A	280	LYS
1	A	283	ARG
1	A	284	GLU
1	A	290	GLN
1	A	291	SER
1	A	293	LEU
1	A	298	VAL
1	A	299	ILE
1	A	304	GLU
1	A	305	ARG
1	A	315	LYS
1	A	316	LEU

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Mol	Chain	Res	Type
1	A	318	ARG
1	A	319	ILE
1	A	324	LEU
1	A	328	THR
1	A	332	ILE
1	A	333	ILE
1	A	335	THR
1	A	336	ILE
1	A	337	SER
1	A	340	SER
1	A	341	LEU
1	A	342	ASN
1	A	343	LEU
1	A	345	GLU
1	A	347	LEU
1	A	351	GLU
1	A	358	ASN
1	A	360	LEU
1	A	362	LYS
1	B	20	GLN
1	B	21	VAL
1	B	24	ARG
1	B	25	CYS
1	B	28	PHE
1	B	33	ARG
1	B	34	LYS
1	B	36	SER
1	B	38	HIS
1	B	40	ILE
1	B	41	VAL
1	B	43	CYS
1	B	44	ASP
1	B	46	VAL
1	B	48	LYS
1	B	50	VAL
1	B	52	VAL
1	B	62	SER
1	B	70	MET
1	B	76	THR
1	B	77	LYS
1	B	78	GLN
1	B	79	ILE

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Mol	Chain	Res	Type
1	B	82	TYR
1	B	85	VAL
1	B	87	CYS
1	B	89	ILE
1	B	94	ILE
1	B	95	MET
1	B	98	ASN
1	B	100	THR
1	B	101	ILE
1	B	104	TYR
1	B	107	THR
1	B	111	LYS
1	B	113	PHE
1	B	114	THR
1	B	119	ARG
1	B	120	SER
1	B	122	ASN
1	B	123	GLU
1	B	124	GLU
1	B	129	GLU
1	B	132	LEU
1	B	139	THR
1	B	141	HIS
1	B	142	GLN
1	B	144	PHE
1	B	146	LYS
1	B	148	THR
1	B	153	GLU
1	B	156	VAL
1	B	157	LYS
1	B	159	SER
1	B	161	LEU
1	B	162	GLU
1	B	165	ASN
1	B	166	GLU
1	B	168	LEU
1	B	169	PHE
1	B	170	ASP
1	B	171	LEU
1	B	172	LEU
1	B	176	SER
1	B	177	ASP

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Mol	Chain	Res	Type
1	B	178	VAL
1	B	181	ARG
1	B	183	GLN
1	B	187	ASP
1	B	195	ILE
1	B	197	LYS
1	B	200	GLU
1	B	204	VAL
1	B	207	LYS
1	B	210	VAL
1	B	213	ILE
1	B	220	LYS
1	B	221	ARG
1	B	222	THR
1	B	227	LEU
1	B	228	MET
1	B	231	TYR
1	B	232	SER
1	B	234	ARG
1	B	236	HIS
1	B	240	SER
1	B	245	MET
1	B	248	THR
1	B	249	THR
1	B	250	ILE
1	B	255	LEU
1	B	256	VAL
1	B	258	ILE
1	B	261	LEU
1	B	262	ASN
1	B	263	LEU
1	B	266	LEU
1	B	269	SER
1	B	270	GLU
1	B	271	ASN
1	B	272	ILE
1	B	274	ARG
1	B	275	SER
1	B	287	ASN
1	B	292	LEU
1	B	293	LEU
1	B	295	LEU

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Mol	Chain	Res	Type
1	B	297	ARG
1	B	302	LEU
1	B	304	GLU
1	B	306	THR
1	B	309	VAL
1	B	311	TYR
1	B	313	GLU
1	B	315	LYS
1	B	316	LEU
1	B	320	LEU
1	B	321	GLN
1	B	329	ARG
1	B	333	ILE
1	B	335	THR
1	B	336	ILE
1	B	337	SER
1	B	340	SER
1	B	341	LEU
1	B	342	ASN
1	B	345	GLU
1	B	346	THR
1	B	347	LEU
1	B	350	LEU
1	B	352	TYR
1	B	357	LYS
1	B	359	ILE
1	B	360	LEU
1	B	361	ASN
1	B	362	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	38	HIS
1	A	141	HIS
1	A	165	ASN
1	A	229	ASN
1	A	290	GLN
1	A	358	ASN
1	B	20	GLN
1	B	150	ASN

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Mol	Chain	Res	Type
1	B	173	ASN
1	B	183	GLN
1	B	212	GLN
1	B	244	HIS
1	B	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 30 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	6LX	B	1375	1	36,40,40	2.39	9 (25%)	44,56,56	1.91	10 (22%)
5	6LX	A	1375	-	36,40,40	2.65	14 (38%)	44,56,56	1.50	7 (15%)
2	ADP	A	601	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	4 (13%)
2	ADP	B	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.51	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	6LX	B	1375	1	-	5/24/28/28	0/4/4/4
5	6LX	A	1375	-	-	7/24/28/28	0/4/4/4
2	ADP	A	601	-	-	3/12/32/32	0/3/3/3
2	ADP	B	601	-	-	5/12/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1375	6LX	OBA-CAS	9.09	1.39	1.23
5	B	1375	6LX	OBA-CAS	8.69	1.38	1.23
5	A	1375	6LX	CAT-CAI	6.08	1.47	1.39
5	A	1375	6LX	CAL-NAK	6.02	1.48	1.34
5	B	1375	6LX	CAL-NAK	5.38	1.47	1.34
5	B	1375	6LX	CAT-CAI	4.44	1.45	1.39
5	B	1375	6LX	OAH-CAI	-3.53	1.30	1.35
5	A	1375	6LX	CAF-CAG	3.40	1.44	1.37
5	A	1375	6LX	CAF-CAE	3.34	1.43	1.36
5	B	1375	6LX	CAF-CAG	2.90	1.43	1.37
5	B	1375	6LX	CAF-CAE	2.73	1.41	1.36
5	A	1375	6LX	CAP-CAE	2.70	1.43	1.38
5	A	1375	6LX	OAH-CAI	-2.59	1.31	1.35
2	B	601	ADP	C5-C4	2.51	1.47	1.40
5	B	1375	6LX	CAP-CAE	2.44	1.42	1.38
5	A	1375	6LX	CBI-CBF	2.44	1.44	1.38
5	B	1375	6LX	CAZ-CAY	2.38	1.59	1.51
5	A	1375	6LX	CAZ-CAY	2.36	1.59	1.51
2	A	601	ADP	C5-C4	2.31	1.47	1.40
5	A	1375	6LX	CBH-CBG	2.27	1.43	1.38
5	A	1375	6LX	CAQ-CAR	2.19	1.45	1.41
5	A	1375	6LX	CBK-CBJ	2.12	1.43	1.38
5	A	1375	6LX	CAQ-CAP	2.11	1.41	1.36
5	B	1375	6LX	CBK-CBJ	2.07	1.43	1.38
5	A	1375	6LX	CAU-NAK	2.04	1.50	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1375	6LX	CAC-CAB-CAJ	6.70	119.73	110.72
5	A	1375	6LX	CAC-CAB-CAJ	4.31	116.53	110.72
5	B	1375	6LX	CAT-CBB-CBG	-3.97	105.04	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1375	6LX	CAQ-CAR-CAG	3.87	120.97	116.50
2	A	601	ADP	N3-C2-N1	-3.70	122.90	128.68
2	B	601	ADP	PA-O3A-PB	-3.60	120.47	132.83
2	B	601	ADP	C3'-C2'-C1'	3.50	106.25	100.98
5	A	1375	6LX	CAQ-CAR-CAG	3.16	120.16	116.50
2	B	601	ADP	N3-C2-N1	-3.16	123.74	128.68
5	A	1375	6LX	OAH-CAG-CAF	3.15	119.80	116.11
2	A	601	ADP	C4-C5-N7	-3.13	106.14	109.40
5	B	1375	6LX	CAT-CAS-CAR	-3.05	117.51	122.29
5	B	1375	6LX	CBC-CAU-NAK	3.00	117.95	113.31
5	B	1375	6LX	CAA-CAB-CAJ	2.97	114.72	110.72
5	A	1375	6LX	CBB-CAT-CAI	2.92	124.15	120.18
5	A	1375	6LX	CAF-CAG-CAR	-2.92	119.81	123.05
5	A	1375	6LX	CBC-CAU-NAK	2.90	117.79	113.31
2	A	601	ADP	C1'-N9-C4	-2.72	121.86	126.64
2	B	601	ADP	C4-C5-N7	-2.72	106.56	109.40
5	A	1375	6LX	CAT-CAS-CAR	-2.56	118.28	122.29
5	B	1375	6LX	CAU-CBC-CBD	2.48	123.38	113.85
5	B	1375	6LX	CBH-CBG-CBF	2.34	121.84	118.17
5	B	1375	6LX	CAP-CAQ-CAR	-2.32	118.29	121.63
5	B	1375	6LX	CAF-CAG-CAR	-2.22	120.59	123.05
2	A	601	ADP	C2-N1-C6	2.19	122.50	118.75

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
5	B	1375	6LX	CAC-CAB-CAJ-CAI
2	A	601	ADP	C5'-O5'-PA-O3A
5	A	1375	6LX	CAI-CAJ-NAK-CAU
5	A	1375	6LX	CAA-CAB-CAJ-CAI
5	A	1375	6LX	CAC-CAB-CAJ-CAI
5	A	1375	6LX	CAC-CAB-CAJ-NAK
2	B	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	C3'-C4'-C5'-O5'
5	B	1375	6LX	CAI-CAT-CBB-CBG
5	B	1375	6LX	CAI-CAJ-NAK-CAU
5	A	1375	6LX	CAA-CAB-CAJ-NAK
5	A	1375	6LX	CAS-CAT-CBB-CBG
2	A	601	ADP	C5'-O5'-PA-O1A

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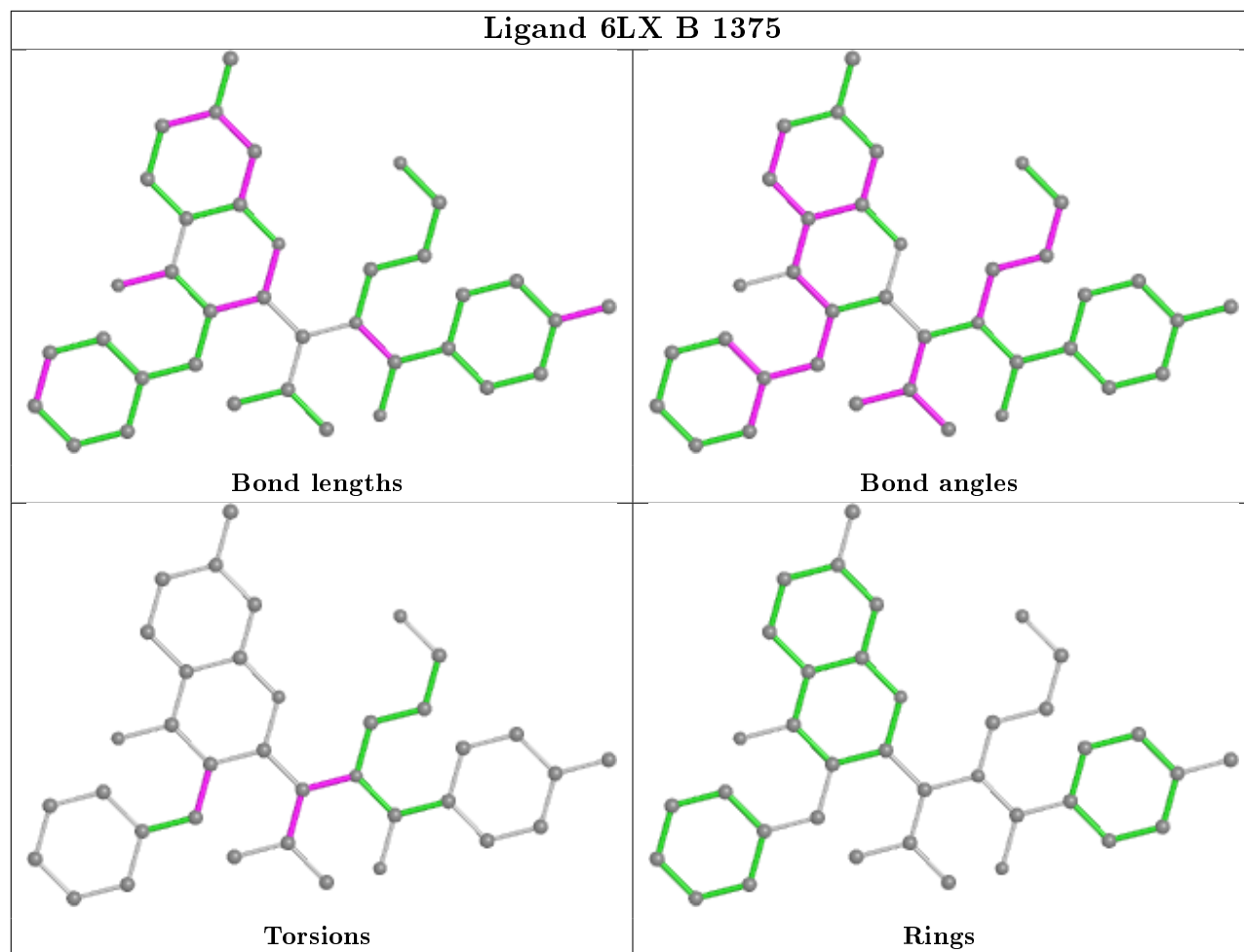
Mol	Chain	Res	Type	Atoms
5	B	1375	6LX	CAB-CAJ-NAK-CAL
5	B	1375	6LX	CAB-CAJ-NAK-CAU
2	A	601	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	C5'-O5'-PA-O3A
5	A	1375	6LX	CAI-CAT-CBB-CBG

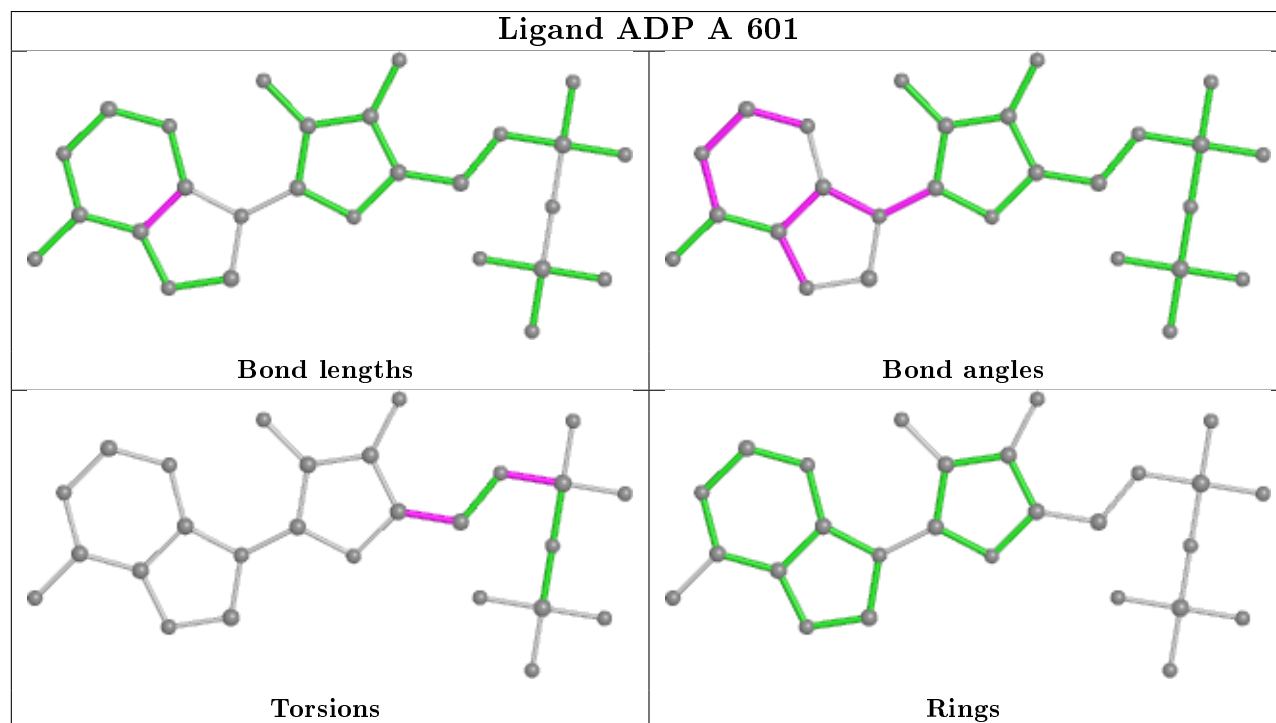
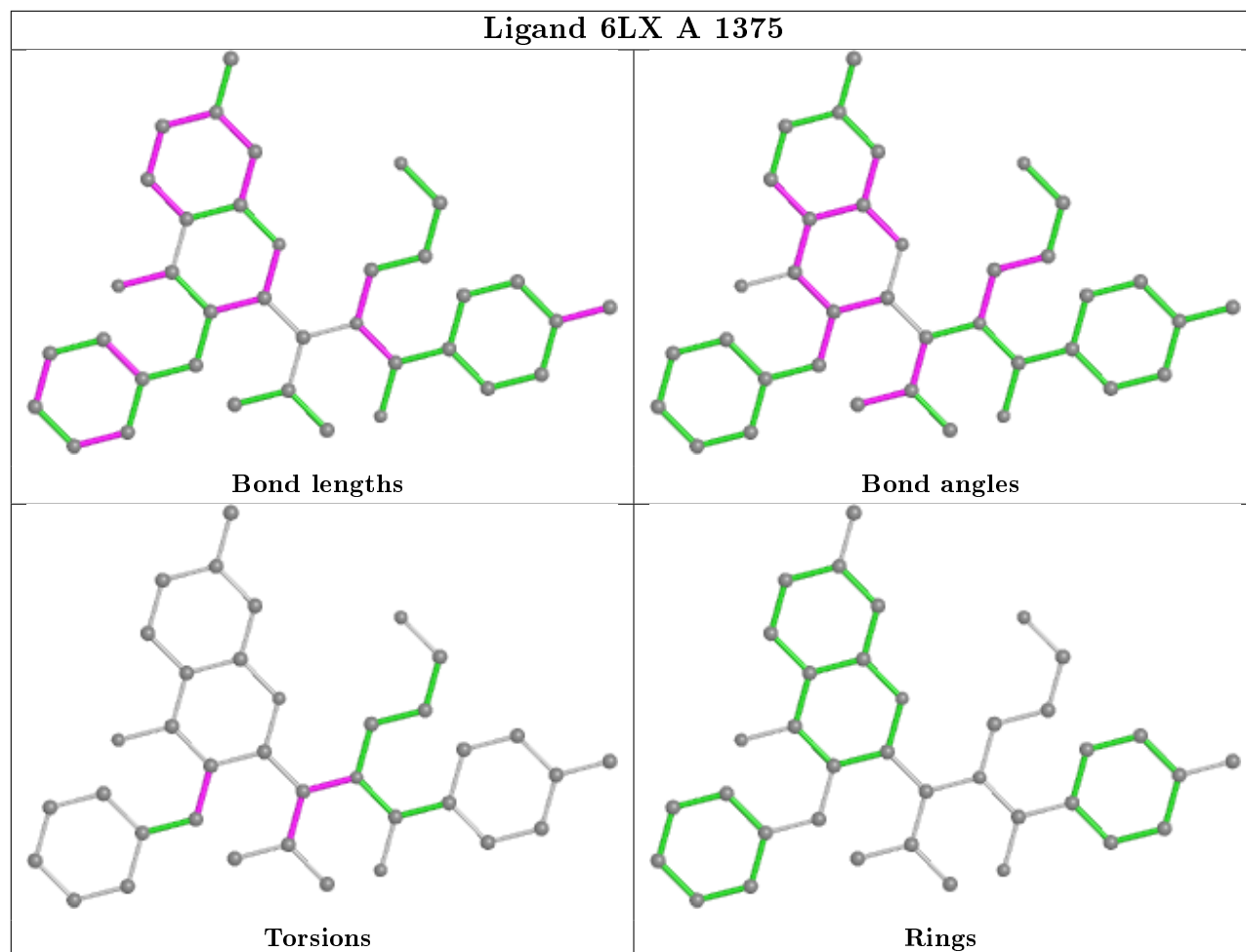
There are no ring outliers.

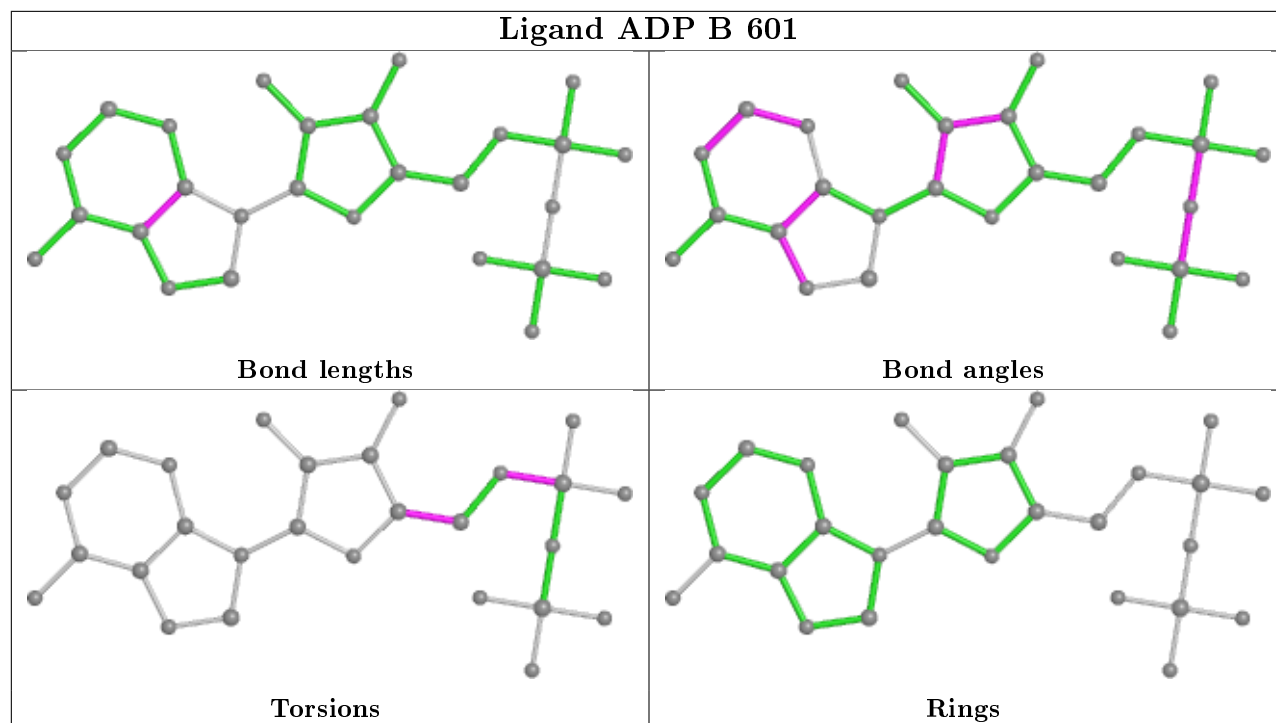
4 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1375	6LX	9	0
5	A	1375	6LX	89	0
2	A	601	ADP	3	0
2	B	601	ADP	21	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

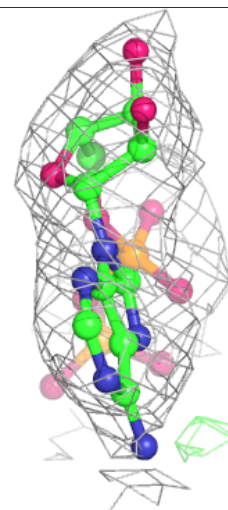
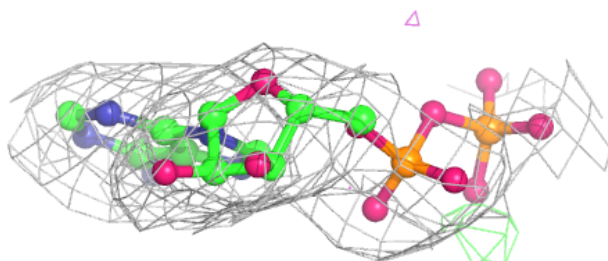
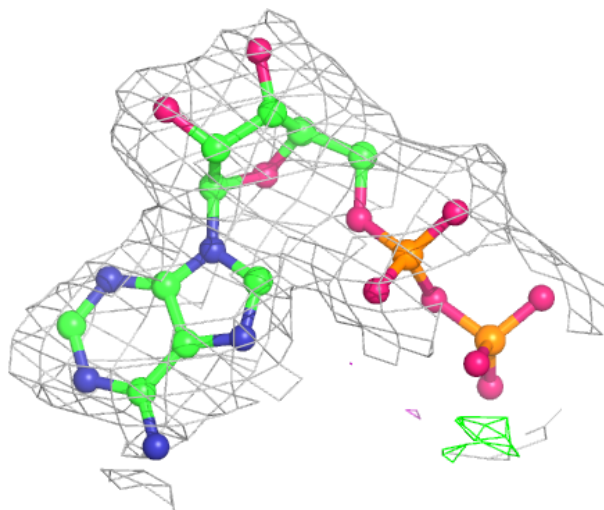
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

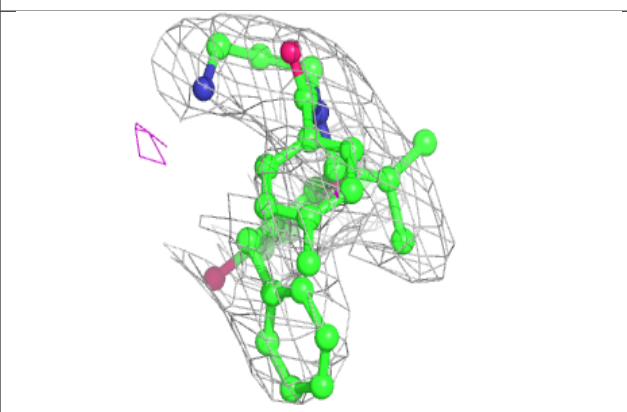
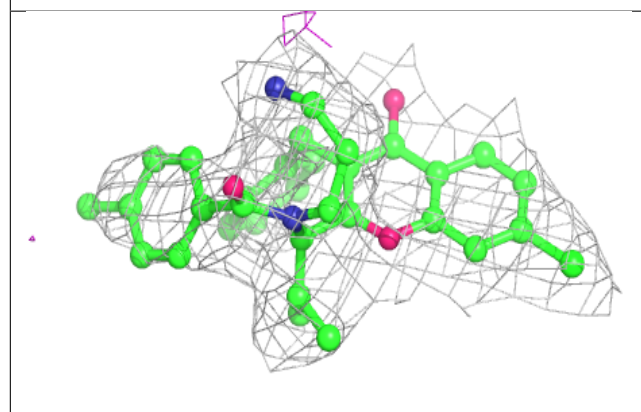
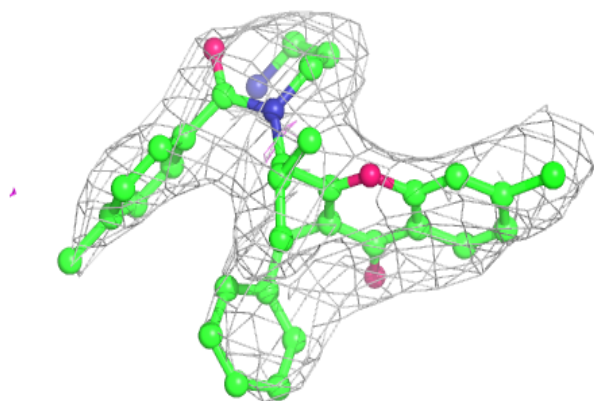
Electron density around ADP B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

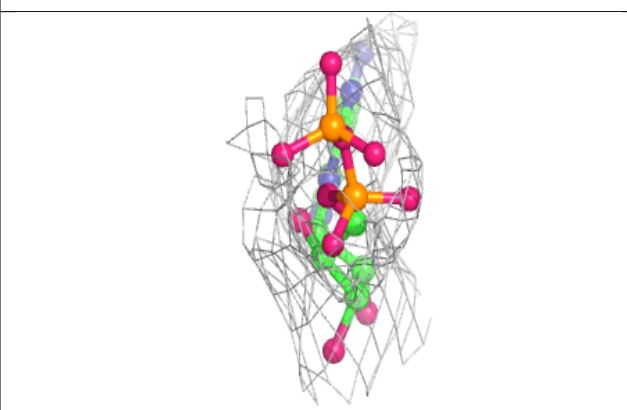
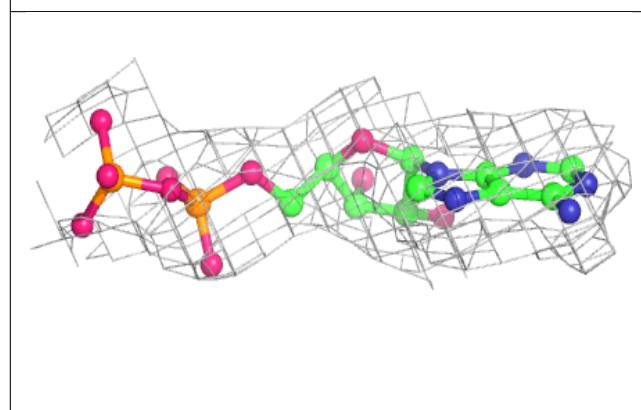
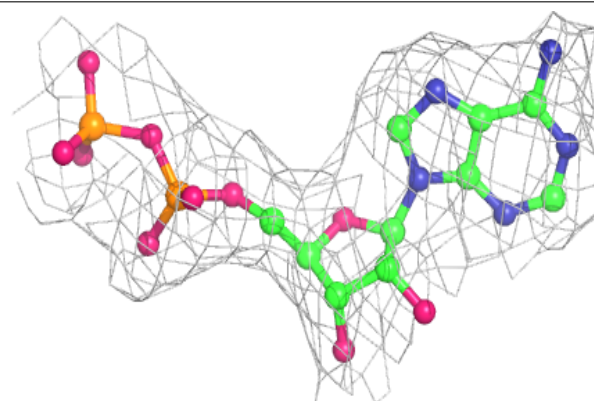


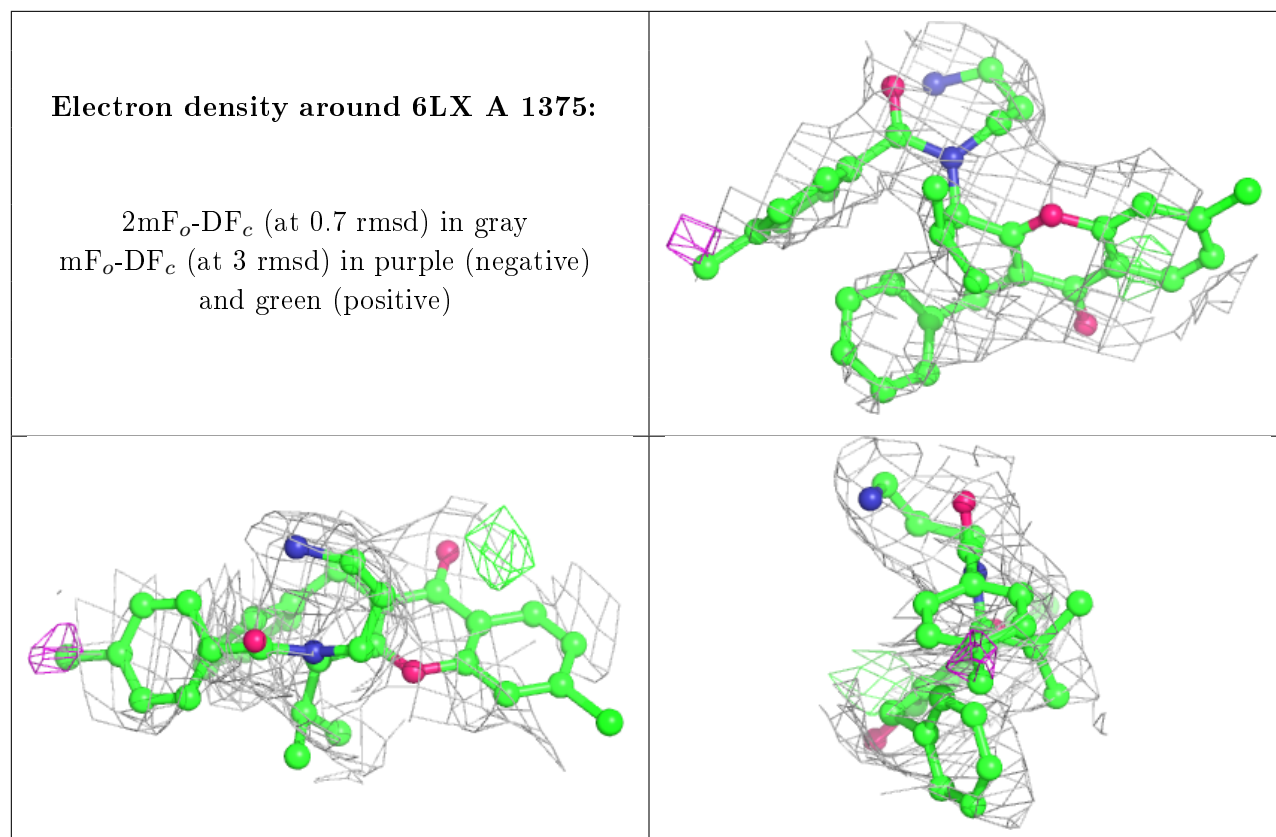
Electron density around 6LX B 1375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP A 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.