



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:32 AM UTC

PDB ID : 4BXN / pdb_00004bxn
Title : Eg5(WT) complex
Authors : Talapatra, S.K.; Anthony, N.G.; Mackay, S.P.; Kozielski, F.
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

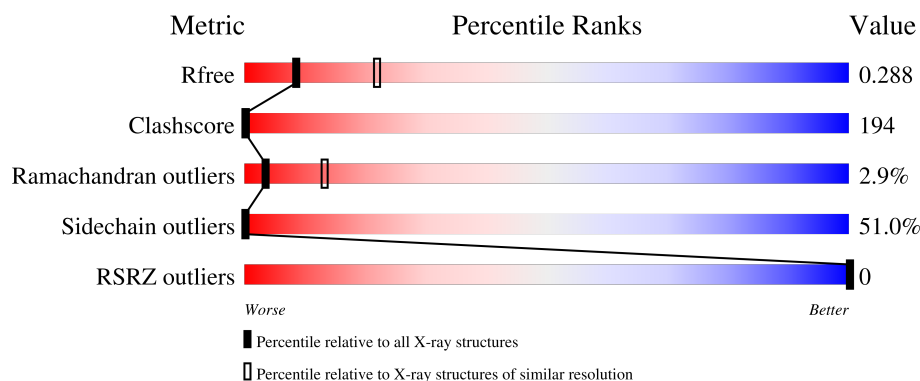
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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	-
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](#)

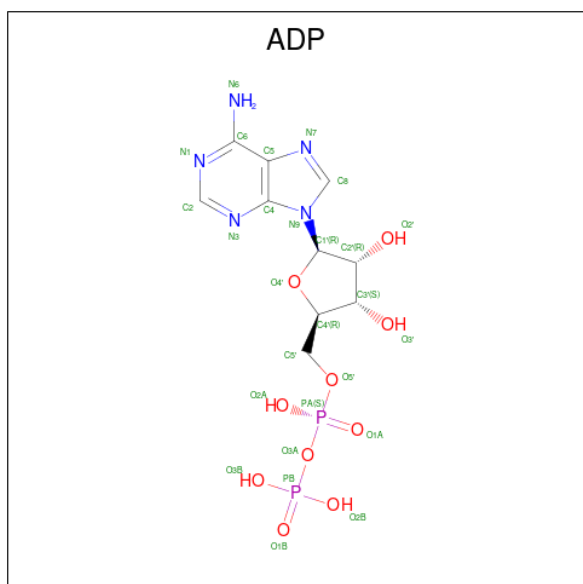
There are 6 unique types of molecules in this entry. The entry contains 5521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

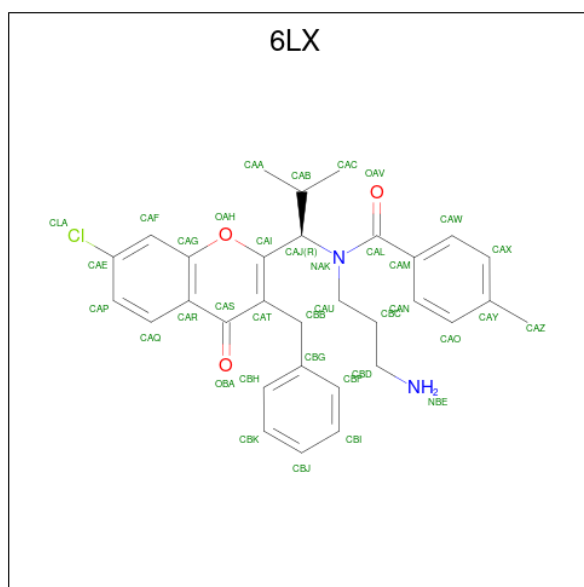


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total Cd 9 9	0	0
3	B	13	Total Cd 13 13	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Cl 5 5	0	0
4	B	3	Total Cl 3 3	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 (CCD ID: 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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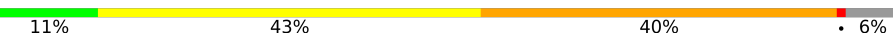
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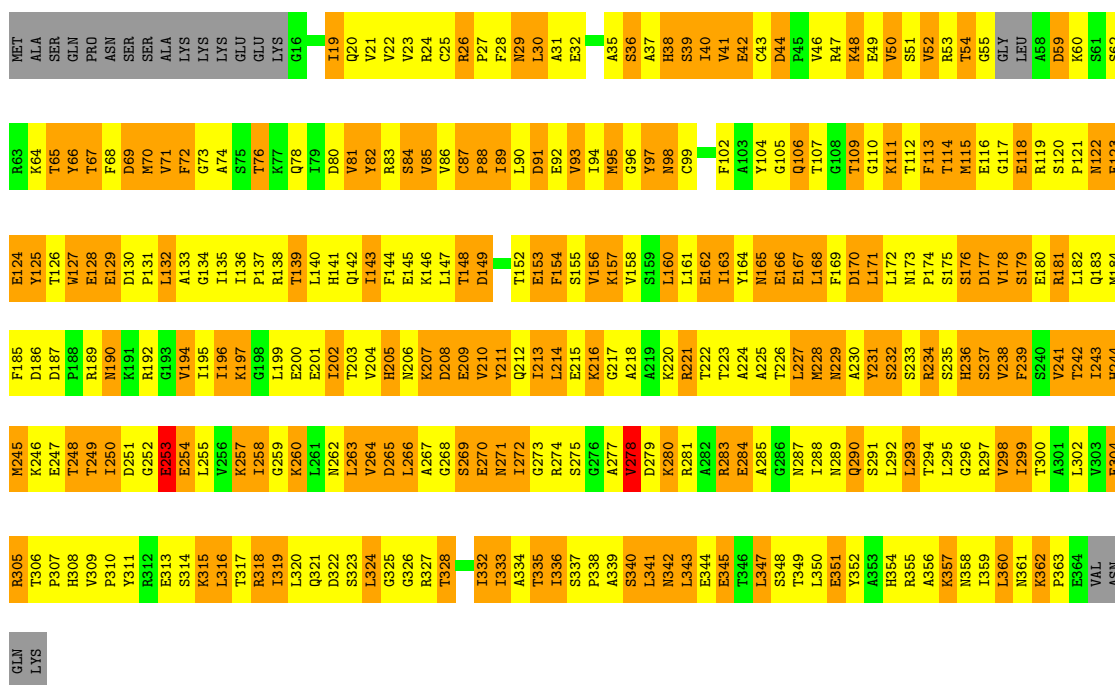
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	26	Total	O	0	0
			26	26		

3 Residue-property plots

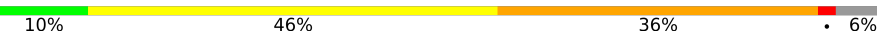
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

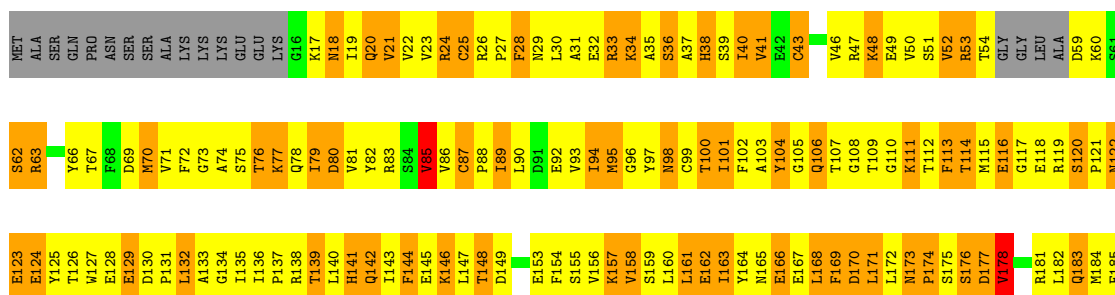
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain A: 



• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain B: 



V309	D186	E247	A219	S291
P310	D187	T248	K220	L292
Y311	P188	T249	R221	L293
	R189	I250	T222	T294
S314	N190	D251	T223	L295
K315	K191	G252	A224	G296
L316	R192	E253	A225	R297
T317	G193	E254	L226	V298
R318	V194	L255	L227	I299
I319	I195	V256	M228	T300
L320	I196	K257	A230	A301
Q321	K197	I258	Y231	E304
D322	G198	G259	S232	R305
S323	L199	K260	R233	T306
L324	E200	L261	R234	H308
	E201	N262	S235	
T328	I202	L263	H236	
R329	T203	V264	S237	
T330	V204	D265	V238	
S331	H205	L266	F239	
I332	N206	A267	S240	
I333	K207	G268	V241	
A334	D208	S269	T242	
T335	E209	I270	I243	
I336	V210	N271	H244	
S337	Y211	L272	M245	
P338	Q212	G273	K246	
A339	I213	R274		
S340	L214	S275		
L341	E215	G276		
N342	K216	A277		
L343		V278		
E344		D279		
E345		K280		
T346		R281		
L347		A282		
S348		R283		
T349		E284		
L350				
E351		N287		
Y352		I288		
A353				
H354		S291		
R355		L292		
A356		L293		
K357		T294		
N358		L295		
I359		G296		
L360		R297		
N361		V298		
K362		I299		
P363		T300		
E364		A301		
VAL		L302		
ASN		V303		
GLN		E304		
LYS		R305		
		T306		

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 27.93 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.1 (27.93-2.79) 97.1 (27.93-2.79)	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 0.279 , 0.288	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)	0.19 , 95.4	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	0.97	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: CD, CL, ADP, 6LX

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	0.47	0/2702	0.90	1/3658 (0.0%)
1	B	0.45	0/2680	0.98	11/3630 (0.3%)
All	All	0.46	0/5382	0.94	12/7288 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASN	C-N-CD	-11.05	79.70	125.00
1	B	251	ASP	N-CA-C	-8.31	102.22	111.28
1	B	276	GLY	N-CA-C	-8.30	103.72	115.43
1	B	278	VAL	N-CA-C	8.21	118.99	110.62
1	A	278	VAL	N-CA-C	-7.75	102.71	110.62
1	B	116	GLU	N-CA-C	6.12	118.03	111.36
1	B	268	GLY	N-CA-C	5.96	118.79	111.93
1	B	337	SER	CA-C-N	5.73	125.27	119.19
1	B	337	SER	C-N-CA	5.73	125.27	119.19
1	B	85	VAL	N-CA-C	5.58	115.78	110.53
1	B	106	GLN	N-CA-C	-5.33	103.49	110.53
1	B	274	ARG	N-CA-C	-5.01	103.97	110.19

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	1057	18
1	B	2642	0	2599	1024	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
4	B	3	0	0	3	0
5	A	37	0	33	91	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	2094	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 194.

All (2094) 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:226:THR:C	1:A:228:MET:HB2	1.15	1.57
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:B:82:TYR:CZ	1:B:86:VAL:HG11	1.46	1.51
1:B:174:PRO:HA	1:B:220:LYS:CD	1.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:226:THR:C	1:A:228:MET:CB	1.91	1.42
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:A:117:GLY:C	5:A:1375:6LX:HAN	1.42	1.41
1:B:24:ARG:NH2	1:B:114:THR:HG23	1.36	1.41
1:B:82:TYR:CD1	1:B:86:VAL:HB	1.55	1.41
1:B:118:GLU:CB	1:B:132:LEU:HD13	1.27	1.41
1:A:160:LEU:HD12	1:A:171:LEU:CD2	1.52	1.40
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:A:252:GLY:CA	1:A:253:GLU:HB3	1.49	1.37
1:B:163:ILE:HB	1:B:236:HIS:CD2	1.58	1.37
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:B:211:TYR:HE1	1:B:215:GLU:CD	1.30	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:28:PHE:CE1	1:A:339:ALA:HB3	1.49	1.32
1:A:224:ALA:O	1:A:228:MET:HG2	1.27	1.32
1:A:294:THR:O	1:A:298:VAL:HG23	1.22	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:O	1:B:347:LEU:CD1	1.77	1.31
1:A:280:LYS:C	1:A:284:GLU:OE2	1.72	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: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
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:195:ILE:HD13	1:B:195:ILE:C	1.56	1.27
1:B:253:GLU:OE2	1:B:255:LEU:HD11	1.29	1.27
1:A:117:GLY:C	5:A:1375:6LX:CAN	2.06	1.27
1:B:195:ILE:HD13	1:B:196:ILE:N	1.50	1.26
1:B:211:TYR:CE1	1:B:215:GLU:CD	2.11	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:30:LEU:C	1:A:30:LEU:HD13	1.62	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:82:TYR:CE1	1:B:86:VAL:HG12	1.49	1.23
1:B:113:PHE:CZ	1:B:118:GLU:HG3	1.72	1.23
1:A:147:LEU:CD1	1:A:154:PHE:CD2	2.22	1.22
1:A:230:ALA:CB	1:A:234:ARG:HB2	1.69	1.22
1:B:352:TYR:CD1	1:B:355:ARG:NH1	2.05	1.22
5:A:1375:6LX:CBF	5:A:1375:6LX:HAJ	1.68	1.22
1:A:88:PRO:O	1:A:91:ASP:OD1	1.55	1.22
1:A:152:THR:HG22	1:A:247:GLU:CD	1.62	1.22
1:A:113:PHE:CE1	1:A:114:THR:HG23	1.75	1.22
1:B:32:GLU:OE1	1:B:339:ALA:HB2	1.40	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PHE:CZ	1:B:241:VAL:CG1	2.15	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:54:THR:OG1	1:A:62:SER:HB2	1.39	1.21
1:A:272:ILE:HD11	1:A:355:ARG:NH1	1.56	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:B:344:GLU:C	1:B:347:LEU:CD1	2.14	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
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:B:40:ILE:C	1:B:52:VAL:HG22	1.68	1.19
1:A:225:ALA:C	1:A:228:MET:HB3	1.67	1.19
1:A:294:THR:O	1:A:298:VAL:CG2	1.89	1.19
1:A:318:ARG:NH1	4:A:1381:CL:CL	2.13	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:A:284:GLU:O	1:A:289:ASN:CG	1.84	1.18
1:A:298:VAL:CG1	1:A:311:TYR:CD1	2.27	1.18
1:B:20:GLN:NE2	1:B:329:ARG:NH1	1.89	1.18
1:B:128:GLU:OE2	1:B:208:ASP:OD1	1.59	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:174:PRO:CA	1:B:220:LYS:CD	1.77	1.18
1:B:40:ILE:O	1:B:52:VAL:HG22	1.42	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:163:ILE:HB	1:B:236:HIS:NE2	1.58	1.16
1:B:211:TYR:HE1	1:B:215:GLU:OE1	0.84	1.16
1:A:298:VAL:HG11	1:A:311:TYR:CD1	1.80	1.16
1:A:27:PRO:CD	1:A:74:ALA:HB1	1.75	1.16
1:A:298:VAL:HG12	1:A:311:TYR:CE1	1.80	1.16
1:A:242:THR:HG23	1:A:260:LYS:CD	1.75	1.16
1:B:40:ILE:C	1:B:52:VAL:CG2	2.19	1.16
1:B:296:GLY:O	1:B:300:THR:CG2	1.93	1.16
1:B:93:VAL:HG21	1:B:261:LEU:CD2	1.76	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:O	1:A:70:MET:SD	2.04	1.15
1:B:22:VAL:HG21	1:B:333:ILE:CG2	1.74	1.15
1:B:40:ILE:H	1:B:40:ILE:CD1	1.58	1.15
1:B:171:LEU:HB3	1:B:220:LYS:HE3	1.21	1.15
1:B:127:TRP:NE1	1:B:128:GLU:OE2	1.80	1.14
1:B:105:GLY:HA3	1:B:109:THR:CB	1.70	1.14
1:B:171:LEU:CB	1:B:177:ASP:OD2	1.93	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
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: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
1:A:294:THR:CB	1:A:314:SER:OG	1.98	1.12
5:A:1375:6LX:HAJ	5:A:1375:6LX:HBF	1.21	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: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: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: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:41:VAL:HG13	1:B:52:VAL:HG21	1.11	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: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: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:A:41:VAL:HG13	1:A:52:VAL:HG21	1.11	1.10
1:A:147:LEU:HD13	1:A:154:PHE:CD2	1.85	1.10
1:B:22:VAL:CG2	1:B:333:ILE:CG2	2.27	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:OG1	1:A:335:THR:HB	1.49	1.10
1:A:152:THR:CG2	1:A:247:GLU:HB2	1.81	1.10
1:A:324:LEU:HD23	1:A:324:LEU:H	0.95	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:192:ARG:HB3	1:B:322:ASP:HA	1.15	1.10
1:B:315:LYS:O	1:B:319:ILE:HG13	1.51	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
1:A:23:VAL:HG21	1:A:68:PHE:HE2	0.96	1.09
1:A:226:THR:HA	1:A:229:ASN:H	1.11	1.09
1:B:121:PRO:C	1:B:122:ASN:OD1	1.94	1.09
1:B:173:ASN:HB2	1:B:176:SER:OG	1.49	1.09
1:A:28:PHE:CZ	1:A:339:ALA:HB2	1.62	1.09
1:A:105:GLY:O	1:A:268:GLY:HA2	1.52	1.09
1:A:115:MET:O	1:A:136:ILE:HG13	1.51	1.09
1:B:82:TYR:CE1	1:B:86:VAL:CB	2.35	1.09
1:B:168:LEU:H	1:B:168:LEU:HD23	1.15	1.09
1:B:112:THR:CG2	1:B:116:GLU:HG3	1.81	1.09
1:A:27:PRO:HD3	1:A:74:ALA:CB	1.83	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: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:HD23	1:A:324:LEU:N	1.58	1.08
1:A:78:GLN:NE2	1:A:132:LEU:O	1.85	1.08
1:B:40:ILE:HD12	1:B:40:ILE:N	1.65	1.08
1:B:100:THR:HG23	1:B:262:ASN:OD1	1.50	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:164:TYR:OH	1:B:230:ALA:HB3	1.50	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:A:114:THR:O	1:A:134:GLY:HA3	1.54	1.07
1:A:152:THR:CG2	1:A:247:GLU:CD	2.26	1.07
1:A:167:GLU:O	1:A:168:LEU:HD12	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:104:TYR:OH	1:B:349:THR:HB	1.54	1.07
1:A:192:ARG:HH12	1:A:325:GLY:HA3	1.19	1.07
1:A:225:ALA:HB1	1:A:231:TYR:HB2	1.33	1.07
1:B:134:GLY:O	1:B:137:PRO:HG2	1.53	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
1:B:266:LEU:N	1:B:266:LEU:HD23	1.69	1.07
1:B:341:LEU:HD22	1:B:341:LEU:H	1.15	1.07
1:A:160:LEU:CD2	1:A:239:PHE:HB2	1.82	1.07
1:B:128:GLU:OE2	1:B:208:ASP:CG	1.98	1.07
1:B:250:ILE:HD13	1:B:250:ILE:N	1.69	1.07
1:A:86:VAL:C	1:A:88:PRO:HD2	1.80	1.06
1:A:105:GLY:HA2	1:A:269:SER:OG	0.89	1.06
1:A:167:GLU:CG	1:A:181:ARG:CB	2.16	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:HZ2	1:B:357:LYS:HB3	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:HH11	1:B:274:ARG:HG3	1.16	1.06
1:A:118:GLU:N	5:A:1375:6LX:HAO	1.68	1.06
1:B:127:TRP:NE1	1:B:128:GLU:CD	2.12	1.06
1:A:242:THR:HG23	1:A:260:LYS:HD3	1.36	1.05
1:B:157:LYS:HE3	1:B:242:THR:HB	1.37	1.05
1:B:344:GLU:C	1:B:347:LEU:HD13	1.77	1.05
1:B:347:LEU:H	1:B:347:LEU:HD12	1.15	1.05
1:A:91:ASP:O	1:A:94:ILE:HG22	1.56	1.05
1:A:225:ALA:HB1	1:A:231:TYR:CB	1.85	1.05
1:A:280:LYS:O	1:A:284:GLU:CD	1.98	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:47:ARG:O	1:A:48:LYS:HG3	1.56	1.05
1:A:167:GLU:HG2	1:A:181:ARG:HB3	1.39	1.05
1:A:120:SER:OG	1:A:130:ASP:OD1	1.75	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:OH	1:A:354:HIS:HB2	1.54	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:174:PRO:N	1:B:220:LYS:CD	2.19	1.04
1:B:134:GLY:O	1:B:137:PRO:HD2	1.55	1.04
1:B:228:MET:N	1:B:228:MET:SD	2.30	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:A:242:THR:CG2	1:A:260:LYS:HG2	1.85	1.04
1:B:41:VAL:N	1:B:52:VAL:HG23	1.71	1.04
1:B:134:GLY:O	1:B:137:PRO:CG	2.04	1.04
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.38	1.04
1:B:239:PHE:HE1	1:B:241:VAL:HG13	1.22	1.04
1:A:102:PHE:CZ	1:A:332:ILE:CG2	2.39	1.04
1:A:147:LEU:HD12	1:A:154:PHE:CD2	1.90	1.04
1:A:245:MET:HE2	1:A:257:LYS:CG	1.87	1.04
1:A:272:ILE:HD13	1:A:355:ARG:NH2	1.73	1.04
1:A:23:VAL:CG2	1:A:68:PHE:HE2	1.71	1.04
1:A:167:GLU:HG3	1:A:181:ARG:HB2	1.38	1.04
1:B:82:TYR:CZ	1:B:86:VAL:CG1	2.19	1.04
1:B:177:ASP:O	1:B:178:VAL:HG13	1.58	1.04
1:B:17:LYS:O	1:B:19:ILE:O	1.76	1.03
1:A:28:PHE:CE2	1:A:32:GLU:HB2	1.92	1.03
1:A:78:GLN:NE2	1:A:133:ALA:C	2.15	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: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:116:GLU:O	5:B:1375:6LX:HBB1	1.58	1.02
1:B:344:GLU:HA	1:B:347:LEU:CD1	1.87	1.02
1:A:242:THR:HG23	1:A:260:LYS:CG	1.88	1.02
1:B:22:VAL:HG22	1:B:332:ILE:O	1.59	1.02
1:B:143:ILE:O	1:B:147:LEU:HD23	1.59	1.02
1:A:285:ALA:C	1:A:289:ASN:HD22	1.67	1.02
1:B:344:GLU:CA	1:B:347:LEU:CD1	2.38	1.02
1:A:207:LYS:O	1:A:210:VAL:CG1	2.06	1.02
1:A:215:GLU:O	5:A:1375:6LX:CLA	2.14	1.02
1:A:245:MET:CB	1:A:257:LYS:HD3	1.90	1.02
1:B:98:ASN:O	1:B:328:THR:OG1	1.75	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLY:HA3	1:B:109:THR:HB	1.39	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:227:LEU:HA	1:B:228:MET:C	1.84	1.01
1:B:304:GLU:HB2	1:B:306:THR:HG22	1.42	1.01
1:B:93:VAL:HG21	1:B:261:LEU:HD23	1.40	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: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: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
1:B:347:LEU:O	1:B:351:GLU:N	1.93	1.01
1:A:41:VAL:HG21	1:A:338:PRO:HA	1.05	1.01
1:B:41:VAL:HA	1:B:52:VAL:HG23	1.06	1.01
1:B:131:PRO:HA	1:B:138:ARG:NH2	1.76	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:152:THR:CG2	1:A:247:GLU:OE1	2.08	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: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:49:GLU:OE1	1:A:67:THR:HA	1.61	0.99
1:A:120:SER:HB2	1:A:124:GLU:CG	1.91	0.99
1:A:118:GLU:N	5:A:1375:6LX:CAN	2.20	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:245:MET:HE2	1:A:257:LYS:HG2	1.40	0.99
1:A:273:GLY:HA3	1:A:280:LYS:HA	1.43	0.99
1:B:41:VAL:HA	1:B:52:VAL:CG2	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:C	1:A:30:LEU:CD1	2.30	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:133:ALA:HB2	5:A:1375:6LX:HAZ2	1.42	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
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:A:284:GLU:C	1:A:289:ASN:ND2	2.21	0.97
1:B:98:ASN:HD21	1:B:260:LYS:HD2	1.24	0.97
1:B:110:GLY:HA2	2:B:601:ADP:C8	1.99	0.97
1:A:225:ALA:C	1:A:231:TYR:HD2	1.72	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:A:227:LEU:N	1:A:228:MET:C	2.23	0.97
1:A:28:PHE:CE2	1:A:339:ALA:CB	2.46	0.97
1:A:156:VAL:HG11	1:A:204:VAL:HB	1.43	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:HD22	1:B:316:LEU:N	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:177:ASP:C	1:B:178:VAL:HG13	1.90	0.96
1:B:40:ILE:H	1:B:40:ILE:HD12	0.80	0.96
1:B:296:GLY:HA2	1:B:299:ILE:HG22	1.44	0.96
1:B:302:LEU:HD23	1:B:302:LEU:H	0.82	0.96
1:A:272:ILE:HG22	1:A:348:SER:HB3	1.43	0.96
1:B:109:THR:O	1:B:335:THR:HB	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PHE:CE1	1:B:241:VAL:HG11	1.97	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:A:167:GLU:C	1:A:168:LEU:CD1	2.38	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:195:ILE:C	1:B:195:ILE:CD1	2.30	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:B:265:ASP:C	1:B:266:LEU:HD23	1.90	0.95
1:A:186:ASP:OD1	1:A:318:ARG:NH2	2.00	0.95
1:A:133:ALA:HA	5:A:1375:6LX:HAO	1.48	0.95
1:A:324:LEU:N	1:A:324:LEU:CD2	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:A:69:ASP:C	1:A:70:MET:SD	2.49	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: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:B:77:LYS:NZ	6:B:2006:HOH:O	1.79	0.94
1:B:127:TRP:HZ2	1:B:208:ASP:HA	1.16	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: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:B:239:PHE:CE1	1:B:241:VAL:HG13	1.93	0.94
1:A:324:LEU:H	1:A:324:LEU:CD2	1.76	0.94
1:B:20:GLN:NE2	1:B:329:ARG:NH2	2.14	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:CD	1:B:339:ALA:CB	2.40	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:A:144:PHE:CE1	1:A:207:LYS:HB3	2.04	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: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:54:THR:HG1	1:A:62:SER:HB2	1.33	0.93
1:A:226:THR:CA	1:A:228:MET:HB3	1.97	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:A:226:THR:O	1:A:228:MET:CB	2.00	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: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:H	1:B:316:LEU:HD22	1.30	0.92
1:B:143:ILE:C	1:B:147:LEU:HD23	1.94	0.92
1:B:211:TYR:O	1:B:215:GLU:N	2.01	0.92
1:A:225:ALA:HA	1:A:231:TYR:CG	2.03	0.92
3:A:1365:CD:CD	1:B:87:CYS:HG	0.87	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:102:PHE:HZ	1:A:332:ILE:HG23	1.15	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:72:PHE:CZ	1:A:81:VAL:CG2	2.38	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: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:A:160:LEU:HD22	1:A:239:PHE:CB	2.00	0.91
1:B:22:VAL:CG2	1:B:333:ILE:HA	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:GLU:C	5:A:1375:6LX:CAY	2.43	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:227:LEU:HA	1:B:229:ASN:N	1.84	0.91
1:B:100:THR:HA	1:B:262:ASN:ND2	1.85	0.91
1:B:110:GLY:CA	2:B:601:ADP:N7	2.34	0.91
1:A:242:THR:HG23	1:A:260:LYS:HG2	1.47	0.91
1:A:336:ILE:HD12	1:A:336:ILE:C	1.95	0.91
1:A:26:ARG:HA	1:A:74:ALA:HA	1.53	0.91
1:A:49:GLU:OE1	1:A:66:TYR:C	2.14	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
1:B:105:GLY:CA	1:B:109:THR:CB	2.49	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:66:TYR:CZ	1:A:354:HIS:HB2	2.06	0.90
1:A:236:HIS:HA	1:A:265:ASP:O	1.72	0.90
1:B:118:GLU:O	1:B:132:LEU:HB2	1.71	0.90
1:A:225:ALA:C	1:A:228:MET:CB	2.39	0.90
1:A:236:HIS:CA	1:A:265:ASP:O	2.19	0.90
1:A:160:LEU:CG	1:A:171:LEU:HD23	2.02	0.90
1:B:52:VAL:O	1:B:53:ARG:O	1.88	0.90
1:B:174:PRO:HB3	1:B:220:LYS:HB2	1.51	0.90
1:A:67:THR:O	1:A:68:PHE:CD1	2.25	0.90
1:B:161:LEU:HD22	1:B:161:LEU:C	1.92	0.89
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:87:CYS:SG	4:A:1377:CL:CL	2.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:CG2	1:A:311:TYR:HE2	1.79	0.89
1:B:32:GLU:CD	1:B:339:ALA:HB2	1.98	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:26:ARG:O	1:B:338:PRO:HG3	1.73	0.89
1:B:197:LYS:HD2	1:B:198:GLY:H	1.02	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:118:GLU:C	1:B:132:LEU:HB3	1.98	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:28:PHE:CG	1:A:339:ALA:HB2	2.07	0.88
1:A:221:ARG:NH2	5:A:1375:6LX:CAP	2.34	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
1:B:143:ILE:HG23	1:B:147:LEU:CD2	1.88	0.88
1:B:227:LEU:CA	1:B:228:MET:C	2.46	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:167:GLU:C	1:A:168:LEU:HD13	1.97	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:A:47:ARG:C	1:A:48:LYS:HG3	1.96	0.88
1:B:76:THR:C	1:B:77:LYS:HE2	1.97	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:51:SER:HA	1:A:64:LYS:O	1.73	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:B:112:THR:O	1:B:116:GLU:HB2	1.72	0.88
1:A:73:GLY:H	1:A:76:THR:CG2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HD1	1:A:114:THR:H	1.16	0.87
1:A:44:ASP:OD2	1:A:47:ARG:HB3	1.72	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:B:134:GLY:C	1:B:137:PRO:HD2	1.97	0.87
1:B:247:GLU:O	1:B:255:LEU:N	2.06	0.87
1:B:296:GLY:C	1:B:300:THR:HG23	1.98	0.87
1:B:342:ASN:C	1:B:346:THR:HG22	1.99	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:CD2	1:B:316:LEU:N	2.30	0.87
1:B:20:GLN:HE21	1:B:329:ARG:HH12	0.90	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: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:A:336:ILE:C	1:A:336:ILE:CD1	2.48	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:B:304:GLU:CD	1:B:304:GLU:H	1.84	0.86
1:A:302:LEU:CG	1:A:311:TYR:OH	2.22	0.86
1:B:20:GLN:HE22	1:B:329:ARG:NH2	1.69	0.86
1:B:183:GLN:OE1	1:B:185:PHE:CE2	2.28	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
1:B:82:TYR:CE1	1:B:86:VAL:HB	2.03	0.86
1:A:66:TYR:OH	1:A:354:HIS:CB	2.23	0.86
1:A:66:TYR:CE1	1:A:354:HIS:HB2	2.10	0.86
1:A:125:TYR:CD1	1:A:125:TYR:N	2.43	0.86
1:A:157:LYS:CG	1:A:203:THR:HG22	2.06	0.86
1:A:105:GLY:C	1:A:269:SER:OG	2.18	0.86
1:A:298:VAL:CG1	1:A:311:TYR:CG	2.58	0.86
1:B:142:GLN:C	1:B:146:LYS:HG3	2.01	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:236:HIS:C	1:A:265:ASP:O	2.19	0.86
1:B:127:TRP:CE2	1:B:128:GLU:CD	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:C	1:B:147:LEU:CD2	2.47	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:73:GLY:N	1:A:76:THR:HG21	1.91	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: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:27:PRO:HD3	1:A:74:ALA:HB1	0.91	0.85
1:A:225:ALA:O	1:A:228:MET:CG	2.25	0.85
1:A:120:SER:HB2	1:A:124:GLU:HG3	1.56	0.85
1:A:133:ALA:HB2	5:A:1375:6LX:HAZ3	1.58	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:249:THR:CG2	1:B:255:LEU:HD21	2.07	0.85
1:B:72:PHE:CB	1:B:76:THR:HG21	2.05	0.85
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
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:192:ARG:HD3	1:B:322:ASP:OD1	1.78	0.84
1:B:250:ILE:HD13	1:B:250:ILE:H	1.36	0.84
1:B:32:GLU:OE1	1:B:339:ALA:CB	2.24	0.84
1:B:135:ILE:O	1:B:139:THR:OG1	1.96	0.84
1:A:41:VAL:HA	1:A:52:VAL:CG2	2.07	0.84
1:A:281:ARG:O	1:A:285:ALA:HB2	1.78	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:A:28:PHE:CE2	1:A:32:GLU:CB	2.60	0.84
1:A:156:VAL:O	1:A:204:VAL:N	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLU:OE2	1:A:37:ALA:N	2.11	0.83
1:A:118:GLU:C	5:A:1375:6LX:CAO	2.51	0.83
1:A:152:THR:HG21	1:A:247:GLU:OE1	1.77	0.83
1:A:226:THR:C	1:A:228:MET:HB3	2.03	0.83
1:A:230:ALA:O	1:A:234:ARG:N	2.11	0.83
1:B:352:TYR:CE1	1:B:355:ARG:NH1	2.45	0.83
1:A:118:GLU:O	5:A:1375:6LX:HAZ3	1.77	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:B:104:TYR:CE1	1:B:334:ALA:HB1	2.12	0.83
1:A:91:ASP:OD2	3:A:1367:CD:CD	1.46	0.83
1:A:234:ARG:NH2	6:A:2013:HOH:O	2.10	0.83
1:B:316:LEU:H	1:B:316:LEU:HD23	1.41	0.83
1:B:174:PRO:C	1:B:220:LYS:HD2	2.02	0.83
1:B:47:ARG:C	1:B:48:LYS:HG3	2.02	0.83
1:B:225:ALA:HA	1:B:231:TYR:CE1	2.14	0.83
1:B:230:ALA:HB1	1:B:234:ARG:NE	1.92	0.83
1:B:53:ARG:C	1:B:54:THR:HG22	2.04	0.82
1:A:67:THR:HG21	1:A:359:ILE:HG22	1.61	0.82
1:A:86:VAL:C	1:A:88:PRO:CD	2.51	0.82
1:A:302:LEU:HG	1:A:311:TYR:OH	1.79	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:A:143:ILE:O	1:A:147:LEU:HG	1.80	0.82
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:B:172:LEU:HG	1:B:173:ASN:N	1.92	0.82
1:A:109:THR:HG21	1:A:335:THR:OG1	1.78	0.82
1:A:197:LYS:HE3	1:B:250:ILE:HG13	1.62	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:B:26:ARG:O	6:B:2002:HOH:O	1.96	0.82
1:B:120:SER:CB	1:B:125:TYR:HB2	2.08	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:22:VAL:CG2	1:B:333:ILE:CA	2.55	0.82
1:B:40:ILE:C	1:B:52:VAL:HG23	1.95	0.82
1:B:82:TYR:OH	1:B:90:LEU:HD22	1.79	0.82
1:B:104:TYR:HE1	1:B:334:ALA:HB1	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HD13	1:B:196:ILE:CA	2.10	0.82
1:A:23:VAL:HG22	1:A:334:ALA:HB3	1.61	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:A:225:ALA:C	1:A:228:MET:CG	2.53	0.82
1:B:234:ARG:HH11	1:B:288:ILE:HD13	1.45	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:20:GLN:N	1:B:330:THR:O	2.12	0.81
1:B:314:SER:HB3	1:B:317:THR:HG23	1.60	0.81
1:A:226:THR:CA	1:A:229:ASN:H	1.91	0.81
1:B:127:TRP:CD1	1:B:128:GLU:CD	2.58	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:47:ARG:HA	1:A:47:ARG:HE	1.44	0.81
1:A:249:THR:HB	1:A:252:GLY:CA	2.10	0.81
1:A:41:VAL:CG2	1:A:338:PRO:CA	2.52	0.81
1:A:65:THR:OG1	1:A:361:ASN:CG	2.24	0.81
1:A:118:GLU:H	1:A:133:ALA:HA	1.42	0.81
1:B:47:ARG:HB2	1:B:49:GLU:OE1	1.81	0.81
1:B:164:TYR:OH	1:B:230:ALA:CB	2.29	0.81
1:A:167:GLU:C	1:A:168:LEU:HD12	2.00	0.81
1:B:127:TRP:CH2	1:B:207:LYS:CG	2.64	0.81
1:B:128:GLU:CD	1:B:208:ASP:OD1	2.22	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:105:GLY:C	1:A:269:SER:H	1.89	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:B:53:ARG:O	1:B:54:THR:CG2	2.30	0.80
1:B:246:LYS:NZ	6:B:2009:HOH:O	2.14	0.80
1:B:164:TYR:HE1	1:B:234:ARG:NE	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:TYR:CE1	1:B:215:GLU:HB2	2.16	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:32:GLU:CD	1:A:37:ALA:HB3	2.08	0.79
1:A:342:ASN:HB2	1:A:345:GLU:CG	2.12	0.79
1:B:32:GLU:O	1:B:37:ALA:HB2	1.83	0.79
1:B:117:GLY:HA3	1:B:134:GLY:H	1.47	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:17:LYS:O	1:B:18:ASN:C	2.25	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: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:A:262:ASN:C	1:A:263:LEU:HD13	2.08	0.79
1:B:227:LEU:HA	1:B:228:MET:HB2	1.64	0.79
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:B:239:PHE:CD1	1:B:263:LEU:HD12	2.18	0.78
1:A:73:GLY:O	1:A:76:THR:CG2	2.31	0.78
1:B:26:ARG:HD2	2:B:601:ADP:C1'	2.13	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: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:38:HIS:N	1:B:38:HIS:ND1	2.32	0.78
1:B:131:PRO:CA	1:B:138:ARG:NH2	2.46	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: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
1:B:136:ILE:HG12	1:B:263:LEU:CD1	2.12	0.78
1:B:83:ARG:O	1:B:87:CYS:HB2	1.84	0.78
1:A:21:VAL:CG2	1:A:357:LYS:HG3	2.13	0.77
1:A:127:TRP:HE3	1:A:128:GLU:OE2	1.61	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:N	1:A:228:MET:HB2	1.98	0.77
1:B:41:VAL:CB	1:B:52:VAL:HG23	2.14	0.77
1:B:311:TYR:HD1	1:B:317:THR:O	1.65	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:265:ASP:C	1:B:266:LEU:CD2	2.57	0.77
1:A:67:THR:HG21	1:A:359:ILE:CG2	2.15	0.77
1:A:123:GLU:O	1:A:124:GLU:OE1	2.03	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:82:TYR:HE1	1:B:86:VAL:HG12	0.94	0.77
1:B:357:LYS:HZ2	1:B:357:LYS:CB	1.95	0.77
1:A:96:GLY:HA2	1:A:258:ILE:O	1.84	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:B:47:ARG:HH12	1:B:364:GLU:CB	1.98	0.77
1:B:136:ILE:CG1	1:B:263:LEU:HD13	2.13	0.77
1:A:21:VAL:HG21	1:A:357:LYS:HB2	1.67	0.77
1:B:40:ILE:CD1	1:B:40:ILE:N	2.30	0.77
1:B:247:GLU:O	1:B:255:LEU:HB2	1.85	0.77
1:B:98:ASN:HD21	1:B:260:LYS:CD	1.98	0.76
1:B:104:TYR:O	1:B:104:TYR:HD1	1.66	0.76
1:A:32:GLU:OE2	1:A:37:ALA:O	2.04	0.76
1:A:284:GLU:O	1:A:289:ASN:CB	2.33	0.76
1:B:121:PRO:O	1:B:124:GLU:CG	2.33	0.76
1:A:49:GLU:CD	1:A:67:THR:HA	2.06	0.76
1:A:114:THR:C	1:A:134:GLY:HA3	2.10	0.76
1:A:116:GLU:C	5:A:1375:6LX:HBB2	2.10	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:156:VAL:O	1:A:203:THR:HA	1.85	0.76
1:B:168:LEU:N	1:B:168:LEU:CD2	2.49	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: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:78:GLN:HE22	1:A:133:ALA:C	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:CE	1:B:250:ILE:HG13	2.16	0.76
1:A:336:ILE:O	1:A:336:ILE:CD1	2.30	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:106:GLN:CB	1:A:345:GLU:HB3	2.16	0.75
1:A:117:GLY:C	5:A:1375:6LX:CAO	2.47	0.75
1:A:225:ALA:CB	1:A:231:TYR:HB2	2.14	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: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:B:304:GLU:O	1:B:305:ARG:HB3	1.84	0.75
1:A:73:GLY:N	1:A:76:THR:CG2	2.48	0.75
1:A:201:GLU:O	1:A:201:GLU:HG2	1.84	0.75
1:B:341:LEU:H	1:B:341:LEU:CD2	1.94	0.75
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:HBI	5:A:1375:6LX:CAX	2.16	0.75
1:B:192:ARG:HG3	1:B:192:ARG:HH11	1.50	0.75
1:B:250:ILE:N	1:B:250:ILE:CD1	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:A:296:GLY:C	1:A:300:THR:HG1	1.93	0.75
1:B:110:GLY:HA2	2:B:601:ADP:N7	1.98	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: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:44:ASP:OD2	1:A:47:ARG:HB2	1.85	0.74
1:A:166:GLU:O	1:A:167:GLU:CD	2.30	0.74
1:A:225:ALA:HA	1:A:231:TYR:CE2	2.12	0.74
1:B:136:ILE:N	1:B:137:PRO:HD2	2.02	0.74
1:A:47:ARG:O	1:A:48:LYS:CG	2.35	0.74
1:A:225:ALA:O	1:A:228:MET:HG3	1.86	0.74
1:A:253:GLU:C	1:A:253:GLU:OE2	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:128:GLU:H	1:A:128:GLU:CD	1.96	0.73
1:A:143:ILE:HD11	1:A:147:LEU:HD11	1.69	0.73
1:A:214:LEU:O	5:A:1375:6LX:CAE	2.36	0.73
1:A:228:MET:HG3	1:A:231:TYR:HD2	1.50	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:86:VAL:HG21	1:B:135:ILE:CG2	2.18	0.73
1:B:121:PRO:O	1:B:124:GLU:HG3	1.87	0.73
1:A:72:PHE:CZ	1:A:81:VAL:N	2.56	0.73
1:B:48:LYS:C	1:B:71:VAL:HG21	2.14	0.73
1:B:118:GLU:C	1:B:132:LEU:HD12	2.13	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:B:142:GLN:C	1:B:146:LYS:CG	2.59	0.73
1:A:248:THR:HG23	1:A:254:GLU:OE2	1.88	0.73
1:A:39:SER:HB3	1:A:338:PRO:C	2.13	0.73
1:A:41:VAL:HA	1:A:52:VAL:HG23	1.71	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:65:THR:HG1	1:A:361:ASN:CG	1.97	0.73
1:A:153:GLU:HG3	1:A:246:LYS:O	1.89	0.73
1:A:167:GLU:O	1:A:168:LEU:CD1	2.32	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:73:GLY:O	1:A:76:THR:HG23	1.88	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:B:28:PHE:HE1	1:B:39:SER:OG	1.72	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:113:PHE:CD1	1:A:113:PHE:C	2.65	0.72
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:186:ASP:CG	1:A:318:ARG:HH22	1.98	0.72
1:A:227:LEU:H	1:A:228:MET:C	1.96	0.72
1:A:296:GLY:O	1:A:300:THR:CB	2.37	0.72
1:A:43:CYS:SG	1:A:73:GLY:HA2	2.29	0.72
1:A:152:THR:HG22	1:A:247:GLU:HG3	1.68	0.72
1:B:98:ASN:ND2	1:B:260:LYS:HD2	2.04	0.72
1:A:249:THR:HB	1:A:252:GLY:HA3	1.69	0.72
1:B:197:LYS:HD2	1:B:197:LYS:C	2.04	0.72
1:A:170:ASP:C	1:A:170:ASP:OD1	2.32	0.72
1:B:76:THR:O	1:B:77:LYS:CE	2.36	0.72
1:B:85:VAL:HG11	1:B:333:ILE:HG21	1.72	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:A:249:THR:O	1:A:252:GLY:C	2.32	0.72
1:B:48:LYS:HD2	1:B:362:LYS:HZ1	1.53	0.72
1:A:96:GLY:CA	1:A:258:ILE:O	2.37	0.72
1:A:202:ILE:HD13	1:A:202:ILE:N	2.04	0.72
1:B:303:VAL:HG21	1:B:357:LYS:HZ2	1.54	0.72
1:B:347:LEU:HD12	1:B:347:LEU:N	2.00	0.72
1:B:41:VAL:N	1:B:52:VAL:CG2	2.40	0.71
1:B:77:LYS:HE2	1:B:77:LYS:HA	1.70	0.71
1:B:177:ASP:C	1:B:178:VAL:CG1	2.63	0.71
1:B:295:LEU:O	1:B:299:ILE:N	2.21	0.71
1:A:227:LEU:H	1:A:229:ASN:N	1.89	0.71
1:A:25:CYS:HB3	1:A:43:CYS:CB	2.20	0.71
1:A:210:VAL:O	1:A:214:LEU:N	2.22	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: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: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:22:VAL:CG2	1:B:332:ILE:O	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:O	1:B:52:VAL:HA	1.89	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:A:113:PHE:O	1:A:117:GLY:HA2	1.90	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:A:91:ASP:C	1:A:94:ILE:HG22	2.15	0.70
1:B:342:ASN:O	1:B:343:LEU:C	2.33	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:A:245:MET:HE2	1:A:257:LYS:HG3	1.70	0.70
1:B:19:ILE:HA	1:B:330:THR:HB	1.73	0.70
1:B:40:ILE:O	1:B:52:VAL:CA	2.39	0.70
1:B:357:LYS:NZ	1:B:357:LYS:CB	2.47	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:125:TYR:H	1:A:125:TYR:HD1	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: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:82:TYR:HE2	1:A:139:THR:HA	1.54	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
1:A:343:LEU:O	1:A:347:LEU:HD23	1.90	0.70
1:B:19:ILE:H	1:B:19:ILE:HD12	1.57	0.70
1:B:112:THR:O	1:B:116:GLU:CB	2.40	0.70
1:A:35:ALA:HB1	1:A:341:LEU:HG	1.71	0.70
1:A:270:GLU:C	1:A:348:SER:OG	2.34	0.70
1:B:81:VAL:CG1	1:B:85:VAL:HG21	2.22	0.70
1:B:172:LEU:CD1	1:B:173:ASN:HD21	2.05	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:47:ARG:HB2	1:B:49:GLU:CD	2.17	0.70
1:B:276:GLY:O	1:B:278:VAL:HG12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:OE1	1:A:129:GLU:CA	2.40	0.69
1:A:28:PHE:CD2	1:A:32:GLU:CB	2.74	0.69
1:A:28:PHE:HE2	1:A:32:GLU:CD	2.00	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:89:ILE:HD13	1:A:99:CYS:HB3	1.73	0.69
1:A:173:ASN:O	1:A:220:LYS:NZ	2.26	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:B:268:GLY:C	1:B:270:GLU:OE2	2.36	0.69
1:A:66:TYR:CE2	1:A:68:PHE:CZ	2.80	0.69
1:A:106:GLN:HA	1:A:268:GLY:CA	2.23	0.69
1:B:20:GLN:NE2	1:B:329:ARG:HH12	1.64	0.69
1:B:73:GLY:C	1:B:75:SER:H	1.94	0.69
1:B:172:LEU:CD1	1:B:173:ASN:HD22	2.04	0.69
1:B:24:ARG:HH21	1:B:114:THR:HG21	1.51	0.69
1:B:104:TYR:HH	1:B:349:THR:HB	1.57	0.69
1:A:72:PHE:CE2	1:A:81:VAL:HG21	2.24	0.69
5:A:1375:6LX:HAW	5:A:1375:6LX:HAC2	1.73	0.69
1:B:26:ARG:HD2	2:B:601:ADP:O4'	1.92	0.69
1:B:106:GLN:CA	1:B:270:GLU:OE1	2.40	0.69
1:B:182:LEU:HD23	1:B:182:LEU:H	1.57	0.69
1:B:183:GLN:CD	1:B:185:PHE:CZ	2.71	0.69
1:B:296:GLY:C	1:B:299:ILE:HG22	2.17	0.69
1:A:186:ASP:HB2	1:A:318:ARG:HH12	1.58	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:A:118:GLU:H	5:A:1375:6LX:CAO	1.90	0.68
1:B:77:LYS:H	1:B:80:ASP:CG	2.01	0.68
1:B:127:TRP:CZ2	1:B:208:ASP:N	2.58	0.68
1:A:83:ARG:O	1:A:88:PRO:HD3	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:30:LEU:O	1:B:30:LEU:HD13	1.92	0.68
1:B:303:VAL:HG21	1:B:357:LYS:NZ	2.08	0.68
1:A:44:ASP:C	1:A:44:ASP:OD1	2.35	0.68
1:B:127:TRP:HH2	1:B:207:LYS:HG2	1.56	0.68
1:B:342:ASN:O	1:B:346:THR:HG22	1.93	0.68
1:B:360:LEU:HD12	1:B:361:ASN:H	1.58	0.68
1:A:104:TYR:CE2	1:A:352:TYR:CG	2.82	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:OE1	1:A:129:GLU:HA	1.92	0.68
1:A:214:LEU:O	5:A:1375:6LX:CAP	2.41	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:B:93:VAL:CG2	1:B:261:LEU:HD23	2.20	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: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:A:118:GLU:CA	5:A:1375:6LX:CAN	2.72	0.68
1:B:172:LEU:HD12	1:B:173:ASN:HD21	1.56	0.68
1:B:234:ARG:HH11	1:B:288:ILE:CD1	2.07	0.68
1:B:239:PHE:HB3	1:B:263:LEU:HD12	1.74	0.68
1:A:105:GLY:C	1:A:269:SER:N	2.52	0.68
1:A:210:VAL:O	1:A:214:LEU:HB2	1.93	0.68
5:A:1375:6LX:CAO	5:A:1375:6LX:HBI	2.24	0.68
1:B:347:LEU:CD1	1:B:347:LEU:H	1.95	0.68
1:A:80:ASP:O	1:A:84:SER:OG	2.11	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: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:25:CYS:O	1:A:73:GLY:C	2.37	0.67
1:A:294:THR:HB	1:A:314:SER:OG	1.93	0.67
1:A:315:LYS:CE	1:A:315:LYS:N	2.57	0.67
1:B:41:VAL:HG12	1:B:52:VAL:HB	1.77	0.67
1:B:341:LEU:HD22	1:B:341:LEU:N	2.00	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:112:THR:HB	2:A:601:ADP:O2A	1.95	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:215:GLU:C	5:A:1375:6LX:CLA	2.74	0.67
1:B:76:THR:HA	1:B:80:ASP:OD2	1.94	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:A:54:THR:O	1:A:55:GLY:C	2.37	0.67
1:A:272:ILE:HG22	1:A:348:SER:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:104:TYR:CD1	1:B:104:TYR:C	2.70	0.66
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:CD2	1:A:347:LEU:N	2.58	0.66
1:B:227:LEU:HB3	1:B:228:MET:C	2.19	0.66
1:A:90:LEU:O	1:A:94:ILE:HB	1.96	0.66
1:A:174:PRO:O	1:A:177:ASP:O	2.13	0.66
1:A:32:GLU:CD	1:A:32:GLU:O	2.38	0.66
1:A:197:LYS:NZ	1:B:250:ILE:HG13	2.11	0.66
1:B:20:GLN:NE2	1:B:329:ARG:HH22	1.92	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:A:67:THR:HG22	1:A:359:ILE:HB	1.76	0.66
1:B:126:THR:C	1:B:130:ASP:OD2	2.39	0.66
1:B:163:ILE:CG2	1:B:236:HIS:CD2	2.78	0.66
1:A:133:ALA:CB	5:A:1375:6LX:HAZ3	2.25	0.66
1:A:170:ASP:OD2	1:A:200:GLU:CB	2.38	0.66
1:A:25:CYS:HB3	1:A:43:CYS:SG	2.36	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:216:LYS:C	5:A:1375:6LX:CLA	2.76	0.66
1:A:236:HIS:CD2	1:A:266:LEU:HD23	2.31	0.66
1:A:342:ASN:HB2	1:A:345:GLU:HG2	1.78	0.66
1:B:82:TYR:HD1	1:B:82:TYR:O	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: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:160:LEU:HD13	1:A:238:VAL:O	1.97	0.65
1:A:168:LEU:HD13	1:A:168:LEU:N	2.11	0.65
1:A:249:THR:CB	1:A:252:GLY:HA3	2.26	0.65
1:A:51:SER:CA	1:A:64:LYS:O	2.43	0.65
1:A:156:VAL:CG1	1:A:204:VAL:H	2.08	0.65
1:B:333:ILE:O	1:B:333:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:SER:HB2	1:B:244:HIS:HB2	1.78	0.65
1:B:173:ASN:O	1:B:174:PRO:C	2.38	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
5:A:1375:6LX:CAN	5:A:1375:6LX:HBF	2.27	0.65
1:A:168:LEU:CD1	1:A:168:LEU:N	2.56	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:B:77:LYS:CE	1:B:77:LYS:HA	2.26	0.65
1:A:73:GLY:C	1:A:76:THR:HG22	2.22	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:170:ASP:C	1:B:170:ASP:OD1	2.40	0.65
1:B:173:ASN:C	1:B:175:SER:N	2.52	0.65
1:B:344:GLU:C	1:B:347:LEU:HD12	2.15	0.65
1:B:121:PRO:O	1:B:122:ASN:OD1	2.14	0.64
1:A:41:VAL:CG2	1:A:338:PRO:O	2.45	0.64
1:A:82:TYR:HE2	1:A:139:THR:CA	2.10	0.64
1:A:351:GLU:O	1:A:355:ARG:HG2	1.97	0.64
1:B:41:VAL:HG21	1:B:338:PRO:HA	1.77	0.64
1:B:104:TYR:OH	1:B:349:THR:CA	2.45	0.64
1:B:270:GLU:N	1:B:270:GLU:CD	2.50	0.64
1:B:343:LEU:C	1:B:346:THR:CG2	2.69	0.64
1:A:82:TYR:CE2	1:A:139:THR:HA	2.32	0.64
1:B:127:TRP:CH2	1:B:207:LYS:C	2.75	0.64
1:B:192:ARG:HH11	1:B:192:ARG:CG	2.09	0.64
1:B:26:ARG:NH1	1:B:27:PRO:O	2.29	0.64
1:B:113:PHE:HE2	1:B:118:GLU:HG3	0.86	0.64
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: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:253:GLU:HG2	1:B:254:GLU:N	2.12	0.64
1:A:49:GLU:OE2	6:A:2004:HOH:O	2.15	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:82:TYR:CD1	1:A:82:TYR:C	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LYS:O	1:B:19:ILE:C	2.41	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:98:ASN:HB2	1:A:323:SER:HA	1.78	0.64
1:A:234:ARG:O	1:A:234:ARG:NE	2.30	0.64
1:A:347:LEU:N	1:A:347:LEU:HD22	2.13	0.64
1:B:24:ARG:HG3	1:B:24:ARG:O	1.97	0.64
1:B:26:ARG:HG2	1:B:26:ARG:HH11	1.63	0.64
1:B:49:GLU:OE1	1:B:49:GLU:N	2.30	0.64
1:B:122:ASN:OD1	1:B:122:ASN:N	2.30	0.64
1:A:26:ARG:HA	1:A:74:ALA:CA	2.26	0.63
1:A:253:GLU:C	1:A:253:GLU:CD	2.65	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: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:B:127:TRP:CZ2	1:B:207:LYS:C	2.76	0.63
1:A:53:ARG:CG	1:A:60:LYS:O	2.47	0.63
1:B:26:ARG:NH1	1:B:26:ARG:HG2	2.14	0.63
1:B:172:LEU:N	1:B:220:LYS:HE2	2.13	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: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:A:114:THR:O	1:A:134:GLY:C	2.42	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
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:131:PRO:C	1:B:138:ARG:HH21	2.07	0.62
1:B:163:ILE:CG1	1:B:236:HIS:NE2	2.62	0.62
1:A:187:ASP:O	1:A:190:ASN:O	2.16	0.62
1:A:214:LEU:HD11	5:A:1375:6LX:HAQ	1.82	0.62
1:A:225:ALA:O	1:A:231:TYR:HD2	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HD12	1:B:245:MET:HE1	1.81	0.62
1:A:139:THR:HG21	1:A:263:LEU:HD21	1.80	0.62
1:A:249:THR:CB	1:A:252:GLY:H	2.07	0.62
1:B:95:MET:HB3	1:B:97:TYR:HD1	1.64	0.62
1:B:117:GLY:HA2	1:B:134:GLY:N	2.15	0.62
1:A:28:PHE:CD2	1:A:32:GLU:HB2	2.33	0.62
1:A:225:ALA:C	1:A:231:TYR:CD2	2.64	0.62
1:A:274:ARG:O	1:A:277:ALA:HB2	1.98	0.62
1:B:164:TYR:HH	1:B:230:ALA:HB3	1.64	0.62
1:B:170:ASP:OD2	1:B:199:LEU:HA	1.98	0.62
1:A:49:GLU:OE1	1:A:67:THR:N	2.32	0.62
1:A:144:PHE:CD2	1:A:207:LYS:HB2	2.34	0.62
1:B:105:GLY:CA	1:B:109:THR:HB	2.23	0.62
1:A:25:CYS:CB	1:A:43:CYS:HB3	2.29	0.62
1:A:43:CYS:HB3	4:A:1376:CL:CL	2.36	0.62
1:A:285:ALA:C	1:A:289:ASN:ND2	2.50	0.62
1:B:221:ARG:HB2	1:B:231:TYR:OH	2.00	0.62
1:B:311:TYR:HD1	1:B:317:THR:C	2.08	0.62
1:A:170:ASP:O	1:A:220:LYS:NZ	2.32	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:OD1	1:B:287:ASN:N	2.30	0.62
1:A:225:ALA:C	1:A:228:MET:HG3	2.21	0.62
1:A:253:GLU:OE2	1:A:254:GLU:N	2.32	0.62
1:A:265:ASP:OD1	1:A:265:ASP:N	2.32	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:17:LYS:O	1:B:19:ILE:N	2.33	0.61
1:B:118:GLU:HB3	1:B:132:LEU:HD13	0.63	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: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:294:THR:O	1:B:298:VAL:N	2.19	0.61
1:B:126:THR:HG22	1:B:129:GLU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:78:GLN:NE2	1:A:132:LEU:C	2.58	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:B:40:ILE:O	1:B:53:ARG:N	2.34	0.61
1:B:43:CYS:HG	3:B:1367:CD:CD	1.33	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:41:VAL:HG12	1:B:52:VAL:CG2	2.31	0.61
1:B:110:GLY:H	2:B:601:ADP:PB	2.23	0.61
1:A:91:ASP:HA	1:A:94:ILE:CG2	2.31	0.61
1:B:118:GLU:C	1:B:132:LEU:CD1	2.74	0.61
1:B:106:GLN:HA	1:B:270:GLU:OE1	2.01	0.60
1:B:249:THR:C	1:B:252:GLY:N	2.59	0.60
1:A:28:PHE:HE2	1:A:32:GLU:HB2	1.56	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:41:VAL:CG1	1:A:52:VAL:HG23	2.30	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: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:110:GLY:HA2	2:B:601:ADP:O2A	2.01	0.60
1:B:164:TYR:CE1	1:B:234:ARG:NE	2.66	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:B:300:THR:HG22	1:B:356:ALA:C	2.25	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:A:284:GLU:C	1:A:289:ASN:CG	2.62	0.60
1:B:128:GLU:HG2	1:B:208:ASP:OD1	2.01	0.60
1:A:47:ARG:C	1:A:48:LYS:CG	2.65	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:261:LEU:CD1	1:B:261:LEU:C	2.74	0.60
1:B:342:ASN:HA	1:B:345:GLU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:HG23	1:B:129:GLU:H	1.67	0.60
1:A:86:VAL:N	1:A:88:PRO:HD2	2.17	0.59
1:A:106:GLN:N	1:A:269:SER:OG	2.34	0.59
1:A:263:LEU:HD13	1:A:263:LEU:N	2.16	0.59
1:A:284:GLU:O	1:A:289:ASN:HB3	2.01	0.59
1:A:177:ASP:OD1	1:A:177:ASP:C	2.45	0.59
1:B:117:GLY:HA3	1:B:133:ALA:HA	1.84	0.59
1:A:160:LEU:CD1	1:A:160:LEU:C	2.75	0.59
1:B:28:PHE:CZ	1:B:339:ALA:HA	2.36	0.59
1:B:83:ARG:O	1:B:88:PRO:HD3	2.02	0.59
1:B:341:LEU:O	1:B:345:GLU:OE1	2.21	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
2:A:601:ADP:O2'	6:A:2029:HOH:O	2.02	0.59
1:B:77:LYS:N	1:B:80:ASP:OD2	2.30	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:183:GLN:O	1:B:197:LYS:N	2.29	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:B:128:GLU:OE1	1:B:128:GLU:N	2.30	0.59
1:B:22:VAL:HG22	1:B:332:ILE:C	2.28	0.59
1:B:221:ARG:CA	1:B:231:TYR:OH	2.51	0.59
1:B:227:LEU:C	1:B:228:MET:SD	2.86	0.59
1:A:67:THR:C	1:A:68:PHE:CD1	2.80	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:24:ARG:HG2	1:B:335:THR:HG22	1.84	0.59
1:B:93:VAL:CG2	1:B:261:LEU:CD2	2.68	0.59
1:B:113:PHE:CD2	1:B:118:GLU:HB2	2.38	0.59
1:B:295:LEU:O	1:B:299:ILE:HB	2.03	0.59
1:B:100:THR:CG2	1:B:262:ASN:CG	2.75	0.58
1:A:28:PHE:CE2	1:A:339:ALA:HB1	2.26	0.58
1:A:37:ALA:HB1	1:A:341:LEU:H	1.68	0.58
1:A:264:VAL:CG2	1:A:265:ASP:N	2.66	0.58
1:B:136:ILE:N	1:B:137:PRO:CD	2.66	0.58
1:A:29:ASN:OD1	1:A:29:ASN:N	2.33	0.58
1:A:134:GLY:C	1:A:137:PRO:HD2	2.28	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:B:143:ILE:C	1:B:147:LEU:HD22	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD2	1:A:347:LEU:H	2.17	0.58
1:B:227:LEU:CB	1:B:228:MET:C	2.75	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:67:THR:CG2	1:A:359:ILE:HG21	2.33	0.58
1:A:104:TYR:CE2	1:A:269:SER:HB3	2.39	0.58
1:A:156:VAL:O	1:A:203:THR:HB	2.03	0.58
1:A:323:SER:O	1:A:328:THR:HB	2.03	0.58
1:B:82:TYR:O	1:B:86:VAL:N	2.34	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:116:GLU:C	5:B:1375:6LX:HBB1	2.28	0.58
1:B:227:LEU:HD23	1:B:229:ASN:HA	1.85	0.58
1:B:274:ARG:HH11	1:B:274:ARG:CG	1.98	0.58
1:A:165:ASN:N	1:A:165:ASN:ND2	2.50	0.58
1:B:192:ARG:CD	1:B:322:ASP:OD1	2.51	0.58
1:A:32:GLU:OE2	1:A:37:ALA:CB	2.52	0.57
1:A:93:VAL:HG23	1:A:99:CYS:HG	1.69	0.57
1:A:162:GLU:HG2	1:A:231:TYR:HE1	1.69	0.57
1:A:213:ILE:O	1:A:216:LYS:CD	2.52	0.57
1:A:281:ARG:CA	1:A:284:GLU:OE2	2.52	0.57
1:B:29:ASN:OD1	1:B:31:ALA:N	2.37	0.57
1:A:109:THR:CB	1:A:335:THR:HB	2.32	0.57
1:A:323:SER:OG	1:A:324:LEU:HD23	2.04	0.57
1:B:261:LEU:HD13	1:B:261:LEU:C	2.30	0.57
1:A:39:SER:HB3	1:A:339:ALA:HA	1.85	0.57
1:A:239:PHE:CD1	1:A:239:PHE:C	2.82	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:B:82:TYR:HD1	1:B:82:TYR:C	2.12	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:A:133:ALA:CB	5:A:1375:6LX:CAZ	2.69	0.57
1:A:184:MET:SD	1:A:184:MET:C	2.87	0.57
1:B:246:LYS:HA	1:B:255:LEU:O	2.04	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:THR:HG21	1:B:360:LEU:O	2.05	0.57
1:A:29:ASN:O	1:A:32:GLU:HB3	2.04	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:133:ALA:CA	5:A:1375:6LX:HAZ3	2.34	0.57
1:A:271:ASN:OD1	1:A:283:ARG:O	2.22	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
1:B:270:GLU:CD	1:B:270:GLU:H	2.13	0.57
5:A:1375:6LX:HAU1	5:A:1375:6LX:OAH	2.03	0.57
1:B:108:GLY:HA2	2:B:601:ADP:H5'1	1.87	0.57
1:B:211:TYR:CZ	1:B:215:GLU:CD	2.79	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:32:GLU:OE2	1:B:339:ALA:CB	2.53	0.57
1:B:82:TYR:CD1	1:B:82:TYR:C	2.83	0.57
1:B:171:LEU:HD22	1:B:220:LYS:CG	2.31	0.57
1:B:183:GLN:NE2	1:B:185:PHE:HZ	2.02	0.57
1:A:105:GLY:C	1:A:268:GLY:HA2	2.26	0.57
1:B:106:GLN:HA	1:B:270:GLU:CD	2.30	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:24:ARG:NE	2:B:601:ADP:HN62	2.02	0.56
1:B:48:LYS:HD2	1:B:362:LYS:NZ	2.19	0.56
1:B:353:ALA:O	1:B:357:LYS:C	2.48	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:28:PHE:CD1	1:A:339:ALA:CB	2.51	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:B:80:ASP:N	1:B:80:ASP:OD1	2.33	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:261:LEU:CD1	1:B:262:ASN:N	2.66	0.56
1:A:26:ARG:NH2	1:A:27:PRO:O	2.38	0.56
1:A:86:VAL:C	1:A:88:PRO:N	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HG3	1:A:203:THR:HG22	1.86	0.56
1:A:214:LEU:HD11	5:A:1375:6LX:CAQ	2.34	0.56
1:A:270:GLU:HA	1:A:345:GLU:HA	1.87	0.56
1:A:342:ASN:OD1	1:A:342:ASN:N	2.38	0.56
1:A:205:HIS:ND1	1:A:205:HIS:N	2.39	0.56
1:A:218:ALA:CB	5:A:1375:6LX:CAE	2.80	0.56
1:B:93:VAL:O	1:B:96:GLY:N	2.38	0.56
1:B:115:MET:O	1:B:136:ILE:HD12	2.05	0.56
1:A:20:GLN:O	1:A:332:ILE:HD12	2.06	0.56
1:A:86:VAL:CA	1:A:88:PRO:HD2	2.36	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:B:192:ARG:CG	1:B:192:ARG:NH1	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:212:GLN:C	1:B:216:LYS:HG3	2.26	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:51:SER:CB	1:A:64:LYS:O	2.54	0.55
1:A:271:ASN:ND2	1:A:284:GLU:HA	2.21	0.55
1:B:163:ILE:CG2	1:B:236:HIS:HD2	2.18	0.55
1:A:82:TYR:HE2	1:A:139:THR:N	2.04	0.55
1:A:175:SER:C	1:A:177:ASP:H	2.15	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: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:167:GLU:CD	1:A:181:ARG:CB	2.80	0.55
1:A:168:LEU:C	1:A:169:PHE:CD1	2.85	0.55
1:A:234:ARG:NH1	1:A:288:ILE:HB	2.19	0.55
1:B:66:TYR:CE2	1:B:350:LEU:HB3	2.41	0.55
1:B:316:LEU:O	1:B:320:LEU:N	2.39	0.55
1:A:98:ASN:CB	1:A:323:SER:HA	2.36	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:B:96:GLY:O	1:B:259:GLY:HA2	2.06	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:A:163:ILE:CG2	1:A:163:ILE:O	2.53	0.55
1:B:304:GLU:CD	1:B:304:GLU:N	2.58	0.55
1:A:156:VAL:O	1:A:203:THR:C	2.50	0.55
1:B:89:ILE:HG21	1:B:101:ILE:HD11	1.88	0.55
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:A:73:GLY:CA	1:A:76:THR:HG22	2.37	0.55
1:A:149:ASP:OD1	1:A:149:ASP:N	2.40	0.55
1:B:77:LYS:HE2	1:B:77:LYS:N	2.22	0.55
1:B:352:TYR:O	1:B:356:ALA:CA	2.55	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:41:VAL:HG23	1:A:338:PRO:CA	2.35	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:B:41:VAL:CG1	1:B:52:VAL:HG23	2.14	0.55
1:B:41:VAL:CG2	1:B:338:PRO:HA	2.37	0.54
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:A:117:GLY:HA3	1:A:137:PRO:HG3	1.89	0.54
1:B:62:SER:O	1:B:63:ARG:CB	2.55	0.54
1:B:234:ARG:O	1:B:267:ALA:CB	2.56	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:32:GLU:OE2	1:A:37:ALA:C	2.49	0.54
1:A:120:SER:OG	1:A:130:ASP:CG	2.50	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:B:53:ARG:O	1:B:54:THR:HB	2.07	0.54
1:B:100:THR:HA	1:B:262:ASN:CG	2.32	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:301:ALA:C	1:B:306:THR:HG23	2.30	0.54
1:B:47:ARG:O	1:B:48:LYS:HG3	2.06	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: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:A:133:ALA:N	5:A:1375:6LX:HAZ3	2.23	0.54
1:A:162:GLU:HG2	1:A:231:TYR:CE1	2.42	0.54
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:239:PHE:CB	1:B:263:LEU:HD12	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:262:ASN:C	1:A:263:LEU:CD1	2.78	0.54
1:B:26:ARG:HD2	2:B:601:ADP:N9	2.23	0.54
1:B:73:GLY:C	1:B:75:SER:N	2.55	0.54
1:B:163:ILE:HG12	1:B:168:LEU:HB3	1.91	0.54
1:B:304:GLU:HB2	1:B:306:THR:CG2	2.27	0.54
1:A:72:PHE:CZ	1:A:76:THR:OG1	2.61	0.53
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:B:35:ALA:O	1:B:36:SER:C	2.49	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:B:221:ARG:O	1:B:225:ALA:N	2.41	0.53
1:A:22:VAL:HB	1:A:333:ILE:HG13	1.91	0.53
1:A:144:PHE:CZ	1:A:207:LYS:CB	2.91	0.53
1:A:299:ILE:CG2	1:A:300:THR:N	2.71	0.53
1:B:78:GLN:HG3	1:B:132:LEU:O	2.08	0.53
1:A:19:ILE:C	1:A:20:GLN:HE21	2.11	0.53
1:A:118:GLU:OE1	1:A:132:LEU:HD13	2.06	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:66:TYR:CD2	1:A:68:PHE:CZ	2.97	0.53
1:A:160:LEU:HD22	1:A:239:PHE:CA	2.39	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: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:HD13	1:B:195:ILE:O	2.03	0.53
1:B:226:THR:O	1:B:228:MET:HB2	2.09	0.53
1:A:119:ARG:HB2	5:A:1375:6LX:CAW	2.38	0.53
1:A:143:ILE:HD13	1:A:243:ILE:HD13	1.90	0.53
1:A:144:PHE:CZ	1:A:207:LYS:HB3	2.42	0.53
1:A:169:PHE:CE1	1:A:181:ARG:HA	2.44	0.53
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.91	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:A:91:ASP:HA	1:A:94:ILE:HG22	1.90	0.53
1:A:94:ILE:O	1:A:245:MET:CE	2.57	0.53
1:A:242:THR:HG21	1:A:260:LYS:HE2	1.91	0.53
1:B:41:VAL:HG12	1:B:52:VAL:CB	2.39	0.53
1:B:231:TYR:CD1	1:B:231:TYR:C	2.87	0.53
1:B:333:ILE:O	1:B:333:ILE:HG12	2.08	0.53
1:B:342:ASN:ND2	1:B:342:ASN:H	2.06	0.53
1:A:50:VAL:HG12	1:A:71:VAL:HG11	1.91	0.53
1:A:66:TYR:HE1	1:A:354:HIS:HB2	1.68	0.53
1:A:236:HIS:O	1:A:265:ASP:C	2.50	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:B:20:GLN:O	1:B:332:ILE:N	2.38	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:323:SER:OG	1:A:324:LEU:CD2	2.57	0.52
1:B:98:ASN:OD1	1:B:323:SER:CB	2.57	0.52
1:B:183:GLN:NE2	1:B:185:PHE:CZ	2.78	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:HE	1:A:234:ARG:CA	2.23	0.52
1:B:25:CYS:SG	1:B:25:CYS:O	2.67	0.52
1:A:109:THR:OG1	1:A:335:THR:CB	2.40	0.52
1:B:30:LEU:HD13	1:B:30:LEU:C	2.35	0.52
1:B:66:TYR:CE2	1:B:350:LEU:HG	2.44	0.52
1:B:106:GLN:O	1:B:109:THR:N	2.43	0.52
1:B:236:HIS:ND1	1:B:236:HIS:C	2.67	0.52
1:A:113:PHE:O	1:A:117:GLY:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TYR:CE1	1:A:292:LEU:HD13	2.45	0.52
1:B:23:VAL:HG13	1:B:23:VAL:O	2.09	0.52
1:B:161:LEU:CD2	1:B:162:GLU:H	2.09	0.52
1:A:184:MET:SD	1:A:185:PHE:N	2.83	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:53:ARG:C	1:B:54:THR:CG2	2.74	0.52
1:B:265:ASP:CA	1:B:266:LEU:HD23	2.38	0.52
1:B:82:TYR:OH	1:B:86:VAL:CG1	2.57	0.52
1:A:154:PHE:N	1:A:154:PHE:CD1	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:172:LEU:H	1:B:220:LYS:HE2	1.71	0.52
1:B:204:VAL:O	1:B:204:VAL:CG2	2.58	0.52
1:A:213:ILE:O	1:A:216:LYS:CG	2.57	0.51
1:A:347:LEU:HD23	1:A:347:LEU:H	1.74	0.51
1:B:32:GLU:OE2	1:B:339:ALA:HB3	2.09	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:A:268:GLY:O	1:A:270:GLU:OE1	2.27	0.51
1:B:127:TRP:CE2	1:B:208:ASP:OD1	2.64	0.51
1:B:134:GLY:N	1:B:137:PRO:HG3	2.24	0.51
1:A:23:VAL:HA	1:A:334:ALA:O	2.11	0.51
1:A:73:GLY:C	1:A:76:THR:CG2	2.83	0.51
1:A:106:GLN:HA	1:A:268:GLY:HA3	1.92	0.51
1:A:148:THR:HG22	1:A:149:ASP:N	2.24	0.51
1:A:167:GLU:CD	1:A:181:ARG:HG3	2.35	0.51
5:A:1375:6LX:CAO	5:A:1375:6LX:CBI	2.89	0.51
1:B:211:TYR:OH	1:B:215:GLU:OE2	2.23	0.51
1:A:42:GLU:C	4:A:1378:CL:CL	2.91	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:229:ASN:ND2	1:A:229:ASN:C	2.69	0.51
1:A:234:ARG:O	1:A:234:ARG:CZ	2.58	0.51
1:A:274:ARG:HG3	1:A:351:GLU:HG2	1.91	0.51
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:B:82:TYR:HH	1:B:90:LEU:HD22	1.72	0.51
1:B:329:ARG:NH1	1:B:329:ARG:HB3	2.20	0.51
1:A:73:GLY:O	1:A:76:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:CG	1:A:207:LYS:HB3	2.44	0.51
1:A:165:ASN:N	1:A:165:ASN:HD22	2.07	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:B:211:TYR:CD1	1:B:211:TYR:C	2.88	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
1:B:195:ILE:HD13	1:B:196:ILE:C	2.36	0.51
2:B:601:ADP:H8	2:B:601:ADP:O5'	1.93	0.51
1:A:35:ALA:HB1	1:A:341:LEU:CD1	2.41	0.51
1:A:160:LEU:HD12	1:A:161:LEU:N	2.25	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:283:ARG:HH21	1:A:344:GLU:CD	2.19	0.51
1:B:207:LYS:HG2	1:B:208:ASP:N	2.23	0.51
1:B:254:GLU:C	1:B:255:LEU:HD13	2.35	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:B:354:HIS:C	1:B:357:LYS:O	2.54	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:B:134:GLY:C	1:B:137:PRO:CD	2.72	0.50
1:A:40:ILE:H	1:A:40:ILE:HD12	1.75	0.50
1:A:111:LYS:O	1:A:115:MET:N	2.33	0.50
1:B:147:LEU:HD22	1:B:147:LEU:H	1.76	0.50
1:A:105:GLY:O	1:A:111:LYS:NZ	2.44	0.50
1:A:113:PHE:O	1:A:117:GLY:C	2.55	0.50
1:A:135:ILE:O	1:A:139:THR:CA	2.60	0.50
1:B:93:VAL:C	1:B:96:GLY:H	2.19	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:26:ARG:HA	1:A:74:ALA:CB	2.42	0.50
1:A:42:GLU:C	4:A:1376:CL:CL	2.92	0.50
1:A:209:GLU:CD	1:A:213:ILE:CD1	2.84	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:89:ILE:CD1	1:A:99:CYS:HB3	2.41	0.50
1:A:148:THR:CG2	1:A:149:ASP:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:106:GLN:CA	1:A:268:GLY:CA	2.90	0.50
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: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:32:GLU:O	1:A:32:GLU:OE1	2.30	0.50
1:A:91:ASP:CA	1:A:94:ILE:HG22	2.41	0.50
1:A:97:TYR:CD1	1:A:97:TYR:N	2.80	0.50
1:A:234:ARG:HE	1:A:234:ARG:C	2.19	0.50
1:A:284:GLU:OE1	1:A:293:LEU:HD11	2.12	0.50
1:B:164:TYR:O	1:B:167:GLU:HG2	2.12	0.50
1:B:195:ILE:CD1	1:B:196:ILE:C	2.84	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:35:ALA:O	1:A:36:SER:CB	2.59	0.49
1:A:164:TYR:CZ	1:A:228:MET:SD	3.05	0.49
1:A:170:ASP:OD1	1:A:170:ASP:O	2.30	0.49
1:A:197:LYS:HZ1	1:B:250:ILE:HG13	1.77	0.49
1:B:183:GLN:HE22	1:B:185:PHE:HZ	1.60	0.49
1:B:256:VAL:C	1:B:257:LYS:HD2	2.37	0.49
1:A:41:VAL:CG2	1:A:338:PRO:C	2.86	0.49
1:A:117:GLY:CA	5:A:1375:6LX:CAN	2.81	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:A:44:ASP:CG	1:A:47:ARG:HB3	2.38	0.49
1:A:162:GLU:CG	1:A:231:TYR:HE1	2.26	0.49
1:A:204:VAL:HG12	1:A:206:ASN:O	2.12	0.49
1:A:126:THR:O	1:A:129:GLU:CB	2.60	0.49
1:A:264:VAL:C	1:A:265:ASP:OD1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LYS:O	1:B:241:VAL:HA	2.12	0.49
1:B:214:LEU:CB	5:B:1375:6LX:HAA2	2.43	0.49
1:A:28:PHE:CE2	1:A:32:GLU:CD	2.83	0.49
1:A:126:THR:O	1:A:130:ASP:N	2.43	0.49
1:B:239:PHE:CD1	1:B:239:PHE:C	2.91	0.49
1:B:293:LEU:O	1:B:352:TYR:OH	2.31	0.49
1:A:88:PRO:C	1:A:91:ASP:OD1	2.46	0.49
1:A:109:THR:CG2	1:A:335:THR:OG1	2.57	0.49
1:A:192:ARG:HH22	1:A:325:GLY:HA3	1.77	0.49
1:B:82:TYR:OH	1:B:139:THR:HG23	2.13	0.49
1:B:120:SER:HB3	1:B:125:TYR:HB2	1.93	0.49
1:B:354:HIS:O	1:B:357:LYS:O	2.31	0.49
1:A:32:GLU:CD	1:A:32:GLU:C	2.81	0.49
1:A:72:PHE:CZ	1:A:81:VAL:CA	2.96	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:B:48:LYS:C	1:B:71:VAL:CG2	2.84	0.49
1:B:78:GLN:CD	1:B:132:LEU:O	2.56	0.49
1:B:264:VAL:CG1	1:B:266:LEU:HD22	2.38	0.49
1:A:28:PHE:HE2	1:A:32:GLU:OE1	1.96	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:40:ILE:CD1	1:B:338:PRO:O	2.61	0.48
1:B:227:LEU:CA	1:B:229:ASN:N	2.66	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:A:27:PRO:CD	1:A:74:ALA:CB	2.65	0.48
1:A:144:PHE:CE2	1:A:207:LYS:CB	2.96	0.48
1:A:245:MET:CE	1:A:257:LYS:HG3	2.39	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: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:304:GLU:O	1:A:305:ARG:HB2	2.14	0.48
1:B:47:ARG:NH2	1:B:363:PRO:O	2.29	0.48
1:B:311:TYR:C	1:B:317:THR:HG1	2.11	0.48
1:B:342:ASN:ND2	1:B:342:ASN:N	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:H	1:A:172:LEU:CD2	2.27	0.48
1:A:351:GLU:CD	1:A:351:GLU:N	2.72	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:94:ILE:O	1:A:245:MET:HE1	2.13	0.48
1:A:104:TYR:CE2	1:A:352:TYR:CD2	3.01	0.48
1:A:131:PRO:C	1:A:138:ARG:HH21	2.21	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:231:TYR:C	1:A:232:SER:OG	2.54	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
1:B:343:LEU:N	1:B:346:THR:HG22	2.28	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:O	1:B:204:VAL:HG23	2.12	0.48
1:A:227:LEU:CA	1:A:228:MET:C	2.87	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:18:ASN:O	1:B:20:GLN:CD	2.57	0.48
1:B:157:LYS:CE	1:B:242:THR:HB	2.27	0.48
1:B:361:ASN:N	1:B:361:ASN:OD1	2.46	0.48
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:22:VAL:HG22	1:B:333:ILE:HG22	1.75	0.47
1:B:100:THR:HG23	1:B:262:ASN:CG	2.29	0.47
1:B:227:LEU:CA	1:B:228:MET:HB2	2.41	0.47
1:B:353:ALA:O	1:B:357:LYS:HG3	2.14	0.47
1:A:168:LEU:C	1:A:169:PHE:HD1	2.21	0.47
1:A:295:LEU:O	1:A:299:ILE:HB	2.14	0.47
1:B:82:TYR:CD1	1:B:82:TYR:O	2.62	0.47
1:B:171:LEU:HA	1:B:177:ASP:OD2	2.13	0.47
1:A:30:LEU:CD1	1:A:31:ALA:N	2.77	0.47
1:A:135:ILE:CG2	1:A:139:THR:OG1	2.63	0.47
1:A:294:THR:C	1:A:298:VAL:HG23	2.21	0.47
5:A:1375:6LX:HAC2	5:A:1375:6LX:CAW	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:A:129:GLU:N	2.48	0.47
1:A:242:THR:CG2	1:A:260:LYS:HE2	2.45	0.47
1:A:271:ASN:ND2	1:A:271:ASN:C	2.72	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:O	1:A:202:ILE:HG12	2.13	0.47
1:A:283:ARG:NH2	1:A:344:GLU:OE2	2.48	0.47
1:B:79:ILE:CD1	1:B:83:ARG:HH21	2.20	0.47
1:A:85:VAL:O	1:A:88:PRO:HG2	2.14	0.47
1:A:102:PHE:CD1	1:A:102:PHE:C	2.93	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:197:LYS:HE2	1:A:197:LYS:HB2	1.51	0.47
1:A:226:THR:C	1:A:229:ASN:N	2.72	0.47
1:A:283:ARG:HD2	1:A:283:ARG:HA	1.64	0.47
1:A:290:GLN:HE21	1:A:290:GLN:HB3	1.54	0.47
1:B:121:PRO:CB	1:B:122:ASN:OD1	2.63	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:H	1:B:250:ILE:CD1	2.08	0.47
1:B:250:ILE:O	6:B:2017:HOH:O	2.21	0.47
1:A:37:ALA:HB2	1:A:341:LEU:HB2	1.97	0.47
1:A:263:LEU:N	1:A:263:LEU:CD1	2.76	0.47
1:B:30:LEU:HA	1:B:33:ARG:HB3	1.97	0.47
1:B:227:LEU:CD2	1:B:229:ASN:HA	2.45	0.47
1:B:249:THR:C	1:B:252:GLY:CA	2.79	0.47
1:B:299:ILE:CG2	1:B:300:THR:N	2.77	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:83:ARG:HA	1:A:87:CYS:CB	2.31	0.46
1:A:236:HIS:ND1	1:A:236:HIS:N	2.63	0.46
1:B:30:LEU:O	1:B:34:LYS:N	2.45	0.46
1:B:113:PHE:HB2	2:B:601:ADP:C8	2.50	0.46
1:B:221:ARG:O	1:B:231:TYR:CE1	2.67	0.46
1:A:70:MET:SD	1:A:70:MET:N	2.80	0.46
5:A:1375:6LX:CAN	5:A:1375:6LX:CBF	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TYR:CZ	1:B:349:THR:HB	2.47	0.46
1:B:118:GLU:H	1:B:132:LEU:C	2.23	0.46
1:B:127:TRP:HZ2	1:B:208:ASP:OD1	1.94	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:HA	1:B:295:LEU:HD13	1.78	0.46
1:B:308:HIS:ND1	1:B:309:VAL:N	2.63	0.46
1:A:66:TYR:OH	1:A:354:HIS:CA	2.63	0.46
1:A:109:THR:HG21	1:A:335:THR:HG1	1.78	0.46
1:A:118:GLU:CD	1:A:132:LEU:HD13	2.39	0.46
1:A:284:GLU:CB	1:A:293:LEU:HD21	2.43	0.46
1:B:166:GLU:OE2	1:B:287:ASN:O	2.34	0.46
1:B:169:PHE:CD1	1:B:169:PHE:N	2.84	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: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:B:173:ASN:C	1:B:175:SER:H	2.16	0.46
1:B:194:VAL:O	1:B:194:VAL:HG23	2.15	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:308:HIS:HE1	1:B:87:CYS:HB3	1.79	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:B:90:LEU:HD12	1:B:90:LEU:C	2.40	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: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:B:135:ILE:C	1:B:137:PRO:HD2	2.41	0.46
1:B:170:ASP:OD1	1:B:171:LEU:N	2.49	0.46
1:A:106:GLN:C	1:A:268:GLY:HA2	2.41	0.46
1:B:165:ASN:N	1:B:288:ILE:HG13	2.32	0.46
1:A:41:VAL:HG21	1:A:338:PRO:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:24:ARG:HG3	1:A:72:PHE:HB3	1.98	0.45
1:A:49:GLU:CD	1:A:67:THR:CA	2.77	0.45
1:B:40:ILE:HG12	1:B:343:LEU:CB	2.46	0.45
1:B:112:THR:O	1:B:116:GLU:CA	2.65	0.45
1:B:268:GLY:N	4:B:1377:CL:CL	2.86	0.45
1:A:38:HIS:O	1:A:340:SER:CB	2.65	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:B:87:CYS:CB	1:B:88:PRO:HD3	2.47	0.45
1:A:233:SER:O	1:A:267:ALA:HA	2.17	0.45
1:A:41:VAL:CA	1:A:52:VAL:CG2	2.89	0.45
1:A:175:SER:O	1:A:176:SER:OG	2.30	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:90:LEU:O	1:A:94:ILE:CB	2.63	0.45
1:A:153:GLU:CG	1:A:246:LYS:O	2.63	0.45
1:A:154:PHE:HA	1:A:244:HIS:O	2.15	0.45
1:A:217:GLY:C	1:A:221:ARG:HE	2.25	0.45
1:A:226:THR:HA	1:A:228:MET:HB3	1.90	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: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:B:294:THR:C	1:B:298:VAL:HG23	2.38	0.45
1:A:153:GLU:O	1:A:246:LYS:N	2.34	0.45
1:B:26:ARG:HH11	1:B:26:ARG:CG	2.27	0.45
1:B:28:PHE:CE1	1:B:39:SER:CB	2.97	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: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:163:ILE:O	1:A:163:ILE:HG22	2.16	0.45
1:A:192:ARG:HG2	1:A:321:GLN:NE2	2.32	0.45
1:A:236:HIS:HA	1:A:266:LEU:HA	1.99	0.45
1:A:250:ILE:H	1:A:250:ILE:HG13	1.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:THR:HG21	1:A:314:SER:N	2.31	0.45
1:B:93:VAL:CG2	1:B:261:LEU:HD22	2.32	0.45
1:B:135:ILE:O	1:B:139:THR:N	2.35	0.45
1:B:173:ASN:O	1:B:176:SER:N	2.46	0.45
1:B:173:ASN:HA	1:B:174:PRO:HD2	1.49	0.45
1:A:117:GLY:CA	5:A:1375:6LX:HAO	2.47	0.44
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: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:78:GLN:CG	1:B:132:LEU:O	2.65	0.44
1:B:226:THR:O	1:B:228:MET:CB	2.64	0.44
1:A:154:PHE:N	1:A:154:PHE:HD1	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:B:41:VAL:HA	1:B:52:VAL:CB	2.45	0.44
1:B:128:GLU:O	1:B:141:HIS:CD2	2.70	0.44
1:A:39:SER:HB3	1:A:339:ALA:CA	2.47	0.44
1:A:118:GLU:CD	1:A:132:LEU:CD1	2.87	0.44
1:A:192:ARG:NH2	1:A:325:GLY:HA3	2.31	0.44
1:A:342:ASN:HB3	1:A:345:GLU:OE2	2.18	0.44
1:A:362:LYS:HD2	1:A:362:LYS:HA	1.44	0.44
1:B:110:GLY:N	2:B:601:ADP:PB	2.89	0.44
1:B:187:ASP:OD1	1:B:187:ASP:C	2.61	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: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:O	1:A:238:VAL:CG2	2.62	0.44
1:B:143:ILE:CA	1:B:146:LYS:HG3	2.47	0.44
1:B:158:VAL:O	1:B:158:VAL:HG22	2.17	0.44
1:B:168:LEU:HD11	1:B:184:MET:HE2	2.00	0.44
1:B:320:LEU:HD23	1:B:320:LEU:HA	1.82	0.44
1:B:337:SER:CB	1:B:342:ASN:OD1	2.62	0.44
1:A:234:ARG:NE	1:A:234:ARG:CA	2.80	0.44
1:B:52:VAL:O	1:B:53:ARG:C	2.59	0.44
1:B:207:LYS:O	1:B:210:VAL:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:19:ILE:HG21	1:B:299:ILE:HD11	1.99	0.44
1:B:62:SER:O	1:B:63:ARG:HB2	2.17	0.44
1:B:160:LEU:HD12	1:B:161:LEU:H	1.83	0.44
1:B:296:GLY:N	1:B:352:TYR:OH	2.51	0.44
1:A:82:TYR:CE2	1:A:138:ARG:C	2.96	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:295:LEU:HB3	1:A:352:TYR:OH	2.18	0.43
1:A:315:LYS:HE2	1:A:315:LYS:CA	2.46	0.43
1:B:300:THR:CG2	1:B:356:ALA:CA	2.42	0.43
1:A:226:THR:C	1:A:228:MET:CA	2.73	0.43
1:A:309:VAL:HG21	1:A:311:TYR:CD2	2.26	0.43
1:B:40:ILE:O	1:B:52:VAL:CB	2.61	0.43
1:B:100:THR:HG22	1:B:262:ASN:CG	2.42	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:A:167:GLU:CD	1:A:181:ARG:CG	2.91	0.43
1:A:272:ILE:HD13	1:A:273:GLY:O	2.18	0.43
5:A:1375:6LX:CBI	5:A:1375:6LX:HAB	2.48	0.43
1:B:225:ALA:CA	1:B:231:TYR:HE1	2.30	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:HG12	2.18	0.43
1:B:302:LEU:C	1:B:305:ARG:H	2.26	0.43
1:A:47:ARG:HE	1:A:47:ARG:CA	2.21	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: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:68:PHE:HB2	1:A:71:VAL:HG22	2.00	0.43
1:A:85:VAL:C	1:A:88:PRO:HD2	2.44	0.43
1:A:131:PRO:HA	1:A:138:ARG:HH22	1.82	0.43
1:A:175:SER:C	1:A:177:ASP:N	2.75	0.43
1:A:284:GLU:HG3	1:A:284:GLU:H	1.47	0.43
1:A:293:LEU:HD13	1:A:293:LEU:HA	1.80	0.43
1:B:98:ASN:CB	1:B:323:SER:HA	2.45	0.43
1:B:240:SER:O	1:B:240:SER:OG	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:THR:H	1:B:252:GLY:HA3	1.84	0.43
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: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: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:B:221:ARG:HH21	1:B:232:SER:HA	1.84	0.43
1:A:326:GLY:O	1:A:327:ARG:C	2.61	0.42
1:B:111:LYS:N	2:B:601:ADP:O1B	2.52	0.42
1:B:221:ARG:HA	1:B:231:TYR:OH	2.19	0.42
1:B:234:ARG:HA	4:B:1377:CL:CL	2.56	0.42
1:A:95:MET:HB3	1:A:97:TYR:CE1	2.54	0.42
1:A:157:LYS:HG3	1:A:203:THR:CG2	2.49	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: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
1:A:144:PHE:CZ	1:A:207:LYS:HA	2.54	0.42
1:A:253:GLU:OE2	1:A:253:GLU:O	2.37	0.42
1:A:355:ARG:HG3	1:A:356:ALA:N	2.33	0.42
5:A:1375:6LX:CBF	5:A:1375:6LX:HAB	2.48	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:A:21:VAL:HG21	1:A:357:LYS:CB	2.45	0.42
1:A:285:ALA:N	1:A:289:ASN:ND2	2.64	0.42
1:B:89:ILE:HG22	1:B:90:LEU:N	2.33	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:A:21:VAL:HA	1:A:332:ILE:O	2.19	0.42
1:A:105:GLY:C	1:A:106:GLN:O	2.61	0.42
1:A:117:GLY:HA2	1:A:134:GLY:CA	2.48	0.42
1:A:118:GLU:C	5:A:1375:6LX:CAX	2.92	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
1:A:194:VAL:HG21	1:A:319:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HB3	1:A:352:TYR:HH	1.84	0.42
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:50:VAL:O	1:A:50:VAL:HG22	2.18	0.42
1:A:140:LEU:O	1:A:143:ILE:HG22	2.20	0.42
1:B:59:ASP:HB3	1:B:60:LYS:H	1.58	0.42
1:A:82:TYR:O	1:A:86:VAL:HB	2.20	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: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: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:A:281:ARG:HA	1:A:284:GLU:CD	2.45	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:69:ASP:OD1	1:B:69:ASP:N	2.52	0.42
1:B:101:ILE:HB	1:B:263:LEU:HA	2.02	0.42
1:B:348:SER:O	1:B:351:GLU:HB3	2.20	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:B:274:ARG:O	1:B:275:SER:C	2.62	0.41
1:A:253:GLU:OE2	1:A:254:GLU:C	2.62	0.41
1:B:21:VAL:HA	1:B:332:ILE:HB	2.01	0.41
1:B:133:ALA:HB1	1:B:137:PRO:CB	2.50	0.41
1:A:48:LYS:HB3	1:A:48:LYS:HE3	1.75	0.41
1:A:225:ALA:CA	1:A:231:TYR:HB2	2.50	0.41
1:A:229:ASN:C	1:A:229:ASN:HD22	2.28	0.41
1:A:242:THR:HG23	1:A:260:LYS:CE	2.45	0.41
5:A:1375:6LX:CBF	5:A:1375:6LX:CAB	2.98	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:109:THR:CG2	1:A:335:THR:CB	2.98	0.41
1:A:217:GLY:CA	5:A:1375:6LX:CAP	2.95	0.41
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:A:93:VAL:HA	1:A:97:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:HG22	1:A:116:GLU:HB2	2.02	0.41
1:B:32:GLU:CD	1:B:339:ALA:HB1	2.39	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:49:GLU:OE1	1:A:67:THR:CB	2.65	0.41
1:A:134:GLY:N	1:A:137:PRO:CG	2.83	0.41
1:A:315:LYS:HE2	1:A:315:LYS:HB3	1.89	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:96:GLY:HA2	1:A:258:ILE:C	2.45	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:B:94:ILE:HD12	1:B:245:MET:CE	2.48	0.41
1:B:104:TYR:CZ	1:B:349:THR:HG22	2.55	0.41
1:B:111:LYS:CE	1:B:266:LEU:O	2.69	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:316:LEU:O	1:B:320:LEU:CG	2.69	0.41
1:A:37:ALA:CB	1:A:341:LEU:H	2.34	0.41
1:A:72:PHE:CZ	1:A:80:ASP:HB3	2.56	0.41
1:A:72:PHE:CE1	1:A:81:VAL:HG13	2.56	0.41
1:A:128:GLU:CD	1:A:128:GLU:N	2.74	0.41
1:A:298:VAL:HG12	1:A:311:TYR:CE2	2.55	0.41
1:A:360:LEU:HD13	1:A:360:LEU:HA	1.86	0.41
1:B:19:ILE:HD12	1:B:19:ILE:N	2.29	0.41
1:B:53:ARG:CG	1:B:54:THR:N	2.84	0.41
1:B:177:ASP:N	1:B:220:LYS:NZ	2.66	0.41
1:B:195:ILE:CD1	1:B:195:ILE:O	2.66	0.41
1:B:294:THR:HG22	1:B:298:VAL:CG2	2.51	0.41
1:A:21:VAL:CG2	1:A:357:LYS:CG	2.94	0.41
1:A:22:VAL:O	1:A:333:ILE:HA	2.21	0.41
1:A:82:TYR:C	1:A:82:TYR:HD1	2.26	0.41
1:A:225:ALA:CB	1:A:231:TYR:CG	3.03	0.41
1:A:231:TYR:C	1:A:232:SER:HG	2.27	0.41
1:A:262:ASN:O	1:A:263:LEU:CD1	2.69	0.41
1:B:161:LEU:O	1:B:237:SER:HA	2.21	0.41
1:B:221:ARG:HA	1:B:224:ALA:HB3	2.03	0.41
1:B:317:THR:HA	1:B:320:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TYR:OH	1:A:269:SER:HB3	2.20	0.40
1:A:160:LEU:HD12	1:A:160:LEU:C	2.46	0.40
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:B:98:ASN:CG	1:B:323:SER:HG	2.06	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:343:LEU:C	1:B:346:THR:HG22	2.46	0.40
1:B:353:ALA:HB1	1:B:359:ILE:HD11	2.03	0.40
1:A:66:TYR:HD1	1:A:66:TYR:HA	1.76	0.40
5:A:1375:6LX:HBFB	5:A:1375:6LX:CAM	2.51	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:275:SER:C	1:B:277:ALA:H	2.26	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:139:THR:H	1:B:139:THR:HG1	1.54	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:93:VAL:O	1:B:96:GLY:CA	2.69	0.40
1:B:222:THR:HG22	1:B:223:THR:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASP:C	1:B:344:GLU:OE2[1_545]	1.44	0.76
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:297:ARG:NH2	4:A:1377:CL:CL[2_564]	1.98	0.22
1:B:33:ARG:CZ	1:B:253:GLU:CG[3_565]	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/368 (93%)	325 (95%)	9 (3%)	9 (3%)	4	15
1	B	341/368 (93%)	318 (93%)	12 (4%)	11 (3%)	3	11
All	All	684/736 (93%)	643 (94%)	21 (3%)	20 (3%)	3	13

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 [i](#)

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%)	132 (46%)	158 (54%)	0	0
1	B	287/322 (89%)	151 (53%)	136 (47%)	0	0
All	All	577/644 (90%)	283 (49%)	294 (51%)	0	0

All (294) 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	48	LYS
1	A	50	VAL
1	A	52	VAL
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	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	132	LEU
1	A	139	THR
1	A	141	HIS
1	A	143	ILE
1	A	146	LYS
1	A	148	THR
1	A	149	ASP
1	A	153	GLU
1	A	154	PHE
1	A	155	SER
1	A	156	VAL
1	A	157	LYS
1	A	158	VAL
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	210	VAL
1	A	211	TYR
1	A	213	ILE

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Mol	Chain	Res	Type
1	A	214	LEU
1	A	216	LYS
1	A	221	ARG
1	A	222	THR
1	A	223	THR
1	A	227	LEU
1	A	228	MET
1	A	229	ASN
1	A	231	TYR
1	A	232	SER
1	A	234	ARG
1	A	235	SER
1	A	236	HIS
1	A	238	VAL
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	253	GLU
1	A	254	GLU
1	A	257	LYS
1	A	258	ILE
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

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Mol	Chain	Res	Type
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
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	357	LYS
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	46	VAL
1	B	48	LYS

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Mol	Chain	Res	Type
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	79	ILE
1	B	80	ASP
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	158	VAL
1	B	159	SER
1	B	161	LEU
1	B	162	GLU
1	B	163	ILE

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Mol	Chain	Res	Type
1	B	166	GLU
1	B	168	LEU
1	B	169	PHE
1	B	170	ASP
1	B	171	LEU
1	B	176	SER
1	B	177	ASP
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	202	ILE
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	241	VAL
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	260	LYS
1	B	261	LEU
1	B	262	ASN
1	B	263	LEU
1	B	266	LEU
1	B	269	SER
1	B	270	GLU

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Mol	Chain	Res	Type
1	B	271	ASN
1	B	272	ILE
1	B	274	ARG
1	B	275	SER
1	B	278	VAL
1	B	287	ASN
1	B	292	LEU
1	B	293	LEU
1	B	295	LEU
1	B	297	ARG
1	B	299	ILE
1	B	302	LEU
1	B	304	GLU
1	B	306	THR
1	B	309	VAL
1	B	311	TYR
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

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

Mol	Chain	Res	Type
1	A	38	HIS
1	A	98	ASN
1	A	165	ASN
1	A	229	ASN
1	A	244	HIS
1	A	290	GLN
1	A	358	ASN
1	B	20	GLN
1	B	150	ASN
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 oligosaccharides 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	$\# Z > 2$
2	ADP	B	601	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	6LX	B	1375	-	40,40,40	2.35	15 (37%)	47,56,56	1.62	8 (17%)
5	6LX	A	1375	-	40,40,40	2.64	18 (45%)	47,56,56	1.20	5 (10%)
2	ADP	A	601	-	28,29,29	1.50	6 (21%)	43,45,45	1.87	11 (25%)

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
2	ADP	B	601	-	-	5/16/32/32	0/3/3/3
5	6LX	B	1375	-	-	3/24/28/28	0/4/4/4
5	6LX	A	1375	-	-	8/24/28/28	0/4/4/4
2	ADP	A	601	-	-	3/16/32/32	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1375	6LX	OBA-CAS	7.57	1.39	1.23
5	A	1375	6LX	CAT-CAI	7.30	1.47	1.35
5	B	1375	6LX	OBA-CAS	7.24	1.38	1.23
5	B	1375	6LX	CAT-CAI	6.01	1.45	1.35
5	A	1375	6LX	CAL-NAK	5.98	1.48	1.34
5	B	1375	6LX	CAL-NAK	5.35	1.47	1.34
2	B	601	ADP	C5-C4	4.75	1.47	1.39
2	A	601	ADP	C5-C4	4.46	1.47	1.39
5	B	1375	6LX	OAH-CAI	-3.79	1.30	1.36
5	A	1375	6LX	CAQ-CAR	3.64	1.45	1.39
5	A	1375	6LX	CAJ-CAI	3.31	1.53	1.49
5	A	1375	6LX	CAF-CAG	3.27	1.44	1.38
5	A	1375	6LX	CBI-CBF	3.02	1.44	1.38
2	A	601	ADP	PA-O3A	2.99	1.62	1.59
5	A	1375	6LX	CAF-CAE	2.97	1.43	1.38
5	A	1375	6LX	OAH-CAI	-2.97	1.31	1.36
5	B	1375	6LX	CAQ-CAR	2.94	1.44	1.39
2	A	601	ADP	C5-C6	2.82	1.48	1.41
5	B	1375	6LX	CAZ-CAY	2.82	1.59	1.51
5	A	1375	6LX	CAZ-CAY	2.79	1.59	1.51
5	A	1375	6LX	CAP-CAE	2.76	1.43	1.38
2	B	601	ADP	C5-C6	2.75	1.48	1.41
5	B	1375	6LX	CAF-CAG	2.71	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1375	6LX	CBB-CAT	2.55	1.54	1.51
2	A	601	ADP	C4-N9	-2.53	1.32	1.37
5	B	1375	6LX	CAP-CAE	2.49	1.42	1.38
5	A	1375	6LX	CBK-CBJ	2.45	1.43	1.38
5	A	1375	6LX	CBH-CBG	2.44	1.43	1.38
5	A	1375	6LX	CAB-CAJ	-2.44	1.48	1.54
5	B	1375	6LX	CBK-CBJ	2.39	1.43	1.38
2	B	601	ADP	C8-N7	2.38	1.36	1.31
2	A	601	ADP	C8-N7	2.35	1.36	1.31
5	B	1375	6LX	CBI-CBF	2.35	1.42	1.38
2	B	601	ADP	C5-N7	-2.25	1.35	1.39
5	B	1375	6LX	CAF-CAE	2.24	1.41	1.38
5	B	1375	6LX	CAJ-CAI	2.17	1.52	1.49
5	A	1375	6LX	CAU-NAK	2.12	1.50	1.46
5	A	1375	6LX	CBK-CBH	2.12	1.42	1.38
5	B	1375	6LX	CBH-CBG	2.06	1.43	1.38
5	B	1375	6LX	CAX-CAW	2.02	1.42	1.38
2	A	601	ADP	C5-N7	-2.02	1.35	1.39
5	B	1375	6LX	CAU-NAK	2.01	1.50	1.46
5	A	1375	6LX	CAC-CAB	2.01	1.59	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-5.83	118.69	126.72
2	A	601	ADP	C5-C4-N3	-4.83	120.07	126.72
5	B	1375	6LX	CBG-CBB-CAT	-4.71	105.04	114.24
2	B	601	ADP	N3-C4-N9	4.59	134.97	127.17
2	A	601	ADP	C4-C5-N7	-3.89	106.14	110.58
2	A	601	ADP	N3-C2-N1	-3.75	122.90	128.58
2	B	601	ADP	C2-N3-C4	3.69	120.84	111.83
2	A	601	ADP	N3-C4-N9	3.66	133.40	127.17
2	A	601	ADP	C2-N3-C4	3.62	120.67	111.83
2	B	601	ADP	C4-C5-N7	-3.51	106.56	110.58
5	B	1375	6LX	CAC-CAB-CAJ	3.50	119.73	110.77
2	A	601	ADP	C4-N9-C8	3.43	109.34	105.74
5	A	1375	6LX	CAG-OAH-CAI	3.34	123.76	117.86
5	B	1375	6LX	CBB-CBG-CBF	-3.30	116.04	120.89
2	B	601	ADP	N3-C2-N1	-3.20	123.74	128.58
5	B	1375	6LX	CBC-CAU-NAK	3.10	117.95	113.25
5	A	1375	6LX	CBC-CAU-NAK	2.99	117.79	113.25
2	A	601	ADP	C6-C5-N7	2.85	137.58	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1375	6LX	OAH-CAG-CAF	2.80	119.80	115.83
2	A	601	ADP	C5-N7-C8	2.72	107.73	103.45
5	B	1375	6LX	CAG-OAH-CAI	2.68	122.59	117.86
5	B	1375	6LX	CAU-CBC-CBD	2.62	123.38	113.72
2	B	601	ADP	C4-N9-C8	2.61	108.48	105.74
2	A	601	ADP	N9-C8-N7	-2.59	110.26	113.94
2	B	601	ADP	C5-N7-C8	2.58	107.51	103.45
2	B	601	ADP	C3'-C2'-C1'	2.53	106.25	101.46
5	B	1375	6LX	CBH-CBG-CBF	2.43	121.84	118.23
2	A	601	ADP	C2-N1-C6	2.30	122.50	118.73
5	A	1375	6LX	CAC-CAB-CAJ	2.25	116.53	110.77
5	A	1375	6LX	CBB-CBG-CBF	-2.22	117.62	120.89
5	B	1375	6LX	CAQ-CAR-CAG	2.10	120.97	118.21
2	B	601	ADP	C6-C5-N7	2.10	136.14	132.09
2	A	601	ADP	C4-N9-C1'	-2.04	121.86	126.63

There are no chirality outliers.

All (19) torsion outliers are listed below:

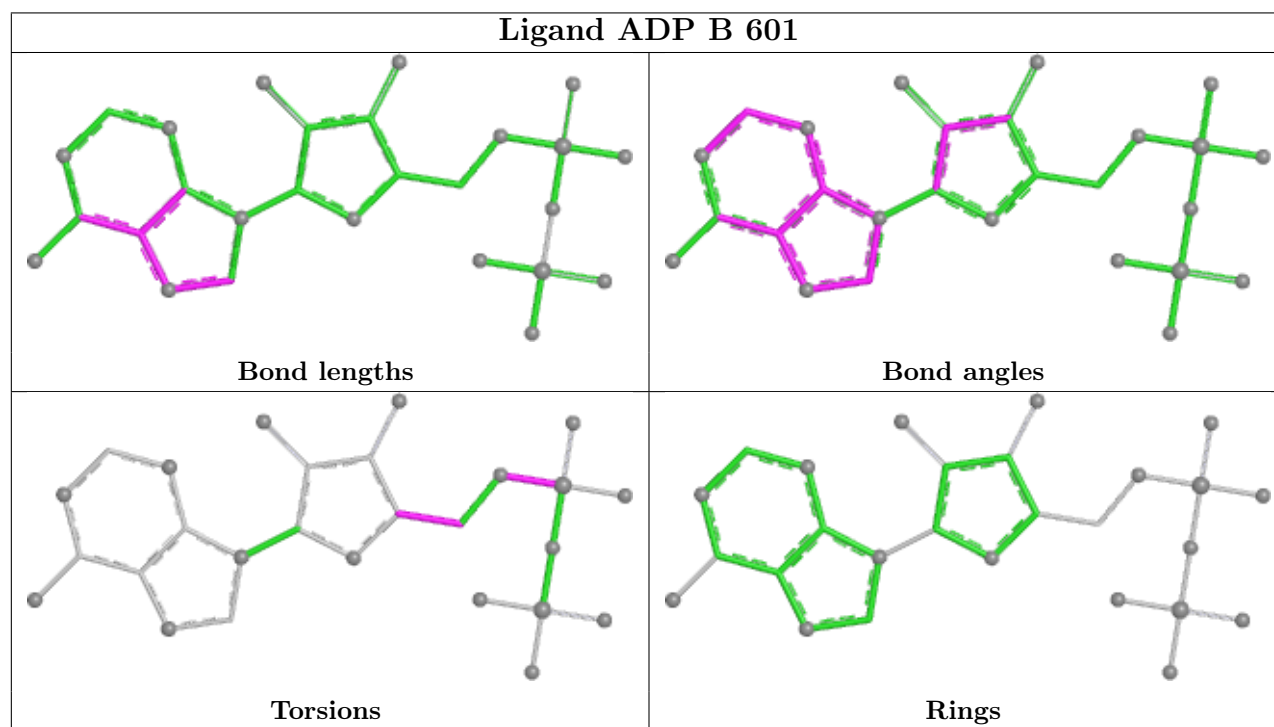
Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
2	B	601	ADP	C5'-O5'-PA-O3A
5	A	1375	6LX	CAI-CAJ-NAK-CAU
5	A	1375	6LX	CAC-CAB-CAJ-CAI
5	A	1375	6LX	CAI-CAT-CBB-CBG
5	A	1375	6LX	CAC-CAB-CAJ-NAK
2	B	601	ADP	O4'-C4'-C5'-O5'
5	A	1375	6LX	CAA-CAB-CAJ-CAI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

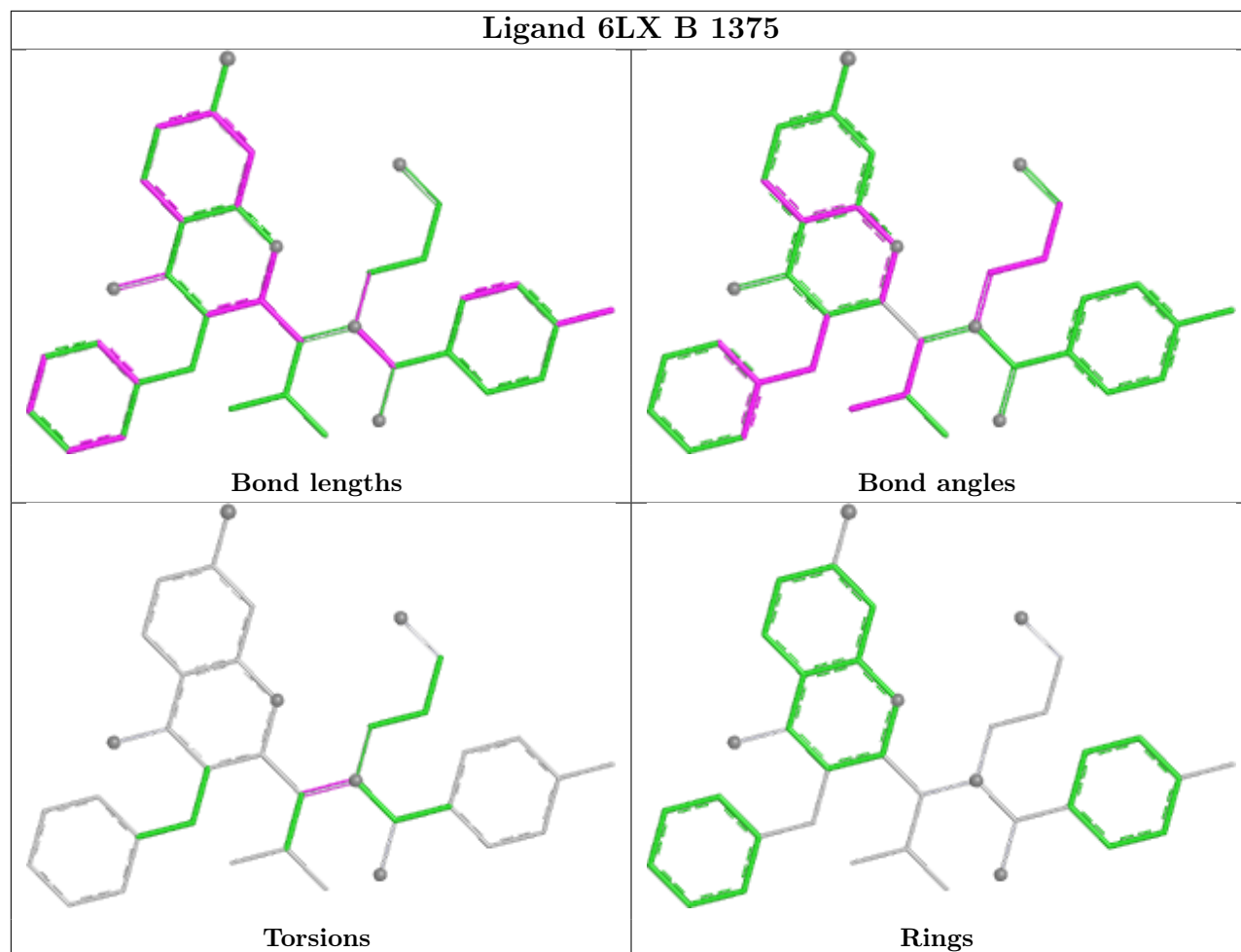
There are no ring outliers.

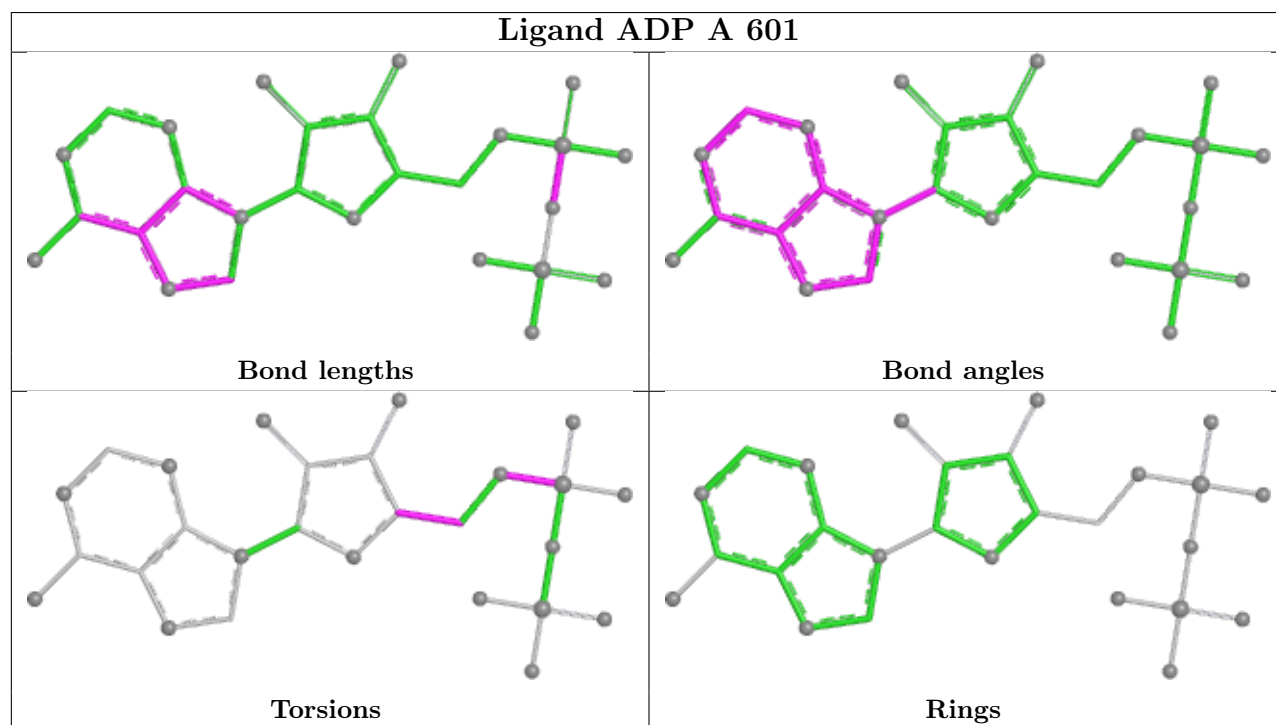
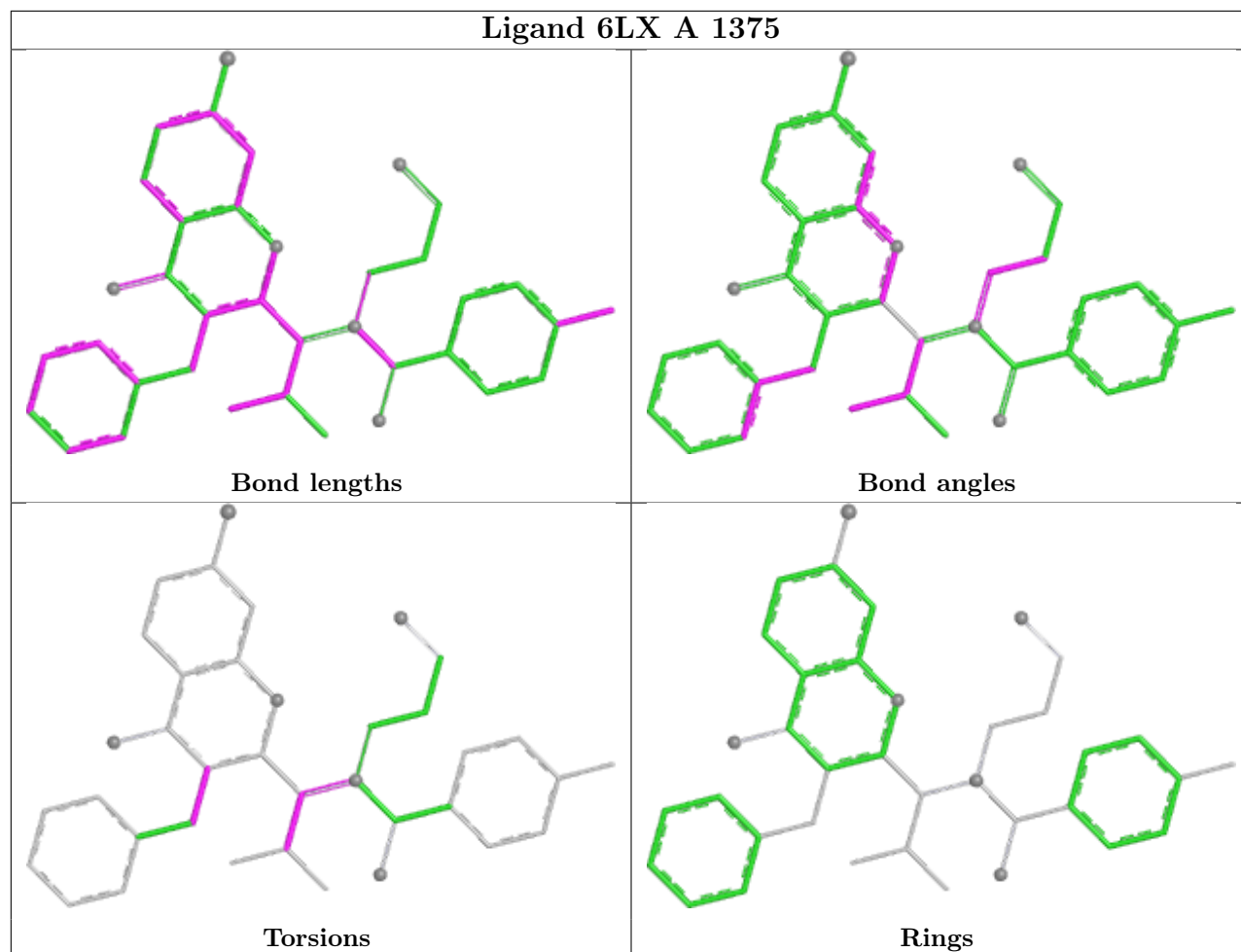
4 monomers are involved in 124 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ADP	21	0
5	B	1375	6LX	9	0
5	A	1375	6LX	91	0
2	A	601	ADP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	347/368 (94%)	-1.48	0 100 100	48, 71, 88, 93	1 (0%)
1	B	345/368 (93%)	-1.47	0 100 100	48, 72, 87, 96	0
All	All	692/736 (94%)	-1.48	0 100 100	48, 72, 88, 96	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	A	1381	1/1	0.95	0.04	80,80,80,80	0
2	ADP	B	601	27/27	0.99	0.03	60,67,69,73	0
3	CD	B	1374	1/1	0.99	0.02	115,115,115,115	0
3	CD	B	1378	1/1	0.99	0.03	106,106,106,106	0
3	CD	B	1379	1/1	0.99	0.03	120,120,120,120	0
2	ADP	A	601	27/27	0.99	0.03	61,66,74,79	0
4	CL	B	1377	1/1	0.99	0.02	67,67,67,67	0

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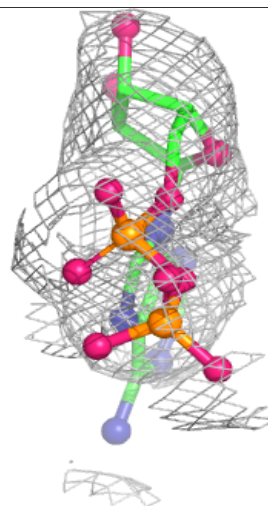
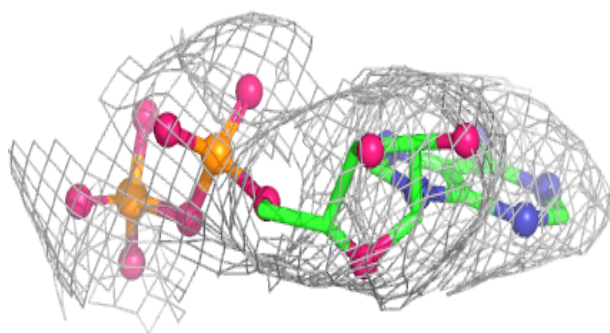
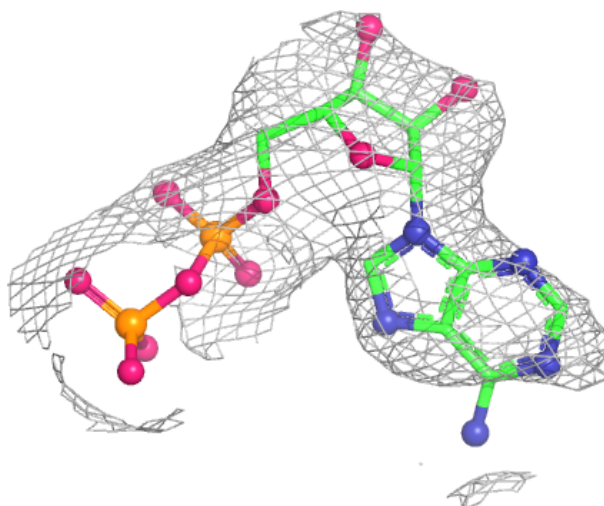
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	1385	1/1	0.99	0.04	83,83,83,83	0
4	CL	B	1386	1/1	0.99	0.02	66,66,66,66	0
5	6LX	A	1375	37/37	0.99	0.04	67,76,80,87	0
5	6LX	B	1375	37/37	0.99	0.04	67,76,80,87	0
3	CD	B	1365	1/1	1.00	0.02	82,82,82,82	0
3	CD	B	1366	1/1	1.00	0.01	90,90,90,90	0
3	CD	B	1367	1/1	1.00	0.02	78,78,78,78	0
3	CD	B	1368	1/1	1.00	0.01	51,51,51,51	0
3	CD	B	1369	1/1	1.00	0.01	80,80,80,80	0
3	CD	B	1370	1/1	1.00	0.01	60,60,60,60	0
3	CD	B	1371	1/1	1.00	0.02	100,100,100,100	0
3	CD	B	1372	1/1	1.00	0.01	115,115,115,115	0
3	CD	B	1373	1/1	1.00	0.01	107,107,107,107	0
3	CD	A	1365	1/1	1.00	0.01	66,66,66,66	0
3	CD	B	1376	1/1	1.00	0.04	30,30,30,30	0
3	CD	A	1366	1/1	1.00	0.02	86,86,86,86	0
3	CD	A	1367	1/1	1.00	0.01	59,59,59,59	0
4	CL	A	1374	1/1	1.00	0.01	54,54,54,54	0
4	CL	A	1376	1/1	1.00	0.02	85,85,85,85	0
4	CL	A	1377	1/1	1.00	0.02	74,74,74,74	0
4	CL	A	1378	1/1	1.00	0.02	84,84,84,84	0
3	CD	A	1368	1/1	1.00	0.01	91,91,91,91	0
3	CD	A	1369	1/1	1.00	0.01	100,100,100,100	0
3	CD	A	1370	1/1	1.00	0.01	69,69,69,69	0
3	CD	A	1371	1/1	1.00	0.03	100,100,100,100	0
3	CD	A	1372	1/1	1.00	0.01	104,104,104,104	0
3	CD	A	1373	1/1	1.00	0.02	112,112,112,112	0

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.

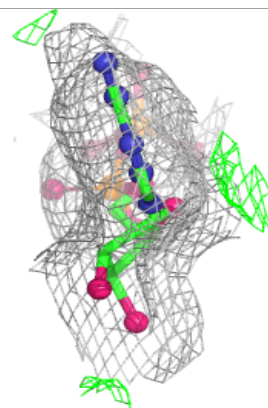
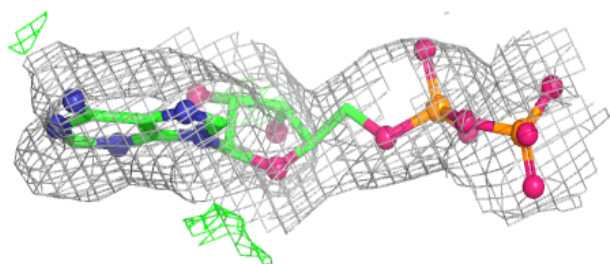
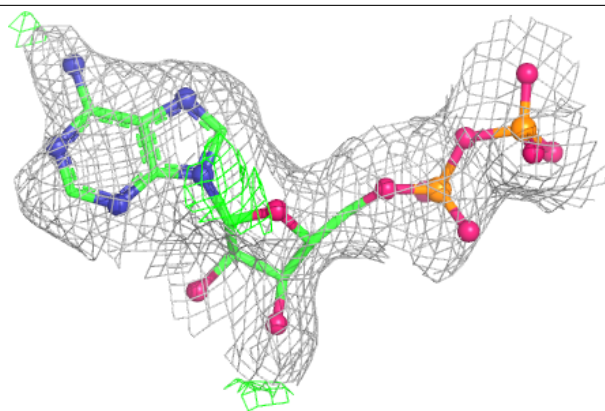
Electron density around ADP B 601:

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

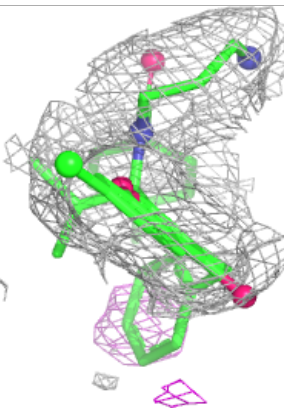
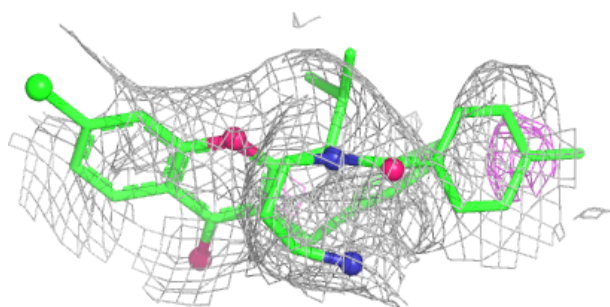
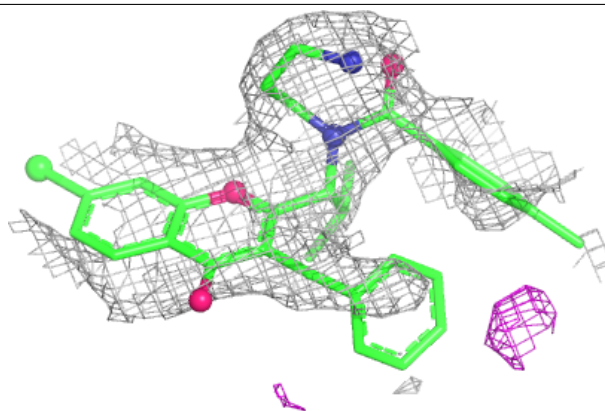


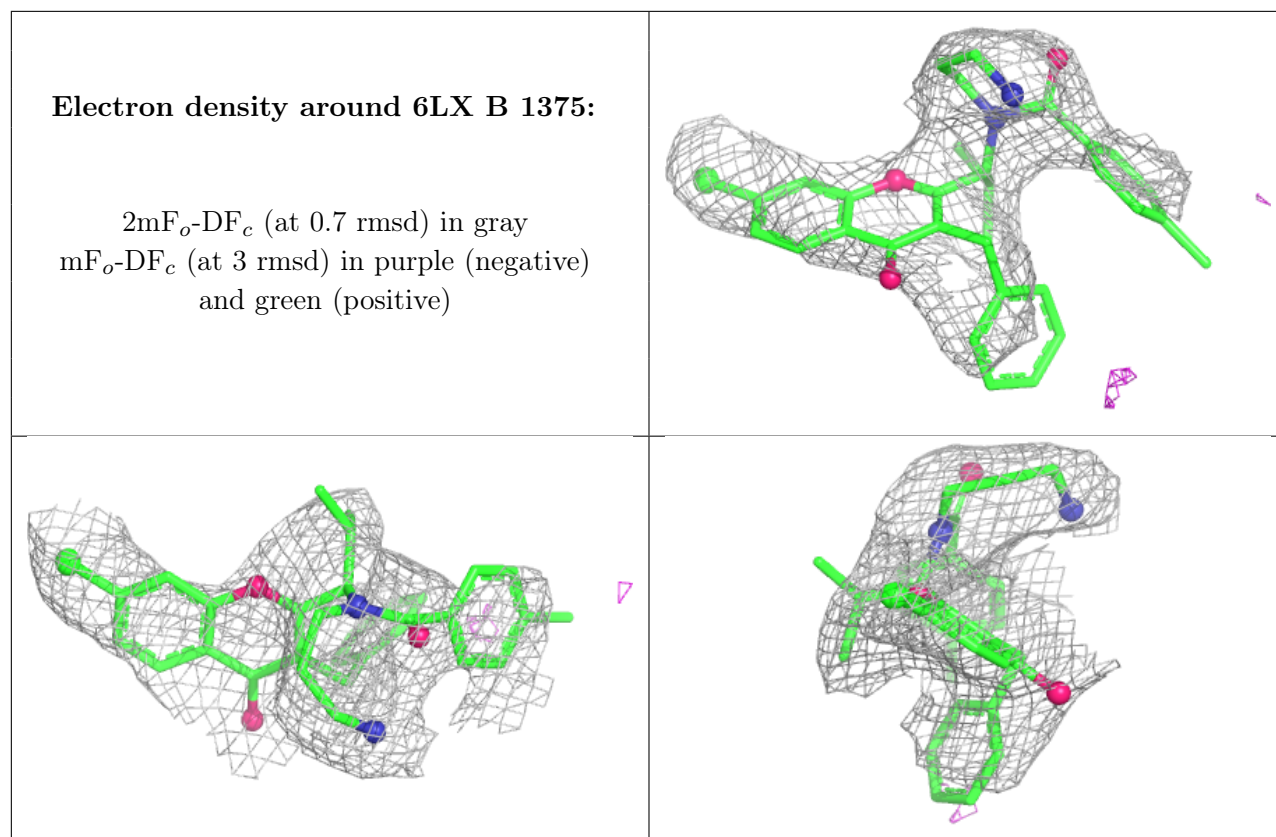
Electron density around ADP A 601:

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

**Electron density around 6LX A 1375:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.