Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:14 PM GMT

PDB ID	:	4BXN
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

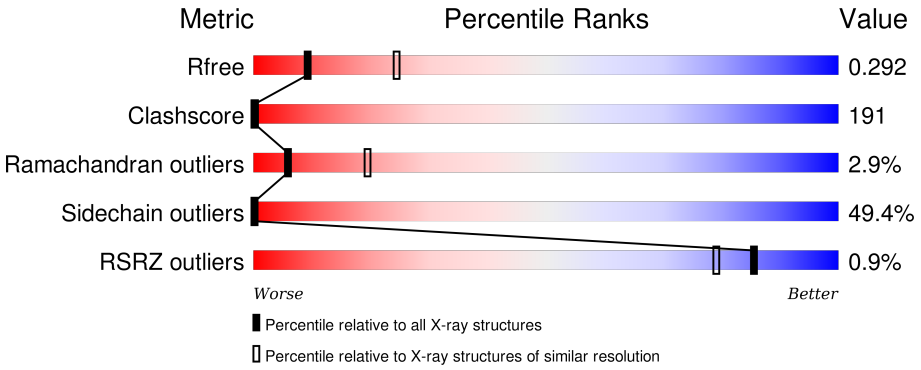
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.79 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	% 12% 44% 38% • 6%
1	B	368	% 10% 48% 35% • 6%

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	-
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

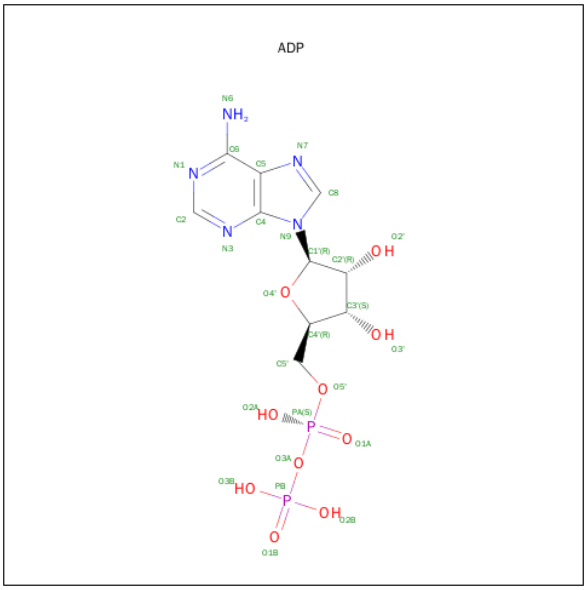
There are 6 unique types of molecules in this entry. The entry contains 5521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called KINESIN-LIKE PROTEIN KIF11.

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

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



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

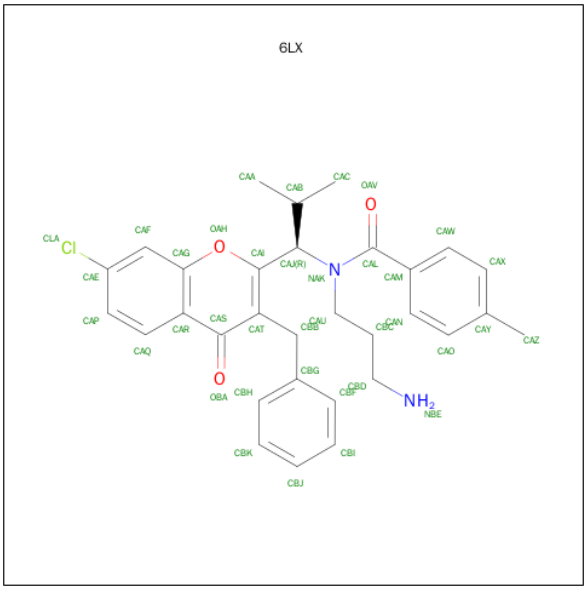
- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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

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

- Molecule 5 is N-(3-AMINOPROPYL)-N-[(1R)-1-(3-BENZYL-7-CHLORO-4-OXO-4H-CHROMEN-2-YL)-2-METHYLPROPYL]-4-METHYLBENZAMIDE (three-letter code: 6LX) (formula: $C_{31}H_{33}ClN_2O_3$).



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

- Molecule 6 is water.

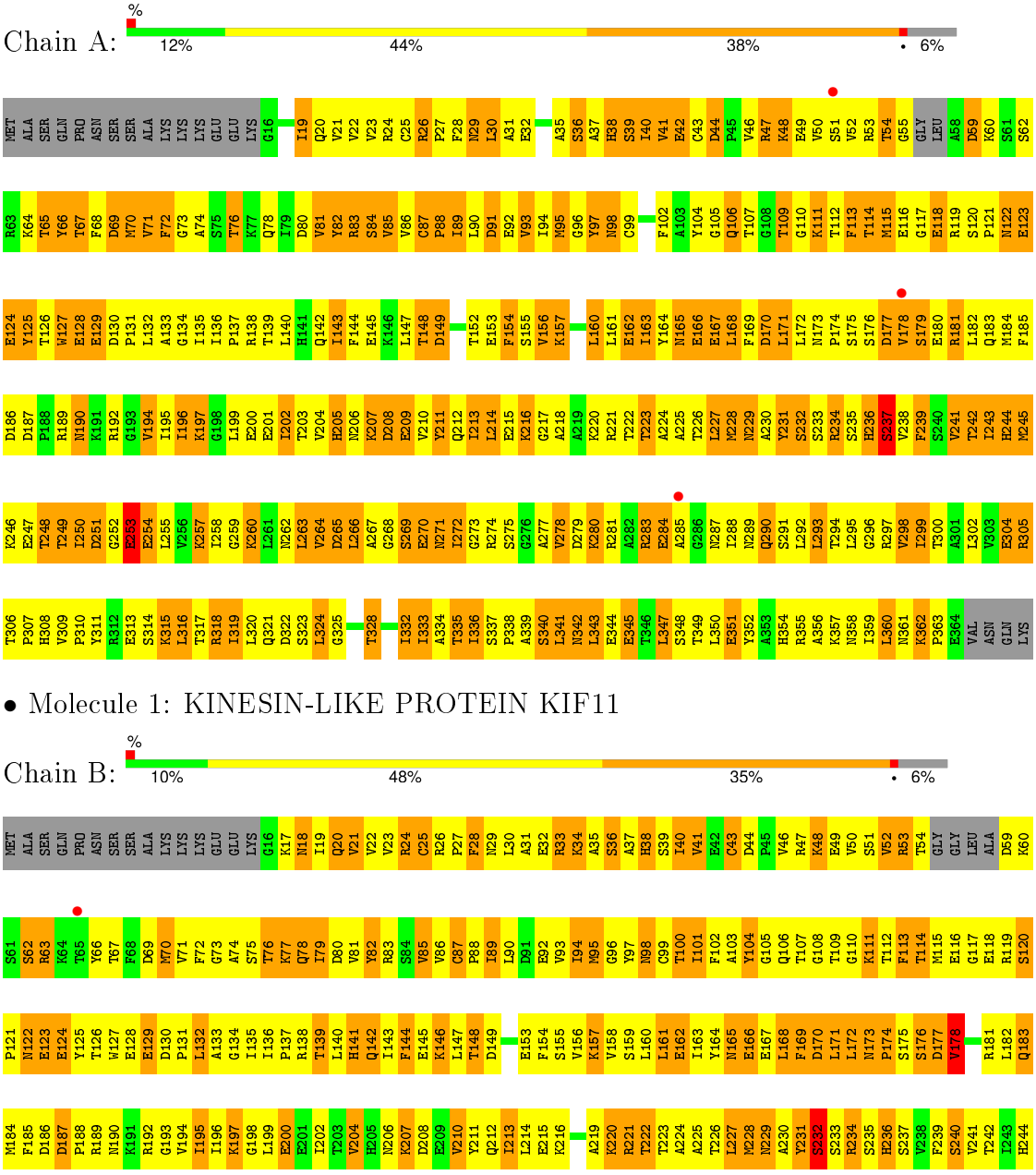
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	32	Total O 32 32	0	0
6	B	26	Total O 26 26	0	0

3 Residue-property plots (i)

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

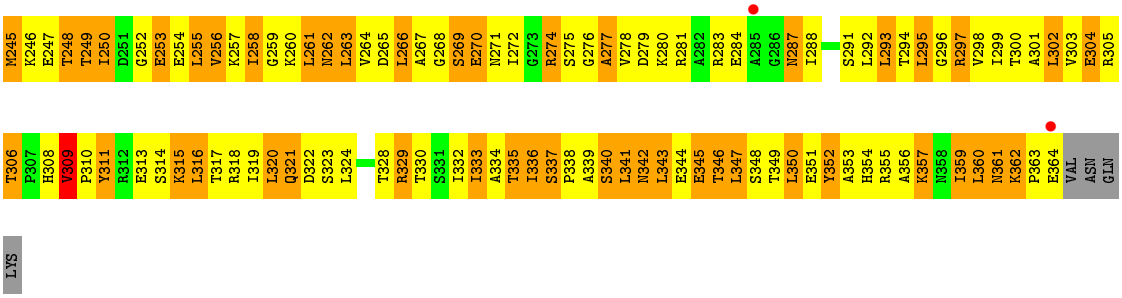
- Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain A:



- Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain B:


M245 K246 E247 T248 T249 I250 D251 G252 E253 E254 L255 V256 K257 I258 G259 K260 L261 N262 L263 V264 D265 L266 A267 G268 S269 E270 N271 I272 G273 R274 S275 G276 A277 V278 D279 K280 R281 A282 R283 E284 A285 G286 N287 I288 S291 L292 L293 T294 L295 G296 R297 V298 I299 T300 A301 L302 V303 E304 R305 T306 P307 H308 V309 P310 Y311 R312 E313 S314 K315 L316 T317 R318 I319 L320 Q321 D322 S323 L324 T328 R329 T330 S331 I332 I333 A334 T335 I336 S337 P338 A339 S340 L341 N342 L343 E344 E345 T346 L347 S348 T349 L350 E351 Y352 A353 H354 R355 A356 K357 N358 I359 L360 N361 K362 P363 E364 VAL ASN GLN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	81.43Å 81.43Å 115.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.93 – 2.79 27.94 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.1 (27.93-2.79) 97.1 (27.94-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.230 , 0.274 0.280 , 0.292	Depositor DCC
R_{free} test set	1059 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	79.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 54.8	EDS
Estimated twinning fraction	0.500 for -H,-K,L 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
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 20599 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5521	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/2702	0.46	0/3658
1	B	0.31	0/2680	0.58	2/3630 (0.1%)
All	All	0.31	0/5382	0.52	2/7288 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1035	17
1	B	2642	0	2599	1009	24
2	A	27	0	12	3	0
2	B	27	0	12	21	0
3	A	9	0	0	1	0
3	B	13	0	0	1	1
4	A	5	0	0	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	3	0
5	A	37	0	33	89	0
5	B	37	0	33	9	0
6	A	32	0	0	12	0
6	B	26	0	0	4	0
All	All	5521	0	5309	2057	30

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 191.

All (2057) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PHE:CE2	1:A:81:VAL:HG22	1.21	1.63
1:A:28:PHE:CE1	1:A:339:ALA:CB	1.80	1.63
1:A:28:PHE:CZ	1:A:339:ALA:CB	1.77	1.62
1:A:211:TYR:CE1	5:A:1375:6LX:HAA1	1.34	1.60
1:B:113:PHE:CE2	1:B:118:GLU:HG3	1.26	1.60
1:B:239:PHE:CE1	1:B:241:VAL:CG1	1.80	1.59
1:A:225:ALA:HA	1:A:231:TYR:CD2	1.13	1.59
1:B:82:TYR:CE1	1:B:86:VAL:CG1	1.79	1.58
1:A:272:ILE:CD1	1:A:355:ARG:NH2	1.69	1.55
1:B:239:PHE:CE1	1:B:241:VAL:HG12	1.34	1.53
1:A:226:THR:C	1:A:228:MET:HB2	1.15	1.52
1:B: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:A:167:GLU:HG3	1:A:181:ARG:CB	1.44	1.47
1:B:127:TRP:CZ2	1:B:208:ASP:HA	1.51	1.45
1:B:174:PRO:CA	1:B:220:LYS:HD2	0.98	1.45
1:A:28:PHE:CE1	1:A:339:ALA:HB2	1.46	1.45
1:B:41:VAL:CA	1:B:52:VAL:HG23	1.44	1.44
1:A:167:GLU:CG	1:A:181:ARG:HB3	1.44	1.43
1:A:272:ILE:HD11	1:A:355:ARG:CZ	1.48	1.43
1:B:22:VAL:CG2	1:B:333:ILE:HG22	1.47	1.43
1:A:102:PHE:CZ	1:A:332:ILE:HG23	1.54	1.43
1:A:160:LEU:CD1	1:A:171:LEU:HD23	1.48	1.43
1:B:239:PHE:CZ	1:B:241:VAL:HG12	1.54	1.43
1:A:105:GLY:CA	1:A:269:SER:OG	1.64	1.42
1:B:143:ILE:CG2	1:B:147:LEU:HD21	1.49	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:THR:CG2	1:B:356:ALA:HA	1.48	1.41
1:B:211:TYR:CE1	1:B:215:GLU:OE1	1.71	1.41
1:B:24:ARG:NH2	1:B:114:THR:HG23	1.36	1.41
1:B:118:GLU:CB	1:B:132:LEU:HD13	1.27	1.41
1:B:82:TYR:CD1	1:B:86:VAL:HB	1.55	1.41
1:A:160:LEU:HD12	1:A:171:LEU:CD2	1.52	1.40
1:A:252:GLY:CA	1:A:253:GLU:HB3	1.49	1.40
1:A:226:THR:C	1:A:228:MET:CB	1.91	1.39
1:B:142:GLN:O	1:B:146:LYS:CG	1.68	1.39
1:A:279:ASP:CB	1:A:283:ARG:HG2	1.50	1.39
1:B:300:THR:HG22	1:B:356:ALA:CA	1.52	1.38
1:A:211:TYR:HE1	5:A:1375:6LX:CAA	1.36	1.37
1:B:163:ILE:HB	1:B:236:HIS:CD2	1.58	1.37
1:A:117:GLY:C	5:A:1375:6LX:HAN	1.42	1.36
1:B:252:GLY:CA	1:B:253:GLU:HB3	1.48	1.36
1:A:72:PHE:CE2	1:A:81:VAL:CG2	2.06	1.36
1:A:272:ILE:CD1	1:A:355:ARG:CZ	2.02	1.35
1:B:113:PHE:CE2	1:B:118:GLU:CG	2.09	1.35
1:A:225:ALA:CA	1:A:231:TYR:CD2	2.05	1.34
1:B:24:ARG:HH21	1:B:114:THR:CG2	1.39	1.34
1:A:152:THR:HG22	1:A:247:GLU:CG	1.54	1.34
1:B:249:THR:OG1	1:B:252:GLY:N	1.57	1.34
1:B:172:LEU:CB	1:B:200:GLU:OE2	1.75	1.34
1:A:280:LYS:O	1:A:284:GLU:CG	1.76	1.33
1:B:197:LYS:HD2	1:B:198:GLY:N	1.42	1.33
1:B:81:VAL:O	1:B:85:VAL:HG23	1.22	1.33
1:B:161:LEU:HD22	1:B:162:GLU:N	1.41	1.33
1:A:224:ALA:O	1:A:228:MET:HG2	1.27	1.32
1:A:28:PHE:CE1	1:A:339:ALA:HB3	1.49	1.32
1:A:294:THR:O	1:A:298:VAL:HG23	1.22	1.32
1:B:344:GLU:O	1:B:347:LEU:CD1	1.77	1.31
1:B:351:GLU:OE1	1:B:355:ARG:NH2	1.60	1.31
1:B:143:ILE:CG2	1:B:147:LEU:CD2	2.08	1.30
1:A:225:ALA:CA	1:A:231:TYR:HD2	1.38	1.30
1:B:211:TYR:HE1	1:B:215:GLU:CD	1.30	1.30
1:B:142:GLN:O	1:B:146:LYS:HG3	1.21	1.30
1:A:225:ALA:O	1:A:228:MET:HB3	1.18	1.29
1:A:116:GLU:O	5:A:1375:6LX:HBB2	1.32	1.29
1:B:143:ILE:HG22	1:B:147:LEU:CD2	1.61	1.29
1:A:280:LYS:O	1:A:284:GLU:HG3	1.13	1.28
1:B:343:LEU:O	1:B:346:THR:HG23	1.27	1.28

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:OH	1:A:350:LEU:O	1.56	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:B:20:GLN:NE2	1:B:329:ARG:NH1	1.89	1.18
1:A:298:VAL:CG1	1:A:311:TYR:CD1	2.27	1.18
1:B:128:GLU:OE2	1:B:208:ASP:OD1	1.59	1.18
1:B: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:73:GLY:O	1:B:75:SER:N	1.75	1.18
1:B:40:ILE:O	1:B:52:VAL:HG22	1.42	1.17
1:A:152:THR:HG22	1:A:247:GLU:CD	1.62	1.17
1:A:78:GLN:NE2	1:A:133:ALA:O	1.78	1.17
1:A:127:TRP:CE3	1:A:128:GLU:OE2	1.97	1.17
1:A:205:HIS:NE2	6:A:2018:HOH:O	1.75	1.17
1: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:298:VAL:HG12	1:A:311:TYR:CE1	1.80	1.16
1:A:27:PRO:CD	1:A:74:ALA:HB1	1.75	1.16
1:B:296:GLY:O	1:B:300:THR:CG2	1.93	1.16
1:A:242:THR:HG23	1:A:260:LYS:CD	1.75	1.16
1:A:284:GLU:O	1:A:289:ASN:CG	1.84	1.16
1:B:93:VAL:HG21	1:B:261:LEU:CD2	1.76	1.16
1:B:22:VAL:HG21	1:B:333:ILE:CG2	1.74	1.15
1:A:69:ASP:O	1:A:70:MET:SD	2.04	1.15
1:B: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:40:ILE:C	1:B:52:VAL:HG22	1.68	1.14
1:A:225:ALA:C	1:A:228:MET:HB3	1.67	1.14
1:B: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:C	1:B:347:LEU:CD1	2.14	1.13
1:B:344:GLU:HA	1:B:347:LEU:HD11	1.18	1.13
1:A:41:VAL:CG2	1:A:338:PRO:HA	1.78	1.12
1:B:112:THR:HG22	1:B:116:GLU:HG3	1.21	1.12
1:A:118:GLU:O	5:A:1375:6LX:CAY	1.97	1.12
5:A:1375:6LX:HBF	5:A:1375:6LX:HAJ	1.21	1.12
1:B:40:ILE:O	1:B:52:VAL:CG2	1.96	1.12
1:A:294:THR:CB	1:A:314:SER:OG	1.98	1.12
1:B:127:TRP:CZ2	1:B:208:ASP:CA	2.32	1.12
1:A:296:GLY:O	1:A:300:THR:OG1	1.68	1.11
1: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: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:B:264:VAL:HG12	1:B:266:LEU:CD2	1.80	1.11
1:B:171:LEU:CB	1:B:220:LYS:HE3	1.79	1.11
1:A:294:THR:OG1	1:A:314:SER:OG	1.66	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:B:40:ILE:C	1:B:52:VAL:CG2	2.19	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:HE2	1.33	1.11
1:B:172:LEU:HB2	1:B:200:GLU:OE2	1.39	1.11
1:A:23:VAL:HG21	1:A:68:PHE:CE2	1.86	1.11
1:B:171:LEU:HB2	1:B:220:LYS:CE	1.80	1.11
1:B:311:TYR:OH	1:B:324:LEU:CB	1.99	1.11
1:A:147:LEU:HD13	1:A:154:PHE:CD2	1.85	1.10
1:A:41:VAL:HG13	1:A:52:VAL:HG21	1.11	1.10
1:B:22:VAL:CG2	1:B:333:ILE:CG2	2.27	1.10
1:A:30:LEU:HD13	1:A:30:LEU:O	1.49	1.10
1:A:109:THR:OG1	1:A:335:THR:HB	1.49	1.10
1:B:118:GLU:CB	1:B:132:LEU:CD1	2.15	1.10
1:A:152:THR:CG2	1:A:247:GLU:HB2	1.81	1.10
1:A:324:LEU:H	1:A:324:LEU:HD23	0.95	1.10
1:A: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:226:THR:HA	1:A:229:ASN:H	1.11	1.09
1:B:173:ASN:HB2	1:B:176:SER:OG	1.49	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:HG21	1:A:68:PHE:HE2	0.96	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:A:28:PHE:CZ	1:A:339:ALA:HB2	1.62	1.09
1:B:168:LEU:H	1:B:168:LEU:HD23	1.15	1.09
1:B:82:TYR:CE1	1:B:86:VAL:CB	2.35	1.09
1:B:112:THR:CG2	1:B:116:GLU:HG3	1.81	1.09
1:A:118:GLU:OE1	1:A:132:LEU:HD12	1.50	1.09
1:A:228:MET:HG3	1:A:231:TYR:CD2	1.86	1.09
1:A: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:27:PRO:HD3	1:A:74:ALA:CB	1.83	1.09
1:A:113:PHE:HE1	1:A:114:THR:HG23	0.94	1.09
1:B:143:ILE:O	1:B:147:LEU:HD22	1.51	1.09
1:A:249:THR:O	1:A:252:GLY:O	1.71	1.09
1:A:324:LEU:N	1:A:324:LEU:HD23	1.58	1.08
1:A:78:GLN:NE2	1:A:132:LEU:O	1.85	1.08
1:B:100:THR:HG23	1:B:262:ASN:OD1	1.50	1.08
1:B:40:ILE:N	1:B:40:ILE:HD12	1.65	1.08
1:B:296:GLY:HA3	1:B:352:TYR:CZ	1.88	1.08
1:B:22:VAL:HG23	1:B:333:ILE:HA	1.11	1.08
1:A:118:GLU:O	5:A:1375:6LX:CAZ	2.02	1.08
1:B:143:ILE:HG22	1:B:147:LEU:HD23	1.18	1.08
1:B:302:LEU:H	1:B:302:LEU:CD2	1.63	1.08
1:B:164:TYR:OH	1:B:230:ALA:HB3	1.50	1.08
1:B:231:TYR:O	1:B:232:SER:HB2	1.48	1.08
1:A:114:THR:O	1:A:134:GLY:HA3	1.54	1.07
1:A:167:GLU:O	1:A:168:LEU:HD12	1.54	1.07
1:B: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:309:VAL:CG2	1:A:311:TYR:CE2	2.36	1.07
1:A:225:ALA:HB1	1:A:231:TYR:HB2	1.33	1.07
1:A:133:ALA:HB2	5:A:1375:6LX:HAZ1	1.12	1.07
1:B:134:GLY:O	1:B:137:PRO:HG2	1.53	1.07
1:B:77:LYS:NZ	6:B:2006:HOH:O	1.79	1.07
1:A:192:ARG:HH12	1:A:325:GLY:HA3	1.19	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:341:LEU:H	1:B:341:LEU:HD22	1.15	1.07
1:B:266:LEU:N	1:B:266:LEU:HD23	1.69	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:CD2	1:A:239:PHE:HB2	1.82	1.07
1:B:250:ILE:HD13	1:B:250:ILE:N	1.69	1.07
1:A:167:GLU:CG	1:A:181:ARG:CB	2.16	1.06
1:A:105:GLY:HA2	1:A:269:SER:OG	0.89	1.06
1:B:82:TYR:CD1	1:B:86:VAL:CB	2.37	1.06
1:A:218:ALA:HB2	5:A:1375:6LX:CAF	1.85	1.06
1:B:344:GLU:CA	1:B:347:LEU:HD11	1.83	1.06
1:B:357:LYS:HZ2	1:B:357:LYS:HB3	1.17	1.06
1:B:343:LEU:O	1:B:346:THR:CG2	2.01	1.06
1:A:236:HIS:O	1:A:265:ASP:O	1.74	1.06
1:A:147:LEU:HD12	1:A:154:PHE:CE2	1.90	1.06
1:B:274:ARG:HG3	1:B:274:ARG:HH11	1.16	1.06
1:A:93:VAL:HG23	1:A:99:CYS:SG	1.96	1.06
1:A:118:GLU:N	5:A:1375:6LX:HAO	1.68	1.06
1:B:157:LYS:HE3	1:B:242:THR:HB	1.37	1.05
1:B:347:LEU:H	1:B:347:LEU:HD12	1.15	1.05
1:A:242:THR:HG23	1:A:260:LYS:HD3	1.36	1.05
1:A:225:ALA:HB1	1:A:231:TYR:CB	1.85	1.05
1:A:226:THR:O	1:A:228:MET:CB	2.00	1.05
1:A:91:ASP:O	1:A:94:ILE:HG22	1.56	1.05
1:A:117:GLY:HA2	1:A:134:GLY:H	1.16	1.05
1:B:41:VAL:CG1	1:B:52:VAL:CG2	2.35	1.05
1:A:167:GLU:HG2	1:A:181:ARG:HB3	1.39	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:B:121:PRO:C	1:B:122:ASN:OD1	1.94	1.05
1:A:120:SER:OG	1:A:130:ASP:OD1	1.75	1.05
1:A:133:ALA:CB	5:A:1375:6LX:HAZ1	1.86	1.04
1: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:A:66:TYR:OH	1:A:354:HIS:HB2	1.54	1.04
1:B:134:GLY:O	1:B:137:PRO:HD2	1.55	1.04
1:B:228:MET:SD	1:B:228:MET:N	2.30	1.04
1:A:28:PHE:CZ	1:A:339:ALA:HB3	1.66	1.04
1:B:239:PHE:HE1	1:B:241:VAL:HG13	1.22	1.04
1:B:136:ILE:HG12	1:B:263:LEU:HD13	1.38	1.04
1:B:134:GLY:O	1:B:137:PRO:CG	2.04	1.04
1:B:41:VAL:N	1:B:52:VAL:HG23	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD12	1:A:154:PHE:CD2	1.90	1.04
1:A:272:ILE:HD13	1:A:355:ARG:NH2	1.73	1.04
1:A:102:PHE:CZ	1:A:332:ILE:CG2	2.39	1.04
1:A:167:GLU:HG3	1:A:181:ARG:HB2	1.38	1.04
1: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:A:23:VAL:CG2	1:A:68:PHE:HE2	1.71	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:249:THR:HB	1:A:252:GLY:H	1.21	1.03
1:A:170:ASP:OD2	1:A:200:GLU:HB2	1.56	1.03
1:B:127:TRP:HZ2	1:B:208:ASP:CA	1.66	1.03
1:A:152:THR:CG2	1:A:247:GLU:CD	2.26	1.03
1:B:269:SER:N	1:B:270:GLU:OE2	1.91	1.03
1:B:102:PHE:HZ	1:B:320:LEU:HD11	1.21	1.03
1:A:211:TYR:CE1	5:A:1375:6LX:CAA	2.22	1.02
1:B:344:GLU:HA	1:B:347:LEU:CD1	1.87	1.02
1:B:116:GLU:O	5:B:1375:6LX:HBB1	1.58	1.02
1:B:143:ILE:O	1:B:147:LEU:HD23	1.59	1.02
1:B:128:GLU:OE2	1:B:208:ASP:CG	1.98	1.02
1:B:22:VAL:HG22	1:B:332:ILE:O	1.59	1.02
1:A:242:THR:HG23	1:A:260:LYS:CG	1.88	1.02
1:B:344:GLU:CA	1:B:347:LEU:CD1	2.38	1.02
1:A:215:GLU:O	5:A:1375:6LX:CLA	2.14	1.02
1:A:207:LYS:O	1:A:210:VAL:CG1	2.06	1.02
1:A:86:VAL:C	1:A:88:PRO:HD2	1.80	1.02
1:A:245:MET:CB	1:A:257:LYS:HD3	1.90	1.02
1:B:105:GLY:HA3	1:B:109:THR:HB	1.39	1.02
1:B:98:ASN:O	1:B:328:THR:OG1	1.75	1.02
1:B:134:GLY:O	1:B:137:PRO:CD	2.08	1.02
1:A:274:ARG:HA	1:A:351:GLU:CG	1.90	1.01
1:B:76:THR:O	1:B:77:LYS:HE2	1.57	1.01
1:B:304:GLU:HB2	1:B:306:THR:HG22	1.42	1.01
1:B:127:TRP:NE1	1:B:128:GLU:CD	2.12	1.01
1:B:139:THR:O	1:B:143:ILE:HG13	1.61	1.01
1:B:168:LEU:O	1:B:182:LEU:CD2	2.07	1.01
1:B:93:VAL:HG21	1:B:261:LEU:HD23	1.40	1.01
1:A:104:TYR:CZ	1:A:269:SER:HB3	1.96	1.01
1:B:347:LEU:O	1:B:351:GLU:N	1.93	1.01
1:B:344:GLU:C	1:B:347:LEU:HD13	1.77	1.01
1:B:249:THR:OG1	1:B:252:GLY:CA	2.08	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HG21	1:A:311:TYR:HE2	1.04	1.01
1:B:316:LEU:O	1:B:320:LEU:HB2	1.60	1.01
1:A:125:TYR:HB2	1:A:129:GLU:HB3	1.38	1.01
1:A:41:VAL:HG21	1:A:338:PRO:HA	1.05	1.01
1:B:131:PRO:HA	1:B:138:ARG:NH2	1.76	1.01
1:B:41:VAL:HA	1:B:52:VAL:HG23	1.06	1.01
1:B:163:ILE:CB	1:B:236:HIS:CD2	2.43	1.01
1:A:280:LYS:O	1:A:284:GLU:CD	1.98	1.00
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:A:30:LEU:C	1:A:30:LEU:CD1	2.30	1.00
1:B:225:ALA:HA	1:B:231:TYR:CD1	1.97	1.00
1:B:353:ALA:O	1:B:357:LYS:O	1.79	1.00
1:A:118:GLU:N	5:A:1375:6LX:CAN	2.20	1.00
1:A:156:VAL:CG1	1:A:204:VAL:HB	1.92	1.00
1:B:227:LEU:HD23	1:B:229:ASN:CB	1.92	1.00
1:A:311:TYR:O	1:A:317:THR:OG1	1.79	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: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:B:174:PRO:CA	1:B:220:LYS:HD3	1.91	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
1:B:294:THR:O	1:B:298:VAL:HG23	1.63	0.98
1:A:135:ILE:O	1:A:139:THR:N	1.95	0.98
1:A:78:GLN:NE2	1:A:133:ALA:C	2.15	0.98
1:B:163:ILE:HD12	1:B:236:HIS:NE2	1.76	0.98
1:A:279:ASP:CB	1:A:283:ARG:CG	2.41	0.98
1:B:127:TRP:CH2	1:B:207:LYS:HG2	1.98	0.98
1:B:127:TRP:CE2	1:B:208:ASP:HA	1.98	0.98
1:A:73:GLY:H	1:A:76:THR:HG21	1.27	0.98
1:A:41:VAL:HG21	1:A:338:PRO:CA	1.92	0.98
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ALA:O	1:A:228:MET:CG	2.11	0.98
1:A:245:MET:HB3	1:A:257:LYS:HD3	1.46	0.98
1:A:320:LEU:O	1:A:324:LEU:CD2	2.12	0.98
1:A:117:GLY:O	5:A:1375:6LX:HAN	1.64	0.98
1:B: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:285:ALA:C	1:A:289:ASN:HD22	1.67	0.97
1:B:126:THR:O	1:B:130:ASP:OD2	1.80	0.97
1:B:171:LEU:CD2	1:B:220:LYS:HG2	1.92	0.97
1:B:227:LEU:HA	1:B:228:MET:C	1.84	0.97
1:A:156:VAL:HG11	1:A:204:VAL:HB	1.43	0.97
1:A:28:PHE:CE2	1:A:339:ALA:CB	2.46	0.97
1:A:23:VAL:CG2	1:A:68:PHE:CE2	2.45	0.97
1:A:156:VAL:HG13	1:A:204:VAL:HG23	1.44	0.97
1:A:249:THR:HB	1:A:252:GLY:N	1.79	0.97
1:B:316:LEU:N	1:B:316:LEU:HD22	1.77	0.97
1:B:123:GLU:OE1	1:B:123:GLU:HA	1.61	0.97
1:A:293:LEU:HB3	1:A:297:ARG:HH21	1.26	0.96
1:B:298:VAL:HG22	1:B:310:PRO:HB2	1.43	0.96
1:A:113:PHE:HD1	1:A:114:THR:N	1.60	0.96
1:A:226:THR:HA	1:A:229:ASN:N	1.80	0.96
1:B:81:VAL:O	1:B:85:VAL:CG2	2.13	0.96
1:B:296:GLY:HA2	1:B:299:ILE:HG22	1.44	0.96
1:B:302:LEU:H	1:B:302:LEU:HD23	0.82	0.96
1:B:40:ILE:H	1:B:40:ILE:HD12	0.80	0.96
1:A:272:ILE:HG22	1:A:348:SER:HB3	1.43	0.96
1:B:109:THR:O	1:B:335:THR:HB	1.64	0.96
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: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:B:106:GLN:CB	1:B:270:GLU:OE1	2.14	0.95
1:A:314:SER:HB2	1:A:317:THR:HG23	1.48	0.95
1:B:296:GLY:HA3	1:B:352:TYR:CE1	2.00	0.95
1:B:352:TYR:HD1	1:B:355:ARG:NH1	1.56	0.95
1:B:168:LEU:HD23	1:B:168:LEU:N	1.82	0.95
1:A:186:ASP:OD1	1:A:318:ARG:NH2	2.00	0.95
1:A:133:ALA:HA	5:A:1375:6LX:HAO	1.48	0.95
1:B:93:VAL:HG21	1:B:261:LEU:HD22	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:N	1:A:324:LEU:CD2	2.30	0.95
1:B:172:LEU:CD1	1:B:173:ASN:ND2	2.30	0.95
1:A:309:VAL:CG2	1:A:311:TYR:CD2	2.49	0.95
5:A:1375:6LX:CAY	5:A:1375:6LX:HBI	1.97	0.94
1:B:300:THR:CA	1:B:356:ALA:O	2.14	0.94
1:A:217:GLY:HA3	5:A:1375:6LX:HAP	1.45	0.94
1:B:131:PRO:HA	1:B:138:ARG:HH22	1.27	0.94
1:B:161:LEU:CD2	1:B:162:GLU:N	2.30	0.94
1:B:357:LYS:NZ	1:B:357:LYS:HB3	1.80	0.94
1:B:127:TRP:HZ2	1:B:208:ASP:HA	1.16	0.94
1:B:41:VAL:CG1	1:B:52:VAL:HG21	1.92	0.94
1:B:53:ARG:O	1:B:54:THR:HG22	1.66	0.94
1:A:118:GLU:OE1	1:A:132:LEU:CD1	2.14	0.94
1:B:143:ILE:HG23	1:B:147:LEU:HD21	0.97	0.94
1:B:239:PHE:CZ	1:B:241:VAL:HG11	2.02	0.94
1:A:118:GLU:H	5:A:1375:6LX:HAO	1.29	0.94
1:B:311:TYR:CD1	1:B:317:THR:O	2.21	0.94
1:B:239:PHE:CE1	1:B:241:VAL:HG13	1.93	0.94
1:B:22:VAL:HG23	1:B:333:ILE:CB	1.97	0.94
1:A:334:ALA:HB1	1:A:349:THR:HG22	1.50	0.94
1:B:20:GLN:NE2	1:B:329:ARG:NH2	2.14	0.94
1:A:324:LEU:H	1:A:324:LEU:CD2	1.76	0.94
1:A:144:PHE:CE1	1:A:207:LYS:HB3	2.04	0.93
1:B:157:LYS:HG3	1:B:242:THR:O	1.67	0.93
1:B:104:TYR:OH	1:B:349:THR:CB	2.15	0.93
1:B:227:LEU:HA	1:B:229:ASN:N	1.84	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:82:TYR:OH	1:A:142:GLN:OE1	1.86	0.93
1:B:164:TYR:HB3	1:B:169:PHE:CE1	2.02	0.93
1:A:226:THR:CA	1:A:228:MET:HB3	1.97	0.93
1:A:284:GLU:C	1:A:289:ASN:ND2	2.21	0.93
1:B:164:TYR:HE1	1:B:234:ARG:CD	1.80	0.93
1:A:54:THR:HG1	1:A:62:SER:HB2	1.33	0.93
1:B:82:TYR:CE1	1:B:86:VAL:HG11	1.67	0.93
1:A:44:ASP:OD2	1:A:47:ARG:CB	2.17	0.93
1:A:102:PHE:CE2	1:A:332:ILE:HG23	2.03	0.93
1:A:225:ALA:C	1:A:231:TYR:HD2	1.72	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:B:174:PRO:N	1:B:220:LYS:HD3	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:H	1:A:202:ILE:HD13	1.34	0.93
1:A:144:PHE:CD1	1:A:207:LYS:HB3	2.04	0.92
1:B:316:LEU:HD22	1:B:316:LEU:H	1.30	0.92
1:A:227:LEU:N	1:A:228:MET:C	2.23	0.92
1:B:211:TYR:O	1:B:215:GLU:N	2.01	0.92
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: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:102:PHE:HZ	1:A:332:ILE:HG23	1.15	0.92
1:A:298:VAL:HG12	1:A:311:TYR:CD1	2.00	0.92
1:A:272:ILE:HG22	1:A:348:SER:CB	2.00	0.92
1:A:281:ARG:N	1:A:284:GLU:OE2	2.03	0.92
1:A:72:PHE:CZ	1:A:81:VAL:CG2	2.38	0.92
1:A: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:102:PHE:HZ	1:A:332:ILE:CG2	1.80	0.92
1:A:118:GLU:HB3	1:A:132:LEU:HB3	1.49	0.92
1:B:195:ILE:C	1:B:195:ILE:CD1	2.30	0.92
1:A:160:LEU:HD22	1:A:239:PHE:CB	2.00	0.91
1:A:167:GLU:C	1:A:168:LEU:CD1	2.38	0.91
1:B:22:VAL:CG2	1:B:333:ILE:HA	1.99	0.91
1:A:90:LEU:O	1:A:94:ILE:N	2.03	0.91
1:A:28:PHE:CD2	1:A:32:GLU:HG2	2.05	0.91
1:B:171:LEU:CB	1:B:220:LYS:HE2	1.99	0.91
1:A:309:VAL:HG23	1:A:311:TYR:HD2	1.35	0.91
1:A:167:GLU:HG3	1:A:181:ARG:HB3	0.94	0.91
1:A:160:LEU:HD13	1:A:161:LEU:N	1.85	0.91
1:B:116:GLU:O	5:B:1375:6LX:CBB	2.18	0.91
1:B:110:GLY:CA	2:B:601:ADP:N7	2.34	0.91
1:B:100:THR:HA	1:B:262:ASN:ND2	1.85	0.91
1:A:242:THR:HG23	1:A:260:LYS:HG2	1.47	0.91
1:A:26:ARG:HA	1:A:74:ALA:HA	1.53	0.91
1:A:217:GLY:N	5:A:1375:6LX:CLA	2.41	0.90
1:B:183:GLN:OE1	1:B:185:PHE:CZ	2.24	0.90
1:A:211:TYR:CZ	5:A:1375:6LX:HAA1	2.05	0.90
1:B:105:GLY:CA	1:B:109:THR:CB	2.49	0.90
1:B:265:ASP:C	1:B:266:LEU:HD23	1.90	0.90
1:B:164:TYR:HB3	1:B:169:PHE:HE1	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:118:GLU:O	1:B:132:LEU:HB2	1.71	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:177:ASP:C	1:B:178:VAL:HG13	1.90	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:69:ASP:C	1:A:70:MET:SD	2.49	0.90
1:A:67:THR:O	1:A:68:PHE:CD1	2.25	0.90
1:A:157:LYS:HG2	1:A:203:THR:HG22	1.55	0.89
1:A:116:GLU:O	5:A:1375:6LX:CBB	2.18	0.89
1:B:127:TRP:CD1	1:B:128:GLU:OE1	2.25	0.89
1:A:109:THR:HG23	1:A:111:LYS:HG2	1.54	0.89
1:A:87:CYS:SG	4:A:1377:CL:CL	2.67	0.89
1:B:274:ARG:HG3	1:B:274:ARG:NH1	1.81	0.89
1:A:230:ALA:CB	1:A:234:ARG:CB	2.35	0.89
1:A:137:PRO:HB3	5:A:1375:6LX:CBK	2.02	0.89
1:B:106:GLN:O	1:B:109:THR:HG23	0.92	0.89
1:A:309:VAL:CG2	1:A:311:TYR:HE2	1.79	0.89
1:B:100:THR:CG2	1:B:262:ASN:OD1	2.19	0.89
1:B:197:LYS:CD	1:B:198:GLY:H	1.85	0.89
1:A:134:GLY:O	1:A:137:PRO:HG2	1.72	0.89
1:B:197:LYS:HD2	1:B:198:GLY:H	1.02	0.89
1:B:26:ARG:O	1:B:338:PRO:HG3	1.73	0.89
1:B:32:GLU:CD	1:B:339:ALA:CB	2.40	0.89
1:B:72:PHE:HB3	1:B:76:THR:CG2	2.03	0.89
1:A:334:ALA:HB1	1:A:349:THR:CG2	2.03	0.89
1:B:112:THR:O	1:B:116:GLU:N	2.05	0.88
1:B:296:GLY:HA2	1:B:299:ILE:CG2	2.03	0.88
1:B:177:ASP:O	1:B:178:VAL:HG22	1.73	0.88
1:A:221:ARG:NH2	5:A:1375:6LX:CAP	2.34	0.88
1:A:28:PHE:CG	1:A:339:ALA:HB2	2.07	0.88
1:B:113:PHE:CE2	1:B:118:GLU:CB	2.56	0.88
1:B:266:LEU:CD2	1:B:266:LEU:N	2.37	0.88
1:B:143:ILE:HG23	1:B:147:LEU:CD2	1.88	0.88
1:A:242:THR:CG2	1:A:260:LYS:CG	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLY:CA	1:A:134:GLY:H	1.87	0.88
1:A:226:THR:CA	1:A:228:MET:CB	2.51	0.88
1:B:239:PHE:CD1	1:B:263:LEU:HD11	2.08	0.88
1:B:102:PHE:HZ	1:B:320:LEU:CD1	1.86	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:19:ILE:O	1:A:20:GLN:NE2	2.07	0.88
1:A:106:GLN:N	1:A:269:SER:H	1.71	0.88
1:A:228:MET:HG3	1:A:231:TYR:CE2	2.09	0.88
1:A:51:SER:HA	1:A:64:LYS:O	1.73	0.88
1:B:112:THR:O	1:B:116:GLU:HB2	1.72	0.88
1:A:213:ILE:HA	1:A:216:LYS:HE2	1.55	0.88
1:A:272:ILE:HD12	1:A:355:ARG:CZ	1.89	0.88
1:A:73:GLY:H	1:A:76:THR:CG2	1.86	0.88
1:A:120:SER:HB2	1:A:124:GLU:HG2	1.56	0.88
1:A:113:PHE:HD1	1:A:114:THR:H	1.16	0.87
1:B:143:ILE:C	1:B:147:LEU:HD23	1.94	0.87
1:A:135:ILE:O	1:A:139:THR:HB	1.72	0.87
1:A:44:ASP:OD2	1:A:47:ARG:HB3	1.72	0.87
1:A:124:GLU:OE2	1:A:125:TYR:CE1	2.27	0.87
1:B:247:GLU:O	1:B:255:LEU:N	2.06	0.87
1:A:152:THR:HG22	1:A:247:GLU:HB2	1.43	0.87
1:B:311:TYR:O	1:B:317:THR:OG1	1.91	0.87
1:B:316:LEU:N	1:B:316:LEU:CD2	2.30	0.87
1:B: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:B:81:VAL:HG12	1:B:85:VAL:HG21	1.55	0.86
1:A:309:VAL:HG23	1:A:311:TYR:CD2	2.06	0.86
1:A:242:THR:HG22	1:A:260:LYS:HG2	1.57	0.86
1:A:118:GLU:C	5:A:1375:6LX:CAY	2.43	0.86
1:B:183:GLN:OE1	1:B:185:PHE:CE2	2.28	0.86
1:B:20:GLN:HE22	1:B:329:ARG:NH2	1.69	0.86
1:A:302:LEU:CG	1:A:311:TYR:OH	2.22	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:336:ILE:C	1:A:336:ILE:HD12	1.95	0.86
1:A:157:LYS:CG	1:A:203:THR:HG22	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:CE1	1:A:354:HIS:HB2	2.10	0.86
1:A:49:GLU:OE1	1:A:66:TYR:C	2.14	0.86
1:A:66:TYR:OH	1:A:354:HIS:CB	2.23	0.86
1:A:125:TYR:N	1:A:125:TYR:CD1	2.43	0.86
1:A:298:VAL:CG1	1:A:311:TYR:CG	2.58	0.86
1:B:311:TYR:OH	1:B:324:LEU:HB3	1.76	0.86
1:A:152:THR:CB	1:A:247:GLU:HB2	2.05	0.86
1:B:127:TRP:CZ2	1:B:207:LYS:HG2	2.10	0.85
1:A:65:THR:OG1	1:A:361:ASN:OD1	1.93	0.85
1:A:270:GLU:O	1:A:348:SER:OG	1.94	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:315:LYS:H	1:A:315:LYS:CE	1.89	0.85
1:A:114:THR:O	1:A:135:ILE:N	2.09	0.85
1:A:73:GLY:N	1:A:76:THR:HG21	1.91	0.85
1:B:296:GLY:CA	1:B:299:ILE:HG22	2.05	0.85
1:B:351:GLU:OE1	1:B:355:ARG:CZ	2.24	0.85
1:A:196:ILE:HG13	1:A:199:LEU:HB2	1.56	0.85
1:A:111:LYS:O	1:A:115:MET:HB2	1.75	0.85
1:A:272:ILE:HG22	1:A:348:SER:CA	2.07	0.85
1:B:113:PHE:HE2	1:B:118:GLU:CG	1.68	0.85
1:B:22:VAL:HG21	1:B:333:ILE:HG22	0.85	0.85
1:A:225:ALA:O	1:A:228:MET:CG	2.25	0.85
1:A:27:PRO:HD3	1:A:74:ALA:HB1	0.91	0.85
1:A:192:ARG:NH1	1:A:325:GLY:HA3	1.91	0.85
1:A:120:SER:HB2	1:A:124:GLU:HG3	1.56	0.85
1:A:249:THR:OG1	1:A:253:GLU:OE1	1.94	0.85
1:A:148:THR:HG22	1:A:149:ASP:OD1	1.77	0.85
1:B:161:LEU:HD22	1:B:161:LEU:C	1.92	0.85
1:B:249:THR:CG2	1:B:255:LEU:HD21	2.07	0.85
1:A:167:GLU:C	1:A:168:LEU:HD13	1.97	0.85
1:A:94:ILE:O	1:A:245:MET:HE1	1.76	0.85
1:B:72:PHE:CB	1:B:76:THR:HG21	2.05	0.85
1:B:172:LEU:HG	1:B:173:ASN:N	1.92	0.84
1:A:214:LEU:HD12	5:A:1375:6LX:CAQ	2.07	0.84
1:B:305:ARG:O	1:B:305:ARG:HG3	1.74	0.84
1:A:28:PHE:CE2	1:A:32:GLU:CG	2.60	0.84
1:A:41:VAL:CG1	1:A:52:VAL:CG2	2.55	0.84
1:B:22:VAL:N	1:B:332:ILE:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:CD	1:B:339:ALA:HB2	1.98	0.84
1:A:54:THR:OG1	1:A:62:SER:CB	2.24	0.84
1:B:250:ILE:H	1:B:250:ILE:HD13	1.36	0.84
1:B:135:ILE:O	1:B:139:THR:OG1	1.96	0.84
1:B:32:GLU:OE1	1:B:339:ALA:CB	2.24	0.84
1:A:281:ARG:O	1:A:285:ALA:HB2	1.78	0.84
1:A:41:VAL:HA	1:A:52:VAL:CG2	2.07	0.84
1:A:113:PHE:HE1	1:A:114:THR:CG2	1.87	0.84
1:B:104:TYR:O	1:B:104:TYR:CD1	2.31	0.84
1:A:230:ALA:HB1	1:A:234:ARG:HB3	1.59	0.84
1:B:118:GLU:C	1:B:132:LEU:HB3	1.98	0.84
1:A:156:VAL:O	1:A:204:VAL:N	2.10	0.84
1:A:28:PHE:CE2	1:A:32:GLU:CB	2.60	0.84
1:A:298:VAL:HG12	1:A:311:TYR:CZ	2.12	0.84
1:A:221:ARG:HH21	5:A:1375:6LX:CAQ	1.83	0.84
1:B:227:LEU:CA	1:B:228:MET:C	2.46	0.84
1:A:32:GLU:OE2	1:A:37:ALA:N	2.11	0.83
1:B:352:TYR:CE1	1:B:355:ARG:NH1	2.45	0.83
1:A:230:ALA:O	1:A:234:ARG:N	2.11	0.83
1:A:152:THR:HG21	1:A:247:GLU:OE1	1.77	0.83
1:B:164:TYR:CE1	1:B:234:ARG:HD2	2.13	0.83
1:A:265:ASP:OD1	6:A:2020:HOH:O	1.94	0.83
1:B:104:TYR:CE1	1:B:334:ALA:HB1	2.12	0.83
1:B:76:THR:C	1:B:77:LYS:HE2	1.97	0.83
1:A:47:ARG:C	1:A:48:LYS:HG3	1.96	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:230:ALA:HB1	1:B:234:ARG:NE	1.92	0.83
1:B:225:ALA:HA	1:B:231:TYR:CE1	2.14	0.83
1:B:134:GLY:C	1:B:137:PRO:HD2	1.97	0.83
1:A:67:THR:HG21	1:A:359:ILE:HG22	1.61	0.82
1:A:302:LEU:HG	1:A:311:TYR:OH	1.79	0.82
1:B:164:TYR:CZ	1:B:230:ALA:HB3	2.14	0.82
1:B:127:TRP:CH2	1:B:207:LYS:O	2.31	0.82
1:B:264:VAL:HG12	1:B:266:LEU:HD22	1.61	0.82
1:B:342:ASN:C	1:B:346:THR:HG22	1.99	0.82
1:A:143:ILE:O	1:A:147:LEU:HG	1.80	0.82
1:B:110:GLY:N	2:B:601:ADP:O3A	2.11	0.82
1:A:113:PHE:O	1:A:117:GLY:CA	2.28	0.82
1:A:298:VAL:CG1	1:A:311:TYR:CE1	2.55	0.82
1:A:109:THR:HG21	1:A:335:THR:OG1	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HH22	5:A:1375:6LX:CAQ	1.88	0.82
1:B:26:ARG:O	6:B:2002:HOH:O	1.96	0.82
1:A:302:LEU:HG	1:A:311:TYR:HH	1.44	0.82
1:A:197:LYS:HE3	1:B:250:ILE:HG13	1.62	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:104:TYR:HE1	1:B:334:ALA:HB1	1.43	0.82
1:B:82:TYR:OH	1:B:90:LEU:HD22	1.79	0.82
1:B:195:ILE:HD13	1:B:196:ILE:CA	2.10	0.82
1:B:24:ARG:HH21	1:B:114:THR:HG23	0.93	0.82
1:A:23:VAL:HG22	1:A:334:ALA:HB3	1.61	0.82
1:A:336:ILE:C	1:A:336:ILE:CD1	2.48	0.82
1:A:161:LEU:HB3	1:A:238:VAL:HG22	1.60	0.82
1:B:296:GLY:C	1:B:300:THR:HG23	1.98	0.82
1:B:234:ARG:HH11	1:B:288:ILE:HD13	1.45	0.82
1:B:304:GLU:H	1:B:304:GLU:CD	1.84	0.82
1:A:78:GLN:OE1	1:A:113:PHE:CE1	2.33	0.81
1:B:66:TYR:CD2	1:B:350:LEU:HG	2.15	0.81
1:A:160:LEU:CD1	1:A:171:LEU:CD2	2.31	0.81
1:B: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:228:MET:O	1:B:229:ASN:CB	2.29	0.81
1:B:187:ASP:OD2	1:B:193:GLY:O	1.99	0.81
1:B:316:LEU:O	1:B:320:LEU:CB	2.28	0.81
1:A:147:LEU:HD13	1:A:154:PHE:CG	2.14	0.81
1:A:105:GLY:C	1:A:269:SER:OG	2.18	0.81
1:B:127:TRP:CE2	1:B:128:GLU:CD	2.54	0.81
1:B:142:GLN:C	1:B:146:LYS:HG3	2.01	0.81
1:A:249:THR:HB	1:A:252:GLY:CA	2.10	0.81
1:A:236:HIS:C	1:A:265:ASP:O	2.19	0.81
1:A:47:ARG:HA	1:A:47:ARG:HE	1.44	0.81
1:A:118:GLU:H	1:A:133:ALA:HA	1.42	0.81
1:A:118:GLU:O	5:A:1375:6LX:HAZ2	1.81	0.81
1:A:41:VAL:CG2	1:A:338:PRO:CA	2.52	0.81
1:B:164:TYR:OH	1:B:230:ALA:CB	2.29	0.81
1:B:47:ARG:HB2	1:B:49:GLU:OE1	1.81	0.81
1:B:127:TRP:CH2	1:B:207:LYS:CG	2.64	0.81
1:B:143:ILE:C	1:B:147:LEU:CD2	2.47	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LEU:N	1:B:302:LEU:CD2	2.30	0.81
1:B:352:TYR:O	1:B:356:ALA:CB	2.28	0.81
1:A:161:LEU:HD12	1:A:169:PHE:O	1.80	0.81
1:A:228:MET:O	1:A:229:ASN:HB3	1.79	0.81
1:B:164:TYR:CE1	1:B:234:ARG:CD	2.63	0.81
1:B:230:ALA:CB	1:B:234:ARG:HE	1.92	0.80
1:B:329:ARG:HB3	1:B:329:ARG:HH11	1.44	0.80
1:B:195:ILE:CD1	1:B:196:ILE:N	2.40	0.80
1:A:214:LEU:CD1	5:A:1375:6LX:CAQ	2.60	0.80
1:B:143:ILE:CG2	1:B:147:LEU:HD23	1.96	0.80
1:A:296:GLY:C	1:A:300:THR:HG1	1.83	0.80
1:B:53:ARG:O	1:B:54:THR:CG2	2.30	0.80
1:B:164:TYR:HE1	1:B:234:ARG:NE	1.78	0.80
1:B:211:TYR:CE1	1:B:215:GLU:HB2	2.16	0.80
1:A:225:ALA:C	1:A:228:MET:CB	2.39	0.80
1:A:160:LEU:CD1	1:A:161:LEU:N	2.44	0.80
1:A:245:MET:HB2	1:A:257:LYS:HD3	1.62	0.80
1:A:310:PRO:HB2	1:A:313:GLU:OE1	1.83	0.80
1:B:113:PHE:CE2	1:B:118:GLU:HB2	2.16	0.79
1:A:28:PHE:CD2	1:A:339:ALA:HB2	2.17	0.79
1:A:342:ASN:HB2	1:A:345:GLU:CG	2.12	0.79
1:B:117:GLY:HA3	1:B:134:GLY:H	1.47	0.79
1:B:32:GLU:O	1:B:37:ALA:HB2	1.83	0.79
1:B:127:TRP:HZ2	1:B:208:ASP:N	1.79	0.79
1:A:314:SER:HB2	1:A:317:THR:CG2	2.11	0.79
1:B:333:ILE:O	1:B:333:ILE:CG1	2.30	0.79
1:B:347:LEU:HA	1:B:350:LEU:HB2	1.65	0.79
1:B:177:ASP:O	1:B:178:VAL:CG1	2.31	0.79
1:A:118:GLU:C	5:A:1375:6LX:CAO	2.51	0.79
1:A:112:THR:O	1:A:116:GLU:N	2.16	0.79
1:A:225:ALA:CB	1:A:231:TYR:CB	2.59	0.79
1:B:227:LEU:HA	1:B:228:MET:HB2	1.64	0.79
1:B: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:B:79:ILE:HD11	1:B:83:ARG:HH21	1.44	0.78
1:A:73:GLY:O	1:A:76:THR:CG2	2.31	0.78
1:A:86:VAL:C	1:A:88:PRO:CD	2.51	0.78
1:B:26:ARG:HD2	2:B:601:ADP:C1'	2.13	0.78
1:B:47:ARG:C	1:B:48:LYS:HG3	2.02	0.78
2:A:601:ADP:O1B	6:A:2009:HOH:O	2.01	0.78
1:B:26:ARG:NE	1:B:108:GLY:O	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ILE:CD1	1:B:236:HIS:NE2	2.46	0.78
1:B:174:PRO:C	1:B:220:LYS:HD2	2.02	0.78
1:B:311:TYR:HH	1:B:324:LEU:CB	1.92	0.78
1:A:218:ALA:HB2	5:A:1375:6LX:HAF	1.65	0.78
1:B:131:PRO:CA	1:B:138:ARG:NH2	2.46	0.78
1:A:165:ASN:HA	6:A:2014:HOH:O	1.83	0.78
1:B:38:HIS:N	1:B:38:HIS:ND1	2.32	0.78
1:A:166:GLU:HB3	6:A:2015:HOH:O	1.84	0.78
1:B:22:VAL:CG2	1:B:333:ILE:CB	2.59	0.78
1:B:53:ARG:C	1:B:54:THR:HG22	2.04	0.78
1:B:172:LEU:HG	1:B:173:ASN:H	1.46	0.78
1:A:218:ALA:CB	5:A:1375:6LX:CAF	2.62	0.78
2:A:601:ADP:O2'	6:A:2029:HOH:O	2.02	0.78
1:B:136:ILE:HG12	1:B:263:LEU:CD1	2.12	0.78
1:A:167:GLU:O	1:A:168:LEU:CD1	2.32	0.78
1:B:83:ARG:O	1:B:87:CYS:HB2	1.84	0.78
1:A: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:A:21:VAL:CG2	1:A:357:LYS:HG3	2.13	0.77
1:B:246:LYS:NZ	6:B:2009:HOH:O	2.14	0.77
1:A:127:TRP:HE3	1:A:128:GLU:OE2	1.61	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:40:ILE:C	1:B:52:VAL:HG23	1.95	0.77
1:A:225:ALA:C	1:A:228:MET:CG	2.53	0.77
1:A:67:THR:HG21	1:A:359:ILE:CG2	2.15	0.77
1:B:247:GLU:N	1:B:255:LEU:O	2.15	0.77
1:A:123:GLU:O	1:A:124:GLU:OE1	2.03	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:CB	1:B:357:LYS:HZ2	1.95	0.77
1:A:118:GLU:CA	5:A:1375:6LX:CAO	2.62	0.77
1:B:127:TRP:CD1	1:B:128:GLU:CD	2.58	0.77
1:B:136:ILE:CG1	1:B:263:LEU:HD13	2.13	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:A:96:GLY:HA2	1:A:258:ILE:O	1.84	0.77
1:B:40:ILE:N	1:B:40:ILE:CD1	2.30	0.77
1:A:21:VAL:HG21	1:A:357:LYS:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:O	1:B:255:LEU:HB2	1.85	0.77
1:B:104:TYR:O	1:B:104:TYR:HD1	1.66	0.76
1:B:98:ASN:HD21	1:B:260:LYS:CD	1.98	0.76
1:A:284:GLU:O	1:A:289:ASN:CB	2.33	0.76
1:A:32:GLU:OE2	1:A:37:ALA:O	2.04	0.76
1:B:121:PRO:O	1:B:124:GLU:CG	2.33	0.76
1:B:192:ARG:CB	1:B:322:ASP:HA	2.08	0.76
5:A:1375:6LX:CBF	5:A:1375:6LX:CAJ	2.57	0.76
1:A:65:THR:OG1	1:A:361:ASN:CG	2.24	0.76
1:A:156:VAL:O	1:A:203:THR:HA	1.85	0.76
1:B:168:LEU:CD2	1:B:168:LEU:N	2.49	0.76
1:B:128:GLU:CD	1:B:208:ASP:OD1	2.22	0.76
1:B:262:ASN:ND2	1:B:262:ASN:N	2.30	0.76
1:A:137:PRO:HB3	5:A:1375:6LX:CBJ	2.15	0.76
1:A:167:GLU:C	1:A:168:LEU:HD12	2.00	0.76
1:B:164:TYR:CB	1:B:169:PHE:HE1	1.98	0.76
1:B:110:GLY:HA3	2:B:601:ADP:N7	1.99	0.76
1:A:336:ILE:O	1:A:336:ILE:CD1	2.30	0.76
1:A:105:GLY:C	1:A:269:SER:H	1.89	0.76
1:A:173:ASN:ND2	1:A:200:GLU:OE2	2.19	0.76
1:B:161:LEU:HD22	1:B:162:GLU:H	1.45	0.76
1:A:152:THR:HB	1:A:247:GLU:HB2	1.67	0.76
1:B:344:GLU:O	1:B:347:LEU:HD12	1.83	0.76
1:A:197:LYS:CE	1:B:250:ILE:HG13	2.16	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: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:B:66:TYR:CZ	1:B:350:LEU:HB3	2.20	0.75
1:B:41:VAL:N	1:B:52:VAL:CG2	2.40	0.75
1:B:96:GLY:HA2	1:B:259:GLY:HA3	1.68	0.75
1:A:230:ALA:HB1	1:A:234:ARG:HB2	0.79	0.75
1:B:304:GLU:O	1:B:305:ARG:HB3	1.84	0.75
1:A:73:GLY:N	1:A:76:THR:CG2	2.48	0.75
1:B:341:LEU:CD2	1:B:341:LEU:H	1.94	0.75
1:A:201:GLU:O	1:A:201:GLU:HG2	1.84	0.75
1:A:87:CYS:N	1:A:88:PRO:HD2	2.01	0.75
5:A:1375:6LX:CAX	5:A:1375:6LX:HBI	2.16	0.75
1:A:117:GLY:CA	5:A:1375:6LX:HAN	2.14	0.75
1:B:192:ARG:HH11	1:B:192:ARG:HG3	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:CD1	1:B:250:ILE:N	2.44	0.75
1:B:128:GLU:CG	1:B:208:ASP:OD1	2.34	0.75
1:A:136:ILE:O	1:A:140:LEU:HB2	1.85	0.75
1:B: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:225:ALA:HA	1:A:231:TYR:CE2	2.12	0.74
1:A:44:ASP:OD2	1:A:47:ARG:HB2	1.85	0.74
1:B:136:ILE:N	1:B:137:PRO:HD2	2.02	0.74
1:A:225:ALA:O	1:A:228:MET:HG3	1.86	0.74
1:B:98:ASN:HB3	1:B:323:SER:HA	1.69	0.74
1:A:47:ARG:O	1:A:48:LYS:CG	2.35	0.74
1:A:227:LEU:N	1:A:228:MET:CB	2.51	0.74
1:B:17:LYS:O	1:B:18:ASN:C	2.25	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
1:A:72:PHE:HE2	1:A:81:VAL:CG2	1.80	0.74
1:A:87:CYS:N	1:A:88:PRO:CD	2.50	0.74
1:B:166:GLU:OE1	1:B:166:GLU:CA	2.35	0.74
1:A:135:ILE:O	1:A:139:THR:CB	2.36	0.74
1:A:262:ASN:C	1:A:263:LEU:HD13	2.08	0.74
1:A:285:ALA:O	1:A:289:ASN:ND2	2.20	0.74
1:B:226:THR:O	1:B:228:MET:HG2	1.88	0.74
1:A: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:A:72:PHE:HZ	1:A:81:VAL:N	1.85	0.73
1:B:117:GLY:HA3	1:B:134:GLY:N	2.03	0.73
1:B:172:LEU:HG	1:B:173:ASN:HD22	1.52	0.73
1:A:67:THR:CG2	1:A:359:ILE:CG2	2.65	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:A:32:GLU:CD	1:A:37:ALA:HB3	2.08	0.73
1:B:90:LEU:HD12	1:B:90:LEU:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLY:HA2	1:B:259:GLY:CA	2.18	0.73
1:A:248:THR:HG23	1:A:254:GLU:OE2	1.88	0.73
1:A:41:VAL:HA	1:A:52:VAL:HG23	1.71	0.73
1:A:227:LEU:N	1:A:229:ASN:N	2.36	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:194:VAL:HG11	1:A:318:ARG:HG3	1.71	0.73
1:A:153:GLU:HG3	1:A:246:LYS:O	1.89	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:73:GLY:O	1:A:76:THR:HG23	1.88	0.73
1:B:147:LEU:HB3	1:B:154:PHE:CD1	2.24	0.73
1:B:110:GLY:CA	2:B:601:ADP:C8	2.71	0.73
1:B:28:PHE:HE1	1:B:39:SER:OG	1.72	0.73
1:A:320:LEU:O	1:A:324:LEU:HD21	1.88	0.73
1:B:113:PHE:CZ	1:B:118:GLU:HG2	2.22	0.72
1:B:172:LEU:HD12	1:B:173:ASN:ND2	2.03	0.72
1:A:296:GLY:O	1:A:300:THR:CB	2.37	0.72
1:A: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:B:265:ASP:C	1:B:266:LEU:CD2	2.57	0.72
1:A:249:THR:HB	1:A:252:GLY:HA3	1.69	0.72
1:B:85:VAL:HG11	1:B:333:ILE:HG21	1.72	0.72
1:B:76:THR:O	1:B:77:LYS:CE	2.36	0.72
1: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:49:GLU:CD	1:A:67:THR:HA	2.06	0.72
1:B:347:LEU:N	1:B:347:LEU:HD12	2.00	0.72
1:B:303:VAL:HG21	1:B:357:LYS:HZ2	1.54	0.72
1:A:202:ILE:HD13	1:A:202:ILE:N	2.04	0.72
1:A:96:GLY:CA	1:A:258:ILE:O	2.37	0.72
1:A:114:THR:C	1:A:134:GLY:HA3	2.10	0.71
1:A:116:GLU:C	5:A:1375:6LX:HBB2	2.10	0.71
1:B:295:LEU:O	1:B:299:ILE:N	2.21	0.71
1:B:77:LYS:HE2	1:B:77:LYS:HA	1.70	0.71
1:A:227:LEU:H	1:A:229:ASN:N	1.89	0.71
1:A:133:ALA:CA	5:A:1375:6LX:HAZ1	2.19	0.71
1:A:210:VAL:O	1:A:214:LEU:N	2.22	0.71
1:A:25:CYS:HB3	1:A:43:CYS:CB	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:78:GLN:HE22	1:A:133:ALA:C	1.94	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:48:LYS:HD2	1:B:362:LYS:HZ1	1.55	0.71
1:B:362:LYS:HG3	1:B:363:PRO:HD2	1.73	0.71
1:B:279:ASP:O	1:B:283:ARG:N	2.21	0.71
1:A:315:LYS:H	1:A:315:LYS:HE3	1.53	0.71
1:A:162:GLU:OE1	1:A:171:LEU:HD11	1.91	0.71
1:B:165:ASN:O	1:B:166:GLU:HB2	1.90	0.71
1:B:22:VAL:CG2	1:B:332:ILE:O	2.37	0.71
1:B:40:ILE:O	1:B:52:VAL:HA	1.89	0.71
1: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:A:117:GLY:C	5:A:1375:6LX:CAO	2.47	0.71
1:B:127:TRP:HH2	1:B:207:LYS:CG	2.03	0.71
1:A:227:LEU:N	1:A:228:MET:CA	2.53	0.71
1:A:25:CYS:HB3	1:A:43:CYS:HB3	1.73	0.70
1:B:352:TYR:O	1:B:356:ALA:HB3	1.89	0.70
1:A:115:MET:O	1:A:136:ILE:CG1	2.35	0.70
1:A:156:VAL:CG1	1:A:204:VAL:HG23	2.21	0.70
1:B:19:ILE:HA	1:B:330:THR:HB	1.73	0.70
1:B: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:225:ALA:HB1	1:A:231:TYR:HB3	1.71	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:294:THR:CG2	1:A:314:SER:OG	2.38	0.70
1:A:194:VAL:HG11	1:A:318:ARG:CG	2.21	0.70
1:A:125:TYR:HD1	1:A:125:TYR:H	1.36	0.70
1:A:206:ASN:HB2	1:A:209:GLU:HB3	1.72	0.70
1:B:245:MET:HG3	1:B:257:LYS:O	1.90	0.70
1:A:156:VAL:HG13	1:A:204:VAL:CG2	2.18	0.70
1:A:156:VAL:CG1	1:A:204:VAL:CG2	2.69	0.70
1:A:343:LEU:O	1:A:347:LEU:HD23	1.90	0.70
1:A:82:TYR:HE2	1:A:139:THR:HA	1.54	0.70
1:B:112:THR:O	1:B:116:GLU:CB	2.40	0.70
1:B:19:ILE:HD12	1:B:19:ILE:H	1.57	0.70
1:A:302:LEU:CG	1:A:311:TYR:HH	2.02	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HB1	1:A:341:LEU:HG	1.71	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:166:GLU:O	1:A:167:GLU:CD	2.30	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: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:276:GLY:O	1:B:278:VAL:HG12	1.91	0.70
1:A:253:GLU:OE2	1:A:253:GLU:C	2.30	0.70
1:A:129:GLU:CA	1:A:129:GLU:OE1	2.40	0.69
1:A:28:PHE:CD2	1:A:32:GLU:CB	2.74	0.69
1:B:77:LYS:HE2	1:B:77:LYS:CA	2.22	0.69
1:A:320:LEU:O	1:A:324:LEU:HD23	1.92	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: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:172:LEU:CD1	1:B:173:ASN:HD22	2.04	0.69
1:A:66:TYR:CE2	1:A:68:PHE:CZ	2.80	0.69
1:B:24:ARG:HH21	1:B:114:THR:HG21	1.51	0.69
1:A:72:PHE:CE2	1:A:81:VAL:HG21	2.24	0.69
5:A:1375:6LX:HAC2	5:A:1375:6LX:HAW	1.73	0.69
1:B: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:H	1:B:182:LEU:HD23	1.57	0.69
1:B:118:GLU:C	1:B:132:LEU:HD12	2.13	0.69
1:B:158:VAL:HG13	1:B:202:ILE:HG22	1.75	0.69
1:B:177:ASP:O	1:B:178:VAL:CG2	2.41	0.69
1:A:186:ASP:HB2	1:A:318:ARG:HH12	1.58	0.69
1:A:128:GLU:CD	1:A:128:GLU:H	1.96	0.69
1:B:48:LYS:C	1:B:71:VAL:HG21	2.14	0.69
1:A:118:GLU:H	5:A:1375:6LX:CAO	1.90	0.68
1:A:168:LEU:CD1	1:A:168:LEU:N	2.56	0.68
1:B:127:TRP:CZ2	1:B:208:ASP:N	2.58	0.68
1:B:142:GLN:C	1:B:146:LYS:CG	2.59	0.68
1:A:83:ARG:O	1:A:88:PRO:HD3	1.93	0.68
1:B:342:ASN:O	1:B:346:THR:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:HIS:HA	1:B:357:LYS:O	1.93	0.68
1:A:162:GLU:OE2	1:A:237:SER:HB2	1.92	0.68
1:B:303:VAL:HG21	1:B:357:LYS:NZ	2.08	0.68
1:B:30:LEU:HD13	1:B:30:LEU:O	1.92	0.68
1:A:39:SER:HB3	1:A:338:PRO:C	2.13	0.68
1:B:127:TRP:HH2	1:B:207:LYS:HG2	1.56	0.68
1:B:360:LEU:HD12	1:B:361:ASN:H	1.58	0.68
1:A:65:THR:HG1	1:A:361:ASN:CG	1.97	0.68
1:A:104:TYR:CE2	1:A:352:TYR:CG	2.82	0.68
1:A:113:PHE:C	1:A:113:PHE:CD1	2.65	0.68
1:A:214:LEU:O	5:A:1375:6LX:CAP	2.41	0.68
1:A:227:LEU:H	1:A:228:MET:C	1.96	0.68
1:A:243:ILE:HG13	1:A:259:GLY:O	1.94	0.68
1:B:105:GLY:HA3	1:B:109:THR:OG1	1.93	0.68
1:B:93:VAL:CG2	1:B:261:LEU:HD23	2.20	0.68
1:B:172:LEU:CG	1:B:173:ASN:HD22	2.07	0.68
1:A:309:VAL:CB	1:A:311:TYR:CE2	2.77	0.68
1:A:129:GLU:HA	1:A:129:GLU:OE1	1.92	0.68
1:A:118:GLU:CA	5:A:1375:6LX:CAN	2.72	0.68
1:A:81:VAL:O	1:A:85:VAL:HG22	1.93	0.68
1:A:32:GLU:OE2	1:A:37:ALA:HB3	1.93	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:B:172:LEU:HD12	1:B:173:ASN:HD21	1.56	0.68
1:A:186:ASP:CG	1:A:318:ARG:HH22	1.98	0.68
5:A:1375:6LX:CAO	5:A:1375:6LX:HBI	2.24	0.68
1:A:210:VAL:O	1:A:214:LEU:HB2	1.93	0.68
1:B:347:LEU:H	1:B:347:LEU:CD1	1.95	0.68
1:A:116:GLU:OE1	5:A:1375:6LX:CAS	2.42	0.68
1:A:133:ALA:HB1	1:A:137:PRO:CG	2.24	0.68
1:A:80:ASP:O	1:A:84:SER:OG	2.11	0.68
1:B:249:THR:O	1:B:252:GLY:N	2.23	0.68
1:B:173:ASN:CB	1:B:176:SER:OG	2.34	0.67
1:A:156:VAL:HG11	1:A:204:VAL:CB	2.20	0.67
1:B:117:GLY:CA	1:B:134:GLY:H	2.05	0.67
1:A:65:THR:OG1	1:A:361:ASN:ND2	2.27	0.67
1:B:197:LYS:C	1:B:197:LYS:HD2	2.04	0.67
1:B:341:LEU:N	1:B:341:LEU:HD22	2.00	0.67
1:B:41:VAL:HG12	1:B:52:VAL:HB	1.77	0.67
1:A:294:THR:HB	1:A:314:SER:OG	1.93	0.67
1:A:93:VAL:HG23	1:A:99:CYS:HG	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASP:C	1:A:170:ASP:OD1	2.32	0.67
1:A:315:LYS:N	1:A:315:LYS:CE	2.57	0.67
1:A:281:ARG:O	1:A:285:ALA:CB	2.41	0.67
1:A:249:THR:O	1:A:252:GLY:C	2.32	0.67
1:A:23:VAL:HG23	1:A:68:PHE:CE2	2.29	0.67
1:A:217:GLY:O	1:A:221:ARG:HG2	1.95	0.67
1:A:245:MET:HB2	1:A:257:LYS:HG2	1.77	0.67
1:A:112:THR:HB	2:A:601:ADP:O2A	1.95	0.67
1:B:288:ILE:HD12	1:B:288:ILE:H	1.59	0.67
1:B:296:GLY:O	1:B:299:ILE:HG22	1.95	0.67
1:B:76:THR:HA	1:B:80:ASP:OD2	1.94	0.67
1:A:272:ILE:HG22	1:A:348:SER:HA	1.75	0.67
1:B:118:GLU:HB3	1:B:132:LEU:CG	2.23	0.67
1:B:172:LEU:HG	1:B:173:ASN:ND2	2.10	0.67
1:B:165:ASN:H	1:B:288:ILE:HG12	1.58	0.67
1:B:165:ASN:HA	1:B:288:ILE:HD11	1.77	0.66
1:A:347:LEU:N	1:A:347:LEU:CD2	2.58	0.66
1:A:28:PHE:CE2	1:A:32:GLU:HG2	2.27	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:B:20:GLN:NE2	1:B:329:ARG:HH22	1.92	0.66
1:A:197:LYS:NZ	1:B:250:ILE:HG13	2.11	0.66
1:A:119:ARG:HB2	5:A:1375:6LX:CAX	2.26	0.66
1:A:218:ALA:CB	5:A:1375:6LX:HAF	2.24	0.66
1:A:284:GLU:HB2	1:A:293:LEU:HD21	1.76	0.66
1:B:177:ASP:C	1:B:178:VAL:CG1	2.63	0.66
1:B:163:ILE:CG2	1:B:236:HIS:CD2	2.78	0.66
1:A:67:THR:HG22	1:A:359:ILE:HB	1.76	0.66
1:B:342:ASN:O	1:B:343:LEU:C	2.33	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:A:91:ASP:C	1:A:94:ILE:HG22	2.15	0.66
1:B:311:TYR:CZ	1:B:321:GLN:HA	2.31	0.66
1:A:116:GLU:O	5:A:1375:6LX:HBF	1.96	0.66
1:A:196:ILE:HG13	1:A:199:LEU:CB	2.26	0.66
1:A: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:226:THR:O	1:B:228:MET:CG	2.44	0.66
1:B:187:ASP:CB	1:B:195:ILE:HG22	2.26	0.66
1:A:236:HIS:CD2	1:A:266:LEU:HD23	2.31	0.66
1:A:125:TYR:HB2	1:A:129:GLU:CB	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PHE:CG	1:B:263:LEU:HD12	2.31	0.65
1:B:174:PRO:HB3	1:B:220:LYS:CB	2.26	0.65
1:A:242:THR:CG2	1:A:260:LYS:CD	2.63	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:156:VAL:CG1	1:A:204:VAL:H	2.08	0.65
1:A:270:GLU:C	1:A:348:SER:OG	2.34	0.65
1:B:333:ILE:HG13	1:B:333:ILE:O	1.96	0.65
1:A:51:SER:CA	1:A:64:LYS:O	2.43	0.65
1:B:155:SER:HB2	1:B:244:HIS:HB2	1.78	0.65
5:A:1375:6LX:HBF	5:A:1375:6LX:CAN	2.27	0.65
1:A:156:VAL:HG13	1:A:204:VAL:H	1.61	0.65
1:A:315:LYS:N	1:A:315:LYS:HE2	2.12	0.65
1:B:47:ARG:HB2	1:B:49:GLU:CD	2.17	0.65
1:B: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:B:172:LEU:HD11	1:B:173:ASN:ND2	2.11	0.65
1:A:78:GLN:OE1	1:A:113:PHE:CZ	2.50	0.65
1:A:28:PHE:HE1	1:A:339:ALA:HB3	1.49	0.65
1:A:105:GLY:O	1:A:268:GLY:CA	2.38	0.65
1:A:28:PHE:HE2	1:A:32:GLU:CD	2.00	0.65
1:B:77:LYS:HA	1:B:77:LYS:CE	2.26	0.65
1:B:112:THR:CG2	1:B:116:GLU:CG	2.66	0.65
1:B:157:LYS:CG	1:B:242:THR:O	2.44	0.65
1:B:268:GLY:C	1:B:270:GLU:OE2	2.36	0.64
1:B:121:PRO:O	1:B:122:ASN:OD1	2.14	0.64
1:B:73:GLY:C	1:B:75:SER:H	1.94	0.64
1:A:351:GLU:O	1:A:355:ARG:HG2	1.97	0.64
1:A:82:TYR:HE2	1:A:139:THR:CA	2.10	0.64
1:A:41:VAL:CG2	1:A:338:PRO:O	2.45	0.64
1:B:104:TYR:OH	1:B:349:THR:CA	2.45	0.64
1:B:41:VAL:HG21	1:B:338:PRO:HA	1.77	0.64
1:A:47:ARG:C	1:A:48:LYS:CG	2.65	0.64
1:A:82:TYR:CE2	1:A:139:THR:HA	2.32	0.64
1:B:192:ARG:CG	1:B:192:ARG:HH11	2.09	0.64
1:B:113:PHE:HE2	1:B:118:GLU:HG3	0.86	0.64
1:B:26:ARG:NH1	1:B:27:PRO:O	2.29	0.64
1:B:270:GLU:OE2	1:B:270:GLU:N	2.30	0.64
1:B:177:ASP:H	1:B:220:LYS:NZ	1.95	0.64
1:B:183:GLN:CD	1:B:185:PHE:CZ	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLY:C	1:B:299:ILE:HG22	2.17	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:113:PHE:CE1	1:A:114:THR:CG2	2.67	0.64
1:A:229:ASN:O	1:A:229:ASN:ND2	2.30	0.64
1:A:49:GLU:OE2	6:A:2004:HOH:O	2.15	0.64
1:B:77:LYS:H	1:B:80:ASP:CG	2.01	0.64
1:A:86:VAL:O	1:A:88:PRO:N	2.31	0.64
1:B:227:LEU:HD23	1:B:229:ASN:CA	2.27	0.64
1:A:347:LEU:N	1:A:347:LEU:HD22	2.13	0.64
1:B:24:ARG:O	1:B:24:ARG:HG3	1.97	0.64
1:B:26:ARG:HH11	1:B:26:ARG:HG2	1.63	0.64
1:A:234:ARG:NE	1:A:234:ARG:O	2.30	0.64
1:A:98:ASN:HB2	1:A:323:SER:HA	1.78	0.64
1:B:122:ASN:N	1:B:122:ASN:OD1	2.30	0.64
1:B:49:GLU:N	1:B:49:GLU:OE1	2.30	0.64
1:A:272:ILE:CG2	1:A:348:SER:HA	2.28	0.63
1:B:225:ALA:CA	1:B:231:TYR:CE1	2.80	0.63
1:A:298:VAL:HG11	1:A:311:TYR:CG	2.27	0.63
1:A:26:ARG:HA	1:A:74:ALA:CA	2.26	0.63
1:A:44:ASP:OD1	1:A:44:ASP:C	2.35	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:26:ARG:HG2	1:B:26:ARG:NH1	2.14	0.63
1:B:172:LEU:N	1:B:220:LYS:HE2	2.13	0.63
1:A:53:ARG:CG	1:A:60:LYS:O	2.47	0.63
1:B:225:ALA:HA	1:B:231:TYR:HD1	1.56	0.63
1:A:211:TYR:OH	5:A:1375:6LX:HAC1	1.98	0.63
1:A:105:GLY:C	1:A:269:SER:N	2.52	0.63
1:B:182:LEU:HB2	1:B:197:LYS:O	1.97	0.63
1:B:249:THR:CB	1:B:252:GLY:HA3	2.29	0.63
1:A:177:ASP:OD1	1:A:179:SER:N	2.31	0.63
1:A:296:GLY:O	1:A:300:THR:N	2.30	0.63
1:B:79:ILE:HG13	1:B:80:ASP:N	2.10	0.63
1:B:304:GLU:OE1	1:B:306:THR:HG23	1.93	0.63
1:B:82:TYR:OH	1:B:86:VAL:HG11	1.97	0.63
1:A:126:THR:O	1:A:129:GLU:HB2	1.99	0.63
1:B:163:ILE:CG1	1:B:236:HIS:NE2	2.62	0.62
1:B:344:GLU:C	1:B:347:LEU:HD12	2.15	0.62
1:A:294:THR:HG21	1:A:314:SER:OG	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HG2	1:A:196:ILE:CG2	2.28	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:A:25:CYS:O	1:A:73:GLY:C	2.37	0.62
1:B:165:ASN:HA	1:B:288:ILE:CD1	2.29	0.62
1:B:252:GLY:HA2	1:B:253:GLU:HB3	0.70	0.62
1:A:187:ASP:O	1:A:190:ASN:O	2.16	0.62
1:A:139:THR:HG21	1:A:263:LEU:HD21	1.80	0.62
1:B:117:GLY:HA2	1:B:134:GLY:N	2.15	0.62
1: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:A:274:ARG:O	1:A:277:ALA:HB2	1.98	0.62
1:A:28:PHE:CD2	1:A:32:GLU:HB2	2.33	0.62
1:B:170:ASP:OD2	1:B:199:LEU:HA	1.98	0.62
1:A:215:GLU:C	5:A:1375:6LX:CLA	2.74	0.62
1:A:144:PHE:CD2	1:A:207:LYS:HB2	2.34	0.62
1:B:105:GLY:CA	1:B:109:THR:HB	2.23	0.62
1:A:49:GLU:OE1	1:A:67:THR:N	2.32	0.62
1:A:43:CYS:HB3	4:A:1376:CL:CL	2.36	0.62
1:A:245:MET:HE2	1:A:257:LYS:HG2	1.82	0.62
1:A:25:CYS:CB	1:A:43:CYS:HB3	2.29	0.62
1:A:54:THR:O	1:A:55:GLY:C	2.37	0.62
1:B:221:ARG:HB2	1:B:231:TYR:OH	2.00	0.62
1:B:104:TYR:C	1:B:104:TYR:CD1	2.70	0.62
1:B:143:ILE:CA	1:B:147:LEU:CD2	2.78	0.62
1:B:287:ASN:N	1:B:287:ASN:OD1	2.30	0.62
1:B:171:LEU:CA	1:B:177:ASP:OD2	2.47	0.62
1:A:170:ASP:O	1:A:220:LYS:NZ	2.32	0.62
1:B:227:LEU:HB3	1:B:228:MET:C	2.19	0.62
1:A:253:GLU:OE2	1:A:254:GLU:N	2.32	0.62
1:A:265:ASP:N	1:A:265:ASP:OD1	2.32	0.62
1: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:245:MET:HB2	1:A:257:LYS:CD	2.28	0.61
1:B:118:GLU:HB3	1:B:132:LEU:HD13	0.63	0.61
1:B:17:LYS:O	1:B:19:ILE:N	2.33	0.61
1:A:184:MET:HG2	1:A:196:ILE:HG23	1.81	0.61
1:B:47:ARG:NH2	1:B:363:PRO:O	2.29	0.61
1:A:32:GLU:CD	1:A:32:GLU:O	2.38	0.61
1:B:85:VAL:HG11	1:B:333:ILE:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HH11	1:B:33:ARG:HB2	1.65	0.61
1:A:41:VAL:HA	1:A:52:VAL:HG22	1.79	0.61
1:B:172:LEU:CG	1:B:173:ASN:ND2	2.63	0.61
1:A:225:ALA:O	1:A:231:TYR:CD2	2.53	0.61
1:B:126:THR:C	1:B:130:ASP:OD2	2.39	0.61
1:B:270:GLU:CD	1:B:270:GLU:N	2.50	0.61
1:B: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
1:B:299:ILE:HA	1:B:302:LEU:HG	1.82	0.61
1:B:220:LYS:O	1:B:224:ALA:CB	2.49	0.61
1:B:222:THR:O	1:B:225:ALA:HB3	2.01	0.61
1:B:161:LEU:HD22	1:B:162:GLU:CA	2.29	0.61
1:A:213:ILE:O	1:A:216:LYS:HD2	2.00	0.61
1:A:245:MET:CE	1:A:257:LYS:CG	2.79	0.61
1:B:40:ILE:O	1:B:53:ARG:N	2.34	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:A:216:LYS:C	5:A:1375:6LX:CLA	2.76	0.61
1:A:225:ALA:C	1:A:228:MET:HG3	2.21	0.61
1:B:110:GLY:H	2:B:601:ADP:PB	2.23	0.61
1:B:41:VAL:HG12	1:B:52:VAL:CG2	2.31	0.61
1:A:91:ASP:HA	1:A:94:ILE:CG2	2.31	0.61
1:B:106:GLN:HA	1:B:270:GLU:OE1	2.01	0.60
1:B:173:ASN:O	1:B:174:PRO:C	2.38	0.60
1:A:161:LEU:N	1:A:238:VAL:O	2.25	0.60
1:A:28:PHE:HE2	1:A:32:GLU:HB2	1.56	0.60
1:A:253:GLU:OE2	1:A:254:GLU:CA	2.49	0.60
1:A:145:GLU:OE1	6:A:2012:HOH:O	2.16	0.60
1:A:271:ASN:HD21	1:A:284:GLU:HA	1.67	0.60
1:A:41:VAL:CG1	1:A:52:VAL:HG23	2.30	0.60
1:B:300:THR:HG22	1:B:356:ALA:HA	0.67	0.60
1:A:309:VAL:HB	1:A:311:TYR:CE2	2.36	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:73:GLY:C	1:A:76:THR:HG22	2.22	0.60
1:B:343:LEU:O	1:B:347:LEU:HD11	2.02	0.60
1:B:170:ASP:C	1:B:170:ASP:OD1	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:CG2	1:A:247:GLU:CB	2.49	0.60
1:A:264:VAL:HG23	1:A:265:ASP:N	2.16	0.60
1:A:25:CYS:SG	4:A:1376:CL:CL	2.97	0.60
1:B:128:GLU:HG2	1:B:208:ASP:OD1	2.01	0.60
1:B:133:ALA:HB1	1:B:137:PRO:CG	2.31	0.60
1:B:342:ASN:HA	1:B:345:GLU:HB2	1.83	0.60
1:B:221:ARG:CB	1:B:231:TYR:OH	2.49	0.60
1:A:252:GLY:HA2	1:A:253:GLU:HB3	0.68	0.60
1:B:126:THR:HG23	1:B:129:GLU:H	1.67	0.60
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:86:VAL:N	1:A:88:PRO:HD2	2.17	0.59
1:B:343:LEU:C	1:B:346:THR:CG2	2.69	0.59
1:B:117:GLY:HA3	1:B:133:ALA:HA	1.84	0.59
1:B:127:TRP:CH2	1:B:207:LYS:C	2.75	0.59
1:B:341:LEU:O	1:B:345:GLU:OE1	2.21	0.59
1:B:83:ARG:O	1:B:88:PRO:HD3	2.02	0.59
1:B:28:PHE:CZ	1:B:339:ALA:HA	2.36	0.59
1:B:231:TYR:O	1:B:232:SER:CB	2.34	0.59
1:A:294:THR:O	1:A:298:VAL:HG22	1.97	0.59
1:B:136:ILE:O	1:B:140:LEU:HG	2.03	0.59
1:B:77:LYS:N	1:B:80:ASP:OD2	2.30	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:17:LYS:O	1:B:19:ILE:C	2.41	0.59
1:B:300:THR:CB	1:B:356:ALA:O	2.50	0.59
1:A:133:ALA:HB1	1:A:137:PRO:CB	2.32	0.59
1:A:82:TYR:C	1:A:82:TYR:CD1	2.76	0.59
1:B:128:GLU:N	1:B:128:GLU:OE1	2.30	0.59
1:B:221:ARG:CA	1:B:231:TYR:OH	2.51	0.59
1:A:228:MET:CG	1:A:231:TYR:CE2	2.85	0.59
1:B:239:PHE:HZ	1:B:241:VAL:HG11	1.64	0.59
1:B:113:PHE:CD2	1:B:118:GLU:HB2	2.38	0.59
1:B:127:TRP:CZ2	1:B:207:LYS:C	2.76	0.59
1:B:93:VAL:CG2	1:B:261:LEU:CD2	2.68	0.59
1:B:295:LEU:O	1:B:299:ILE:HB	2.03	0.59
1:B:24:ARG:HG2	1:B:335:THR:HG22	1.84	0.59
1:A:28:PHE:CE2	1:A:339:ALA:HB1	2.26	0.58
1:A:37:ALA:HB1	1:A:341:LEU:H	1.68	0.58
1:B:136:ILE:N	1:B:137:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:CG2	1:A:265:ASP:N	2.66	0.58
1:A:135:ILE:HG22	1:A:139:THR:OG1	2.03	0.58
1:A:29:ASN:OD1	1:A:29:ASN:N	2.33	0.58
1:B:214:LEU:CD1	5:B:1375:6LX:CBK	2.82	0.58
1:A:185:PHE:O	1:A:195:ILE:N	2.30	0.58
1:A:347:LEU:H	1:A:347:LEU:CD2	2.17	0.58
1:A:28:PHE:HE2	1:A:32:GLU:CB	2.09	0.58
1:B:131:PRO:C	1:B:138:ARG:HH21	2.07	0.58
1:B:353:ALA:O	1:B:357:LYS:N	2.35	0.58
1:A:114:THR:O	1:A:134:GLY:C	2.42	0.58
1:A:126:THR:O	1:A:129:GLU:N	2.36	0.58
1:A:156:VAL:O	1:A:203:THR:HB	2.03	0.58
1:A:104:TYR:CE2	1:A:269:SER:HB3	2.39	0.58
1:B:116:GLU:HB3	5:B:1375:6LX:NBE	2.18	0.58
1:B:210:VAL:HG13	1:B:214:LEU:HG	1.86	0.58
1:B:82:TYR:O	1:B:86:VAL:N	2.34	0.58
1:A:67:THR:CG2	1:A:359:ILE:HG21	2.33	0.58
1:A:323:SER:O	1:A:328:THR:HB	2.03	0.58
1:B:274:ARG:CG	1:B:274:ARG:HH11	1.98	0.58
1:B:227:LEU:HD23	1:B:229:ASN:HA	1.85	0.58
1:B:192:ARG:CD	1:B:322:ASP:OD1	2.51	0.58
1:B:43:CYS:HG	3:B:1367:CD:CD	1.37	0.58
1:A:165:ASN:ND2	1:A:165:ASN:N	2.50	0.58
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:A:32:GLU:OE2	1:A:37:ALA:CB	2.52	0.57
1:B:29:ASN:OD1	1:B:31:ALA:N	2.37	0.57
1:A: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:A:270:GLU:N	1:A:270:GLU:OE1	2.37	0.57
1:A:39:SER:HB3	1:A:339:ALA:HA	1.85	0.57
1:B:177:ASP:O	1:B:178:VAL:CB	2.52	0.57
1:A:320:LEU:O	1:A:324:LEU:CG	2.51	0.57
1:A:320:LEU:O	1:A:324:LEU:HG	2.04	0.57
1:A:104:TYR:CG	1:A:105:GLY:N	2.72	0.57
1:B:344:GLU:CA	1:B:347:LEU:HD13	2.24	0.57
1:B:246:LYS:HA	1:B:255:LEU:O	2.04	0.57
1:A:302:LEU:CD2	1:A:311:TYR:OH	2.52	0.57
1:B:311:TYR:HD1	1:B:317:THR:C	2.08	0.57
1:A:192:ARG:HH12	1:A:325:GLY:CA	2.06	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:116:GLU:HB3	5:A:1375:6LX:HBC1	1.85	0.57
1:A:131:PRO:HA	1:A:138:ARG:NH2	2.19	0.57
1:A:271:ASN:OD1	1:A:283:ARG:O	2.22	0.57
1:A:272:ILE:CG2	1:A:348:SER:CA	2.82	0.57
1:A:29:ASN:O	1:A:32:GLU:HB3	2.04	0.57
1:B:127:TRP:CE2	1:B:128:GLU:OE2	2.53	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:A:147:LEU:CD1	1:A:154:PHE:HD2	2.09	0.57
1:B:183:GLN:NE2	1:B:185:PHE:HZ	2.02	0.57
1:B:171:LEU:HD22	1:B:220:LYS:CG	2.31	0.57
1:B:32:GLU:OE2	1:B:339:ALA:CB	2.53	0.57
1:A:196:ILE:HG13	1:A:199:LEU:HG	1.87	0.57
1:B:261:LEU:HD13	1:B:262:ASN:H	1.70	0.57
1:A:133:ALA:HB1	1:A:137:PRO:HB2	1.87	0.57
1:A:164:TYR:HE2	1:A:231:TYR:HH	1.48	0.57
1:A:245:MET:HB2	1:A:257:LYS:CG	2.35	0.57
1:B:220:LYS:O	1:B:224:ALA:N	2.32	0.57
1:B:227:LEU:CA	1:B:229:ASN:N	2.66	0.57
1:B: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:267:ALA:HB1	4:B:1377:CL:CL	2.41	0.56
1:A:252:GLY:CA	1:A:253:GLU:CB	2.36	0.56
1:A:214:LEU:CD1	5:A:1375:6LX:HAQ	2.35	0.56
1:A:28:PHE:CD1	1:A:339:ALA:CB	2.51	0.56
1:B:239:PHE:CE1	1:B:263:LEU:HD11	2.39	0.56
1:B:80:ASP:OD1	1:B:80:ASP:N	2.33	0.56
1:B:261:LEU:CD1	1:B:262:ASN:N	2.66	0.56
1: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:211:TYR:CD1	1:B:215:GLU:OE1	2.51	0.56
1:A:302:LEU:HD21	1:A:311:TYR:OH	2.05	0.56
1:A:214:LEU:HD11	5:A:1375:6LX:CAQ	2.34	0.56
1:A:157:LYS:HG3	1:A:203:THR:HG22	1.86	0.56
1:A:342:ASN:N	1:A:342:ASN:OD1	2.38	0.56
1:A:270:GLU:HA	1:A:345:GLU:HA	1.87	0.56
1:A:26:ARG:NH2	1:A:27:PRO:O	2.38	0.56
1:A:245:MET:HE2	1:A:257:LYS:CG	2.35	0.56
1:B:118:GLU:C	1:B:132:LEU:CD1	2.74	0.56
1:A:205:HIS:ND1	1:A:205:HIS:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ALA:CB	5:A:1375:6LX:CAE	2.80	0.56
1:B:115:MET:O	1:B:136:ILE:HD12	2.05	0.56
1:B:93:VAL:O	1:B:96:GLY:N	2.38	0.56
1:B:249:THR:C	1:B:252:GLY:N	2.59	0.56
1:A:226:THR:CA	1:A:229:ASN:N	2.59	0.56
1:A:86:VAL:CA	1:A:88:PRO:HD2	2.36	0.56
1:A:20:GLN:O	1:A:332:ILE:HD12	2.06	0.56
1:A:302:LEU:CD2	1:A:311:TYR:HH	2.19	0.56
1:B:192:ARG:NH1	1:B:192:ARG:CG	2.69	0.56
1:A:106:GLN:CA	1:A:268:GLY:HA2	2.35	0.56
1:B:219:ALA:O	1:B:223:THR:N	2.28	0.56
1:A:321:GLN:O	1:A:325:GLY:N	2.31	0.56
1:A:165:ASN:ND2	1:A:165:ASN:H	2.03	0.56
1:A:116:GLU:O	5:A:1375:6LX:CBF	2.53	0.56
1:B:93:VAL:HG11	1:B:261:LEU:HB2	1.87	0.56
1:A:271:ASN:ND2	1:A:284:GLU:HA	2.21	0.55
1:B:163:ILE:CG2	1:B:236:HIS:HD2	2.18	0.55
1:A:51:SER:CB	1:A:64:LYS:O	2.54	0.55
1:A:82:TYR:HE2	1:A:139:THR:N	2.04	0.55
1:A:308:HIS:CE1	1:B:87:CYS:HB3	2.41	0.55
1:B:264:VAL:CG1	1:B:266:LEU:HD21	2.25	0.55
1:B:111:LYS:HE2	1:B:266:LEU:O	2.06	0.55
1:A:196:ILE:HG13	1:A:199:LEU:CG	2.37	0.55
1:B:66:TYR:CE2	1:B:350:LEU:HB3	2.41	0.55
1:A:234:ARG:NH1	1:A:288:ILE:HB	2.19	0.55
1:B:316:LEU:O	1:B:320:LEU:N	2.39	0.55
1:A:214:LEU:HD12	5:A:1375:6LX:CAP	2.36	0.55
1:A:137:PRO:HB3	5:A:1375:6LX:CBH	2.36	0.55
1:A:228:MET:N	1:A:228:MET:SD	2.79	0.55
1:B:261:LEU:CD1	1:B:261:LEU:C	2.74	0.55
1:B:300:THR:HG22	1:B:356:ALA:C	2.25	0.55
1:A:354:HIS:O	1:A:357:LYS:O	2.24	0.55
1:A:98:ASN:CB	1:A:323:SER:HA	2.36	0.55
1:A:245:MET:CE	1:A:257:LYS:HG2	2.36	0.55
1:B:96:GLY:O	1:B:259:GLY:HA2	2.06	0.55
1:A:160:LEU:HG	1:A:171:LEU:HD23	1.85	0.55
1:A:163:ILE:CG2	1:A:163:ILE:O	2.53	0.55
1:B:89:ILE:HG21	1:B:101:ILE:HD11	1.88	0.55
1:B:211:TYR:O	1:B:215:GLU:CB	2.55	0.55
1:B:121:PRO:O	1:B:124:GLU:HG2	2.04	0.55
1:A:73:GLY:CA	1:A:76:THR:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:TYR:O	1:B:356:ALA:CA	2.55	0.55
1:B:77:LYS:HE2	1:B:77:LYS:N	2.22	0.55
1:A:149:ASP:OD1	1:A:149:ASP:N	2.40	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:177:ASP:OD1	1:A:177:ASP:C	2.45	0.55
1:A:144:PHE:CE2	1:A:207:LYS:HB2	2.42	0.55
1:A:272:ILE:HG21	1:A:348:SER:O	2.07	0.55
1:A:41:VAL:HG23	1:A:338:PRO:CA	2.35	0.55
1:B:41:VAL:CG1	1:B:52:VAL:HG23	2.14	0.55
1:B:118:GLU:CA	1:B:132:LEU:HB3	2.37	0.54
1:B:41:VAL:CG2	1:B:338:PRO:HA	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:234:ARG:O	1:B:267:ALA:CB	2.56	0.54
1:A:253:GLU:CD	1:A:253:GLU:C	2.65	0.54
1:B:62:SER:O	1:B:63:ARG:CB	2.55	0.54
1:A:104:TYR:CD1	1:A:105:GLY:N	2.74	0.54
1:A:274:ARG:CD	1:A:347:LEU:HD12	2.36	0.54
1:A:160:LEU:C	1:A:160:LEU:CD1	2.75	0.54
1:B:239:PHE:HZ	1:B:241:VAL:CG1	2.06	0.54
1:B:227:LEU:C	1:B:228:MET:SD	2.86	0.54
1:B:232:SER:H	1:B:235:SER:CB	2.21	0.54
1:A:218:ALA:HB2	5:A:1375:6LX:CAE	2.33	0.54
1:A:285:ALA:C	1:A:289:ASN:ND2	2.50	0.54
1:B:165:ASN:N	1:B:288:ILE:CG1	2.67	0.54
1:B:53:ARG:O	1:B:54:THR:HB	2.07	0.54
1:A:67:THR:C	1:A:68:PHE:CD1	2.80	0.54
1:B:247:GLU:O	1:B:255:LEU:CB	2.53	0.54
1:A:192:ARG:NH2	1:A:322:ASP:HA	2.23	0.54
1:B:353:ALA:O	1:B:357:LYS:CG	2.55	0.54
1:B:47:ARG:O	1:B:48:LYS:HG3	2.06	0.54
1:B:188:PRO:HG2	1:B:189:ARG:HD2	1.90	0.54
1:A:162:GLU:HG2	1:A:231:TYR:CE1	2.42	0.54
1:A:72:PHE:HZ	1:A:81:VAL:H	1.55	0.54
1:B:106:GLN:O	1:B:109:THR:CB	2.53	0.54
1:B:157:LYS:HE3	1:B:242:THR:CB	2.24	0.54
1:B:100:THR:CG2	1:B:262:ASN:CG	2.75	0.54
1:B:239:PHE:CB	1:B:263:LEU:HD12	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:MET:HE3	1:A:257:LYS:CG	2.37	0.54
1:A:35:ALA:HB1	1:A:341:LEU:CG	2.36	0.54
1:B:127:TRP:CE2	1:B:128:GLU:HG3	2.43	0.54
1:B:213:ILE:HG22	1:B:214:LEU:N	2.22	0.54
1:B:211:TYR:CE1	1:B:215:GLU:CB	2.88	0.54
1:B:245:MET:O	1:B:256:VAL:HA	2.08	0.54
1:A:134:GLY:C	1:A:137:PRO:HD2	2.28	0.54
1:B:143:ILE:C	1:B:147:LEU:HD22	2.24	0.54
1:B:163:ILE:HG12	1:B:168:LEU:HB3	1.91	0.54
1:B:26:ARG:HD2	2:B:601:ADP:N9	2.23	0.54
1:B:227:LEU:CB	1:B:228:MET:C	2.75	0.54
1:B:304:GLU:HB2	1:B:306:THR:CG2	2.27	0.54
1:A:143:ILE:CD1	1:A:147:LEU:HD11	2.36	0.53
1:A:156:VAL:O	1:A:203:THR:CB	2.55	0.53
1:A:351:GLU:HB3	1:A:355:ARG:HH21	1.72	0.53
1:A:72:PHE:CZ	1:A:76:THR:OG1	2.61	0.53
1:B:343:LEU:O	1:B:347:LEU:CD1	2.56	0.53
1:B:221:ARG:HB2	1:B:231:TYR:HH	1.72	0.53
1:A:134:GLY:O	1:A:137:PRO:HD2	2.08	0.53
1:B:113:PHE:HB2	2:B:601:ADP:N7	2.24	0.53
1:A:136:ILE:N	1:A:137:PRO:CD	2.71	0.53
1:A:181:ARG:H	1:A:181:ARG:CD	2.20	0.53
1:A:78:GLN:NE2	1:A:132:LEU:C	2.58	0.53
1:B:221:ARG:O	1:B:225:ALA:N	2.41	0.53
1:A:144:PHE:CZ	1:A:207:LYS:CB	2.91	0.53
1:A: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:B:116:GLU:C	5:B:1375:6LX:HBB1	2.28	0.53
1:A:22:VAL:HB	1:A:333:ILE:HG13	1.91	0.53
1:A:118:GLU:OE1	1:A:132:LEU:HD13	2.06	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:148:THR:HG22	1:A:149:ASP:N	2.24	0.53
1:A:304:GLU:O	1:A:305:ARG:CB	2.56	0.53
1:A:160:LEU:HD22	1:A:239:PHE:CA	2.39	0.53
1:B:103:ALA:O	1:B:266:LEU:HG	2.09	0.53
1:B:164:TYR:HB3	1:B:169:PHE:CZ	2.42	0.53
1:B:26:ARG:O	1:B:338:PRO:CG	2.53	0.53
1:B:226:THR:O	1:B:228:MET:HB2	2.09	0.53
1:A:66:TYR:CD2	1:A:68:PHE:CZ	2.97	0.53
1:B:195:ILE:O	1:B:195:ILE:HD13	2.03	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:O	1:B:37:ALA:CB	2.53	0.53
1:A:119:ARG:HB2	5:A:1375:6LX:CAW	2.38	0.53
1:A:169:PHE:CE1	1:A:181:ARG:HA	2.44	0.53
1:A:144:PHE:CZ	1:A:207:LYS:HB3	2.42	0.53
1:A:143:ILE:HD13	1:A:243:ILE:HD13	1.90	0.53
1:B: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:B:261:LEU:C	1:B:261:LEU:HD13	2.30	0.53
1:B:333:ILE:HG12	1:B:333:ILE:O	2.08	0.53
1:B:342:ASN:H	1:B:342:ASN:ND2	2.06	0.53
1:B:41:VAL:HG12	1:B:52:VAL:CB	2.39	0.53
1:A:242:THR:HG21	1:A:260:LYS:HE2	1.91	0.53
1:A:239:PHE:C	1:A:239:PHE:CD1	2.82	0.53
1:A:270:GLU:CA	1:A:345:GLU:HA	2.39	0.53
1:A:347:LEU:O	1:A:351:GLU:OE2	2.27	0.53
1:B:20:GLN:O	1:B:332:ILE:N	2.38	0.53
1:B:82:TYR:C	1:B:82:TYR:HD1	2.12	0.53
1:A:66:TYR:HE1	1:A:354:HIS:HB2	1.68	0.53
1:A:50:VAL:HG12	1:A:71:VAL:HG11	1.91	0.53
1:B:227:LEU:HA	1:B:228:MET:CB	2.19	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:A:184:MET:C	1:A:184:MET:SD	2.87	0.52
1:A:86:VAL:C	1:A:88:PRO:N	2.63	0.52
1:B:183:GLN:NE2	1:B:185:PHE:CZ	2.78	0.52
1:B:98:ASN:OD1	1:B:323:SER:CB	2.57	0.52
1:A:323:SER:OG	1:A:324:LEU:CD2	2.57	0.52
1:A:104:TYR:HE2	1:A:352:TYR:CG	2.28	0.52
1:A:231:TYR:O	1:A:232:SER:OG	2.27	0.52
1:A:234:ARG:HE	1:A:234:ARG:CA	2.23	0.52
1:B:25:CYS:O	1:B:25:CYS:SG	2.67	0.52
1:A:109:THR:OG1	1:A:335:THR:CB	2.40	0.52
1:B:106:GLN:O	1:B:109:THR:N	2.43	0.52
1:B:265:ASP:CA	1:B:266:LEU:HD23	2.38	0.52
1:B:66:TYR:CE2	1:B:350:LEU:HG	2.44	0.52
1:B:82:TYR:C	1:B:82:TYR:CD1	2.83	0.52
1:A:70:MET:SD	1:A:70:MET:N	2.80	0.52
1:A:113:PHE:O	1:A:117:GLY:N	2.42	0.52
1:A:105:GLY:C	1:A:268:GLY:HA2	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLN:HA	1:B:270:GLU:CD	2.30	0.52
1:B:127:TRP:CZ2	1:B:207:LYS:O	2.62	0.52
1:B:252:GLY:CA	1:B:253:GLU:CB	2.32	0.52
1:A:104:TYR:CE1	1:A:292:LEU:HD13	2.45	0.52
1:B:161:LEU:CD2	1:B:162:GLU:H	2.09	0.52
1:B:23:VAL:HG13	1:B:23:VAL:O	2.09	0.52
1:A:245:MET:CE	1:A:257:LYS:HG3	2.39	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:82:TYR:OH	1:B:86:VAL:CG1	2.57	0.52
1:A:154:PHE:CD1	1:A:154:PHE:N	2.78	0.52
1:A:352:TYR:HA	1:A:355:ARG:HG2	1.91	0.52
1:B:82:TYR:HH	1:B:90:LEU:HD22	1.72	0.52
1:B:172:LEU:H	1:B:220:LYS:HE2	1.71	0.52
1:A:230:ALA:CA	1:A:234:ARG:HB2	2.37	0.52
1:B:204:VAL:CG2	1:B:204:VAL:O	2.58	0.52
1:A:213:ILE:O	1:A:216:LYS:CG	2.57	0.51
1:A:347:LEU:H	1:A:347:LEU:HD23	1.74	0.51
1:B:127:TRP:CE2	1:B:128:GLU:CG	2.93	0.51
1:B:32:GLU:OE2	1:B:339:ALA:HB3	2.09	0.51
1:B:301:ALA:O	1:B:306:THR:CG2	2.53	0.51
1:B:304:GLU:N	1:B:304:GLU:CD	2.58	0.51
1: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:106:GLN:HA	1:A:268:GLY:HA3	1.92	0.51
5:A:1375:6LX:CBI	5:A:1375:6LX:CAO	2.89	0.51
1:A:23:VAL:HA	1:A:334:ALA:O	2.11	0.51
1:B:211:TYR:CZ	1:B:215:GLU:CD	2.79	0.51
1:B:211:TYR:OH	1:B:215:GLU:OE2	2.23	0.51
1:B:164:TYR:CB	1:B:169:PHE:CE1	2.80	0.51
1:A:106:GLN:CB	1:A:345:GLU:CB	2.88	0.51
1:A:274:ARG:HG3	1:A:351:GLU:HG2	1.91	0.51
1:B:329:ARG:HB3	1:B:329:ARG:NH1	2.20	0.51
1:B:53:ARG:CG	1:B:54:THR:H	2.22	0.51
1:B:79:ILE:CD1	1:B:83:ARG:NH2	2.50	0.51
1:A:234:ARG:CZ	1:A:234:ARG:O	2.58	0.51
1:A:144:PHE:CG	1:A:207:LYS:HB3	2.44	0.51
1:A:73:GLY:O	1:A:76:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:HD22	1:A:165:ASN:N	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:A:110:GLY:O	1:A:113:PHE:HD1	1.93	0.51
1:A:134:GLY:O	1:A:137:PRO:CD	2.59	0.51
2:B:601:ADP:H8	2:B:601:ADP:O5'	1.93	0.51
1:A:160:LEU:HD12	1:A:161:LEU:N	2.25	0.51
1:A:168:LEU:C	1:A:169:PHE:CD1	2.85	0.51
1:A:274:ARG:HG3	1:A:351:GLU:CG	2.40	0.51
1:A:35:ALA:HB1	1:A:341:LEU:CD1	2.41	0.51
1:B:207:LYS:HG2	1:B:208:ASP:N	2.23	0.51
1:A:236:HIS:CD2	1:A:266:LEU:CD2	2.94	0.51
1:A:109:THR:HG21	1:A:335:THR:CB	2.41	0.50
1:B:143:ILE:HA	1:B:146:LYS:HG3	1.93	0.50
1:A:194:VAL:HG11	1:A:318:ARG:HG2	1.93	0.50
1:B:81:VAL:HG12	1:B:85:VAL:CG2	2.35	0.50
1:B:28:PHE:CD1	1:B:39:SER:OG	2.57	0.50
1:A:316:LEU:O	1:A:320:LEU:HG	2.10	0.50
1:A:111:LYS:O	1:A:115:MET:N	2.33	0.50
1:B:147:LEU:H	1:B:147:LEU:HD22	1.76	0.50
1:A:175:SER:C	1:A:177:ASP:H	2.15	0.50
1:A:40:ILE:H	1:A:40:ILE:HD12	1.75	0.50
1:A:105:GLY:O	1:A:111:LYS:NZ	2.44	0.50
1:A:135:ILE:O	1:A:139:THR:CA	2.60	0.50
1:B:165:ASN:CA	1:B:288:ILE:HD11	2.41	0.50
1:B:296:GLY:HA2	1:B:299:ILE:HG21	1.91	0.50
1:A:156:VAL:O	1:A:203:THR:C	2.50	0.50
1:B:127:TRP:CH2	1:B:207:LYS:HG3	2.45	0.50
1:A:26:ARG:HA	1:A:74:ALA:CB	2.42	0.50
1:B:121:PRO:HB2	1:B:122:ASN:OD1	2.11	0.50
1:B:173:ASN:C	1:B:175:SER:N	2.52	0.50
1:B:178:VAL:HG23	1:B:178:VAL:O	2.12	0.50
1:B:314:SER:HB3	1:B:317:THR:CG2	2.39	0.50
1:A: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
1:A:105:GLY:O	1:A:106:GLN:O	2.30	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:A:106:GLN:CA	1:A:268:GLY:CA	2.90	0.50
1:B:78:GLN:OE1	1:B:132:LEU:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:OD1	1:B:187:ASP:O	2.30	0.50
1:A:284:GLU:OE1	1:A:293:LEU:HD11	2.12	0.50
1:A:91:ASP:CA	1:A:94:ILE:HG22	2.41	0.50
1:A:32:GLU:OE1	1:A:32:GLU:O	2.30	0.50
1:B:164:TYR:O	1:B:167:GLU:HG2	2.12	0.50
1:B:249:THR:CA	1:B:252:GLY:HA3	2.42	0.50
1:A:97:TYR:N	1:A:97:TYR:CD1	2.80	0.50
1:B:144:PHE:O	1:B:148:THR:CB	2.53	0.50
1:A:126:THR:OG1	1:A:129:GLU:HB2	2.12	0.50
1:A:164:TYR:CZ	1:A:228:MET:SD	3.05	0.49
1:A:35:ALA:O	1:A:36:SER:CB	2.59	0.49
1:B:183:GLN:HE22	1:B:185:PHE:HZ	1.60	0.49
1:B:22:VAL:HG22	1:B:332:ILE:C	2.28	0.49
1:A:197:LYS:HZ1	1:B:250:ILE:HG13	1.77	0.49
1:A:170:ASP:O	1:A:170:ASP:OD1	2.30	0.49
1:A:117:GLY:CA	5:A:1375:6LX:CAN	2.81	0.49
1:A:28:PHE:CE2	1:A:32:GLU:CD	2.83	0.49
1:A:32:GLU:OE2	1:A:37:ALA:C	2.49	0.49
1:B:160:LEU:HD12	1:B:161:LEU:N	2.26	0.49
1:B:141:HIS:HA	1:B:207:LYS:HE3	1.93	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:296:GLY:CA	1:B:352:TYR:OH	2.60	0.49
1:B:301:ALA:C	1:B:306:THR:HG23	2.30	0.49
1:B:145:GLU:O	1:B:149:ASP:HB2	2.12	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:B:100:THR:HA	1:B:262:ASN:CG	2.32	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:126:THR:O	1:A:129:GLU:CB	2.60	0.49
1:A:262:ASN:C	1:A:263:LEU:CD1	2.78	0.49
1:B:214:LEU:CB	5:B:1375:6LX:HAA2	2.43	0.49
1:B:157:LYS:O	1:B:241:VAL:HA	2.12	0.49
1:A:250:ILE:HA	6:A:2019:HOH:O	2.13	0.49
1:A:28:PHE:HE2	1:A:32:GLU:OE1	1.96	0.49
1:B:293:LEU:O	1:B:352:TYR:OH	2.31	0.49
1:A:126:THR:O	1:A:130:ASP:N	2.43	0.49
1:A:109:THR:CG2	1:A:335:THR:OG1	2.57	0.49
1:B:82:TYR:OH	1:B:139:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLY:C	1:B:75:SER:N	2.55	0.49
1:A:192:ARG:HH22	1:A:325:GLY:HA3	1.77	0.49
1:B:354:HIS:O	1:B:357:LYS:O	2.31	0.49
1:B:120:SER:HB3	1:B:125:TYR:HB2	1.93	0.49
1:A:166:GLU:O	1:A:167:GLU:OE1	2.30	0.49
1:A:72:PHE:CZ	1:A:81:VAL:CA	2.96	0.49
1:B:264:VAL:CG1	1:B:266:LEU:HD22	2.38	0.49
1:A:185:PHE:O	1:A:195:ILE:HG13	2.13	0.49
1:B:35:ALA:O	1:B:36:SER:C	2.49	0.49
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:104:TYR:HE2	1:A:352:TYR:CB	2.26	0.48
1:B:274:ARG:O	1:B:277:ALA:N	2.46	0.48
1:B:299:ILE:HG23	1:B:300:THR:N	2.27	0.48
1:B:40:ILE:CD1	1:B:338:PRO:O	2.61	0.48
1:B:227:LEU:H	1:B:227:LEU:HD12	1.78	0.48
1:A:294:THR:HG21	1:A:314:SER:CB	2.43	0.48
1:A:144:PHE:CE2	1:A:207:LYS:CB	2.96	0.48
1:A:27:PRO:CD	1:A:74:ALA:CB	2.65	0.48
1:A:161:LEU:O	1:A:238:VAL:N	2.43	0.48
1:A:78:GLN:O	1:A:81:VAL:HG23	2.13	0.48
1:A:32:GLU:OE1	1:A:37:ALA:HB3	2.13	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:B:342:ASN:ND2	1:B:342:ASN:N	2.61	0.48
1:A:19:ILE:C	1:A:20:GLN:HE21	2.11	0.48
1:A:304:GLU:O	1:A:305:ARG:HB2	2.14	0.48
1:A:160:LEU:H	1:A:172:LEU:CD2	2.27	0.48
1:B:131:PRO:CA	1:B:138:ARG:HH22	2.09	0.48
1:B:295:LEU:O	1:B:299:ILE:CB	2.60	0.48
1:A:120:SER:OG	1:A:130:ASP:CG	2.50	0.48
1:A:104:TYR:CE2	1:A:352:TYR:CD2	3.01	0.48
1:A:134:GLY:O	1:A:138:ARG:HG3	2.13	0.48
1:A:156:VAL:CG1	1:A:204:VAL:N	2.76	0.48
1:A:225:ALA:CB	1:A:231:TYR:HB3	2.39	0.48
1:A:281:ARG:HA	1:A:284:GLU:OE2	2.12	0.48
1:B:343:LEU:N	1:B:346:THR:HG22	2.28	0.48
1:B:231:TYR:C	1:B:231:TYR:CD1	2.87	0.48
1:B:187:ASP:OD1	1:B:190:ASN:N	2.35	0.48
1:A:152:THR:CG2	1:A:247:GLU:CG	2.51	0.48
1:A:236:HIS:O	1:A:265:ASP:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLY:N	1:A:76:THR:HG22	2.28	0.48
1:B:110:GLY:HA2	2:B:601:ADP:H8	1.74	0.48
1:B:204:VAL:HG23	1:B:204:VAL:O	2.12	0.48
1:A:136:ILE:O	1:A:140:LEU:HD23	2.13	0.48
1:A:164:TYR:CE2	1:A:231:TYR:OH	2.58	0.48
1:A:232:SER:HB3	6:A:2009:HOH:O	2.14	0.48
1:B:157:LYS:CE	1:B:242:THR:HB	2.27	0.48
1:B:361:ASN:OD1	1:B:361:ASN:N	2.46	0.48
1:A:109:THR:HG21	1:A:335:THR:HG1	1.77	0.47
1:B:22:VAL:HG22	1:B:333:ILE:HG22	1.75	0.47
1:A:308:HIS:ND1	1:B:88:PRO:HG3	2.29	0.47
1:B:227:LEU:CA	1:B:228:MET:HB2	2.41	0.47
1:B:353:ALA:O	1:B:357:LYS:HG3	2.14	0.47
1:A:125:TYR:N	1:A:125:TYR:HD1	1.96	0.47
1:A:295:LEU:O	1:A:299:ILE:HB	2.14	0.47
1:B:236:HIS:ND1	1:B:236:HIS:C	2.67	0.47
1:B:82:TYR:CD1	1:B:82:TYR:O	2.62	0.47
1:B:171:LEU:HA	1:B:177:ASP:OD2	2.13	0.47
1:A:135:ILE:CG2	1:A:139:THR:OG1	2.63	0.47
5:A:1375:6LX:CAW	5:A:1375:6LX:HAC2	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
1:A:30:LEU:CD1	1:A:31:ALA:N	2.77	0.47
1:B:30:LEU:HD13	1:B:30:LEU:C	2.35	0.47
1:B:98:ASN:HD21	1:B:260:LYS:CG	2.27	0.47
1:A:66:TYR:CZ	1:A:350:LEU:O	2.60	0.47
1:B:95:MET:HB3	1:B:97:TYR:CD1	2.47	0.47
1:A:242:THR:CG2	1:A:260:LYS:HE2	2.45	0.47
1:B:122:ASN:HB2	1:B:123:GLU:H	1.51	0.47
1:A:129:GLU:N	1:A:129:GLU:OE1	2.48	0.47
1:A:112:THR:HG23	1:A:116:GLU:HG3	1.97	0.47
1:A:283:ARG:NH2	1:A:344:GLU:OE2	2.48	0.47
1:B:53:ARG:C	1:B:54:THR:CG2	2.74	0.47
1:B:79:ILE:CD1	1:B:83:ARG:HH21	2.20	0.47
1:A:202:ILE:HG12	1:A:202:ILE:O	2.13	0.47
1:A:121:PRO:O	1:A:122:ASN:HB2	2.14	0.47
1:A:117:GLY:O	5:A:1375:6LX:CAN	2.43	0.47
1:A:85:VAL:O	1:A:88:PRO:HG2	2.14	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:283:ARG:HA	1:A:283:ARG:HD2	1.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:254:GLU:C	1:B:255:LEU:HD13	2.35	0.47
1:A:290:GLN:HE21	1:A:290:GLN:HB3	1.54	0.47
1:A:197:LYS:HB2	1:A:197:LYS:HE2	1.51	0.47
1:B:250:ILE:CD1	1:B:250:ILE:H	2.08	0.47
1:B:250:ILE:O	6:B:2017:HOH:O	2.21	0.47
1:B:121:PRO:CB	1:B:122:ASN:OD1	2.63	0.47
1:A:174:PRO:HB3	1:A:220:LYS:HD2	1.97	0.47
1:A:37:ALA:HB2	1:A:341:LEU:HB2	1.97	0.47
1:A:263:LEU:CD1	1:A:263:LEU:N	2.76	0.47
1:B:299:ILE:CG2	1:B:300:THR:N	2.77	0.47
1:B:227:LEU:CD2	1:B:229:ASN:HA	2.45	0.47
1:B:30:LEU:HA	1:B:33:ARG:HB3	1.97	0.47
1:A:167:GLU:CD	1:A:181:ARG:HG3	2.35	0.47
1:B:264:VAL:CG1	1:B:266:LEU:CD2	2.73	0.47
1:A:47:ARG:O	1:A:48:LYS:CB	2.62	0.47
1:A:42:GLU:C	4:A:1378:CL:CL	2.91	0.46
1:A:285:ALA:N	1:A:289:ASN:ND2	2.64	0.46
1:A:73:GLY:C	1:A:76:THR:CG2	2.83	0.46
1:A:83:ARG:HA	1:A:87:CYS:CB	2.31	0.46
1:B:113:PHE:HB2	2:B:601:ADP:C8	2.50	0.46
1:B:134:GLY:C	1:B:137:PRO:CD	2.72	0.46
1:B:221:ARG:O	1:B:231:TYR:CE1	2.67	0.46
1:B:353:ALA:O	1:B:357:LYS:C	2.48	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
5:A:1375:6LX:CBF	5:A:1375:6LX:CAN	2.93	0.46
1:A:229:ASN:C	1:A:229:ASN:ND2	2.69	0.46
1:B:127:TRP:HZ2	1:B:208:ASP:OD1	1.94	0.46
1:B:104:TYR:CZ	1:B:349:THR:HB	2.47	0.46
1:A:114:THR:HA	1:A:134:GLY:HA2	1.97	0.46
1:A:167:GLU:CG	1:A:181:ARG:CG	2.89	0.46
1:B:295:LEU:HD13	1:B:295:LEU:HA	1.78	0.46
1:B:224:ALA:O	1:B:228:MET:HG2	2.16	0.46
1:B:308:HIS:ND1	1:B:309:VAL:N	2.63	0.46
1:A:284:GLU:CB	1:A:293:LEU:HD21	2.43	0.46
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:66:TYR:OH	1:A:354:HIS:CA	2.63	0.46
1:A:119:ARG:HB2	5:A:1375:6LX:HAX	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:HD11	1:A:355:ARG:HH12	1.66	0.46
1:A:81:VAL:O	1:A:85:VAL:CG2	2.59	0.46
1:A:39:SER:HB3	1:A:339:ALA:N	2.30	0.46
1:B:234:ARG:HD3	1:B:288:ILE:HD13	1.98	0.46
1:B:346:THR:O	1:B:349:THR:OG1	2.25	0.46
1:B:211:TYR:CD1	1:B:211:TYR:C	2.88	0.46
1:A:178:VAL:O	1:A:179:SER:HB2	2.15	0.46
1:A:51:SER:HB3	1:A:64:LYS:O	2.16	0.46
1:B:280:LYS:O	1:B:284:GLU:O	2.34	0.46
1:B:194:VAL:O	1:B:194:VAL:HG23	2.15	0.46
1:A:209:GLU:CD	1:A:213:ILE:CD1	2.84	0.46
1:A:308:HIS:HE1	1:B:87:CYS:HB3	1.79	0.46
1:B:195:ILE:HD13	1:B:196:ILE:C	2.36	0.46
1:A:144:PHE:CG	1:A:207:LYS:CB	2.98	0.46
1:A:283:ARG:HH21	1:A:344:GLU:CD	2.19	0.46
1:A:196:ILE:CG1	1:A:199:LEU:HG	2.46	0.46
1:A:274:ARG:O	1:A:280:LYS:HG3	2.16	0.46
1:B:299:ILE:CA	1:B:302:LEU:HG	2.44	0.46
1:B:354:HIS:C	1:B:357:LYS:O	2.54	0.46
1:A:126:THR:N	1:A:129:GLU:HB2	2.31	0.46
1:A:167:GLU:CD	1:A:181:ARG:CB	2.80	0.46
1:B:40:ILE:HD13	1:B:41:VAL:N	2.30	0.46
1:B:170:ASP:OD1	1:B:171:LEU:N	2.49	0.46
1:B:47:ARG:CB	1:B:49:GLU:OE1	2.60	0.46
1:B:165:ASN:N	1:B:288:ILE:HG13	2.32	0.46
1:A:163:ILE:HG22	1:A:163:ILE:O	2.16	0.46
1:A:113:PHE:O	1:A:117:GLY:C	2.55	0.45
1:A:164:TYR:HE2	1:A:231:TYR:OH	1.97	0.45
1:B:242:THR:HG23	1:B:260:LYS:HG2	1.98	0.45
1:B:93:VAL:C	1:B:96:GLY:H	2.19	0.45
1:A:42:GLU:C	4:A:1376:CL:CL	2.92	0.45
1:B:157:LYS:HA	1:B:202:ILE:O	2.16	0.45
1:B:195:ILE:CD1	1:B:196:ILE:C	2.84	0.45
1:A: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:A:24:ARG:HG3	1:A:72:PHE:HB3	1.98	0.45
1:B:112:THR:O	1:B:116:GLU:CA	2.65	0.45
1:B:268:GLY:N	4:B:1377:CL:CL	2.86	0.45
1:B:40:ILE:HG12	1:B:343:LEU:CB	2.46	0.45
1:A:78:GLN:OE1	1:A:114:THR:HG22	2.17	0.45
1:B:87:CYS:CB	1:B:88:PRO:HD3	2.47	0.45

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:264:VAL:C	1:A:265:ASP:OD1	2.56	0.44
1:B:48:LYS:C	1:B:71:VAL:CG2	2.84	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:HD1	1:A:154:PHE:N	2.15	0.44
1:B:96:GLY:O	1:B:258:ILE:O	2.36	0.44
1:A:88:PRO:C	1:A:91:ASP:OD1	2.46	0.44
1:B:128:GLU:O	1:B:141:HIS:CD2	2.70	0.44
1:B:239:PHE:C	1:B:239:PHE:CD1	2.91	0.44
1:B:41:VAL:HA	1:B:52:VAL:CB	2.45	0.44
1:A:178:VAL:O	1:A:179:SER:CB	2.64	0.44
1:A:342:ASN:HB3	1:A:345:GLU:OE2	2.18	0.44
1:A:39:SER:HB3	1:A:339:ALA:CA	2.47	0.44
1:B:110:GLY:N	2:B:601:ADP:PB	2.89	0.44
1:B:78:GLN:CD	1:B:132:LEU:O	2.56	0.44
1:A:192:ARG:NH2	1:A:325:GLY:HA3	2.31	0.44
1:A:362:LYS:HA	1:A:362:LYS:HD2	1.44	0.44
1:A:228:MET:HB3	1:A:229:ASN:H	1.62	0.44
1:A:238:VAL:CG2	1:A:238:VAL:O	2.62	0.44
1:A:106:GLN:CA	1:A:269:SER:H	2.28	0.44
1:B:143:ILE:CA	1:B:146:LYS:HG3	2.47	0.44
1:B:158:VAL:HG22	1:B:158:VAL:O	2.17	0.44
1:B:337:SER:CB	1:B:342:ASN:OD1	2.62	0.44
1:A:23:VAL:CG2	1:A:68:PHE:CD2	2.99	0.44
1:B:320:LEU:HA	1:B:320:LEU:HD23	1.82	0.44
1:A:178:VAL:HG11	6:A:2031:HOH:O	2.18	0.44
1:B:297:ARG:HG3	1:B:298:VAL:N	2.31	0.44
1:A:121:PRO:O	1:A:122:ASN:CB	2.64	0.44
1:B:207:LYS:O	1:B:210:VAL:HB	2.18	0.44
1:A:234:ARG:CA	1:A:234:ARG:NE	2.80	0.44
1:B:318:ARG:O	1:B:321:GLN:CG	2.65	0.44
1:A:241:VAL:HG12	1:A:241:VAL:O	2.18	0.44
1:A:114:THR:HA	1:A:134:GLY:HA3	2.00	0.44
1:A:245:MET:HE3	1:A:257:LYS:HG3	2.00	0.44
1:B:160:LEU:HD12	1:B:161:LEU:H	1.83	0.44
1:B:19:ILE:HG21	1:B:299:ILE:HD11	1.99	0.44
1:B:296:GLY:N	1:B:352:TYR:OH	2.51	0.44
1:A:230:ALA:CB	1:A:234:ARG:HB3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:SER:O	1:B:63:ARG:HB2	2.17	0.44
1:A:355:ARG:HG3	1:A:356:ALA:N	2.33	0.44
1:B:359:ILE:H	1:B:359:ILE:HG12	1.73	0.44
1:A:117:GLY:CA	5:A:1375:6LX:CAO	2.96	0.43
1:A:156:VAL:HG12	1:A:204:VAL:N	2.33	0.43
1:A:156:VAL:HG12	1:A:204:VAL:H	1.82	0.43
1:A:295:LEU:HB3	1:A:352:TYR:OH	2.18	0.43
1:B:300:THR:CG2	1:B:356:ALA:CA	2.42	0.43
1:A:315:LYS:CA	1:A:315:LYS:HE2	2.46	0.43
1:B:133:ALA:HB1	1:B:137:PRO:HG3	2.00	0.43
1:B:202:ILE:O	1:B:202:ILE:HG22	2.18	0.43
1:B:40:ILE:O	1:B:52:VAL:CB	2.61	0.43
1:A:309:VAL:HG21	1:A:311:TYR:CD2	2.26	0.43
1:B:94:ILE:HD12	1:B:245:MET:CE	2.48	0.43
5:A:1375:6LX:CBI	5:A:1375:6LX:HAB	2.48	0.43
1:A:131:PRO:C	1:A:138:ARG:HH21	2.21	0.43
1:A:231:TYR:C	1:A:232:SER:OG	2.54	0.43
1:A:272:ILE:HD13	1:A:273:GLY:O	2.18	0.43
1:A:351:GLU:N	1:A:351:GLU:CD	2.72	0.43
1:B:270:GLU:CD	1:B:270:GLU:H	2.13	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:CG1	1:A:241:VAL:O	2.66	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:230:ALA:O	1:A:234:ARG:HB2	2.18	0.43
1:A:323:SER:O	1:A:328:THR:CB	2.65	0.43
1:A:47:ARG:CA	1:A:47:ARG:HE	2.21	0.43
1:A:131:PRO:HA	1:A:138:ARG:HH22	1.82	0.43
1:A:227:LEU:CA	1:A:228:MET:C	2.87	0.43
1:A:284:GLU: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:52:VAL:O	1:B:52:VAL:CG1	2.67	0.43
1:A:68:PHE:HB2	1:A:71:VAL:HG22	2.00	0.43
1:B:249:THR:H	1:B:252:GLY:HA3	1.84	0.43
1:B:240:SER:O	1:B:240:SER:OG	2.30	0.43
1:A:352:TYR:CA	1:A:355:ARG:HG2	2.49	0.43
1:B:137:PRO:HB3	5:B:1375:6LX:CBJ	2.49	0.43
1:B:18:ASN:O	1:B:20:GLN:CD	2.57	0.43
1:A:246:LYS:HA	1:A:255:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:THR:HG23	1:B:262:ASN:CG	2.29	0.43
1:B:40:ILE:HG12	1:B:343:LEU:HA	2.00	0.43
1:A:168:LEU:C	1:A:169:PHE:HD1	2.21	0.43
1:A:270:GLU:CB	1:A:345:GLU:HA	2.49	0.43
1:A:272:ILE:CG2	1:A:348:SER:O	2.67	0.43
1:A:152:THR:HG22	1:A:247:GLU:OE1	1.85	0.43
1:A:110:GLY:O	1:A:113:PHE:CD1	2.71	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:294:THR:C	1:A:298:VAL:HG23	2.21	0.43
1:A:196:ILE:HD11	1:A:199:LEU:HG	2.01	0.43
1:B:111:LYS:N	2:B:601:ADP:O1B	2.52	0.42
1:B:234:ARG:HA	4:B:1377:CL:CL	2.56	0.42
1:B:168:LEU:HD11	1:B:184:MET:HE2	2.01	0.42
1:B:221:ARG:HA	1:B:231:TYR:OH	2.19	0.42
1:A:157:LYS:HG3	1:A:203:THR:CG2	2.49	0.42
1:A:271:ASN:ND2	1:A:271:ASN:C	2.72	0.42
1:A:274:ARG:O	1:A:277:ALA:CB	2.67	0.42
1:B:342:ASN:HD22	1:B:343:LEU:N	2.10	0.42
1:B:248:THR:HA	1:B:253:GLU:O	2.19	0.42
1:A:95:MET:HB3	1:A:97:TYR:CE1	2.54	0.42
1:B:301:ALA:HA	1:B:304:GLU:HG2	1.78	0.42
1:A:306:THR:CG2	1:A:307:PRO:HD2	2.48	0.42
5:A:1375:6LX:HAB	5:A:1375:6LX:CBF	2.48	0.42
1:A:144:PHE:CZ	1:A:207:LYS:HA	2.54	0.42
1: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:253:GLU:OE2	1:A:253:GLU:O	2.37	0.42
1:B:317:THR:HG1	1:B:318:ARG:N	2.17	0.42
1:B:299:ILE:CG2	1:B:356:ALA:HB1	2.49	0.42
1:B:110:GLY:HA2	2:B:601:ADP:PA	2.58	0.42
1:B:89:ILE:HG22	1:B:90:LEU:N	2.33	0.42
1:A:21:VAL:HG21	1:A:357:LYS:CB	2.45	0.42
1:A:117:GLY:HA2	1:A:134:GLY:CA	2.48	0.42
1:A:296:GLY:HA2	1:A:299:ILE:HG22	2.01	0.42
1:A:102:PHE:C	1:A:102:PHE:CD1	2.93	0.42
1:A:21:VAL:HA	1:A:332:ILE:O	2.19	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
1:A:126:THR:O	1:A:129:GLU:CA	2.67	0.42
1:A:306:THR:HA	1:A:307:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:O	1:A:143:ILE:HG22	2.20	0.42
1:A:50:VAL:O	1:A:50:VAL:HG22	2.18	0.42
1:B:59:ASP:HB3	1:B:60:LYS:H	1.58	0.42
1:A:133:ALA:N	5:A:1375:6LX:HAZ1	2.33	0.42
1:A:223:THR:CG2	1:A:224:ALA:N	2.83	0.42
1:A:226:THR:C	1:A:229:ASN:N	2.72	0.42
1:A:82:TYR:O	1:A:86:VAL:HB	2.20	0.42
1:B:300:THR:HG22	1:B:356:ALA:CB	2.39	0.42
1:B:72:PHE:CE2	1:B:81:VAL:HG13	2.55	0.42
1:B:86:VAL:HG21	1:B:135:ILE:HG21	2.01	0.42
1: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:A:277:ALA:HB3	1:A:279:ASP:O	2.20	0.42
1:A:281:ARG:O	1:A:285:ALA:CA	2.68	0.42
1:B:120:SER:OG	1:B:125:TYR:CB	2.65	0.42
1:B:276:GLY:O	1:B:278:VAL:N	2.53	0.42
1:A:25:CYS:O	1:A:73:GLY:O	2.38	0.42
1:B:101:ILE:HB	1:B:263:LEU:HA	2.02	0.42
1:B:118:GLU:H	1:B:132:LEU:C	2.23	0.42
1:B:348:SER:O	1:B:351:GLU:HB3	2.20	0.42
1:B:69:ASP:OD1	1:B:69:ASP:N	2.52	0.42
1:B:234:ARG:NH1	1:B:288:ILE:CD1	2.79	0.41
1:A:242:THR:CG2	1:A:260:LYS:CE	2.98	0.41
1:A:118:GLU:CD	1:A:132:LEU:HD13	2.39	0.41
1:B:133:ALA:HB1	1:B:137:PRO:CB	2.50	0.41
1:B:21:VAL:HA	1:B:332:ILE:HB	2.01	0.41
1:B:221:ARG:CG	1:B:222:THR:N	2.83	0.41
5:A:1375:6LX:CBF	5:A:1375:6LX:CAB	2.98	0.41
1:A:225:ALA:CA	1:A:231:TYR:HB2	2.50	0.41
1:A:242:THR:HG23	1:A:260:LYS:CE	2.45	0.41
1:A:48:LYS:HB3	1:A:48:LYS:HE3	1.75	0.41
1:B:210:VAL:CG1	1:B:214:LEU:CD1	2.98	0.41
1:A:27:PRO:N	1:A:74:ALA:HB1	2.31	0.41
1:A:109:THR:CG2	1:A:335:THR:CB	2.98	0.41
1:A:42:GLU:CA	4:A:1378:CL:CL	3.05	0.41
1:A:217:GLY:CA	5:A:1375:6LX:CAP	2.95	0.41
1:B:344:GLU:HG3	1:B:345:GLU:N	2.35	0.41
1:B:90:LEU:HD12	1:B:90:LEU:C	2.40	0.41
1:B:318:ARG:O	1:B:321:GLN:HG2	2.20	0.41
1:A:112:THR:HG22	1:A:116:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:VAL:HA	1:A:97:TYR:O	2.20	0.41
1:A:134:GLY:N	1:A:137:PRO:CG	2.83	0.41
1:B:135:ILE:C	1:B:137:PRO:HD2	2.41	0.41
1:B:22:VAL:HG12	1:B:70:MET:CB	2.50	0.41
1:B:22:VAL:O	1:B:333:ILE:HA	2.21	0.41
1:A:49:GLU:OE1	1:A:67:THR:CB	2.65	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:315:LYS:HB3	1:A:315:LYS:HE2	1.89	0.41
1:A:113:PHE:CD1	1:A:114:THR:HG23	2.43	0.41
1:A:213:ILE:CA	1:A:216:LYS:HE2	2.38	0.41
1:A:106:GLN:C	1:A:268:GLY:HA2	2.41	0.41
1:B: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:94:ILE:O	1:A:245:MET:CE	2.57	0.41
1:A:72:PHE:CE1	1:A:81:VAL:HG13	2.56	0.41
1:A:72:PHE:CZ	1:A:80:ASP:HB3	2.56	0.41
1:A:37:ALA:CB	1:A:341:LEU:H	2.34	0.41
1:A:41:VAL:HG21	1:A:338:PRO:C	2.40	0.41
1:B:53:ARG:CG	1:B:54:THR:N	2.84	0.41
1:B:19:ILE:N	1:B:19:ILE:HD12	2.29	0.41
1:B:177:ASP:N	1:B:220:LYS:NZ	2.66	0.41
1:A:298:VAL:HG12	1:A:311:TYR:CE2	2.55	0.41
1:B:195:ILE:CD1	1:B:195:ILE:O	2.66	0.41
1:B:212:GLN:C	1:B:216:LYS:HG3	2.26	0.41
1:B:294:THR:HG22	1:B:298:VAL:CG2	2.51	0.41
1:A:360:LEU:HD13	1:A:360:LEU:HA	1.86	0.41
1:A:225:ALA:CB	1:A:231:TYR:CG	3.03	0.41
1:A:262:ASN:O	1:A:263:LEU:CD1	2.69	0.41
1: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:A:21:VAL:CG2	1:A:357:LYS:CG	2.94	0.41
1:A:49:GLU:CD	1:A:67:THR:CA	2.77	0.41
1:B:317:THR:HA	1:B:320:LEU:HB2	2.02	0.41
1:A:22:VAL:O	1:A:333:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TYR:OH	1:A:269:SER:HB3	2.20	0.40
1:B:299:ILE:HG23	1:B:356:ALA:HB1	2.02	0.40
1:B:190:ASN:OD1	1:B:192:ARG:HB2	2.21	0.40
1:A:192:ARG:HH22	1:A:325:GLY:CA	2.35	0.40
1:B:353:ALA:HB1	1:B:359:ILE:HD11	2.03	0.40
1:A:175:SER:O	1:A:177:ASP:N	2.54	0.40
5:A:1375:6LX:CAM	5:A:1375:6LX:HBF	2.51	0.40
1:A:66:TYR:HA	1:A:66:TYR:HD1	1.76	0.40
1:B:23:VAL:HG23	1:B:336:ILE:HD11	2.03	0.40
1:B:164:TYR:O	1:B:167:GLU:CG	2.69	0.40
1:B: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:B:186:ASP:HA	1:B:194:VAL:HG12	2.02	0.40
1:A:270:GLU:HB3	1:A:345:GLU:HA	2.03	0.40
1:B:164:TYR:CD1	1:B:234:ARG:HD2	2.56	0.40
1:A:192:ARG:HG2	1:A:321:GLN:HE21	1.87	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 (30) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASP:CA	1:B:344:GLU:OE2[1_545]	1.77	0.43
1:A:206:ASN:CB	1:B:344:GLU:OE1[1_545]	1.81	0.39
1:A:59:ASP:CG	1:A:287:ASN:ND2[3_565]	1.82	0.38
1:A:123:GLU:OE2	1:A:189:ARG:NH1[3_555]	1.83	0.37
1:A:206:ASN:OD1	1:B:274:ARG:CD[1_545]	1.84	0.36
1:B:33:ARG:NH1	1:B:253:GLU:OE1[3_565]	1.85	0.35
1:A:212:GLN:NE2	1:B:345:GLU:OE1[1_545]	1.96	0.24
1:B:33:ARG:CZ	1:B:253:GLU:CG[3_565]	1.98	0.22
1:B:297:ARG:NH2	4:A:1377:CL:CL[2_564]	1.98	0.22
1:B:60:LYS:CB	1:B:287:ASN:CB[3_465]	2.07	0.13
1:A:59:ASP:OD2	1:A:287:ASN:CG[3_565]	2.12	0.08
1:B:33:ARG:NH2	1:B:253:GLU:CB[3_565]	2.12	0.08
1:A:208:ASP:N	1:B:344:GLU:OE2[1_545]	2.14	0.06
1:A:27:PRO:CB	1:A:253:GLU:N[3_555]	2.18	0.02
1:A:208:ASP:CB	1:B:344:GLU:OE2[1_545]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	343/368 (93%)	325 (95%)	9 (3%)	9 (3%)	7 22
1	B	341/368 (93%)	318 (93%)	12 (4%)	11 (3%)	5 17
All	All	684/736 (93%)	643 (94%)	21 (3%)	20 (3%)	6 19

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

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

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

Mol	Chain	Res	Type
1	A	19	ILE
1	A	26	ARG
1	A	29	ASN
1	A	30	LEU
1	A	36	SER
1	A	38	HIS
1	A	39	SER
1	A	40	ILE

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Mol	Chain	Res	Type
1	A	41	VAL
1	A	42	GLU
1	A	44	ASP
1	A	46	VAL
1	A	47	ARG
1	A	48	LYS
1	A	54	THR
1	A	59	ASP
1	A	65	THR
1	A	66	TYR
1	A	67	THR
1	A	69	ASP
1	A	70	MET
1	A	71	VAL
1	A	72	PHE
1	A	76	THR
1	A	81	VAL
1	A	82	TYR
1	A	83	ARG
1	A	84	SER
1	A	85	VAL
1	A	89	ILE
1	A	91	ASP
1	A	92	GLU
1	A	93	VAL
1	A	95	MET
1	A	97	TYR
1	A	98	ASN
1	A	107	THR
1	A	109	THR
1	A	111	LYS
1	A	113	PHE
1	A	114	THR
1	A	115	MET
1	A	118	GLU
1	A	123	GLU
1	A	124	GLU
1	A	125	TYR
1	A	127	TRP
1	A	128	GLU
1	A	129	GLU
1	A	143	ILE

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Mol	Chain	Res	Type
1	A	148	THR
1	A	149	ASP
1	A	154	PHE
1	A	155	SER
1	A	156	VAL
1	A	157	LYS
1	A	160	LEU
1	A	162	GLU
1	A	163	ILE
1	A	165	ASN
1	A	166	GLU
1	A	167	GLU
1	A	168	LEU
1	A	170	ASP
1	A	171	LEU
1	A	177	ASP
1	A	178	VAL
1	A	181	ARG
1	A	182	LEU
1	A	183	GLN
1	A	190	ASN
1	A	194	VAL
1	A	196	ILE
1	A	197	LYS
1	A	202	ILE
1	A	205	HIS
1	A	207	LYS
1	A	208	ASP
1	A	209	GLU
1	A	211	TYR
1	A	213	ILE
1	A	214	LEU
1	A	216	LYS
1	A	222	THR
1	A	223	THR
1	A	227	LEU
1	A	228	MET
1	A	229	ASN
1	A	231	TYR
1	A	232	SER
1	A	234	ARG
1	A	235	SER

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Mol	Chain	Res	Type
1	A	236	HIS
1	A	237	SER
1	A	239	PHE
1	A	241	VAL
1	A	242	THR
1	A	243	ILE
1	A	244	HIS
1	A	245	MET
1	A	248	THR
1	A	249	THR
1	A	250	ILE
1	A	251	ASP
1	A	253	GLU
1	A	254	GLU
1	A	257	LYS
1	A	260	LYS
1	A	263	LEU
1	A	264	VAL
1	A	265	ASP
1	A	266	LEU
1	A	269	SER
1	A	270	GLU
1	A	271	ASN
1	A	272	ILE
1	A	275	SER
1	A	278	VAL
1	A	280	LYS
1	A	283	ARG
1	A	284	GLU
1	A	290	GLN
1	A	291	SER
1	A	293	LEU
1	A	298	VAL
1	A	299	ILE
1	A	304	GLU
1	A	305	ARG
1	A	315	LYS
1	A	316	LEU
1	A	318	ARG
1	A	319	ILE
1	A	324	LEU
1	A	328	THR

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Mol	Chain	Res	Type
1	A	332	ILE
1	A	333	ILE
1	A	335	THR
1	A	336	ILE
1	A	337	SER
1	A	340	SER
1	A	341	LEU
1	A	342	ASN
1	A	343	LEU
1	A	345	GLU
1	A	347	LEU
1	A	351	GLU
1	A	358	ASN
1	A	360	LEU
1	A	362	LYS
1	B	20	GLN
1	B	21	VAL
1	B	24	ARG
1	B	25	CYS
1	B	28	PHE
1	B	33	ARG
1	B	34	LYS
1	B	36	SER
1	B	38	HIS
1	B	40	ILE
1	B	41	VAL
1	B	43	CYS
1	B	44	ASP
1	B	46	VAL
1	B	48	LYS
1	B	50	VAL
1	B	52	VAL
1	B	62	SER
1	B	70	MET
1	B	76	THR
1	B	77	LYS
1	B	78	GLN
1	B	79	ILE
1	B	82	TYR
1	B	85	VAL
1	B	87	CYS
1	B	89	ILE

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Mol	Chain	Res	Type
1	B	94	ILE
1	B	95	MET
1	B	98	ASN
1	B	100	THR
1	B	101	ILE
1	B	104	TYR
1	B	107	THR
1	B	111	LYS
1	B	113	PHE
1	B	114	THR
1	B	119	ARG
1	B	120	SER
1	B	122	ASN
1	B	123	GLU
1	B	124	GLU
1	B	129	GLU
1	B	132	LEU
1	B	139	THR
1	B	141	HIS
1	B	142	GLN
1	B	144	PHE
1	B	146	LYS
1	B	148	THR
1	B	153	GLU
1	B	156	VAL
1	B	157	LYS
1	B	159	SER
1	B	161	LEU
1	B	162	GLU
1	B	165	ASN
1	B	166	GLU
1	B	168	LEU
1	B	169	PHE
1	B	170	ASP
1	B	171	LEU
1	B	172	LEU
1	B	176	SER
1	B	177	ASP
1	B	178	VAL
1	B	181	ARG
1	B	183	GLN
1	B	187	ASP

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Mol	Chain	Res	Type
1	B	195	ILE
1	B	197	LYS
1	B	200	GLU
1	B	204	VAL
1	B	207	LYS
1	B	210	VAL
1	B	213	ILE
1	B	220	LYS
1	B	221	ARG
1	B	222	THR
1	B	227	LEU
1	B	228	MET
1	B	231	TYR
1	B	232	SER
1	B	234	ARG
1	B	236	HIS
1	B	240	SER
1	B	245	MET
1	B	248	THR
1	B	249	THR
1	B	250	ILE
1	B	255	LEU
1	B	256	VAL
1	B	258	ILE
1	B	261	LEU
1	B	262	ASN
1	B	263	LEU
1	B	266	LEU
1	B	269	SER
1	B	270	GLU
1	B	271	ASN
1	B	272	ILE
1	B	274	ARG
1	B	275	SER
1	B	287	ASN
1	B	292	LEU
1	B	293	LEU
1	B	295	LEU
1	B	297	ARG
1	B	302	LEU
1	B	304	GLU
1	B	306	THR

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

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	38	HIS
1	A	141	HIS
1	A	165	ASN
1	A	229	ASN
1	A	290	GLN
1	A	358	ASN
1	B	20	GLN
1	B	150	ASN
1	B	173	ASN
1	B	183	GLN
1	B	212	GLN
1	B	244	HIS

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Mol	Chain	Res	Type
1	B	321	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	6LX	A	1375	-	38,40,40	2.47	15 (39%)	44,56,56	1.42	7 (15%)
2	ADP	A	601	3	22,29,29	0.94	1 (4%)	27,45,45	2.14	5 (18%)
5	6LX	B	1375	-	38,40,40	2.14	10 (26%)	44,56,56	1.93	9 (20%)
2	ADP	B	601	3	22,29,29	1.01	1 (4%)	27,45,45	1.94	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1375	6LX	OAH-CAI	-3.80	1.30	1.35
5	A	1375	6LX	OAH-CAI	-2.76	1.31	1.35
5	A	1375	6LX	CAB-CAJ	-2.27	1.48	1.54
5	A	1375	6LX	CAQ-CAP	2.12	1.41	1.36
5	B	1375	6LX	CBJ-CBK	2.14	1.43	1.38
5	A	1375	6LX	CBJ-CBK	2.18	1.43	1.38
5	A	1375	6LX	CAQ-CAR	2.20	1.45	1.41
5	A	1375	6LX	CAZ-CAY	2.27	1.59	1.51
5	B	1375	6LX	CAZ-CAY	2.29	1.59	1.51
5	A	1375	6LX	CBH-CBG	2.32	1.43	1.38
5	B	1375	6LX	CAU-NAK	2.34	1.50	1.46
5	B	1375	6LX	CAP-CAE	2.38	1.42	1.38
5	A	1375	6LX	CAU-NAK	2.45	1.50	1.46
5	A	1375	6LX	CBI-CBF	2.51	1.44	1.38
5	B	1375	6LX	CAF-CAE	2.54	1.41	1.36
5	A	1375	6LX	CAP-CAE	2.63	1.43	1.38
5	B	1375	6LX	CAF-CAG	2.87	1.43	1.37
2	A	601	ADP	C5-C4	2.90	1.47	1.40
5	A	1375	6LX	CAF-CAE	3.10	1.43	1.36
2	B	601	ADP	C5-C4	3.13	1.47	1.40
5	A	1375	6LX	CAF-CAG	3.35	1.44	1.37
5	B	1375	6LX	CAS-CAR	3.85	1.46	1.41
5	A	1375	6LX	CAS-CAR	4.51	1.47	1.41
5	B	1375	6LX	CAT-CAI	4.76	1.45	1.39
5	A	1375	6LX	CAT-CAI	6.50	1.47	1.39
5	B	1375	6LX	CAL-NAK	7.05	1.47	1.35
5	A	1375	6LX	CAL-NAK	7.90	1.48	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ADP	N3-C2-N1	-7.83	122.90	128.89
2	B	601	ADP	N3-C2-N1	-6.73	123.74	128.89
5	B	1375	6LX	CAT-CBB-CBG	-3.75	105.04	113.64
2	B	601	ADP	PA-O3A-PB	-3.64	120.47	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ADP	C4-C5-N7	-3.64	106.14	109.48
2	A	601	ADP	C1'-N9-C4	-3.37	121.86	126.94
5	B	1375	6LX	CAT-CAS-CAR	-3.33	117.51	122.33
2	B	601	ADP	C4-C5-N7	-3.17	106.56	109.48
2	B	601	ADP	C2'-C1'-N9	-3.01	109.69	114.29
2	A	601	ADP	C2'-C1'-N9	-2.92	109.84	114.29
5	A	1375	6LX	CAT-CAS-CAR	-2.80	118.28	122.33
5	B	1375	6LX	CAP-CAQ-CAR	-2.11	118.29	121.49
5	A	1375	6LX	CAM-CAL-NAK	2.09	121.89	118.73
2	A	601	ADP	C2-N1-C6	2.09	122.50	118.77
5	A	1375	6LX	CAA-CAB-CAJ	2.09	113.05	110.57
5	B	1375	6LX	CBF-CBG-CBH	2.32	121.84	118.13
5	B	1375	6LX	CAU-CBC-CBD	2.49	123.38	113.88
5	A	1375	6LX	OAH-CAG-CAF	2.84	119.80	116.18
5	A	1375	6LX	CBB-CAT-CAI	2.89	124.15	120.19
5	B	1375	6LX	CAB-CAJ-NAK	2.94	118.11	113.40
5	A	1375	6LX	CBC-CAU-NAK	2.98	117.79	113.52
5	B	1375	6LX	CBC-CAU-NAK	3.09	117.95	113.52
5	B	1375	6LX	CAA-CAB-CAJ	3.50	114.72	110.57
5	A	1375	6LX	CAC-CAB-CAJ	5.03	116.53	110.57
5	B	1375	6LX	CAC-CAB-CAJ	7.73	119.73	110.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 122 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.02	3 (0%)	85	79	49, 71, 88, 93	1 (0%)
1	B	345/368 (93%)	-0.05	3 (0%)	85	79	48, 72, 87, 96	0
All	All	692/736 (94%)	-0.04	6 (0%)	85	79	48, 72, 88, 96	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	ALA	3.2
1	B	285	ALA	3.0
1	A	178	VAL	2.8
1	B	364	GLU	2.8
1	B	65	THR	2.7
1	A	51	SER	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	6LX	A	1375	37/37	0.78	0.21	1.33	67,76,80,87	0
5	6LX	B	1375	37/37	0.85	0.21	0.52	67,76,80,87	0
4	CL	A	1374	1/1	0.96	0.13	-0.40	54,54,54,54	0
2	ADP	B	601	27/27	0.94	0.14	-0.41	60,67,69,73	0
3	CD	A	1367	1/1	0.98	0.10	-1.05	59,59,59,59	0
3	CD	B	1370	1/1	0.99	0.14	-1.13	60,60,60,60	0
4	CL	A	1377	1/1	0.98	0.09	-1.15	74,74,74,74	0
2	ADP	A	601	27/27	0.90	0.12	-1.29	61,66,74,79	0
4	CL	A	1376	1/1	0.85	0.13	-1.31	85,85,85,85	0
3	CD	B	1374	1/1	0.98	0.09	-1.38	115,115,115,115	0
3	CD	A	1368	1/1	0.97	0.11	-1.44	91,91,91,91	0
3	CD	B	1368	1/1	0.99	0.08	-1.49	51,51,51,51	0
3	CD	A	1371	1/1	0.98	0.07	-1.96	100,100,100,100	0
3	CD	A	1370	1/1	0.99	0.08	-2.08	69,69,69,69	0
3	CD	A	1365	1/1	0.97	0.12	-2.12	66,66,66,66	0
4	CL	A	1378	1/1	0.89	0.11	-2.19	84,84,84,84	0
3	CD	B	1365	1/1	0.98	0.06	-2.19	82,82,82,82	0
3	CD	B	1369	1/1	0.96	0.10	-2.20	80,80,80,80	0
3	CD	A	1369	1/1	0.98	0.07	-2.63	100,100,100,100	0
3	CD	B	1378	1/1	0.90	0.03	-2.79	106,106,106,106	0
3	CD	B	1367	1/1	0.98	0.04	-3.03	78,78,78,78	0
3	CD	B	1376	1/1	0.98	0.06	-	30,30,30,30	0
4	CL	B	1385	1/1	0.82	0.17	-	83,83,83,83	0
3	CD	A	1372	1/1	0.94	0.14	-	104,104,104,104	0
3	CD	B	1379	1/1	0.93	0.04	-	120,120,120,120	0
3	CD	B	1366	1/1	0.97	0.07	-	90,90,90,90	0
3	CD	A	1373	1/1	0.98	0.07	-	112,112,112,112	0
3	CD	B	1372	1/1	0.96	0.04	-	115,115,115,115	0
3	CD	B	1373	1/1	0.98	0.04	-	107,107,107,107	0
4	CL	A	1381	1/1	0.91	0.07	-	80,80,80,80	0
3	CD	A	1366	1/1	0.96	0.04	-	86,86,86,86	0
4	CL	B	1386	1/1	0.98	0.19	-	66,66,66,66	0
4	CL	B	1377	1/1	0.94	0.08	-	67,67,67,67	0
3	CD	B	1371	1/1	0.99	0.02	-	100,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.