W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 01:07 PM EDT

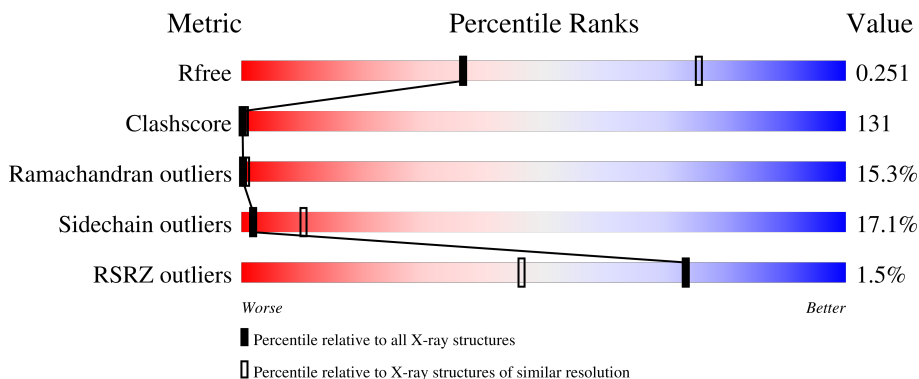|		
PDB ID	:	1RFQ
Title	:	Actin Crystal Dynamics: Structural Implications for F-actin Nucleation, Polymerization and Branching Mediated by the Anti-parallel Dimer
Authors	:	Reutzel, R.; Yoshioka, C.; Govindasamy, L.; Yarmola, E.G.; Agbandje-McKenna, M.; Bubb, M.R.; McKenna, R.
Deposited on	:	2003-11-10
Resolution	:	3.00 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Rfree		0.251
Clashscore		131
Ramachandran outliers		15.3%
Sidechain outliers		17.1%
RSRZ outliers		1.5%

Worse ← → *Better*

▉ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	375	13% 58% 23% · ·
1	B	375	3% / 8% 59% 26% · ·

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
3	ATP	A	376	-	-	X	-
3	ATP	B	386	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5824 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total 2829	C 1794	N 476	O 540	S 19	0	0	0
1	B	361	Total 2829	C 1794	N 476	O 540	S 19	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
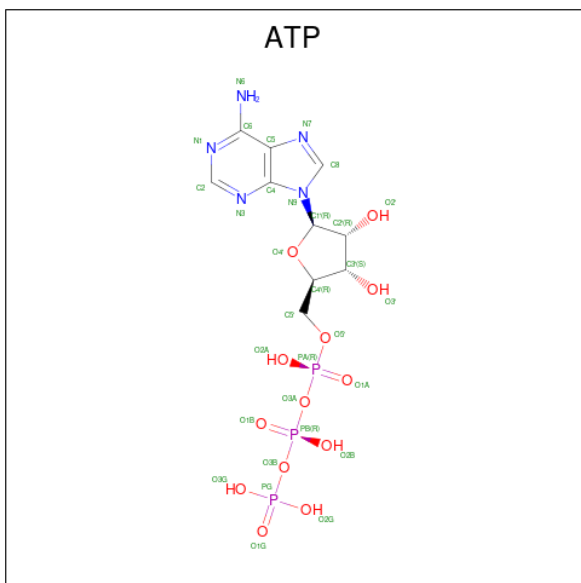
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 4 is LATRUNCULIN A (three-letter code: LAR) (formula: $C_{22}H_{31}NO_5S$).
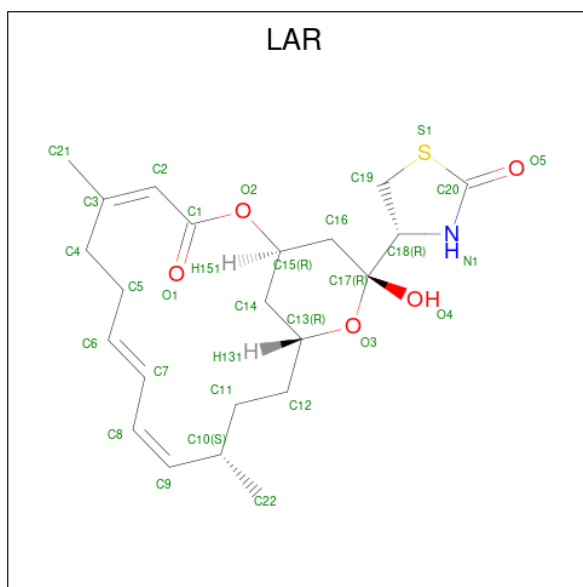
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 29	C 22	N 1	O 5	S 1	0	0
4	B	1	Total 29	C 22	N 1	O 5	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	22	Total 22	O 22	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Actin, alpha skeletal muscle

- Molecule 1: Actin, alpha skeletal muscle

G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 L242

P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300 G301 G302

T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360 E361 Y362

D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 K373 C374 F375

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	101.50Å 101.50Å 104.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 46.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 98.6 (46.35-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.261 0.205 , 0.251	Depositor DCC
R_{free} test set	2858 reflections (13.57%)	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 125.7	EDS
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.089 for -h,-l,-k 0.088 for -h,l,k 0.094 for l,-k,h 0.096 for -l,-k,-h 0.368 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5824	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, LAR, ATP

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	0.63	2/2891 (0.1%)	1.03	20/3919 (0.5%)
1	B	0.64	2/2891 (0.1%)	1.02	18/3919 (0.5%)
All	All	0.63	4/5782 (0.1%)	1.02	38/7838 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	SER	N-CA	16.41	1.79	1.46
1	B	200	PHE	N-CA	11.99	1.70	1.46
1	B	25	ASP	C-N	-6.15	1.20	1.34
1	A	374	CYS	CB-SG	-5.57	1.72	1.81

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	PHE	CB-CG-CD1	12.53	129.57	120.80
1	B	200	PHE	CB-CG-CD2	-11.75	112.57	120.80
1	A	272	ALA	C-N-CA	-10.81	99.61	122.30
1	A	200	PHE	CB-CG-CD2	9.51	127.46	120.80
1	A	270	GLU	N-CA-CB	9.40	127.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	SER	C-N-CA	-9.35	98.32	121.70
1	A	375	PHE	CA-CB-CG	-8.97	92.38	113.90
1	A	372	ARG	CA-C-N	-8.90	97.62	117.20
1	A	200	PHE	C-N-CA	8.68	143.39	121.70
1	B	230	ALA	C-N-CA	-8.50	100.45	121.70
1	B	70	PRO	CA-C-N	-8.49	98.52	117.20
1	B	200	PHE	CA-C-N	-8.28	98.98	117.20
1	B	199	SER	C-N-CA	-8.15	101.33	121.70
1	A	200	PHE	CB-CG-CD1	-8.06	115.15	120.80
1	A	235	SER	N-CA-C	-8.05	89.26	111.00
1	A	374	CYS	C-N-CA	-7.87	102.02	121.70
1	A	270	GLU	N-CA-C	-7.83	89.86	111.00
1	B	70	PRO	O-C-N	7.32	134.40	122.70
1	A	198	TYR	CB-CA-C	7.25	124.90	110.40
1	B	200	PHE	CA-CB-CG	7.17	131.10	113.90
1	A	372	ARG	O-C-N	7.04	133.96	122.70
1	B	26	ALA	N-CA-CB	-6.73	100.68	110.10
1	A	372	ARG	C-N-CA	6.71	138.47	121.70
1	A	374	CYS	CA-C-N	6.64	131.80	117.20
1	A	198	TYR	CA-CB-CG	6.63	126.00	113.40
1	B	73	HIS	C-N-CA	-6.55	108.53	122.30
1	A	270	GLU	C-N-CA	-6.33	105.88	121.70
1	B	71	ILE	CA-C-N	-6.29	103.37	117.20
1	A	375	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	B	130	PRO	CA-N-CD	-5.91	103.23	111.50
1	A	153	LEU	CA-CB-CG	-5.87	101.80	115.30
1	B	270	GLU	CA-C-N	-5.76	104.53	117.20
1	A	356	TRP	CB-CA-C	-5.59	99.21	110.40
1	B	24	ASP	C-N-CA	5.50	135.44	121.70
1	B	200	PHE	C-N-CA	5.48	135.41	121.70
1	B	349	LEU	O-C-N	-5.39	114.08	122.70
1	B	93	GLU	N-CA-C	-5.36	96.52	111.00
1	B	200	PHE	O-C-N	5.28	131.15	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	TYR	Sidechain
1	A	234	SER	Peptide,Mainchain
1	A	372	ARG	Mainchain
1	B	91	TYR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2829	0	2794	703	0
1	B	2829	0	2793	838	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	9	0
3	B	31	0	12	10	0
4	A	29	0	31	2	0
4	B	29	0	31	10	0
5	A	22	0	0	6	0
5	B	22	0	0	6	0
All	All	5824	0	5673	1501	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 131.

All (1501) 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:373:LYS:NZ	1:B:373:LYS:CA	1.67	1.54
1:B:200:PHE:N	1:B:200:PHE:CA	1.70	1.52
1:A:235:SER:N	1:A:235:SER:CA	1.79	1.44
1:B:103:THR:O	1:B:356:TRP:CZ3	1.71	1.44
1:B:21:PHE:CB	1:B:24:ASP:OD2	1.65	1.43
1:A:235:SER:N	1:A:236:LEU:HD13	1.37	1.38
1:A:372:ARG:HG3	1:B:372:ARG:CB	1.50	1.38
1:B:71:ILE:CD1	1:B:82:MET:CE	2.04	1.34
1:B:235:SER:C	1:B:236:LEU:HD23	1.48	1.33
1:A:373:LYS:NZ	1:B:373:LYS:HA	0.96	1.29
1:B:39:ARG:HB3	5:B:391:HOH:O	1.29	1.27
1:B:103:THR:O	1:B:356:TRP:CH2	1.90	1.24
1:A:235:SER:H	1:A:236:LEU:CD1	1.51	1.22
1:B:39:ARG:C	5:B:391:HOH:O	1.79	1.18
1:B:71:ILE:HD12	1:B:82:MET:CE	1.64	1.18
1:A:269:MET:HG3	1:A:270:GLU:H	1.12	1.15
1:A:198:TYR:CZ	1:A:248:ILE:HG21	1.81	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:CE	1:B:373:LYS:HA	1.59	1.14
1:B:150:GLY:HA2	1:B:293:LEU:HA	1.30	1.14
1:B:71:ILE:HD11	1:B:82:MET:CE	1.73	1.14
1:A:198:TYR:CE1	1:A:248:ILE:HD13	1.82	1.14
1:B:71:ILE:CD1	1:B:82:MET:HE2	1.80	1.11
1:B:71:ILE:CD1	1:B:82:MET:HE1	1.71	1.10
1:B:155:SER:HB3	1:B:304:THR:HG22	1.27	1.10
1:A:217:CYS:SG	1:A:258:PRO:HD3	1.92	1.10
1:A:373:LYS:NZ	1:B:373:LYS:CB	2.15	1.09
1:A:123:MET:HB3	1:A:129:VAL:HG21	1.28	1.09
1:A:169:TYR:CE2	1:A:374:CYS:SG	2.46	1.09
1:B:71:ILE:HD12	1:B:82:MET:HE1	1.10	1.08
1:A:123:MET:HB3	1:A:129:VAL:CG2	1.82	1.06
1:B:235:SER:HB3	1:B:236:LEU:CD2	1.85	1.06
1:A:34:ILE:HA	1:A:70:PRO:HD3	1.34	1.06
1:A:374:CYS:CB	5:A:381:HOH:O	2.01	1.06
1:B:263:GLN:O	1:B:266:PHE:CD1	2.09	1.05
1:B:133:TYR:N	1:B:356:TRP:CZ3	2.24	1.05
1:A:372:ARG:HG3	1:B:372:ARG:HB2	1.08	1.05
1:A:373:LYS:HG3	1:B:372:ARG:HG3	1.38	1.05
1:B:21:PHE:HB2	1:B:24:ASP:CG	1.77	1.04
1:A:372:ARG:HG3	1:B:372:ARG:HB3	1.34	1.04
1:B:91:TYR:O	1:B:95:ARG:HD2	1.58	1.04
1:B:267:ILE:HG22	1:B:268:GLY:N	1.72	1.03
1:B:263:GLN:O	1:B:266:PHE:HD1	1.40	1.03
1:B:149:THR:HG23	1:B:167:GLU:H	1.24	1.03
1:B:286:ASP:OD2	1:B:288:ASP:HB3	1.59	1.03
1:A:318:THR:HA	1:A:321:ALA:HB3	1.37	1.02
1:A:198:TYR:OH	1:A:248:ILE:CG2	2.07	1.02
1:B:236:LEU:HD23	1:B:236:LEU:N	1.74	1.01
1:B:76:ILE:HD12	1:B:76:ILE:H	1.19	1.00
1:B:154:ASP:HA	1:B:300:SER:O	1.61	1.00
1:B:318:THR:HA	1:B:321:ALA:HB3	1.41	1.00
1:B:260:THR:HG23	1:B:266:PHE:CD1	1.97	1.00
1:A:235:SER:H	1:A:236:LEU:HD13	0.85	0.99
1:A:198:TYR:OH	1:A:248:ILE:HG23	1.59	0.99
1:A:133:TYR:OH	1:A:375:PHE:N	1.96	0.99
1:A:373:LYS:CD	1:B:373:LYS:HA	1.92	0.98
1:B:349:LEU:CD1	1:B:352:PHE:N	2.27	0.98
1:B:61:LYS:HD2	1:B:65:LEU:HD22	1.43	0.98
1:B:103:THR:O	1:B:356:TRP:HZ3	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:HG3	1:B:129:VAL:HG21	1.43	0.97
1:B:178:LEU:HD21	1:B:277:THR:HG21	1.44	0.97
1:A:372:ARG:HA	1:B:372:ARG:HD2	1.45	0.97
1:B:133:TYR:N	1:B:356:TRP:HZ3	1.58	0.97
1:B:199:SER:C	1:B:200:PHE:CA	2.33	0.97
1:B:116:ARG:HG2	1:B:371:HIS:CE1	2.00	0.97
1:B:159:VAL:HG12	1:B:160:THR:H	1.30	0.97
1:B:325:MET:HE3	1:B:325:MET:HA	1.43	0.96
1:A:372:ARG:CG	1:B:372:ARG:HB2	1.93	0.96
1:A:373:LYS:HG3	1:B:372:ARG:CG	1.95	0.96
1:A:242:LEU:HD12	1:A:243:PRO:HD2	1.46	0.96
1:B:39:ARG:CB	5:B:391:HOH:O	1.93	0.96
1:B:212:ILE:HG23	1:B:216:LEU:HD23	1.47	0.96
1:B:222:ASP:O	1:B:226:GLU:HB3	1.65	0.96
1:B:142:LEU:HD22	1:B:165:ILE:HD13	1.44	0.95
1:B:297:ASN:HB2	1:B:329:ILE:HG23	1.47	0.95
1:B:103:THR:C	1:B:356:TRP:CH2	2.39	0.95
1:B:252:ASN:HD21	1:B:256:ARG:HH21	1.12	0.95
1:B:39:ARG:CA	5:B:391:HOH:O	2.06	0.95
1:B:260:THR:HG23	1:B:266:PHE:CG	2.01	0.95
1:A:92:ASN:H	1:A:92:ASN:HD22	1.08	0.95
1:B:21:PHE:HB2	1:B:24:ASP:OD2	0.78	0.95
1:B:39:ARG:O	5:B:391:HOH:O	1.79	0.95
1:B:235:SER:HB3	1:B:236:LEU:HD21	1.49	0.95
1:A:264:PRO:HG2	1:A:273:GLY:HA2	1.47	0.94
1:A:113:LYS:HA	1:A:116:ARG:NH1	1.83	0.94
1:B:110:LEU:HD11	1:B:175:ILE:HD12	1.50	0.94
1:A:234:SER:C	1:A:235:SER:CA	2.36	0.94
1:A:286:ASP:O	1:A:289:ILE:HG12	1.66	0.93
1:A:169:TYR:CD2	1:A:374:CYS:HB3	2.03	0.93
1:B:78:ASN:CG	1:B:81:ASP:HB2	1.87	0.93
1:A:180:LEU:O	1:A:181:ALA:HB2	1.68	0.93
1:A:373:LYS:CD	1:B:373:LYS:CA	2.45	0.93
1:A:372:ARG:HA	1:B:372:ARG:CD	1.98	0.92
1:B:349:LEU:HD12	1:B:352:PHE:N	1.83	0.92
1:B:229:THR:O	1:B:229:THR:HG22	1.68	0.92
1:A:92:ASN:H	1:A:92:ASN:ND2	1.66	0.91
1:A:259:GLU:O	1:A:263:GLN:HG2	1.69	0.91
1:B:133:TYR:H	1:B:356:TRP:HZ3	0.98	0.91
1:B:349:LEU:HD12	1:B:352:PHE:H	1.31	0.90
1:B:190:MET:HG2	1:B:209:VAL:HG21	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ALA:O	1:B:231:ALA:C	2.01	0.90
1:B:317:ILE:HD12	1:B:318:THR:H	1.34	0.90
1:A:37:ARG:HG2	1:A:38:PRO:HD2	1.53	0.90
1:A:185:LEU:H	1:A:185:LEU:HD12	1.35	0.90
1:A:371:HIS:HB3	1:B:369:ILE:HD13	1.51	0.90
1:B:70:PRO:HG2	1:B:85:ILE:HD11	1.51	0.90
1:A:208:ILE:HG22	1:A:212:ILE:HD11	1.53	0.89
1:B:202:THR:N	1:B:205:GLU:OE1	2.05	0.89
1:A:242:LEU:HB3	1:A:246:GLN:O	1.73	0.89
1:B:317:ILE:HD12	1:B:318:THR:N	1.88	0.89
1:B:349:LEU:CD1	1:B:352:PHE:H	1.83	0.88
1:A:346:LEU:HA	1:A:349:LEU:HD12	1.55	0.88
1:B:147:ARG:CZ	1:B:330:ILE:HG12	2.04	0.88
1:A:373:LYS:HD2	1:B:373:LYS:N	1.86	0.88
1:B:71:ILE:HD11	1:B:82:MET:HE2	1.46	0.88
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.57	0.87
1:B:302:GLY:O	1:B:305:MET:HG2	1.73	0.87
1:B:260:THR:HA	1:B:266:PHE:CE1	2.08	0.87
1:A:235:SER:N	1:A:235:SER:C	2.28	0.87
1:B:223:PHE:CE2	1:B:266:PHE:CZ	2.63	0.87
1:A:358:THR:OG1	1:A:361:GLU:HG3	1.75	0.86
1:A:200:PHE:HD2	1:A:205:GLU:CG	1.87	0.86
1:A:219:VAL:HG11	1:A:309:ILE:HA	1.55	0.86
1:A:269:MET:HG3	1:A:270:GLU:N	1.88	0.86
1:B:153:LEU:HD12	1:B:161:HIS:O	1.75	0.86
1:B:223:PHE:CE2	1:B:266:PHE:HZ	1.92	0.86
1:B:189:LEU:HD23	1:B:209:VAL:HG13	1.57	0.86
1:B:31:PHE:HB2	1:B:32:PRO:HD2	1.56	0.85
1:A:373:LYS:CG	1:B:372:ARG:HG3	2.06	0.85
1:B:260:THR:HG23	1:B:266:PHE:HB2	1.58	0.85
1:A:31:PHE:HB2	1:A:32:PRO:HD2	1.56	0.85
1:A:287:ILE:HA	1:A:290:ARG:HH21	1.41	0.85
1:A:148:THR:O	1:A:168:GLY:N	2.10	0.85
1:B:76:ILE:H	1:B:76:ILE:CD1	1.89	0.84
1:B:65:LEU:HB3	1:B:67:LEU:HD22	1.57	0.84
1:B:164:PRO:HB2	1:B:171:LEU:HD12	1.57	0.84
1:A:198:TYR:CZ	1:A:248:ILE:CG2	2.58	0.84
1:B:223:PHE:CD2	1:B:263:GLN:OE1	2.31	0.84
1:B:105:LEU:HB2	1:B:134:VAL:HG22	1.59	0.84
1:A:62:ARG:HG3	1:A:63:GLY:N	1.91	0.84
1:A:92:ASN:HD22	1:A:92:ASN:N	1.71	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HA	1:A:70:PRO:CD	2.09	0.83
1:B:267:ILE:HG22	1:B:268:GLY:H	1.39	0.83
1:A:37:ARG:HG3	1:A:52:SER:OG	1.77	0.83
1:B:260:THR:HG23	1:B:266:PHE:CB	2.08	0.83
1:A:194:THR:HA	1:A:198:TYR:O	1.79	0.83
1:B:219:VAL:HG23	1:B:258:PRO:HB2	1.61	0.83
1:A:116:ARG:HH11	1:A:116:ARG:HB3	1.43	0.83
1:A:372:ARG:HB2	5:A:389:HOH:O	1.79	0.82
1:A:235:SER:N	1:A:236:LEU:CD1	2.23	0.82
1:A:34:ILE:HG22	1:A:69:TYR:HA	1.60	0.82
1:A:270:GLU:HA	1:A:270:GLU:OE1	1.77	0.82
1:A:373:LYS:HE3	1:B:372:ARG:HG3	1.61	0.82
1:B:21:PHE:CG	1:B:24:ASP:OD2	2.32	0.82
1:A:250:ILE:HD13	1:A:250:ILE:H	1.45	0.82
1:B:147:ARG:NH1	1:B:330:ILE:HG12	1.95	0.82
1:B:76:ILE:HD12	1:B:76:ILE:N	1.94	0.82
1:B:136:ILE:H	1:B:136:ILE:HD12	1.42	0.81
1:A:133:TYR:OH	1:A:375:PHE:CA	2.28	0.81
1:B:274:ILE:HD12	1:B:275:HIS:H	1.45	0.81
1:A:154:ASP:CG	1:A:300:SER:OG	2.17	0.81
1:A:185:LEU:HB3	1:A:257:CYS:SG	2.20	0.81
1:B:118:LYS:NZ	1:B:118:LYS:HB2	1.95	0.81
1:B:264:PRO:HB3	1:B:269:MET:HB2	1.62	0.81
1:B:333:PRO:HG2	1:B:334:GLU:OE2	1.80	0.81
1:B:18:LYS:HG3	1:B:30:VAL:HG22	1.63	0.81
1:B:6:THR:O	1:B:102:PRO:HD2	1.80	0.81
1:B:70:PRO:O	1:B:77:THR:OG1	1.99	0.81
1:B:183:ARG:NH1	1:B:206:ARG:HH22	1.77	0.81
1:A:124:PHE:O	1:A:128:ASN:HA	1.80	0.81
1:A:373:LYS:HD2	1:B:373:LYS:CA	2.08	0.81
1:B:67:LEU:N	1:B:67:LEU:HD23	1.94	0.81
1:A:117:GLU:HB3	1:A:367:PRO:HB3	1.62	0.80
1:A:372:ARG:CG	1:B:372:ARG:CB	2.47	0.80
1:B:38:PRO:HD3	1:B:53:TYR:HE2	1.45	0.80
1:B:182:GLY:H	1:B:303:THR:HG21	1.42	0.80
1:A:287:ILE:HA	1:A:290:ARG:HG3	1.63	0.80
1:B:37:ARG:HD3	1:B:52:SER:HB3	1.64	0.80
1:A:198:TYR:HE1	1:A:248:ILE:HD13	1.44	0.80
1:A:234:SER:O	1:A:235:SER:CA	2.29	0.80
1:B:61:LYS:HD2	1:B:65:LEU:CD2	2.10	0.80
1:B:372:ARG:HG3	1:B:372:ARG:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLY:HA3	3:A:376:ATP:O3G	1.81	0.80
1:A:235:SER:N	1:A:236:LEU:N	2.29	0.79
1:A:116:ARG:NH1	1:A:116:ARG:HB3	1.96	0.79
1:B:267:ILE:CG2	1:B:268:GLY:N	2.45	0.79
1:A:93:GLU:HG3	1:A:94:LEU:HD12	1.65	0.79
1:B:19:ALA:HB3	1:B:29:ALA:HB3	1.63	0.79
1:B:75:ILE:HG22	1:B:76:ILE:O	1.83	0.79
1:B:27:PRO:HB3	1:B:340:TRP:CE2	2.18	0.79
1:A:113:LYS:HA	1:A:116:ARG:HH12	1.47	0.79
1:A:94:LEU:O	1:A:96:VAL:HG13	1.83	0.79
1:A:280:ASN:N	1:A:280:ASN:HD22	1.80	0.79
1:B:236:LEU:CD2	1:B:236:LEU:N	2.45	0.79
1:A:303:THR:O	1:A:305:MET:N	2.17	0.78
1:B:349:LEU:HD11	1:B:352:PHE:N	1.96	0.78
1:B:349:LEU:CD1	1:B:351:THR:HB	2.14	0.78
1:A:194:THR:HG22	1:A:199:SER:O	1.83	0.78
1:B:218:TYR:CE2	1:B:254:ARG:HG2	2.18	0.78
1:B:235:SER:HB3	1:B:236:LEU:HD23	1.64	0.78
1:A:169:TYR:CZ	1:A:374:CYS:SG	2.74	0.78
1:B:116:ARG:HG2	1:B:371:HIS:HE1	1.48	0.78
1:A:372:ARG:HA	1:B:372:ARG:NE	1.97	0.78
1:B:156:GLY:HA3	3:B:386:ATP:O3G	1.85	0.77
1:B:139:VAL:O	1:B:142:LEU:HB3	1.84	0.77
1:A:71:ILE:HG13	1:A:82:MET:HE3	1.67	0.77
1:A:200:PHE:CD2	1:A:205:GLU:CG	2.66	0.77
1:B:285:CYS:HB3	1:B:289:ILE:HD11	1.67	0.77
1:A:169:TYR:CD2	1:A:374:CYS:CB	2.67	0.77
1:A:287:ILE:HG23	1:A:288:ASP:H	1.48	0.77
1:B:156:GLY:HA3	3:B:386:ATP:PG	2.24	0.77
1:B:346:LEU:O	1:B:349:LEU:CD2	2.32	0.77
1:B:216:LEU:HD22	1:B:216:LEU:H	1.48	0.77
1:B:334:GLU:C	1:B:336:LYS:H	1.87	0.77
1:B:235:SER:C	1:B:236:LEU:CD2	2.44	0.77
1:B:230:ALA:C	1:B:232:SER:N	2.32	0.77
1:A:98:PRO:C	1:A:100:GLU:H	1.88	0.76
1:A:154:ASP:OD1	1:A:300:SER:OG	2.02	0.76
1:B:186:THR:HG23	1:B:209:VAL:HG11	1.67	0.76
1:A:316:GLU:OE2	1:A:316:GLU:HA	1.84	0.76
1:B:37:ARG:HG2	1:B:52:SER:HA	1.67	0.76
1:A:200:PHE:CD2	1:A:205:GLU:HG2	2.20	0.76
1:A:218:TYR:CE2	1:A:254:ARG:HB3	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PHE:HE2	1:B:356:TRP:CZ2	2.02	0.76
1:A:60:SER:O	1:A:61:LYS:HD3	1.86	0.75
1:A:226:GLU:HG3	1:A:255:PHE:CZ	2.21	0.75
1:A:359:LYS:O	1:A:363:ASP:HB2	1.86	0.75
1:B:337:TYR:HB2	1:B:341:ILE:HD11	1.66	0.75
1:A:89:THR:HA	1:A:93:GLU:HB3	1.67	0.75
1:A:337:TYR:HB2	1:A:341:ILE:HD11	1.65	0.75
1:A:373:LYS:NZ	1:B:373:LYS:CG	2.48	0.75
1:A:82:MET:O	1:A:85:ILE:HB	1.85	0.75
1:B:103:THR:C	1:B:356:TRP:HH2	1.89	0.75
1:B:142:LEU:HD21	1:B:148:THR:C	2.05	0.75
1:B:233:SER:C	1:B:235:SER:H	1.87	0.75
1:A:279:TYR:CE1	1:A:320:LEU:HB2	2.22	0.75
1:A:76:ILE:HD12	1:A:76:ILE:H	1.51	0.75
1:A:91:TYR:O	1:A:93:GLU:N	2.19	0.75
1:A:218:TYR:HE2	1:A:254:ARG:HB3	1.52	0.75
1:B:140:LEU:HD22	1:B:343:GLY:HA2	1.68	0.75
1:A:71:ILE:HG13	1:A:82:MET:CE	2.16	0.75
1:A:197:GLY:O	1:A:198:TYR:CG	2.39	0.75
1:A:121:GLN:CD	1:A:125:GLU:HG3	2.07	0.74
1:A:190:MET:SD	1:A:206:ARG:HA	2.27	0.74
1:A:200:PHE:HA	1:A:205:GLU:OE1	1.85	0.74
1:A:345:ILE:HG22	1:A:349:LEU:HD11	1.69	0.74
1:B:91:TYR:C	1:B:93:GLU:H	1.89	0.74
1:A:99:GLU:HA	1:A:129:VAL:HA	1.68	0.74
1:B:72:GLU:CD	1:B:77:THR:HG21	2.07	0.74
1:A:352:PHE:O	1:A:355:MET:HB2	1.87	0.74
1:A:238:LYS:C	1:A:249:THR:HG22	2.08	0.74
1:A:247:VAL:O	1:A:248:ILE:HG13	1.88	0.74
1:A:255:PHE:O	1:A:259:GLU:HB2	1.88	0.74
1:A:368:SER:HA	1:A:371:HIS:CD2	2.22	0.74
1:A:200:PHE:HA	1:A:205:GLU:CD	2.08	0.74
1:A:78:ASN:OD1	1:A:80:ASP:HB2	1.88	0.73
1:A:274:ILE:HG13	1:A:275:HIS:H	1.52	0.73
1:B:349:LEU:HG	1:B:352:PHE:HB2	1.70	0.73
1:B:21:PHE:CD2	1:B:24:ASP:OD2	2.41	0.73
1:A:372:ARG:CA	1:B:372:ARG:HD2	2.18	0.73
1:B:274:ILE:CD1	1:B:275:HIS:H	2.01	0.73
1:A:260:THR:HG23	1:A:266:PHE:HB2	1.70	0.73
1:B:242:LEU:CD1	1:B:244:ASP:H	2.02	0.73
1:B:274:ILE:HG13	1:B:275:HIS:ND1	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ARG:CG	1:B:372:ARG:O	2.34	0.73
1:A:250:ILE:HD13	1:A:250:ILE:N	2.03	0.73
1:B:105:LEU:O	1:B:134:VAL:HG13	1.88	0.73
1:A:239:SER:N	1:A:249:THR:HG22	2.03	0.73
1:B:325:MET:HG3	1:B:326:LYS:O	1.87	0.73
1:A:54:VAL:HA	1:A:58:ALA:HB2	1.71	0.73
1:B:274:ILE:CG1	1:B:275:HIS:H	2.02	0.73
1:B:188:TYR:HE2	1:B:257:CYS:HA	1.54	0.72
1:B:243:PRO:C	1:B:245:GLY:H	1.91	0.72
1:A:189:LEU:HD23	1:A:209:VAL:HG12	1.71	0.72
1:B:186:THR:HG23	1:B:209:VAL:CG1	2.18	0.72
1:B:325:MET:HG2	1:B:327:ILE:HD11	1.72	0.72
1:A:70:PRO:HG2	1:A:85:ILE:HD11	1.71	0.72
1:A:149:THR:HG23	1:A:165:ILE:O	1.89	0.72
1:B:123:MET:O	1:B:127:PHE:HB2	1.90	0.72
1:B:269:MET:C	1:B:271:SER:H	1.91	0.72
1:B:93:GLU:O	1:B:95:ARG:HG2	1.89	0.72
1:B:94:LEU:HD12	1:B:94:LEU:H	1.52	0.72
1:B:183:ARG:HH11	1:B:206:ARG:NH2	1.86	0.72
1:A:97:ALA:O	1:A:100:GLU:HB3	1.90	0.72
1:B:273:GLY:O	1:B:276:GLU:HB3	1.89	0.72
1:A:13:GLY:HA3	3:A:376:ATP:PB	2.30	0.71
1:B:36:GLY:HA3	1:B:67:LEU:HB3	1.70	0.71
1:A:264:PRO:HG2	1:A:273:GLY:CA	2.18	0.71
1:B:183:ARG:NH1	1:B:206:ARG:NH2	2.38	0.71
1:B:260:THR:CG2	1:B:266:PHE:HB2	2.20	0.71
1:A:83:GLU:C	1:A:85:ILE:H	1.92	0.71
1:A:374:CYS:CA	5:A:381:HOH:O	2.34	0.71
1:B:58:ALA:HA	1:B:61:LYS:HE2	1.73	0.71
1:B:38:PRO:HD3	1:B:53:TYR:CE2	2.25	0.71
1:B:151:ILE:O	1:B:297:ASN:HA	1.91	0.71
1:B:187:ASP:OD1	1:B:206:ARG:NH2	2.23	0.71
1:A:123:MET:HB3	1:A:129:VAL:HG22	1.70	0.71
1:A:188:TYR:CE2	1:A:257:CYS:HA	2.26	0.71
1:A:317:ILE:HG13	1:A:321:ALA:HB2	1.72	0.71
1:B:326:LYS:O	1:B:327:ILE:HD13	1.89	0.71
1:A:219:VAL:HG21	1:A:309:ILE:HB	1.71	0.71
1:B:207:GLU:OE2	1:B:210:ARG:NH2	2.23	0.71
1:B:218:TYR:CE2	1:B:255:PHE:HB3	2.25	0.71
1:B:319:ALA:C	1:B:320:LEU:HD12	2.11	0.71
1:A:287:ILE:HG23	1:A:288:ASP:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TYR:N	1:B:356:TRP:CE3	2.59	0.71
1:B:185:LEU:HB3	1:B:257:CYS:SG	2.30	0.71
1:A:318:THR:CA	1:A:321:ALA:HB3	2.20	0.70
1:B:181:ALA:H	1:B:184:ASP:HB2	1.55	0.70
1:B:325:MET:HE3	1:B:325:MET:CA	2.19	0.70
1:B:346:LEU:O	1:B:349:LEU:HD21	1.91	0.70
1:A:210:ARG:NH1	1:A:214:GLU:OE2	2.25	0.70
1:B:152:VAL:HG12	1:B:298:VAL:HB	1.74	0.70
1:B:185:LEU:HD12	1:B:185:LEU:H	1.56	0.70
1:B:189:LEU:HA	1:B:192:ILE:HD11	1.73	0.70
1:B:223:PHE:CE1	1:B:259:GLU:HG2	2.25	0.70
1:A:373:LYS:HE3	1:B:372:ARG:CG	2.21	0.70
1:B:235:SER:CB	1:B:236:LEU:HD23	2.22	0.70
1:B:235:SER:CA	1:B:236:LEU:HD23	2.21	0.70
1:B:156:GLY:HA2	3:B:386:ATP:O1A	1.92	0.70
1:A:9:VAL:HG21	1:A:344:SER:HA	1.74	0.70
1:A:242:LEU:HD12	1:A:243:PRO:CD	2.22	0.70
1:B:159:VAL:HG12	1:B:160:THR:N	2.05	0.70
1:A:200:PHE:HD2	1:A:205:GLU:CD	1.94	0.69
1:B:117:GLU:HB3	1:B:367:PRO:HB2	1.73	0.69
1:B:132:MET:HA	1:B:356:TRP:CZ3	2.27	0.69
1:B:29:ALA:O	1:B:30:VAL:HG23	1.92	0.69
1:B:109:PRO:HG3	1:B:136:ILE:CG2	2.22	0.69
1:B:302:GLY:HA2	1:B:336:LYS:HG3	1.73	0.69
1:B:39:ARG:HD2	1:B:64:ILE:O	1.92	0.69
1:A:76:ILE:HD12	1:A:76:ILE:N	2.08	0.69
1:A:7:ALA:CB	1:A:102:PRO:HB2	2.22	0.69
1:A:176:MET:HE2	1:A:277:THR:HA	1.73	0.69
1:B:195:GLU:C	1:B:197:GLY:H	1.94	0.69
1:B:144:ALA:HB2	1:B:342:GLY:CA	2.22	0.69
1:A:368:SER:HA	1:A:371:HIS:NE2	2.06	0.69
1:B:138:ALA:CB	1:B:163:VAL:HG21	2.23	0.69
1:B:223:PHE:O	1:B:227:MET:HB2	1.92	0.69
1:A:98:PRO:O	1:A:100:GLU:N	2.26	0.69
1:A:187:ASP:HA	1:A:190:MET:CE	2.22	0.69
1:B:202:THR:OG1	1:B:204:ALA:HB3	1.93	0.68
1:B:216:LEU:HD22	1:B:216:LEU:N	2.07	0.68
1:A:252:ASN:C	1:A:256:ARG:HG3	2.14	0.68
1:B:140:LEU:HD13	1:B:343:GLY:HA3	1.75	0.68
1:A:99:GLU:C	1:A:130:PRO:HD3	2.13	0.68
1:B:108:ALA:HB3	1:B:111:ASN:HB2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:SER:HA	1:B:338:SER:OG	1.94	0.68
1:A:27:PRO:HD3	1:A:340:TRP:CE3	2.29	0.68
1:A:359:LYS:O	1:A:363:ASP:N	2.20	0.68
1:B:133:TYR:CD1	1:B:134:VAL:N	2.62	0.68
1:B:370:VAL:HG22	1:B:370:VAL:O	1.92	0.68
1:A:7:ALA:HB2	1:A:102:PRO:HB2	1.76	0.68
1:B:76:ILE:O	1:B:77:THR:HG23	1.93	0.68
1:B:132:MET:C	1:B:356:TRP:CE3	2.67	0.68
1:B:242:LEU:HD23	1:B:248:ILE:HD11	1.75	0.68
1:A:176:MET:HG3	1:A:277:THR:O	1.94	0.68
1:A:200:PHE:CD2	1:A:205:GLU:HB3	2.29	0.68
1:A:373:LYS:NZ	1:B:373:LYS:HG3	2.09	0.68
1:B:27:PRO:HD3	1:B:340:TRP:CZ3	2.28	0.68
1:A:113:LYS:O	1:A:117:GLU:HG3	1.94	0.68
1:A:263:GLN:C	1:A:265:SER:H	1.97	0.68
1:A:238:LYS:HG3	1:A:239:SER:N	2.09	0.68
1:B:17:VAL:HG23	1:B:33:SER:HB2	1.75	0.68
1:A:14:SER:OG	1:A:74:GLY:N	2.27	0.68
1:A:209:VAL:O	1:A:212:ILE:HB	1.93	0.68
1:A:222:ASP:CG	1:A:225:ASN:HB2	2.14	0.67
1:A:373:LYS:CE	1:B:372:ARG:HG3	2.23	0.67
1:B:32:PRO:HG2	1:B:55:GLY:HA2	1.76	0.67
1:B:217:CYS:SG	1:B:258:PRO:HD3	2.34	0.67
1:B:262:PHE:HE2	1:B:316:GLU:HG3	1.58	0.67
1:A:315:LYS:HG3	1:A:316:GLU:N	2.08	0.67
1:B:317:ILE:O	1:B:320:LEU:N	2.27	0.67
1:A:246:GLN:NE2	1:A:248:ILE:HD11	2.09	0.67
1:A:372:ARG:CG	1:B:372:ARG:HB3	2.17	0.67
1:A:374:CYS:HA	5:A:381:HOH:O	1.94	0.67
1:A:104:LEU:HD23	1:A:105:LEU:N	2.08	0.67
1:A:218:TYR:O	1:A:258:PRO:HG3	1.95	0.67
1:A:61:LYS:O	1:A:65:LEU:HD13	1.94	0.67
1:A:180:LEU:O	1:A:181:ALA:CB	2.34	0.67
1:B:116:ARG:O	1:B:118:LYS:N	2.28	0.67
1:B:149:THR:HG23	1:B:167:GLU:N	2.05	0.67
1:B:325:MET:HG3	1:B:326:LYS:N	2.10	0.67
1:A:121:GLN:NE2	1:A:125:GLU:HG3	2.10	0.67
1:A:277:THR:HA	1:A:280:ASN:HB2	1.75	0.67
1:B:250:ILE:HD13	1:B:250:ILE:H	1.60	0.67
1:A:227:MET:CE	1:A:256:ARG:HD3	2.25	0.66
1:B:89:THR:O	1:B:93:GLU:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PRO:HB3	1:A:269:MET:HG2	1.76	0.66
1:A:287:ILE:N	1:A:290:ARG:NH2	2.43	0.66
1:B:369:ILE:HD12	1:B:372:ARG:HD3	1.77	0.66
1:A:373:LYS:HG3	1:B:372:ARG:CB	2.24	0.66
1:B:58:ALA:HB1	1:B:67:LEU:HD13	1.76	0.66
1:B:124:PHE:O	1:B:128:ASN:N	2.27	0.66
1:B:154:ASP:O	1:B:160:THR:HA	1.95	0.66
1:B:230:ALA:O	1:B:232:SER:N	2.27	0.66
1:B:107:GLU:HG2	1:B:135:ALA:C	2.15	0.66
1:B:186:THR:HG21	4:B:387:LAR:S1	2.36	0.66
1:B:223:PHE:CD1	1:B:259:GLU:HG2	2.31	0.66
1:B:275:HIS:ND1	1:B:275:HIS:N	2.43	0.66
1:B:62:ARG:HD3	1:B:203:THR:OG1	1.94	0.66
1:B:239:SER:HA	1:B:248:ILE:O	1.96	0.66
1:A:295:ALA:HA	1:A:328:LYS:H	1.59	0.65
1:B:171:LEU:O	1:B:175:ILE:HG13	1.96	0.65
1:B:349:LEU:HD12	1:B:351:THR:HB	1.77	0.65
1:B:215:LYS:HB3	1:B:216:LEU:HD22	1.78	0.65
1:B:289:ILE:HD12	1:B:290:ARG:N	2.11	0.65
1:A:314:GLN:NE2	1:A:318:THR:HG21	2.11	0.65
1:B:187:ASP:HA	1:B:190:MET:CE	2.27	0.65
1:A:203:THR:HA	1:A:206:ARG:HH12	1.62	0.65
1:B:67:LEU:HD23	1:B:67:LEU:H	1.59	0.65
1:B:60:SER:O	1:B:61:LYS:HG2	1.97	0.65
1:B:88:HIS:O	1:B:93:GLU:HG2	1.96	0.65
1:A:183:ARG:HG2	1:A:187:ASP:OD2	1.97	0.65
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.77	0.65
1:B:91:TYR:C	1:B:93:GLU:N	2.45	0.65
1:B:128:ASN:ND2	1:B:359:LYS:HE3	2.12	0.65
1:B:229:THR:O	1:B:229:THR:CG2	2.41	0.65
1:B:61:LYS:HB2	1:B:65:LEU:HB2	1.79	0.65
1:B:325:MET:O	1:B:326:LYS:HB2	1.96	0.65
1:A:340:TRP:CZ3	1:A:344:SER:HB2	2.31	0.65
1:B:70:PRO:HG2	1:B:85:ILE:CD1	2.25	0.65
1:B:76:ILE:HG22	1:B:77:THR:H	1.62	0.65
1:B:119:MET:O	1:B:123:MET:HB2	1.97	0.65
1:B:233:SER:C	1:B:235:SER:N	2.50	0.65
1:B:260:THR:HA	1:B:266:PHE:CD1	2.32	0.65
1:B:242:LEU:HD12	1:B:244:ASP:H	1.62	0.65
1:B:349:LEU:CG	1:B:352:PHE:HB2	2.27	0.65
1:A:113:LYS:HD3	1:B:364:GLU:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:HD11	1:B:82:MET:HE3	1.76	0.64
1:A:219:VAL:CG1	1:A:309:ILE:HA	2.27	0.64
1:B:156:GLY:O	1:B:303:THR:OG1	2.15	0.64
1:A:234:SER:C	1:A:236:LEU:H	2.00	0.64
1:A:143:TYR:CD1	1:A:346:LEU:HD11	2.33	0.64
1:A:143:TYR:C	1:A:145:SER:H	2.00	0.64
1:A:190:MET:HG2	1:A:209:VAL:HG11	1.79	0.64
1:A:200:PHE:CE2	1:A:208:ILE:HD12	2.33	0.64
1:A:133:TYR:OH	1:A:375:PHE:HA	1.98	0.64
1:B:352:PHE:CE2	1:B:356:TRP:CE2	2.86	0.64
1:B:11:ASP:HB3	1:B:18:LYS:HE2	1.78	0.64
1:B:250:ILE:HD13	1:B:250:ILE:N	2.12	0.64
1:B:190:MET:CG	1:B:209:VAL:HG21	2.28	0.64
1:A:142:LEU:HD22	1:A:165:ILE:HD12	1.80	0.64
1:A:195:GLU:OE2	1:A:195:GLU:HA	1.98	0.64
1:A:256:ARG:HH11	1:A:256:ARG:HB3	1.63	0.64
1:A:275:HIS:CD2	1:A:316:GLU:HB3	2.33	0.64
1:A:32:PRO:HG2	1:A:55:GLY:HA2	1.80	0.64
1:B:337:TYR:O	1:B:341:ILE:HG13	1.97	0.64
1:B:199:SER:O	1:B:200:PHE:CA	2.46	0.63
1:A:320:LEU:HD23	1:A:320:LEU:N	2.14	0.63
1:A:330:ILE:HD12	1:A:330:ILE:N	2.13	0.63
1:B:61:LYS:CD	1:B:65:LEU:HD22	2.24	0.63
1:A:299:MET:O	1:A:299:MET:HG3	1.97	0.63
1:B:19:ALA:HA	1:B:340:TRP:HE1	1.64	0.63
1:B:352:PHE:CE2	1:B:356:TRP:CZ2	2.86	0.63
1:A:89:THR:CA	1:A:93:GLU:HB3	2.28	0.63
1:A:187:ASP:HA	1:A:190:MET:HE1	1.79	0.63
1:B:37:ARG:HA	1:B:53:TYR:CD2	2.33	0.63
1:B:94:LEU:HD12	1:B:94:LEU:N	2.13	0.63
1:B:202:THR:HG1	1:B:204:ALA:HB3	1.63	0.63
1:B:282:ILE:HG21	1:B:294:TYR:CE2	2.34	0.63
1:A:259:GLU:OE1	1:A:259:GLU:HA	1.99	0.63
1:A:323:SER:OG	1:A:324:THR:N	2.31	0.63
1:B:289:ILE:HD13	1:B:293:LEU:HD13	1.79	0.63
1:B:290:ARG:O	1:B:294:TYR:HB2	1.99	0.63
1:A:263:GLN:O	1:A:265:SER:N	2.28	0.63
1:A:70:PRO:HB3	1:A:81:ASP:HB2	1.80	0.63
1:A:219:VAL:HG23	1:A:306:TYR:HB3	1.80	0.63
1:A:374:CYS:HB3	5:A:381:HOH:O	1.81	0.63
1:B:325:MET:HA	1:B:325:MET:CE	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HD23	1:A:104:LEU:C	2.19	0.63
1:A:190:MET:O	1:A:194:THR:HG23	1.99	0.63
1:B:90:PHE:HA	1:B:96:VAL:HG22	1.81	0.63
1:A:239:SER:CA	1:A:249:THR:HG22	2.29	0.62
1:B:18:LYS:HD3	1:B:18:LYS:N	2.13	0.62
1:B:133:TYR:CE2	1:B:355:MET:HB3	2.33	0.62
1:B:136:ILE:HD12	1:B:136:ILE:N	2.13	0.62
1:B:349:LEU:HD13	1:B:351:THR:HB	1.78	0.62
1:A:54:VAL:CA	1:A:58:ALA:HB2	2.29	0.62
1:A:220:ALA:HB2	1:A:255:PHE:HB2	1.81	0.62
1:A:287:ILE:HA	1:A:290:ARG:NH2	2.14	0.62
1:B:210:ARG:O	1:B:214:GLU:HG3	1.98	0.62
1:A:35:VAL:HG12	1:A:36:GLY:N	2.14	0.62
1:A:61:LYS:HB2	1:A:65:LEU:HD13	1.81	0.62
1:B:110:LEU:CD1	1:B:175:ILE:HD12	2.24	0.62
1:B:228:ALA:C	1:B:230:ALA:H	2.03	0.62
1:B:343:GLY:C	1:B:345:ILE:H	2.02	0.62
1:B:210:ARG:NH1	1:B:214:GLU:OE1	2.33	0.62
1:A:78:ASN:HB3	1:A:81:ASP:OD2	1.99	0.62
1:B:118:LYS:HA	1:B:121:GLN:HE22	1.64	0.62
1:B:124:PHE:HZ	1:B:357:ILE:O	1.83	0.62
1:B:212:ILE:HG23	1:B:216:LEU:CD2	2.24	0.62
1:A:253:GLU:HA	1:A:256:ARG:HB2	1.82	0.62
1:B:118:LYS:HB2	1:B:118:LYS:HZ3	1.62	0.62
1:B:132:MET:C	1:B:356:TRP:HE3	2.04	0.62
1:B:136:ILE:H	1:B:136:ILE:CD1	2.13	0.62
1:A:371:HIS:CB	1:B:369:ILE:HD13	2.26	0.62
1:B:242:LEU:HD12	1:B:243:PRO:HD2	1.81	0.62
1:A:76:ILE:HG23	1:A:82:MET:HE3	1.80	0.61
1:A:172:PRO:HD2	1:A:173:HIS:CE1	2.34	0.61
1:A:198:TYR:CE1	1:A:248:ILE:HG21	2.33	0.61
1:B:39:ARG:CZ	1:B:63:GLY:O	2.48	0.61
1:B:94:LEU:H	1:B:94:LEU:CD1	2.13	0.61
1:A:121:GLN:HA	1:A:362:TYR:OH	2.00	0.61
1:B:180:LEU:HD12	1:B:184:ASP:CB	2.30	0.61
1:A:9:VAL:HG21	1:A:344:SER:CA	2.29	0.61
1:A:152:VAL:HG12	1:A:153:LEU:H	1.65	0.61
1:B:325:MET:HG3	1:B:326:LYS:H	1.64	0.61
1:B:53:TYR:HB3	1:B:61:LYS:HE3	1.82	0.61
1:B:195:GLU:C	1:B:197:GLY:N	2.53	0.61
1:B:318:THR:HA	1:B:321:ALA:CB	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HG23	1:A:82:MET:CE	2.30	0.61
1:B:248:ILE:HD12	1:B:248:ILE:N	2.15	0.61
1:B:297:ASN:HB2	1:B:329:ILE:CG2	2.27	0.61
1:B:67:LEU:H	1:B:67:LEU:CD2	2.13	0.61
1:B:78:ASN:OD1	1:B:81:ASP:HB2	2.00	0.61
1:B:90:PHE:O	1:B:96:VAL:N	2.33	0.61
1:B:142:LEU:HD21	1:B:148:THR:CA	2.31	0.61
1:A:9:VAL:HB	1:A:340:TRP:CE2	2.36	0.61
1:A:307:PRO:C	1:A:309:ILE:H	2.04	0.61
1:B:90:PHE:O	1:B:95:ARG:N	2.33	0.61
1:B:242:LEU:HD12	1:B:243:PRO:CD	2.30	0.61
1:A:88:HIS:ND1	1:A:92:ASN:HB2	2.15	0.61
1:B:105:LEU:HB2	1:B:134:VAL:CG2	2.30	0.61
1:A:185:LEU:O	1:A:188:TYR:HB3	2.00	0.61
1:B:218:TYR:CD2	1:B:255:PHE:HB3	2.36	0.61
1:A:374:CYS:HB2	5:A:381:HOH:O	1.83	0.60
1:A:287:ILE:CA	1:A:290:ARG:HH21	2.13	0.60
1:B:299:MET:HB2	1:B:335:ARG:HD2	1.83	0.60
1:B:335:ARG:HG2	1:B:335:ARG:HH21	1.65	0.60
1:B:349:LEU:O	1:B:350:SER:C	2.37	0.60
1:B:358:THR:HG23	1:B:361:GLU:OE1	2.01	0.60
1:B:369:ILE:O	1:B:369:ILE:HG13	2.01	0.60
1:A:91:TYR:C	1:A:93:GLU:H	2.04	0.60
1:A:188:TYR:HE2	1:A:257:CYS:HA	1.64	0.60
1:A:257:CYS:N	1:A:258:PRO:HD2	2.16	0.60
1:A:326:LYS:NZ	1:A:328:LYS:HB2	2.17	0.60
1:A:358:THR:HG1	1:A:361:GLU:HG3	1.67	0.60
1:A:123:MET:CE	1:A:129:VAL:HG11	2.31	0.60
1:A:224:GLU:OE2	1:A:224:GLU:HA	2.01	0.60
1:B:219:VAL:CG2	1:B:258:PRO:HB2	2.29	0.60
1:B:230:ALA:C	1:B:232:SER:H	2.03	0.60
1:B:242:LEU:HD12	1:B:243:PRO:N	2.17	0.60
1:A:306:TYR:O	1:A:309:ILE:HG22	2.01	0.60
1:B:357:ILE:CD1	1:B:370:VAL:HG23	2.32	0.60
1:B:67:LEU:N	1:B:67:LEU:CD2	2.62	0.60
1:B:180:LEU:HD12	1:B:184:ASP:HB3	1.82	0.60
1:A:256:ARG:O	1:A:259:GLU:HB3	2.02	0.60
1:B:189:LEU:O	1:B:192:ILE:HG13	2.01	0.60
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.65	0.60
1:A:83:GLU:C	1:A:85:ILE:N	2.55	0.60
1:B:252:ASN:H	1:B:252:ASN:HD22	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASP:O	1:B:17:VAL:HA	2.02	0.60
1:B:27:PRO:HB3	1:B:340:TRP:CD2	2.37	0.60
1:B:53:TYR:CD2	1:B:65:LEU:HD11	2.36	0.60
1:B:187:ASP:HA	1:B:190:MET:HE2	1.83	0.60
1:A:157:ASP:HA	3:A:376:ATP:H4'	1.82	0.59
1:A:227:MET:HA	1:A:255:PHE:HZ	1.66	0.59
1:B:118:LYS:HA	1:B:121:GLN:NE2	2.17	0.59
1:A:235:SER:C	1:A:236:LEU:HD13	2.23	0.59
1:A:239:SER:HA	1:A:249:THR:HG22	1.83	0.59
1:B:53:TYR:CB	1:B:61:LYS:HE3	2.31	0.59
1:B:59:GLN:HG3	1:B:60:SER:N	2.17	0.59
1:B:213:LYS:HG2	1:B:214:GLU:N	2.16	0.59
1:B:362:TYR:CE1	1:B:367:PRO:HG3	2.37	0.59
1:A:89:THR:HA	1:A:93:GLU:CB	2.32	0.59
1:A:183:ARG:HH11	1:A:183:ARG:HB3	1.66	0.59
1:B:80:ASP:C	1:B:83:GLU:HG3	2.23	0.59
1:B:346:LEU:O	1:B:349:LEU:HD23	2.01	0.59
1:A:97:ALA:HB3	1:A:100:GLU:CD	2.21	0.59
1:A:269:MET:CG	1:A:270:GLU:H	1.95	0.59
1:A:234:SER:O	1:A:235:SER:HA	2.03	0.59
1:B:35:VAL:HB	1:B:81:ASP:OD2	2.02	0.59
1:B:274:ILE:HD12	1:B:275:HIS:N	2.16	0.59
1:A:88:HIS:O	1:A:93:GLU:HB3	2.03	0.59
1:A:200:PHE:HD2	1:A:205:GLU:HG2	1.55	0.59
1:A:264:PRO:O	1:A:269:MET:HB3	2.02	0.59
1:B:111:ASN:HD21	1:B:115:ASN:CB	2.15	0.59
1:B:134:VAL:O	1:B:373:LYS:NZ	2.36	0.59
1:A:98:PRO:HG2	1:A:99:GLU:H	1.67	0.59
1:A:147:ARG:HE	1:A:296:ASN:HB3	1.68	0.59
1:A:61:LYS:CB	1:A:65:LEU:HD13	2.32	0.59
1:A:186:THR:O	1:A:190:MET:HG3	2.03	0.59
1:A:275:HIS:O	1:A:278:THR:HB	2.03	0.59
1:B:213:LYS:O	1:B:217:CYS:HB2	2.02	0.59
1:B:189:LEU:O	1:B:193:LEU:HD13	2.02	0.59
1:A:314:GLN:O	1:A:318:THR:HG23	2.03	0.58
1:B:159:VAL:CG1	1:B:160:THR:H	2.09	0.58
1:B:307:PRO:C	1:B:309:ILE:H	2.05	0.58
1:A:37:ARG:HG2	1:A:38:PRO:CD	2.31	0.58
1:B:61:LYS:CB	1:B:65:LEU:HB2	2.33	0.58
1:A:198:TYR:CE1	1:A:248:ILE:CD1	2.73	0.58
1:B:97:ALA:O	1:B:101:HIS:CD2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASN:HB2	1:B:176:MET:HB2	1.85	0.58
1:B:223:PHE:HE2	1:B:266:PHE:CZ	2.18	0.58
1:B:349:LEU:HD12	1:B:351:THR:CA	2.34	0.58
1:B:334:GLU:C	1:B:336:LYS:N	2.57	0.58
1:A:117:GLU:HB3	1:A:367:PRO:CB	2.33	0.58
1:A:297:ASN:HB2	1:A:329:ILE:HA	1.86	0.58
1:B:133:TYR:OH	1:B:373:LYS:HG2	2.03	0.58
1:B:210:ARG:HH11	1:B:214:GLU:CD	2.07	0.58
1:B:128:ASN:HD21	1:B:359:LYS:HE3	1.68	0.58
1:A:138:ALA:O	1:A:140:LEU:N	2.36	0.58
1:A:162:ASN:O	1:A:164:PRO:HD3	2.02	0.58
1:A:169:TYR:CD2	1:A:374:CYS:SG	2.96	0.58
1:A:269:MET:CE	1:A:269:MET:HA	2.33	0.58
1:A:373:LYS:HG3	1:B:372:ARG:HB2	1.84	0.58
1:B:289:ILE:HD12	1:B:289:ILE:C	2.23	0.58
1:A:200:PHE:CG	1:A:205:GLU:HB3	2.38	0.58
1:B:19:ALA:HA	1:B:340:TRP:NE1	2.19	0.58
1:B:196:ARG:HH22	1:B:251:GLY:HA3	1.69	0.58
1:A:88:HIS:O	1:A:93:GLU:N	2.37	0.57
1:A:143:TYR:C	1:A:145:SER:N	2.56	0.57
1:A:259:GLU:HG3	1:A:263:GLN:HG3	1.85	0.57
1:A:260:THR:HG23	1:A:266:PHE:CB	2.35	0.57
1:A:163:VAL:HG12	1:A:165:ILE:HG13	1.86	0.57
1:A:223:PHE:CE1	1:A:259:GLU:HG2	2.38	0.57
1:B:37:ARG:HD2	1:B:51:ASP:O	2.04	0.57
1:A:135:ALA:CB	1:A:140:LEU:HD21	2.34	0.57
1:A:200:PHE:CD2	1:A:205:GLU:CB	2.87	0.57
1:A:93:GLU:HG3	1:A:94:LEU:CD1	2.35	0.57
1:A:234:SER:C	1:A:236:LEU:N	2.58	0.57
1:A:262:PHE:CE2	1:A:316:GLU:HG3	2.40	0.57
1:B:357:ILE:HD11	1:B:370:VAL:HG23	1.85	0.57
1:A:291:LYS:HG2	1:A:292:ASP:N	2.19	0.57
1:B:37:ARG:CD	1:B:51:ASP:O	2.51	0.57
1:B:61:LYS:O	1:B:63:GLY:N	2.37	0.57
1:A:61:LYS:HB2	1:A:65:LEU:HD22	1.87	0.57
1:A:98:PRO:C	1:A:100:GLU:N	2.56	0.57
1:B:17:VAL:CG2	1:B:33:SER:HB2	2.34	0.57
1:B:130:PRO:O	1:B:358:THR:HA	2.04	0.57
1:A:366:GLY:O	1:A:369:ILE:HG22	2.04	0.57
1:B:56:ASP:O	1:B:59:GLN:HB3	2.04	0.57
1:B:173:HIS:N	1:B:173:HIS:ND1	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:HG3	1:B:239:SER:H	1.70	0.57
1:A:138:ALA:O	1:A:141:SER:N	2.38	0.57
1:A:252:ASN:OD1	1:A:256:ARG:NE	2.37	0.57
1:B:91:TYR:N	1:B:91:TYR:CD1	2.73	0.57
1:B:172:PRO:HA	1:B:175:ILE:HD12	1.86	0.57
1:B:227:MET:SD	1:B:255:PHE:CZ	2.98	0.57
1:A:9:VAL:HB	1:A:340:TRP:NE1	2.19	0.57
1:A:183:ARG:NH1	1:A:183:ARG:CB	2.68	0.57
1:B:155:SER:OG	1:B:303:THR:HB	2.05	0.57
1:B:180:LEU:O	1:B:181:ALA:HB2	2.04	0.57
1:A:22:ALA:C	1:A:24:ASP:H	2.08	0.57
1:A:185:LEU:H	1:A:185:LEU:CD1	2.13	0.57
1:A:337:TYR:O	1:A:338:SER:C	2.43	0.57
1:B:79:TRP:CE3	1:B:118:LYS:HG2	2.39	0.57
1:A:121:GLN:OE1	1:A:125:GLU:HG3	2.04	0.56
1:B:155:SER:HA	1:B:160:THR:OG1	2.04	0.56
1:B:203:THR:HA	1:B:206:ARG:HB3	1.87	0.56
1:B:208:ILE:O	1:B:212:ILE:HD12	2.04	0.56
1:A:200:PHE:HD2	1:A:205:GLU:OE2	1.88	0.56
1:A:208:ILE:HG22	1:A:212:ILE:CD1	2.33	0.56
1:A:259:GLU:HG3	1:A:263:GLN:CG	2.35	0.56
1:B:9:VAL:HB	1:B:340:TRP:CE2	2.40	0.56
1:B:142:LEU:HD22	1:B:165:ILE:CD1	2.28	0.56
1:B:282:ILE:HG21	1:B:294:TYR:CD2	2.40	0.56
1:B:325:MET:CG	1:B:326:LYS:H	2.16	0.56
1:A:27:PRO:HB3	1:A:340:TRP:CE2	2.40	0.56
1:A:100:GLU:O	1:A:100:GLU:HG2	2.05	0.56
1:A:133:TYR:CZ	1:A:375:PHE:HA	2.41	0.56
1:A:187:ASP:O	1:A:188:TYR:C	2.44	0.56
1:A:223:PHE:HB2	1:A:259:GLU:OE2	2.06	0.56
1:A:263:GLN:HG3	1:A:266:PHE:CZ	2.40	0.56
1:A:287:ILE:CA	1:A:290:ARG:NH2	2.68	0.56
1:A:359:LYS:HE2	1:A:363:ASP:OD2	2.05	0.56
1:B:59:GLN:HB2	4:B:387:LAR:C9	2.34	0.56
1:B:140:LEU:HD13	1:B:343:GLY:CA	2.36	0.56
1:B:149:THR:CG2	1:B:166:TYR:HA	2.35	0.56
1:A:227:MET:SD	1:A:255:PHE:CE1	2.98	0.56
1:A:229:THR:O	1:A:233:SER:N	2.38	0.56
1:B:218:TYR:HD2	1:B:254:ARG:O	1.88	0.56
1:B:223:PHE:CE2	1:B:263:GLN:OE1	2.59	0.56
1:A:64:ILE:HD12	1:A:64:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:TYR:HB2	1:A:309:ILE:HB	1.87	0.56
1:B:37:ARG:HD3	1:B:52:SER:CB	2.35	0.56
1:B:305:MET:HA	1:B:335:ARG:NH1	2.20	0.56
1:A:200:PHE:CE2	1:A:208:ILE:CD1	2.89	0.56
1:B:66:THR:O	1:B:68:LYS:HE2	2.06	0.56
1:B:142:LEU:HD22	1:B:165:ILE:HG21	1.86	0.56
1:B:181:ALA:H	1:B:184:ASP:CB	2.17	0.56
1:A:71:ILE:HD11	1:A:76:ILE:HG13	1.87	0.56
1:A:189:LEU:HD23	1:A:209:VAL:CG1	2.34	0.56
1:B:117:GLU:HG2	1:B:367:PRO:O	2.05	0.56
1:B:157:ASP:OD1	1:B:183:ARG:HB2	2.05	0.56
1:A:9:VAL:HG21	1:A:344:SER:N	2.21	0.56
1:A:79:TRP:HA	1:A:82:MET:CB	2.35	0.56
1:A:157:ASP:HA	1:A:182:GLY:HA3	1.87	0.56
1:A:317:ILE:O	1:A:319:ALA:N	2.39	0.56
1:B:223:PHE:CE2	1:B:266:PHE:CE2	2.94	0.56
1:B:316:GLU:O	1:B:320:LEU:HD13	2.06	0.56
1:A:209:VAL:CA	1:A:212:ILE:HD12	2.35	0.56
1:B:53:TYR:CE2	1:B:65:LEU:HD11	2.41	0.55
1:B:104:LEU:HD12	1:B:347:ALA:HB2	1.88	0.55
1:B:286:ASP:O	1:B:289:ILE:HG13	2.06	0.55
1:A:250:ILE:N	1:A:250:ILE:CD1	2.69	0.55
1:A:280:ASN:N	1:A:280:ASN:ND2	2.52	0.55
1:B:38:PRO:CD	1:B:53:TYR:HE2	2.17	0.55
1:B:54:VAL:HG11	1:B:88:HIS:HB2	1.88	0.55
1:B:314:GLN:HE22	1:B:318:THR:HG21	1.70	0.55
1:A:62:ARG:HG3	1:A:63:GLY:H	1.71	0.55
1:A:189:LEU:O	1:A:190:MET:C	2.45	0.55
1:A:367:PRO:O	1:A:370:VAL:HG12	2.06	0.55
1:B:235:SER:CB	1:B:236:LEU:CD2	2.70	0.55
1:B:349:LEU:HD11	1:B:352:PHE:CA	2.35	0.55
1:B:199:SER:O	1:B:200:PHE:CB	2.54	0.55
1:A:203:THR:HA	1:A:206:ARG:NH1	2.21	0.55
1:B:131:ALA:HA	1:B:358:THR:HA	1.87	0.55
1:B:208:ILE:HG22	1:B:212:ILE:CD1	2.36	0.55
1:B:274:ILE:HD12	1:B:313:MET:HE1	1.88	0.55
1:A:152:VAL:HG12	1:A:153:LEU:N	2.22	0.55
1:B:243:PRO:C	1:B:245:GLY:N	2.59	0.55
1:B:334:GLU:O	1:B:336:LYS:N	2.37	0.55
1:A:89:THR:C	1:A:93:GLU:HB3	2.26	0.55
1:A:216:LEU:N	1:A:216:LEU:HD22	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:HD21	1:B:115:ASN:HB2	1.72	0.55
1:B:223:PHE:CZ	1:B:266:PHE:CE2	2.95	0.55
1:A:297:ASN:O	1:A:330:ILE:N	2.28	0.55
1:A:299:MET:O	1:A:335:ARG:HD2	2.06	0.55
1:B:188:TYR:CZ	1:B:192:ILE:HD13	2.41	0.55
1:A:170:ALA:O	1:A:171:LEU:HD23	2.05	0.55
1:A:238:LYS:HG3	1:A:239:SER:H	1.71	0.55
1:A:267:ILE:O	1:A:267:ILE:HG13	2.07	0.55
1:A:295:ALA:O	1:A:328:LYS:HB3	2.07	0.55
1:A:373:LYS:CD	1:B:373:LYS:C	2.75	0.55
1:B:272:ALA:HB3	1:B:277:THR:HG22	1.87	0.55
1:A:27:PRO:HB3	1:A:340:TRP:CD2	2.42	0.55
1:A:247:VAL:C	1:A:248:ILE:HG13	2.25	0.55
1:A:289:ILE:O	1:A:290:ARG:C	2.45	0.55
1:B:21:PHE:HE2	1:B:28:ARG:CZ	2.20	0.55
1:B:247:VAL:C	1:B:248:ILE:HD12	2.27	0.55
1:A:205:GLU:HA	1:A:208:ILE:CD1	2.37	0.54
1:A:285:CYS:O	1:A:290:ARG:CZ	2.55	0.54
1:A:307:PRO:O	1:A:309:ILE:N	2.40	0.54
1:B:98:PRO:HG2	1:B:99:GLU:H	1.72	0.54
1:B:212:ILE:O	1:B:216:LEU:HD22	2.07	0.54
1:B:259:GLU:O	1:B:261:LEU:N	2.40	0.54
1:B:362:TYR:C	1:B:364:GLU:H	2.10	0.54
1:A:122:ILE:O	1:A:123:MET:C	2.44	0.54
1:A:373:LYS:H	1:B:372:ARG:HE	1.54	0.54
1:B:164:PRO:HB2	1:B:171:LEU:CD1	2.33	0.54
1:A:185:LEU:HA	1:A:188:TYR:HB3	1.90	0.54
1:A:251:GLY:O	1:A:253:GLU:N	2.40	0.54
1:A:275:HIS:HB3	1:A:313:MET:SD	2.47	0.54
1:B:69:TYR:H	1:B:69:TYR:HD1	1.56	0.54
1:B:71:ILE:HD12	1:B:82:MET:HE2	1.58	0.54
1:B:242:LEU:HD11	1:B:244:ASP:HB2	1.89	0.54
1:A:176:MET:HE2	1:A:277:THR:CA	2.38	0.54
1:B:150:GLY:HA2	1:B:293:LEU:CA	2.19	0.54
1:B:259:GLU:OE2	1:B:262:PHE:HB2	2.06	0.54
1:A:28:ARG:HG2	1:A:28:ARG:NH1	2.23	0.54
1:A:135:ALA:HB3	1:A:140:LEU:HD21	1.88	0.54
1:A:273:GLY:O	1:A:277:THR:HG23	2.07	0.54
1:A:325:MET:HE2	1:A:326:LYS:O	2.08	0.54
1:A:227:MET:O	1:A:230:ALA:HB3	2.08	0.54
1:A:337:TYR:O	1:A:341:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ALA:O	1:B:152:VAL:HG21	2.08	0.54
1:B:217:CYS:HA	1:B:254:ARG:O	2.08	0.54
1:B:252:ASN:OD1	1:B:256:ARG:NE	2.40	0.54
1:B:337:TYR:C	1:B:341:ILE:HG13	2.28	0.54
1:A:218:TYR:CZ	1:A:255:PHE:HB3	2.43	0.54
1:B:227:MET:SD	1:B:252:ASN:HB2	2.48	0.54
1:A:59:GLN:C	1:A:59:GLN:CD	2.67	0.54
1:A:156:GLY:HA3	3:A:376:ATP:PG	2.47	0.54
1:A:211:ASP:OD2	1:A:215:LYS:HE2	2.07	0.54
1:B:39:ARG:NE	1:B:66:THR:HG23	2.23	0.54
1:B:120:THR:HG23	1:B:132:MET:HE1	1.90	0.54
1:B:217:CYS:HB3	1:B:306:TYR:CE1	2.43	0.54
1:B:278:THR:O	1:B:281:SER:HB3	2.08	0.54
1:B:208:ILE:O	1:B:211:ASP:HB3	2.08	0.53
1:B:332:PRO:O	1:B:335:ARG:HG2	2.07	0.53
1:A:122:ILE:O	1:A:123:MET:O	2.26	0.53
1:B:349:LEU:HD12	1:B:351:THR:CB	2.37	0.53
1:B:14:SER:O	1:B:71:ILE:HG22	2.09	0.53
1:B:32:PRO:HB2	1:B:34:ILE:CG1	2.37	0.53
1:B:224:GLU:O	1:B:228:ALA:N	2.42	0.53
1:B:277:THR:O	1:B:280:ASN:HB2	2.08	0.53
1:A:185:LEU:HB3	1:A:257:CYS:HG	1.72	0.53
1:A:240:TYR:O	1:A:242:LEU:N	2.41	0.53
1:A:156:GLY:HA2	3:A:376:ATP:O1A	2.09	0.53
1:A:317:ILE:O	1:A:317:ILE:HD12	2.08	0.53
1:B:98:PRO:C	1:B:100:GLU:H	2.12	0.53
1:B:243:PRO:O	1:B:245:GLY:N	2.40	0.53
1:B:268:GLY:O	1:B:269:MET:C	2.43	0.53
1:B:305:MET:HA	1:B:335:ARG:HH11	1.72	0.53
1:B:336:LYS:NZ	3:B:386:ATP:N7	2.48	0.53
1:A:235:SER:H	1:A:236:LEU:HD11	1.63	0.53
1:B:132:MET:HE2	1:B:357:ILE:HB	1.89	0.53
1:B:314:GLN:NE2	1:B:318:THR:OG1	2.41	0.53
1:A:226:GLU:HG2	1:A:255:PHE:CD1	2.42	0.53
1:B:209:VAL:HG12	1:B:210:ARG:N	2.23	0.53
1:B:223:PHE:CZ	1:B:266:PHE:CZ	2.96	0.53
1:B:301:GLY:CA	1:B:304:THR:HG23	2.39	0.53
1:B:318:THR:C	1:B:320:LEU:H	2.12	0.53
1:A:79:TRP:O	1:A:82:MET:HB3	2.08	0.53
1:A:86:TRP:O	1:A:90:PHE:CD1	2.62	0.53
1:A:313:MET:O	1:A:316:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:HG	1:B:222:ASP:OD1	2.09	0.53
1:B:282:ILE:O	1:B:285:CYS:HB2	2.09	0.53
1:B:305:MET:O	1:B:307:PRO:N	2.42	0.53
1:A:22:ALA:O	1:A:24:ASP:N	2.41	0.53
1:A:202:THR:OG1	1:A:205:GLU:HG3	2.08	0.53
1:A:289:ILE:HG13	1:A:290:ARG:H	1.74	0.53
1:B:91:TYR:O	1:B:93:GLU:N	2.42	0.53
1:B:143:TYR:O	1:B:145:SER:N	2.42	0.53
1:A:262:PHE:CE2	1:A:274:ILE:HD11	2.44	0.53
1:B:27:PRO:HB3	1:B:340:TRP:CZ2	2.44	0.53
1:B:131:ALA:HA	1:B:357:ILE:O	2.09	0.53
1:B:319:ALA:O	1:B:320:LEU:HD12	2.09	0.53
1:A:14:SER:HA	1:A:71:ILE:CG2	2.39	0.52
1:A:151:ILE:HG22	1:A:151:ILE:O	2.09	0.52
1:B:12:ASN:O	1:B:13:GLY:C	2.45	0.52
1:B:132:MET:C	1:B:356:TRP:CZ3	2.82	0.52
1:B:132:MET:CA	1:B:356:TRP:CE3	2.92	0.52
1:A:85:ILE:O	1:A:86:TRP:C	2.47	0.52
1:A:269:MET:HA	1:A:269:MET:HE3	1.90	0.52
1:B:209:VAL:O	1:B:212:ILE:N	2.41	0.52
1:B:287:ILE:HA	1:B:290:ARG:CD	2.40	0.52
1:A:97:ALA:HB3	1:A:100:GLU:HB3	1.91	0.52
1:B:34:ILE:HD12	1:B:34:ILE:O	2.10	0.52
1:B:76:ILE:HG22	1:B:77:THR:N	2.23	0.52
1:B:99:GLU:HB2	1:B:128:ASN:O	2.10	0.52
1:B:235:SER:O	1:B:236:LEU:HD23	2.05	0.52
1:B:260:THR:CG2	1:B:266:PHE:CD1	2.83	0.52
1:A:103:THR:O	1:A:356:TRP:HZ3	1.92	0.52
1:A:198:TYR:HE1	1:A:248:ILE:CD1	2.16	0.52
1:B:37:ARG:HA	1:B:53:TYR:CE2	2.44	0.52
1:B:61:LYS:HD2	1:B:65:LEU:HD13	1.90	0.52
1:B:79:TRP:O	1:B:81:ASP:N	2.42	0.52
1:B:355:MET:CE	1:B:374:CYS:SG	2.97	0.52
1:A:91:TYR:C	1:A:93:GLU:N	2.63	0.52
1:A:116:ARG:NH1	1:A:116:ARG:CB	2.72	0.52
1:B:182:GLY:H	1:B:303:THR:CG2	2.16	0.52
1:B:188:TYR:O	1:B:191:LYS:N	2.34	0.52
1:B:207:GLU:CD	1:B:210:ARG:HH21	2.12	0.52
1:B:299:MET:HG2	1:B:331:ALA:HA	1.91	0.52
1:B:332:PRO:O	1:B:335:ARG:HB3	2.10	0.52
1:B:362:TYR:HE1	1:B:367:PRO:HG3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:CE1	1:A:375:PHE:HA	2.44	0.52
1:B:79:TRP:O	1:B:80:ASP:C	2.48	0.52
1:B:150:GLY:HA3	1:B:296:ASN:HB2	1.91	0.52
1:B:229:THR:HA	1:B:232:SER:HB2	1.91	0.52
1:A:124:PHE:O	1:A:128:ASN:CA	2.56	0.52
1:A:177:ARG:O	1:A:177:ARG:HG2	2.10	0.52
1:A:193:LEU:C	1:A:195:GLU:N	2.61	0.52
1:B:92:ASN:N	1:B:92:ASN:ND2	2.56	0.52
1:B:330:ILE:HG22	1:B:332:PRO:HD3	1.91	0.52
1:A:142:LEU:CD2	1:A:165:ILE:HD12	2.39	0.52
1:A:175:ILE:O	1:A:175:ILE:HG22	2.09	0.52
1:B:75:ILE:HG23	1:B:115:ASN:HD21	1.73	0.52
1:A:199:SER:O	1:A:200:PHE:HB2	2.08	0.52
1:A:234:SER:C	1:A:236:LEU:HD22	2.30	0.52
1:B:161:HIS:NE2	1:B:177:ARG:HG3	2.25	0.52
1:B:200:PHE:N	1:B:200:PHE:CB	2.65	0.52
1:A:143:TYR:O	1:A:145:SER:N	2.43	0.52
1:A:215:LYS:HB2	1:A:216:LEU:HD22	1.92	0.52
1:A:136:ILE:O	1:A:137:GLN:C	2.48	0.51
1:A:219:VAL:HG21	1:A:309:ILE:HD13	1.92	0.51
1:A:317:ILE:CG1	1:A:321:ALA:HB2	2.39	0.51
1:B:80:ASP:O	1:B:83:GLU:HG3	2.10	0.51
1:B:107:GLU:HB3	1:B:134:VAL:CG1	2.41	0.51
1:A:370:VAL:HG13	1:A:371:HIS:ND1	2.25	0.51
1:B:73:HIS:HD2	1:B:159:VAL:HG22	1.75	0.51
1:B:89:THR:O	1:B:90:PHE:C	2.48	0.51
1:A:287:ILE:N	1:A:290:ARG:HH22	2.08	0.51
1:B:268:GLY:O	1:B:270:GLU:N	2.43	0.51
1:A:350:SER:CA	1:A:353:GLN:HE21	2.23	0.51
1:B:116:ARG:C	1:B:118:LYS:H	2.14	0.51
1:A:6:THR:O	1:A:102:PRO:HD2	2.11	0.51
1:A:7:ALA:C	1:A:8:LEU:HG	2.30	0.51
1:A:76:ILE:HG21	1:A:82:MET:HG2	1.92	0.51
1:A:122:ILE:HG23	1:A:126:THR:CG2	2.40	0.51
1:A:252:ASN:CG	1:A:256:ARG:HE	2.14	0.51
1:A:358:THR:HG23	1:A:361:GLU:OE1	2.11	0.51
1:B:58:ALA:HB1	1:B:67:LEU:CD1	2.39	0.51
1:B:59:GLN:HE21	4:B:387:LAR:H223	1.76	0.51
1:B:132:MET:O	1:B:357:ILE:HB	2.11	0.51
1:B:262:PHE:CE2	1:B:274:ILE:HD11	2.46	0.51
1:A:79:TRP:HA	1:A:82:MET:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:HD21	1:B:148:THR:HA	1.92	0.51
1:B:149:THR:HG22	1:B:166:TYR:HA	1.91	0.51
1:B:227:MET:HG2	1:B:255:PHE:HE1	1.76	0.51
1:B:192:ILE:HG13	1:B:193:LEU:HD13	1.93	0.51
1:B:306:TYR:O	1:B:309:ILE:HB	2.10	0.51
1:A:279:TYR:CD1	1:A:320:LEU:HB2	2.45	0.51
1:B:32:PRO:HB2	1:B:34:ILE:HG13	1.92	0.51
1:B:152:VAL:CG2	1:B:163:VAL:HB	2.41	0.51
1:B:274:ILE:CG1	1:B:275:HIS:N	2.73	0.51
1:A:64:ILE:HG13	1:A:65:LEU:HD12	1.93	0.51
1:A:70:PRO:HG2	1:A:85:ILE:CD1	2.39	0.51
1:A:190:MET:CG	1:A:209:VAL:HG21	2.40	0.51
1:B:80:ASP:HA	1:B:83:GLU:OE1	2.10	0.51
1:B:142:LEU:CD2	1:B:165:ILE:HD13	2.29	0.51
1:B:142:LEU:CD2	1:B:165:ILE:HG21	2.41	0.51
1:B:222:ASP:HB2	1:B:226:GLU:H	1.74	0.51
1:B:223:PHE:HD2	1:B:263:GLN:OE1	1.91	0.51
1:B:332:PRO:HB3	1:B:333:PRO:HD2	1.93	0.51
1:A:166:TYR:C	1:A:168:GLY:N	2.63	0.50
1:A:181:ALA:O	1:A:183:ARG:N	2.43	0.50
1:A:212:ILE:O	1:A:216:LEU:HD23	2.11	0.50
1:B:88:HIS:CE1	1:B:93:GLU:OE2	2.63	0.50
1:B:132:MET:CE	1:B:357:ILE:HD12	2.42	0.50
1:B:307:PRO:C	1:B:309:ILE:N	2.64	0.50
1:A:64:ILE:HG13	1:A:65:LEU:CD1	2.41	0.50
1:A:62:ARG:CG	1:A:63:GLY:N	2.67	0.50
1:A:287:ILE:CG2	1:A:288:ASP:H	2.21	0.50
1:B:182:GLY:C	1:B:184:ASP:H	2.14	0.50
1:B:188:TYR:CE2	1:B:257:CYS:HA	2.40	0.50
1:B:329:ILE:O	1:B:330:ILE:C	2.48	0.50
1:B:338:SER:N	1:B:341:ILE:HD12	2.27	0.50
1:A:218:TYR:HE2	1:A:254:ARG:CB	2.21	0.50
1:A:234:SER:O	1:A:236:LEU:N	2.40	0.50
1:B:147:ARG:NH2	1:B:330:ILE:HG21	2.26	0.50
1:B:172:PRO:O	1:B:173:HIS:C	2.49	0.50
1:B:305:MET:O	1:B:307:PRO:CD	2.60	0.50
1:A:85:ILE:HG22	1:A:86:TRP:N	2.27	0.50
1:B:109:PRO:HG3	1:B:136:ILE:HG22	1.93	0.50
1:B:133:TYR:HB2	1:B:356:TRP:CE3	2.47	0.50
1:B:305:MET:O	1:B:307:PRO:HD3	2.12	0.50
1:A:181:ALA:O	1:A:184:ASP:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:O	1:A:278:THR:N	2.45	0.50
1:A:9:VAL:O	1:A:19:ALA:HA	2.11	0.50
1:A:263:GLN:C	1:A:265:SER:N	2.61	0.50
1:B:250:ILE:N	1:B:250:ILE:CD1	2.74	0.50
1:A:183:ARG:HB3	1:A:183:ARG:NH1	2.26	0.50
1:B:17:VAL:O	1:B:30:VAL:HA	2.12	0.50
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.94	0.50
1:A:317:ILE:O	1:A:320:LEU:N	2.45	0.50
1:A:337:TYR:O	1:A:340:TRP:N	2.45	0.50
1:B:193:LEU:C	1:B:195:GLU:H	2.14	0.50
1:A:73:HIS:O	1:A:159:VAL:HG11	2.12	0.49
1:B:40:HIS:CE1	5:B:402:HOH:O	2.64	0.49
1:B:111:ASN:OD1	1:B:112:PRO:HD2	2.11	0.49
1:B:218:TYR:N	1:B:258:PRO:HG3	2.26	0.49
1:A:223:PHE:CD1	1:A:259:GLU:HG2	2.47	0.49
1:A:314:GLN:NE2	1:A:318:THR:CG2	2.75	0.49
1:B:59:GLN:HB2	4:B:387:LAR:H91	1.94	0.49
1:B:301:GLY:C	1:B:304:THR:HG23	2.31	0.49
1:B:151:ILE:HD11	1:B:164:PRO:HG3	1.94	0.49
1:A:5:THR:O	1:A:102:PRO:HG2	2.12	0.49
1:A:73:HIS:HA	1:A:159:VAL:HG13	1.94	0.49
1:A:282:ILE:C	1:A:284:LYS:H	2.15	0.49
1:B:79:TRP:CZ3	1:B:118:LYS:HG2	2.47	0.49
1:B:142:LEU:CD2	1:B:148:THR:HA	2.43	0.49
1:B:283:MET:C	1:B:285:CYS:H	2.15	0.49
1:B:335:ARG:HG2	1:B:335:ARG:NH2	2.26	0.49
1:A:373:LYS:HD3	1:B:373:LYS:C	2.33	0.49
1:B:193:LEU:C	1:B:195:GLU:N	2.66	0.49
1:B:196:ARG:NH2	1:B:251:GLY:HA3	2.27	0.49
1:B:365:ALA:O	1:B:366:GLY:O	2.30	0.49
1:A:149:THR:OG1	1:A:167:GLU:N	2.41	0.49
1:A:160:THR:O	1:A:178:LEU:N	2.42	0.49
1:B:144:ALA:HB2	1:B:342:GLY:HA3	1.94	0.49
1:A:149:THR:HG1	1:A:167:GLU:N	2.10	0.49
1:A:207:GLU:OE2	1:A:210:ARG:NE	2.45	0.49
1:A:227:MET:HA	1:A:255:PHE:CZ	2.48	0.49
1:B:82:MET:SD	1:B:85:ILE:HD12	2.52	0.49
1:B:86:TRP:O	1:B:89:THR:HB	2.13	0.49
1:A:53:TYR:HB3	1:A:57:GLU:OE1	2.12	0.49
1:A:200:PHE:CD2	1:A:205:GLU:OE2	2.66	0.49
1:A:305:MET:HE2	1:A:336:LYS:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:C	1:B:18:LYS:HD3	2.33	0.49
1:B:32:PRO:HB2	1:B:34:ILE:HD11	1.95	0.49
1:B:37:ARG:HA	1:B:53:TYR:HD2	1.78	0.49
1:B:59:GLN:CG	1:B:60:SER:N	2.75	0.49
1:B:80:ASP:CA	1:B:83:GLU:HG3	2.43	0.49
1:B:139:VAL:O	1:B:142:LEU:N	2.46	0.49
1:A:220:ALA:HB2	1:A:255:PHE:CB	2.42	0.49
1:A:262:PHE:CD2	1:A:274:ILE:HD11	2.48	0.49
1:A:321:ALA:HB1	1:A:327:ILE:HD11	1.95	0.49
1:B:262:PHE:CE2	1:B:316:GLU:HG3	2.43	0.49
1:A:79:TRP:O	1:A:80:ASP:C	2.50	0.49
1:A:79:TRP:CZ2	1:A:115:ASN:OD1	2.66	0.49
1:A:314:GLN:O	1:A:317:ILE:HG23	2.12	0.49
1:A:317:ILE:C	1:A:319:ALA:N	2.66	0.49
1:B:9:VAL:HG21	1:B:344:SER:HA	1.94	0.49
1:B:85:ILE:O	1:B:88:HIS:HB3	2.13	0.49
1:B:224:GLU:O	1:B:227:MET:N	2.46	0.49
1:A:188:TYR:CD2	1:A:257:CYS:HA	2.48	0.48
1:A:248:ILE:HG22	1:A:249:THR:N	2.28	0.48
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.95	0.48
1:A:290:ARG:O	1:A:291:LYS:C	2.50	0.48
1:B:315:LYS:O	1:B:317:ILE:N	2.46	0.48
1:A:189:LEU:O	1:A:192:ILE:N	2.46	0.48
1:A:189:LEU:HD12	1:A:192:ILE:HD11	1.93	0.48
1:A:198:TYR:CD1	1:A:248:ILE:HD13	2.41	0.48
1:B:37:ARG:HB3	1:B:38:PRO:CD	2.43	0.48
1:B:97:ALA:O	1:B:101:HIS:HD2	1.96	0.48
1:B:132:MET:CA	1:B:356:TRP:CZ3	2.95	0.48
1:B:132:MET:HE3	1:B:357:ILE:HD12	1.95	0.48
1:A:180:LEU:C	1:A:180:LEU:HD12	2.33	0.48
1:B:117:GLU:HG2	1:B:367:PRO:C	2.33	0.48
1:B:210:ARG:HB2	4:B:387:LAR:C20	2.43	0.48
1:B:333:PRO:C	1:B:335:ARG:H	2.16	0.48
1:A:61:LYS:HB2	1:A:65:LEU:CD1	2.43	0.48
1:A:213:LYS:O	1:A:217:CYS:HB2	2.13	0.48
1:A:235:SER:CA	1:A:236:LEU:HD13	2.43	0.48
1:B:91:TYR:O	1:B:95:ARG:CD	2.47	0.48
1:B:315:LYS:O	1:B:316:GLU:C	2.52	0.48
1:B:359:LYS:NZ	1:B:363:ASP:OD1	2.36	0.48
1:B:188:TYR:O	1:B:189:LEU:C	2.51	0.48
1:A:287:ILE:O	1:A:289:ILE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG12	1:A:36:GLY:H	1.78	0.48
1:A:183:ARG:HB2	1:A:183:ARG:CZ	2.43	0.48
1:A:246:GLN:HE21	1:A:248:ILE:HD11	1.78	0.48
1:A:289:ILE:CG1	1:A:290:ARG:H	2.27	0.48
1:B:90:PHE:HB3	1:B:96:VAL:HG23	1.96	0.48
1:B:153:LEU:HD11	1:B:160:THR:HG22	1.95	0.48
1:A:59:GLN:C	1:A:61:LYS:H	2.17	0.48
1:A:183:ARG:O	1:A:187:ASP:OD2	2.32	0.48
1:A:210:ARG:O	1:A:213:LYS:HB3	2.13	0.48
1:A:298:VAL:HG12	1:A:299:MET:H	1.79	0.48
1:B:31:PHE:HB2	1:B:32:PRO:CD	2.37	0.48
1:B:132:MET:HA	1:B:356:TRP:CE3	2.48	0.48
1:B:325:MET:CG	1:B:327:ILE:HD11	2.42	0.48
1:A:23:GLY:O	1:A:24:ASP:C	2.52	0.48
1:B:162:ASN:ND2	1:B:278:THR:OG1	2.47	0.48
1:B:212:ILE:O	1:B:213:LYS:C	2.52	0.48
1:B:313:MET:O	1:B:314:GLN:C	2.52	0.48
1:A:79:TRP:HA	1:A:82:MET:HB3	1.95	0.48
1:A:123:MET:HE2	1:A:129:VAL:HG11	1.94	0.48
1:A:186:THR:HG21	4:A:377:LAR:S1	2.54	0.48
1:A:313:MET:O	1:A:314:GLN:C	2.52	0.48
1:B:132:MET:HE2	1:B:132:MET:O	2.13	0.48
1:B:161:HIS:CE1	1:B:177:ARG:HB2	2.48	0.48
1:B:172:PRO:HA	1:B:175:ILE:CD1	2.43	0.48
1:B:232:SER:O	1:B:233:SER:C	2.53	0.48
1:B:255:PHE:O	1:B:259:GLU:HB3	2.14	0.48
1:B:285:CYS:O	1:B:290:ARG:NE	2.27	0.48
1:B:312:ARG:NE	1:B:316:GLU:OE1	2.39	0.48
1:A:201:VAL:HG22	1:A:201:VAL:O	2.14	0.47
1:A:219:VAL:HG21	1:A:309:ILE:CB	2.42	0.47
1:B:58:ALA:CA	1:B:61:LYS:HE2	2.41	0.47
1:B:299:MET:SD	1:B:299:MET:N	2.87	0.47
1:A:71:ILE:HG13	1:A:82:MET:HE1	1.94	0.47
1:A:280:ASN:HD22	1:A:280:ASN:H	1.61	0.47
1:B:107:GLU:OE2	1:B:135:ALA:HA	2.13	0.47
1:B:229:THR:C	1:B:232:SER:HB2	2.35	0.47
1:B:274:ILE:O	1:B:277:THR:N	2.47	0.47
1:B:317:ILE:HD13	1:B:327:ILE:HG21	1.96	0.47
1:A:98:PRO:HG2	1:A:99:GLU:OE1	2.14	0.47
1:A:303:THR:C	1:A:305:MET:N	2.68	0.47
1:A:9:VAL:HG12	1:A:340:TRP:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ALA:HB3	1:A:100:GLU:CB	2.44	0.47
1:A:113:LYS:HG3	1:B:364:GLU:OE2	2.13	0.47
1:A:189:LEU:O	1:A:192:ILE:HG12	2.13	0.47
1:A:223:PHE:O	1:A:227:MET:N	2.33	0.47
1:B:12:ASN:O	1:B:13:GLY:O	2.31	0.47
1:B:172:PRO:HD2	1:B:173:HIS:CE1	2.48	0.47
1:B:193:LEU:N	1:B:193:LEU:CD1	2.76	0.47
1:A:93:GLU:C	1:A:93:GLU:OE1	2.52	0.47
1:A:93:GLU:CG	1:A:94:LEU:HD12	2.41	0.47
1:A:123:MET:C	1:A:129:VAL:HG22	2.34	0.47
1:A:124:PHE:HE1	1:A:130:PRO:O	1.98	0.47
1:A:136:ILE:HB	1:A:139:VAL:HG23	1.96	0.47
1:A:295:ALA:HA	1:A:328:LYS:N	2.28	0.47
1:B:13:GLY:HA3	3:B:386:ATP:O2B	2.14	0.47
1:B:343:GLY:C	1:B:345:ILE:N	2.67	0.47
1:A:90:PHE:CD1	1:A:90:PHE:N	2.83	0.47
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.49	0.47
1:A:352:PHE:O	1:A:353:GLN:C	2.53	0.47
1:B:61:LYS:HD2	1:B:65:LEU:CD1	2.44	0.47
1:B:110:LEU:HD11	1:B:175:ILE:CD1	2.32	0.47
1:B:124:PHE:HA	1:B:129:VAL:HG23	1.96	0.47
1:A:140:LEU:HD12	1:A:339:VAL:CG1	2.44	0.47
1:A:160:THR:HB	1:A:178:LEU:O	2.15	0.47
1:B:92:ASN:ND2	1:B:92:ASN:H	2.12	0.47
1:B:187:ASP:HA	1:B:190:MET:HE3	1.97	0.47
1:B:279:TYR:CE1	1:B:294:TYR:OH	2.68	0.47
1:A:11:ASP:HB3	1:A:18:LYS:HB2	1.95	0.47
1:A:226:GLU:HG3	1:A:255:PHE:CE1	2.50	0.47
1:A:318:THR:HA	1:A:321:ALA:CB	2.27	0.47
1:B:338:SER:HA	1:B:341:ILE:HD12	1.96	0.47
1:A:141:SER:OG	1:A:339:VAL:HG22	2.15	0.47
1:B:120:THR:HG23	1:B:132:MET:SD	2.54	0.47
1:B:186:THR:C	1:B:188:TYR:N	2.65	0.47
1:B:253:GLU:HA	1:B:256:ARG:CB	2.45	0.47
1:B:259:GLU:OE2	1:B:263:GLN:NE2	2.47	0.47
1:A:189:LEU:O	1:A:191:LYS:N	2.48	0.47
1:A:279:TYR:C	1:A:281:SER:H	2.18	0.47
1:A:350:SER:HA	1:A:353:GLN:HE21	1.79	0.47
1:B:170:ALA:O	1:B:172:PRO:HD3	2.14	0.47
1:B:185:LEU:HD12	1:B:185:LEU:N	2.29	0.47
1:B:229:THR:CA	1:B:232:SER:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:TYR:C	1:B:364:GLU:N	2.68	0.47
1:B:370:VAL:O	1:B:370:VAL:CG2	2.63	0.47
1:A:81:ASP:HA	1:A:84:LYS:HB3	1.97	0.46
1:A:166:TYR:C	1:A:168:GLY:H	2.18	0.46
1:B:118:LYS:HB2	1:B:118:LYS:HZ2	1.76	0.46
1:B:164:PRO:HG2	1:B:174:ALA:O	2.15	0.46
1:A:11:ASP:HA	1:A:106:THR:HG21	1.97	0.46
1:A:285:CYS:O	1:A:286:ASP:C	2.53	0.46
1:B:107:GLU:HG2	1:B:136:ILE:N	2.30	0.46
1:B:157:ASP:HA	3:B:386:ATP:H4'	1.97	0.46
1:A:11:ASP:HA	1:A:106:THR:CG2	2.46	0.46
1:A:99:GLU:HB3	1:A:127:PHE:O	2.15	0.46
1:A:122:ILE:HG23	1:A:126:THR:HG21	1.95	0.46
1:A:130:PRO:HG2	1:A:131:ALA:H	1.81	0.46
1:A:217:CYS:SG	1:A:258:PRO:CD	2.85	0.46
1:A:226:GLU:CG	1:A:255:PHE:CE1	2.98	0.46
1:A:315:LYS:O	1:A:316:GLU:C	2.54	0.46
1:B:242:LEU:HD11	1:B:244:ASP:CB	2.45	0.46
1:A:290:ARG:O	1:A:293:LEU:N	2.47	0.46
1:A:368:SER:HB2	1:B:365:ALA:O	2.14	0.46
1:B:21:PHE:HD2	1:B:24:ASP:OD2	1.97	0.46
1:B:29:ALA:HB2	1:B:94:LEU:HD11	1.98	0.46
1:B:133:TYR:CB	1:B:356:TRP:CZ3	2.99	0.46
1:B:264:PRO:O	1:B:267:ILE:N	2.37	0.46
1:A:21:PHE:HE2	1:A:28:ARG:HE	1.62	0.46
1:A:291:LYS:O	1:A:294:TYR:HB2	2.15	0.46
1:A:299:MET:O	1:A:299:MET:CG	2.63	0.46
1:A:299:MET:CE	1:A:304:THR:HB	2.45	0.46
1:B:114:ALA:O	1:B:118:LYS:NZ	2.48	0.46
1:B:119:MET:HA	1:B:122:ILE:HB	1.98	0.46
1:B:151:ILE:HD13	1:B:163:VAL:C	2.36	0.46
1:A:163:VAL:HG12	1:A:165:ILE:CG1	2.46	0.46
1:A:222:ASP:O	1:A:226:GLU:HB3	2.16	0.46
1:A:307:PRO:C	1:A:309:ILE:N	2.68	0.46
1:B:13:GLY:O	1:B:14:SER:C	2.53	0.46
1:B:123:MET:HA	1:B:127:PHE:CD1	2.50	0.46
1:B:133:TYR:HE2	1:B:355:MET:HB3	1.78	0.46
1:B:150:GLY:O	1:B:165:ILE:HD12	2.16	0.46
1:A:262:PHE:CZ	1:A:274:ILE:HD11	2.50	0.46
1:B:11:ASP:C	1:B:13:GLY:H	2.18	0.46
1:B:170:ALA:C	1:B:172:PRO:HD3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:THR:O	1:B:204:ALA:C	2.52	0.46
1:B:337:TYR:O	1:B:340:TRP:N	2.49	0.46
1:B:354:GLN:HE21	1:B:355:MET:CE	2.28	0.46
1:A:276:GLU:O	1:A:279:TYR:N	2.48	0.46
1:A:276:GLU:C	1:A:278:THR:N	2.69	0.46
1:B:53:TYR:CG	1:B:61:LYS:HE3	2.51	0.46
1:A:309:ILE:HG23	1:A:310:ALA:N	2.30	0.46
1:A:325:MET:HE3	1:A:326:LYS:H	1.80	0.46
1:B:21:PHE:O	1:B:22:ALA:C	2.55	0.46
1:B:314:GLN:HE22	1:B:318:THR:CG2	2.28	0.46
1:A:218:TYR:O	1:A:258:PRO:CG	2.63	0.46
1:A:248:ILE:CG2	1:A:249:THR:N	2.78	0.46
1:B:349:LEU:HD12	1:B:351:THR:C	2.35	0.46
1:A:113:LYS:CA	1:A:116:ARG:HH12	2.23	0.45
1:A:325:MET:CE	1:A:326:LYS:N	2.79	0.45
1:B:79:TRP:C	1:B:81:ASP:N	2.69	0.45
1:B:116:ARG:C	1:B:118:LYS:N	2.70	0.45
1:B:306:TYR:CE1	3:B:386:ATP:H2	2.34	0.45
1:A:13:GLY:CA	3:A:376:ATP:PB	3.01	0.45
1:A:320:LEU:N	1:A:320:LEU:CD2	2.73	0.45
1:A:367:PRO:O	1:A:369:ILE:N	2.49	0.45
1:B:72:GLU:N	1:B:75:ILE:O	2.40	0.45
1:B:105:LEU:CB	1:B:134:VAL:HG22	2.40	0.45
1:B:121:GLN:HE21	1:B:121:GLN:HB3	1.59	0.45
1:B:121:GLN:HB2	1:B:362:TYR:OH	2.15	0.45
1:B:257:CYS:HB3	1:B:258:PRO:CD	2.47	0.45
1:B:261:LEU:O	1:B:274:ILE:HG12	2.16	0.45
1:A:10:CYS:HA	1:A:18:LYS:O	2.16	0.45
1:A:218:TYR:CD2	1:A:254:ARG:HB3	2.51	0.45
1:A:371:HIS:CD2	1:B:365:ALA:HB1	2.51	0.45
1:B:61:LYS:C	1:B:63:GLY:N	2.69	0.45
1:B:142:LEU:HD13	1:B:165:ILE:HD12	1.99	0.45
1:B:164:PRO:CB	1:B:171:LEU:HD12	2.39	0.45
1:B:227:MET:SD	1:B:255:PHE:HZ	2.38	0.45
1:B:262:PHE:CD1	1:B:262:PHE:N	2.85	0.45
1:B:156:GLY:O	1:B:181:ALA:HB1	2.15	0.45
1:B:299:MET:SD	1:B:329:ILE:HG22	2.56	0.45
1:A:88:HIS:O	1:A:93:GLU:CB	2.63	0.45
1:A:90:PHE:CE2	1:A:98:PRO:HB3	2.52	0.45
1:A:164:PRO:HB2	1:A:171:LEU:HD12	1.99	0.45
1:B:29:ALA:O	1:B:30:VAL:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:N	1:B:193:LEU:HD12	2.32	0.45
1:A:51:ASP:CG	1:A:52:SER:H	2.19	0.45
1:A:64:ILE:CD1	1:A:65:LEU:HD12	2.46	0.45
1:A:83:GLU:O	1:A:85:ILE:N	2.49	0.45
1:A:88:HIS:CG	1:A:92:ASN:HB2	2.52	0.45
1:A:172:PRO:O	1:A:174:ALA:N	2.50	0.45
1:A:314:GLN:HE22	1:A:318:THR:HG21	1.81	0.45
1:A:371:HIS:O	1:B:372:ARG:HD2	2.16	0.45
1:B:86:TRP:O	1:B:89:THR:CB	2.65	0.45
1:B:90:PHE:CA	1:B:96:VAL:HG22	2.45	0.45
1:B:106:THR:HA	1:B:135:ALA:O	2.17	0.45
1:B:228:ALA:O	1:B:230:ALA:N	2.49	0.45
1:A:59:GLN:HG3	1:A:60:SER:N	2.31	0.45
1:A:87:HIS:ND1	1:A:87:HIS:C	2.70	0.45
1:A:106:THR:HG22	1:A:140:LEU:HD11	1.99	0.45
1:A:113:LYS:H	1:A:113:LYS:HG2	1.45	0.45
1:A:210:ARG:HG2	1:A:214:GLU:OE2	2.17	0.45
1:A:317:ILE:O	1:A:320:LEU:HG	2.16	0.45
1:B:186:THR:O	1:B:188:TYR:N	2.50	0.45
1:B:191:LYS:O	1:B:193:LEU:N	2.50	0.45
1:A:215:LYS:CB	1:A:216:LEU:HD22	2.46	0.45
1:A:264:PRO:CG	1:A:273:GLY:HA2	2.33	0.45
1:A:286:ASP:O	1:A:287:ILE:C	2.55	0.45
1:A:366:GLY:O	1:A:369:ILE:CG2	2.65	0.45
1:B:27:PRO:HD3	1:B:340:TRP:CE3	2.51	0.45
1:B:283:MET:O	1:B:285:CYS:N	2.50	0.45
1:B:346:LEU:C	1:B:348:SER:H	2.18	0.45
1:A:35:VAL:CG1	1:A:36:GLY:N	2.79	0.45
1:A:54:VAL:CG2	1:A:55:GLY:N	2.80	0.45
1:A:140:LEU:HD12	1:A:339:VAL:HG13	1.98	0.45
1:A:263:GLN:HB2	1:A:266:PHE:CD2	2.52	0.45
1:A:317:ILE:CD1	1:A:321:ALA:HB2	2.47	0.45
1:B:130:PRO:O	1:B:359:LYS:N	2.50	0.45
1:B:133:TYR:HB3	1:B:356:TRP:CZ3	2.52	0.45
1:B:164:PRO:HG3	1:B:281:SER:OG	2.16	0.45
1:B:208:ILE:HG22	1:B:212:ILE:HD12	1.99	0.45
1:B:305:MET:CE	1:B:336:LYS:HB2	2.47	0.45
1:B:337:TYR:O	1:B:338:SER:C	2.55	0.45
1:A:240:TYR:O	1:A:247:VAL:HA	2.16	0.45
1:B:91:TYR:O	1:B:92:ASN:C	2.55	0.45
1:B:299:MET:HG3	1:B:331:ALA:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PRO:HB3	1:B:64:ILE:HD11	1.98	0.44
1:B:88:HIS:HE1	1:B:93:GLU:OE2	1.99	0.44
1:B:104:LEU:N	1:B:356:TRP:HH2	2.14	0.44
1:B:123:MET:O	1:B:124:PHE:C	2.55	0.44
1:B:133:TYR:CB	1:B:356:TRP:CE3	3.01	0.44
1:B:189:LEU:HA	1:B:192:ILE:CD1	2.44	0.44
1:A:154:ASP:OD2	1:A:300:SER:OG	2.35	0.44
1:A:179:ASP:O	1:A:180:LEU:HB3	2.17	0.44
1:B:69:TYR:CD1	1:B:69:TYR:N	2.81	0.44
1:B:122:ILE:O	1:B:123:MET:C	2.55	0.44
1:B:287:ILE:HA	1:B:290:ARG:CG	2.47	0.44
1:A:99:GLU:HB2	1:A:128:ASN:O	2.16	0.44
1:A:269:MET:HG3	1:A:270:GLU:O	2.17	0.44
1:B:39:ARG:CD	1:B:64:ILE:O	2.64	0.44
1:B:111:ASN:HD21	1:B:115:ASN:HB3	1.81	0.44
1:A:18:LYS:N	1:A:18:LYS:HD3	2.32	0.44
1:A:72:GLU:O	1:A:73:HIS:HB2	2.17	0.44
1:A:180:LEU:HB2	1:A:184:ASP:OD1	2.17	0.44
1:A:373:LYS:CD	1:B:372:ARG:HG3	2.47	0.44
1:B:155:SER:O	1:B:303:THR:OG1	2.35	0.44
1:B:203:THR:HA	1:B:206:ARG:CB	2.47	0.44
1:B:218:TYR:CD2	1:B:254:ARG:O	2.68	0.44
1:B:264:PRO:CB	1:B:269:MET:HB2	2.41	0.44
1:B:274:ILE:HG13	1:B:275:HIS:H	1.80	0.44
1:A:6:THR:HG22	1:A:7:ALA:O	2.18	0.44
1:A:103:THR:O	1:A:356:TRP:CZ3	2.71	0.44
1:A:210:ARG:O	1:A:214:GLU:N	2.48	0.44
1:A:338:SER:O	1:A:339:VAL:C	2.56	0.44
1:A:187:ASP:HA	1:A:190:MET:HE2	1.97	0.44
1:A:352:PHE:HA	1:A:355:MET:CG	2.46	0.44
1:B:109:PRO:HB2	1:B:161:HIS:ND1	2.33	0.44
1:B:298:VAL:HA	1:B:330:ILE:O	2.17	0.44
1:A:98:PRO:HB2	1:A:127:PHE:HB3	1.98	0.44
1:A:112:PRO:O	1:A:115:ASN:HB3	2.18	0.44
1:B:72:GLU:HB2	1:B:77:THR:CG2	2.48	0.44
1:B:286:ASP:O	1:B:288:ASP:N	2.51	0.44
1:B:287:ILE:HA	1:B:290:ARG:HG3	1.99	0.44
1:B:207:GLU:OE2	4:B:387:LAR:O4	2.34	0.44
1:B:280:ASN:O	1:B:284:LYS:HG3	2.17	0.44
1:B:358:THR:N	1:B:361:GLU:HB2	2.33	0.44
1:A:74:GLY:O	1:A:75:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:SER:O	1:A:234:SER:OG	2.31	0.44
1:A:256:ARG:HH11	1:A:256:ARG:CB	2.30	0.44
1:A:35:VAL:HG13	1:A:53:TYR:O	2.17	0.43
1:A:157:ASP:CA	3:A:376:ATP:H4'	2.48	0.43
1:A:239:SER:HA	1:A:249:THR:CG2	2.47	0.43
1:A:287:ILE:H	1:A:290:ARG:HH22	1.65	0.43
1:A:334:GLU:O	1:A:336:LYS:N	2.51	0.43
1:B:9:VAL:HB	1:B:340:TRP:CZ2	2.53	0.43
1:B:89:THR:HG22	1:B:90:PHE:N	2.33	0.43
1:B:242:LEU:CD1	1:B:243:PRO:HD2	2.46	0.43
1:B:297:ASN:H	1:B:330:ILE:HD12	1.83	0.43
1:B:349:LEU:CD1	1:B:352:PHE:HB2	2.48	0.43
1:B:354:GLN:HE21	1:B:355:MET:HE1	1.83	0.43
1:A:100:GLU:O	1:A:100:GLU:CG	2.67	0.43
1:A:263:GLN:N	1:A:264:PRO:HD3	2.33	0.43
1:B:56:ASP:CA	1:B:59:GLN:HB3	2.48	0.43
1:B:142:LEU:HD13	1:B:165:ILE:CD1	2.48	0.43
1:B:187:ASP:CG	1:B:206:ARG:NH2	2.71	0.43
1:A:226:GLU:HG3	1:A:255:PHE:CE2	2.51	0.43
1:B:9:VAL:HB	1:B:340:TRP:NE1	2.33	0.43
1:B:292:ASP:OD1	1:B:292:ASP:N	2.48	0.43
1:A:210:ARG:O	1:A:213:LYS:N	2.52	0.43
1:A:313:MET:O	1:A:316:GLU:HB2	2.18	0.43
1:B:133:TYR:CZ	1:B:373:LYS:HG2	2.52	0.43
1:B:216:LEU:H	1:B:216:LEU:CD2	2.24	0.43
1:B:227:MET:SD	1:B:255:PHE:CE1	3.12	0.43
1:A:61:LYS:HB2	1:A:65:LEU:CD2	2.47	0.43
1:A:89:THR:O	1:A:93:GLU:HG3	2.19	0.43
1:A:368:SER:CA	1:A:371:HIS:CD2	3.00	0.43
1:B:172:PRO:O	1:B:175:ILE:N	2.51	0.43
1:A:257:CYS:N	1:A:258:PRO:CD	2.80	0.43
1:A:317:ILE:O	1:A:318:THR:C	2.56	0.43
1:B:9:VAL:CG2	1:B:344:SER:HA	2.49	0.43
1:B:34:ILE:HA	1:B:70:PRO:HD2	2.01	0.43
1:B:90:PHE:HB2	1:B:91:TYR:CE1	2.54	0.43
1:B:185:LEU:H	1:B:185:LEU:CD1	2.29	0.43
1:B:192:ILE:HG21	1:B:256:ARG:HD2	2.00	0.43
1:A:6:THR:O	1:A:101:HIS:ND1	2.51	0.43
1:A:31:PHE:HB2	1:A:32:PRO:CD	2.36	0.43
1:B:70:PRO:HB2	1:B:71:ILE:H	1.29	0.43
1:B:143:TYR:C	1:B:145:SER:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:CD1	1:B:184:ASP:HB3	2.48	0.43
1:B:301:GLY:O	1:B:304:THR:HG23	2.18	0.43
1:A:120:THR:O	1:A:121:GLN:C	2.57	0.43
1:A:141:SER:O	1:A:144:ALA:HB3	2.19	0.43
1:A:302:GLY:O	1:A:305:MET:HB2	2.19	0.43
1:A:303:THR:O	1:A:304:THR:C	2.57	0.43
1:B:73:HIS:CD2	1:B:159:VAL:HG22	2.53	0.43
1:B:89:THR:O	1:B:91:TYR:N	2.52	0.43
1:B:126:THR:O	1:B:127:PHE:CG	2.72	0.43
1:B:156:GLY:HA3	3:B:386:ATP:O2G	2.19	0.43
1:B:301:GLY:HA3	1:B:304:THR:HG23	2.00	0.43
1:B:329:ILE:HD13	1:B:329:ILE:N	2.34	0.43
1:A:76:ILE:N	1:A:76:ILE:CD1	2.80	0.43
1:A:121:GLN:O	1:A:125:GLU:HB2	2.18	0.43
1:A:210:ARG:HA	1:A:213:LYS:HB3	2.00	0.43
1:A:289:ILE:O	1:A:291:LYS:N	2.52	0.43
1:B:55:GLY:O	1:B:58:ALA:HB3	2.19	0.43
1:B:78:ASN:ND2	1:B:81:ASP:HB2	2.32	0.43
1:B:202:THR:O	1:B:206:ARG:N	2.48	0.43
1:A:201:VAL:O	1:A:201:VAL:CG2	2.66	0.43
1:A:209:VAL:O	1:A:213:LYS:N	2.32	0.43
1:A:345:ILE:O	1:A:348:SER:N	2.52	0.43
1:B:132:MET:N	1:B:357:ILE:O	2.51	0.43
1:B:177:ARG:O	1:B:177:ARG:HG2	2.19	0.43
1:B:218:TYR:H	1:B:258:PRO:HG3	1.84	0.43
1:B:219:VAL:CG1	1:B:312:ARG:NH1	2.82	0.43
1:A:151:ILE:HG22	1:A:297:ASN:ND2	2.34	0.42
1:A:241:GLU:HA	1:A:247:VAL:HG12	2.01	0.42
1:A:153:LEU:H	1:A:299:MET:HA	1.84	0.42
1:A:262:PHE:C	1:A:264:PRO:HD3	2.39	0.42
1:A:287:ILE:O	1:A:288:ASP:C	2.56	0.42
1:B:36:GLY:O	1:B:53:TYR:HD2	2.01	0.42
1:B:122:ILE:O	1:B:123:MET:O	2.36	0.42
1:B:139:VAL:O	1:B:142:LEU:CB	2.63	0.42
1:B:190:MET:HG2	1:B:209:VAL:CG2	2.36	0.42
1:B:336:LYS:HE3	3:B:386:ATP:N7	2.33	0.42
1:A:76:ILE:H	1:A:76:ILE:CD1	2.27	0.42
1:A:121:GLN:NE2	1:A:121:GLN:C	2.73	0.42
1:A:142:LEU:HD12	1:A:147:ARG:HB2	2.02	0.42
1:B:53:TYR:HB2	1:B:65:LEU:HD21	2.01	0.42
1:B:188:TYR:O	1:B:191:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:MET:O	1:B:290:ARG:CZ	2.67	0.42
1:B:294:TYR:HD1	1:B:327:ILE:HD12	1.83	0.42
1:B:322:PRO:O	1:B:323:SER:C	2.58	0.42
1:A:218:TYR:HA	1:A:307:PRO:HD2	2.01	0.42
1:A:226:GLU:HG2	1:A:255:PHE:CG	2.55	0.42
1:A:358:THR:HG23	1:A:361:GLU:CD	2.39	0.42
1:B:78:ASN:O	1:B:81:ASP:CB	2.68	0.42
1:B:123:MET:HG3	1:B:129:VAL:CG2	2.31	0.42
1:B:153:LEU:HD11	1:B:160:THR:CG2	2.49	0.42
1:B:178:LEU:N	1:B:178:LEU:HD12	2.34	0.42
1:B:242:LEU:HG	1:B:244:ASP:HB3	2.02	0.42
1:B:253:GLU:C	1:B:255:PHE:N	2.73	0.42
1:A:39:ARG:O	1:A:40:HIS:HB2	2.19	0.42
1:A:252:ASN:OD1	1:A:253:GLU:N	2.53	0.42
1:A:117:GLU:OE1	1:A:367:PRO:HB2	2.19	0.42
1:A:306:TYR:CZ	3:A:376:ATP:H2	2.37	0.42
1:B:121:GLN:O	1:B:122:ILE:C	2.57	0.42
1:B:190:MET:SD	1:B:206:ARG:HG3	2.59	0.42
1:B:222:ASP:C	1:B:224:GLU:H	2.22	0.42
1:B:283:MET:C	1:B:285:CYS:N	2.72	0.42
1:A:14:SER:HA	1:A:71:ILE:HG22	2.01	0.42
1:A:27:PRO:HB3	1:A:340:TRP:CG	2.54	0.42
1:A:183:ARG:NH1	1:A:183:ARG:HB2	2.34	0.42
1:A:263:GLN:HB2	1:A:266:PHE:CG	2.54	0.42
1:A:289:ILE:HG12	1:A:289:ILE:H	1.73	0.42
1:A:338:SER:N	1:A:341:ILE:HD12	2.34	0.42
1:B:193:LEU:O	1:B:195:GLU:N	2.52	0.42
1:B:210:ARG:HA	1:B:213:LYS:HB3	2.02	0.42
1:B:211:ASP:O	1:B:215:LYS:HB2	2.20	0.42
1:B:262:PHE:C	1:B:263:GLN:HG2	2.40	0.42
1:B:311:ASP:OD1	1:B:311:ASP:N	2.47	0.42
1:B:328:LYS:C	1:B:329:ILE:HD13	2.39	0.42
1:B:349:LEU:CD1	1:B:351:THR:CB	2.91	0.42
1:A:161:HIS:HA	1:A:176:MET:O	2.20	0.42
1:B:15:GLY:O	1:B:16:LEU:HG	2.19	0.42
1:B:82:MET:O	1:B:85:ILE:HB	2.19	0.42
1:B:276:GLU:O	1:B:279:TYR:HB3	2.19	0.42
1:B:362:TYR:O	1:B:364:GLU:N	2.52	0.42
1:A:27:PRO:HB3	1:A:340:TRP:CD1	2.55	0.42
1:A:297:ASN:HB2	1:A:329:ILE:HG23	2.01	0.42
1:A:330:ILE:N	1:A:330:ILE:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LYS:N	1:B:18:LYS:CD	2.82	0.42
1:B:56:ASP:HA	1:B:59:GLN:HB3	2.01	0.42
1:B:123:MET:HB3	1:B:124:PHE:H	1.67	0.42
1:B:126:THR:O	1:B:127:PHE:CD1	2.73	0.42
1:B:149:THR:HG22	1:B:165:ILE:O	2.20	0.42
1:B:172:PRO:HD2	1:B:173:HIS:HE1	1.84	0.42
1:B:186:THR:O	1:B:187:ASP:C	2.57	0.42
1:B:317:ILE:H	1:B:317:ILE:HG13	1.71	0.42
1:B:335:ARG:O	1:B:335:ARG:HG3	2.19	0.42
1:A:133:TYR:CD1	1:A:134:VAL:N	2.88	0.42
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.87	0.42
1:A:200:PHE:CB	1:A:205:GLU:HB3	2.50	0.42
1:A:276:GLU:C	1:A:278:THR:H	2.24	0.42
1:A:91:TYR:HB3	1:A:92:ASN:HD22	1.85	0.41
1:A:176:MET:HE2	1:A:280:ASN:HB2	2.01	0.41
1:A:335:ARG:HG2	1:A:335:ARG:HH21	1.85	0.41
1:B:111:ASN:ND2	1:B:115:ASN:HB2	2.34	0.41
1:B:131:ALA:HB1	1:B:356:TRP:HB3	2.02	0.41
1:B:207:GLU:CD	4:B:387:LAR:HO4	2.24	0.41
1:B:274:ILE:O	1:B:275:HIS:C	2.58	0.41
1:B:283:MET:O	1:B:290:ARG:NH1	2.53	0.41
1:A:7:ALA:HA	1:A:102:PRO:HD2	2.01	0.41
1:A:123:MET:HE3	1:A:129:VAL:HG11	2.00	0.41
1:A:316:GLU:OE2	1:A:316:GLU:CA	2.58	0.41
1:B:10:CYS:HB3	1:B:105:LEU:HD23	2.01	0.41
1:B:21:PHE:O	1:B:24:ASP:HB2	2.20	0.41
1:B:70:PRO:CG	1:B:85:ILE:HD11	2.36	0.41
1:A:35:VAL:HB	1:A:81:ASP:HB3	2.02	0.41
1:A:36:GLY:HA3	1:A:67:LEU:HD23	2.01	0.41
1:A:86:TRP:O	1:A:90:PHE:CE1	2.73	0.41
1:A:111:ASN:O	1:A:116:ARG:NH2	2.53	0.41
1:A:354:GLN:OE1	1:A:372:ARG:NH1	2.49	0.41
1:A:359:LYS:O	1:A:360:GLN:C	2.57	0.41
1:B:37:ARG:HD3	1:B:51:ASP:O	2.20	0.41
1:B:61:LYS:CD	1:B:65:LEU:HD13	2.49	0.41
1:B:238:LYS:HD2	1:B:238:LYS:HA	1.74	0.41
1:A:93:GLU:OE1	1:A:93:GLU:O	2.38	0.41
1:A:97:ALA:HB1	1:A:99:GLU:OE2	2.19	0.41
1:A:267:ILE:O	1:A:267:ILE:CG1	2.69	0.41
1:A:350:SER:C	1:A:352:PHE:N	2.73	0.41
1:B:141:SER:CA	1:B:338:SER:OG	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:HB2	4:B:387:LAR:O5	2.19	0.41
1:B:299:MET:CG	1:B:331:ALA:CB	2.99	0.41
1:A:171:LEU:O	1:A:175:ILE:HG13	2.21	0.41
1:A:277:THR:O	1:A:281:SER:HB2	2.20	0.41
1:A:303:THR:C	1:A:305:MET:H	2.23	0.41
1:B:98:PRO:C	1:B:100:GLU:N	2.74	0.41
1:B:175:ILE:HG22	1:B:176:MET:N	2.35	0.41
1:B:228:ALA:C	1:B:230:ALA:N	2.72	0.41
1:B:259:GLU:C	1:B:261:LEU:N	2.73	0.41
1:B:269:MET:HB3	1:B:271:SER:HB3	2.02	0.41
1:A:22:ALA:C	1:A:24:ASP:N	2.73	0.41
1:A:159:VAL:HG22	3:A:376:ATP:O2G	2.19	0.41
1:A:210:ARG:CZ	1:A:210:ARG:HB3	2.50	0.41
1:A:312:ARG:O	1:A:316:GLU:HG2	2.21	0.41
1:B:59:GLN:NE2	4:B:387:LAR:H223	2.33	0.41
1:B:120:THR:HG23	1:B:132:MET:CE	2.50	0.41
1:B:189:LEU:HD12	1:B:192:ILE:CD1	2.50	0.41
1:B:209:VAL:O	1:B:212:ILE:HB	2.20	0.41
1:B:219:VAL:HG12	1:B:312:ARG:NH1	2.36	0.41
1:B:308:GLY:C	1:B:310:ALA:H	2.22	0.41
1:A:64:ILE:C	1:A:65:LEU:HD12	2.40	0.41
1:A:90:PHE:O	1:A:95:ARG:N	2.54	0.41
1:A:137:GLN:O	1:A:138:ALA:O	2.39	0.41
1:A:252:ASN:HB2	1:A:256:ARG:CD	2.51	0.41
1:A:262:PHE:HE2	1:A:316:GLU:HG3	1.85	0.41
1:A:291:LYS:HG2	1:A:292:ASP:OD1	2.20	0.41
1:A:325:MET:CE	1:A:326:LYS:H	2.34	0.41
1:B:16:LEU:HD11	4:B:387:LAR:O1	2.20	0.41
1:B:162:ASN:ND2	1:B:278:THR:HA	2.35	0.41
1:B:170:ALA:O	1:B:171:LEU:HD23	2.20	0.41
1:B:188:TYR:O	1:B:191:LYS:CB	2.69	0.41
1:B:253:GLU:HA	1:B:256:ARG:HB3	2.01	0.41
1:B:308:GLY:C	1:B:310:ALA:N	2.72	0.41
1:A:14:SER:HA	1:A:71:ILE:HG21	2.02	0.41
1:A:111:ASN:HD21	1:A:115:ASN:HD22	1.69	0.41
1:A:141:SER:HA	1:A:338:SER:HB3	2.02	0.41
1:A:183:ARG:HA	4:A:377:LAR:O5	2.20	0.41
1:A:206:ARG:CB	1:A:206:ARG:HH11	2.34	0.41
1:A:206:ARG:HH11	1:A:206:ARG:HB2	1.84	0.41
1:A:320:LEU:HG	1:A:320:LEU:H	1.52	0.41
1:A:337:TYR:C	1:A:341:ILE:HG13	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:HA3	1:B:27:PRO:HA	2.01	0.41
1:B:76:ILE:HD11	1:B:119:MET:HE1	2.03	0.41
1:B:93:GLU:HB3	1:B:94:LEU:HD12	2.02	0.41
1:B:176:MET:HG2	1:B:281:SER:HB2	2.03	0.41
1:B:354:GLN:HG2	1:B:355:MET:HE1	2.02	0.41
1:B:369:ILE:O	1:B:369:ILE:CG1	2.68	0.41
1:A:137:GLN:HA	1:A:339:VAL:HG13	2.02	0.41
1:A:183:ARG:CB	1:A:183:ARG:CZ	2.99	0.41
1:A:191:LYS:C	1:A:193:LEU:H	2.24	0.41
1:B:26:ALA:HA	1:B:27:PRO:HD2	1.98	0.41
1:B:32:PRO:HB2	1:B:34:ILE:CD1	2.50	0.41
1:B:104:LEU:CA	1:B:356:TRP:HH2	2.33	0.41
1:B:180:LEU:HD12	1:B:184:ASP:HB2	2.02	0.41
1:B:244:ASP:O	1:B:246:GLN:N	2.39	0.41
1:A:52:SER:HB2	1:A:84:LYS:HG2	2.02	0.40
1:A:90:PHE:H	1:A:90:PHE:HD1	1.69	0.40
1:A:104:LEU:C	1:A:104:LEU:CD2	2.88	0.40
1:A:117:GLU:HG2	1:A:371:HIS:CE1	2.56	0.40
1:A:200:PHE:CD2	1:A:205:GLU:CD	2.84	0.40
1:A:227:MET:HE1	1:A:256:ARG:HD3	2.01	0.40
1:A:289:ILE:HG13	1:A:290:ARG:N	2.35	0.40
1:A:312:ARG:O	1:A:315:LYS:HG2	2.21	0.40
1:A:326:LYS:HZ2	1:A:328:LYS:HB2	1.84	0.40
1:A:329:ILE:C	1:A:330:ILE:HD12	2.42	0.40
1:A:373:LYS:HD2	1:B:373:LYS:C	2.40	0.40
1:B:150:GLY:H	1:B:293:LEU:HG	1.86	0.40
1:B:197:GLY:O	1:B:198:TYR:CG	2.75	0.40
1:A:85:ILE:O	1:A:89:THR:N	2.49	0.40
1:A:129:VAL:HG23	1:A:129:VAL:O	2.21	0.40
1:A:317:ILE:O	1:A:321:ALA:N	2.36	0.40
1:B:14:SER:HB2	1:B:158:GLY:H	1.86	0.40
1:B:36:GLY:HA3	1:B:67:LEU:CB	2.47	0.40
1:B:288:ASP:OD1	1:B:289:ILE:N	2.54	0.40
1:B:336:LYS:CE	3:B:386:ATP:N7	2.84	0.40
1:A:176:MET:SD	1:A:280:ASN:O	2.80	0.40
1:A:185:LEU:HD12	1:A:185:LEU:N	2.18	0.40
1:B:38:PRO:HA	1:B:64:ILE:HG12	2.03	0.40
1:B:141:SER:HG	1:B:339:VAL:HG22	1.86	0.40
1:B:242:LEU:CG	1:B:244:ASP:HB3	2.51	0.40
1:A:193:LEU:O	1:A:194:THR:C	2.58	0.40
1:B:37:ARG:O	1:B:65:LEU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:SER:HA	1:B:160:THR:HG23	2.04	0.40
1:B:164:PRO:HB3	1:B:293:LEU:HD23	2.02	0.40
1:B:239:SER:OG	1:B:247:VAL:HB	2.20	0.40
1:B:338:SER:CA	1:B:341:ILE:HD12	2.51	0.40
1:A:123:MET:CB	1:A:129:VAL:HG22	2.47	0.40
1:A:332:PRO:HA	1:A:333:PRO:HD2	1.97	0.40
1:B:152:VAL:HG23	1:B:163:VAL:HB	2.02	0.40
1:B:263:GLN:C	1:B:266:PHE:CD1	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/375 (95%)	223 (62%)	84 (24%)	50 (14%)	0	1
1	B	357/375 (95%)	210 (59%)	88 (25%)	59 (16%)	0	0
All	All	714/750 (95%)	433 (61%)	172 (24%)	109 (15%)	0	1

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	TYR
1	A	92	ASN
1	A	99	GLU
1	A	138	ALA
1	A	139	VAL
1	A	173	HIS
1	A	182	GLY
1	A	252	ASN
1	A	290	ARG
1	A	304	THR

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Mol	Chain	Res	Type
1	A	310	ALA
1	A	348	SER
1	B	25	ASP
1	B	70	PRO
1	B	116	ARG
1	B	117	GLU
1	B	123	MET
1	B	144	ALA
1	B	172	PRO
1	B	217	CYS
1	B	274	ILE
1	B	307	PRO
1	B	310	ALA
1	B	323	SER
1	B	326	LYS
1	A	60	SER
1	A	123	MET
1	A	179	ASP
1	A	189	LEU
1	A	287	ILE
1	A	288	ASP
1	A	303	THR
1	A	318	THR
1	A	323	SER
1	A	335	ARG
1	A	345	ILE
1	A	368	SER
1	A	371	HIS
1	A	373	LYS
1	B	13	GLY
1	B	24	ASP
1	B	62	ARG
1	B	182	GLY
1	B	192	ILE
1	B	209	VAL
1	B	229	THR
1	B	244	ASP
1	B	260	THR
1	B	312	ARG
1	B	316	GLU
1	B	366	GLY
1	A	125	GLU

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Mol	Chain	Res	Type
1	A	190	MET
1	A	241	GLU
1	A	286	ASP
1	A	353	GLN
1	B	12	ASN
1	B	89	THR
1	B	91	TYR
1	B	124	PHE
1	B	213	LYS
1	B	220	ALA
1	B	233	SER
1	B	284	LYS
1	B	287	ILE
1	B	304	THR
1	B	324	THR
1	B	325	MET
1	B	335	ARG
1	B	349	LEU
1	A	144	ALA
1	A	180	LEU
1	A	181	ALA
1	A	277	THR
1	A	308	GLY
1	A	367	PRO
1	B	77	THR
1	B	80	ASP
1	B	90	PHE
1	B	98	PRO
1	B	109	PRO
1	B	173	HIS
1	B	181	ALA
1	B	183	ARG
1	B	197	GLY
1	B	275	HIS
1	B	306	TYR
1	B	330	ILE
1	B	344	SER
1	B	363	ASP
1	A	62	ARG
1	A	98	PRO
1	A	130	PRO
1	A	172	PRO

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Mol	Chain	Res	Type
1	A	233	SER
1	A	291	LYS
1	A	299	MET
1	B	311	ASP
1	B	315	LYS
1	A	188	TYR
1	A	305	MET
1	A	314	GLN
1	B	30	VAL
1	B	110	LEU
1	A	38	PRO
1	A	274	ILE
1	A	23	GLY
1	B	85	ILE
1	B	267	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/318 (96%)	261 (85%)	46 (15%)	3	14
1	B	307/318 (96%)	248 (81%)	59 (19%)	1	8
All	All	614/636 (96%)	509 (83%)	105 (17%)	2	10

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	54	VAL
1	A	59	GLN
1	A	62	ARG
1	A	64	ILE
1	A	71	ILE
1	A	81	ASP
1	A	90	PHE

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Mol	Chain	Res	Type
1	A	92	ASN
1	A	99	GLU
1	A	113	LYS
1	A	121	GLN
1	A	126	THR
1	A	141	SER
1	A	151	ILE
1	A	154	ASP
1	A	159	VAL
1	A	173	HIS
1	A	177	ARG
1	A	180	LEU
1	A	193	LEU
1	A	195	GLU
1	A	196	ARG
1	A	211	ASP
1	A	213	LYS
1	A	216	LEU
1	A	217	CYS
1	A	225	ASN
1	A	234	SER
1	A	236	LEU
1	A	246	GLN
1	A	250	ILE
1	A	256	ARG
1	A	263	GLN
1	A	266	PHE
1	A	271	SER
1	A	280	ASN
1	A	288	ASP
1	A	289	ILE
1	A	317	ILE
1	A	320	LEU
1	A	327	ILE
1	A	334	GLU
1	A	354	GLN
1	A	358	THR
1	A	375	PHE
1	B	25	ASP
1	B	39	ARG
1	B	56	ASP
1	B	59	GLN

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Mol	Chain	Res	Type
1	B	66	THR
1	B	67	LEU
1	B	69	TYR
1	B	72	GLU
1	B	76	ILE
1	B	81	ASP
1	B	90	PHE
1	B	92	ASN
1	B	99	GLU
1	B	118	LYS
1	B	119	MET
1	B	121	GLN
1	B	128	ASN
1	B	129	VAL
1	B	130	PRO
1	B	132	MET
1	B	141	SER
1	B	149	THR
1	B	151	ILE
1	B	154	ASP
1	B	172	PRO
1	B	188	TYR
1	B	192	ILE
1	B	195	GLU
1	B	200	PHE
1	B	202	THR
1	B	216	LEU
1	B	218	TYR
1	B	223	PHE
1	B	234	SER
1	B	236	LEU
1	B	242	LEU
1	B	243	PRO
1	B	250	ILE
1	B	252	ASN
1	B	262	PHE
1	B	263	GLN
1	B	270	GLU
1	B	271	SER
1	B	275	HIS
1	B	288	ASP
1	B	292	ASP

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Mol	Chain	Res	Type
1	B	294	TYR
1	B	297	ASN
1	B	299	MET
1	B	303	THR
1	B	304	THR
1	B	311	ASP
1	B	318	THR
1	B	324	THR
1	B	326	LYS
1	B	329	ILE
1	B	349	LEU
1	B	372	ARG
1	B	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	59	GLN
1	A	92	ASN
1	A	111	ASN
1	A	115	ASN
1	A	121	GLN
1	A	246	GLN
1	A	280	ASN
1	A	297	ASN
1	A	314	GLN
1	A	353	GLN
1	A	360	GLN
1	A	371	HIS
1	B	59	GLN
1	B	73	HIS
1	B	92	ASN
1	B	101	HIS
1	B	115	ASN
1	B	121	GLN
1	B	128	ASN
1	B	162	ASN
1	B	280	ASN
1	B	314	GLN
1	B	354	GLN
1	B	360	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 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	#$|Z| > 2$
4	LAR	B	387	-	30,31,31	1.28	5 (16%)	32,43,43	1.59	3 (9%)
3	ATP	A	376	2	26,33,33	2.23	9 (34%)	31,52,52	2.99	8 (25%)
4	LAR	A	377	-	30,31,31	1.30	4 (13%)	32,43,43	1.64	4 (12%)
3	ATP	B	386	2	26,33,33	2.20	10 (38%)	31,52,52	3.13	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LAR	B	387	-	-	4/23/51/51	0/2/3/3
3	ATP	A	376	2	-	2/18/38/38	0/3/3/3
4	LAR	A	377	-	-	3/23/51/51	0/2/3/3
3	ATP	B	386	2	-	2/18/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	376	ATP	O4'-C1'	5.54	1.48	1.41
3	B	386	ATP	O5'-C5'	-4.82	1.26	1.44
3	B	386	ATP	O4'-C1'	4.80	1.47	1.41
3	A	376	ATP	O5'-C5'	-4.69	1.26	1.44
3	B	386	ATP	C4-N3	3.92	1.41	1.35
3	A	376	ATP	C4-N3	3.81	1.40	1.35
4	A	377	LAR	C18-N1	3.59	1.51	1.46
4	B	387	LAR	C18-N1	3.32	1.51	1.46
3	A	376	ATP	PA-O5'	-2.93	1.47	1.59
3	B	386	ATP	PA-O5'	-2.87	1.47	1.59
3	A	376	ATP	PB-O1B	-2.86	1.40	1.50
3	B	386	ATP	C8-N7	-2.76	1.29	1.34
3	A	376	ATP	C8-N7	-2.68	1.29	1.34
3	B	386	ATP	C2-N3	2.68	1.36	1.32
3	B	386	ATP	C3'-C4'	-2.61	1.46	1.53
3	A	376	ATP	C2-N3	2.60	1.36	1.32
3	B	386	ATP	PB-O1B	-2.46	1.42	1.50
3	B	386	ATP	C6-C5	2.40	1.52	1.43
4	B	387	LAR	O3-C13	2.36	1.50	1.44
4	A	377	LAR	C21-C3	2.25	1.56	1.50
4	B	387	LAR	C22-C10	2.23	1.61	1.53
4	A	377	LAR	C22-C10	2.17	1.61	1.53
3	A	376	ATP	C6-C5	2.13	1.51	1.43
3	B	386	ATP	PB-O2B	-2.10	1.45	1.55
3	A	376	ATP	PA-O1A	-2.10	1.43	1.50
4	B	387	LAR	O2-C1	2.06	1.38	1.34
4	A	377	LAR	O3-C13	2.06	1.49	1.44
4	B	387	LAR	C21-C3	2.03	1.55	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	386	ATP	O5'-C5'-C4'	12.12	150.71	108.99
3	A	376	ATP	O5'-C5'-C4'	11.13	147.30	108.99
3	B	386	ATP	O5'-PA-O1A	-7.25	80.74	109.07
3	A	376	ATP	O5'-PA-O1A	-7.13	81.21	109.07
3	A	376	ATP	PA-O5'-C5'	5.90	156.26	121.68
4	A	377	LAR	C19-S1-C20	5.52	94.96	92.00
3	B	386	ATP	PA-O5'-C5'	5.45	153.66	121.68
4	B	387	LAR	C19-S1-C20	5.27	94.83	92.00
3	B	386	ATP	C5'-C4'-C3'	-4.87	96.93	115.18
3	A	376	ATP	C5'-C4'-C3'	-4.15	99.64	115.18

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	377	LAR	C3-C2-C1	3.65	136.50	127.46
4	B	387	LAR	C3-C2-C1	3.41	135.90	127.46
3	B	386	ATP	O4'-C4'-C3'	3.36	111.76	105.11
4	B	387	LAR	O5-C20-N1	3.17	130.27	126.81
3	A	376	ATP	O4'-C4'-C3'	2.68	110.43	105.11
4	A	377	LAR	O5-C20-N1	2.63	129.68	126.81
3	B	386	ATP	C3'-C2'-C1'	2.21	104.31	100.98
3	A	376	ATP	C3'-C2'-C1'	2.19	104.27	100.98
3	B	386	ATP	C1'-N9-C4	-2.13	122.90	126.64
4	A	377	LAR	C21-C3-C2	-2.07	116.54	122.77
3	A	376	ATP	C4-C5-N7	2.05	111.54	109.40
3	B	386	ATP	O2B-PB-O1B	2.03	122.28	112.24
3	A	376	ATP	O2B-PB-O1B	2.02	122.25	112.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	387	LAR	O3-C17-C18-C19
4	B	387	LAR	O2-C1-C2-C3
3	A	376	ATP	PG-O3B-PB-O2B
3	B	386	ATP	PG-O3B-PB-O2B
3	B	386	ATP	PA-O3A-PB-O2B
4	B	387	LAR	O1-C1-C2-C3
3	A	376	ATP	PA-O3A-PB-O2B
4	A	377	LAR	O2-C1-C2-C3
4	A	377	LAR	C4-C5-C6-C7
4	B	387	LAR	C4-C5-C6-C7
4	A	377	LAR	C10-C11-C12-C13

There are no ring outliers.

4 monomers are involved in 31 short contacts:

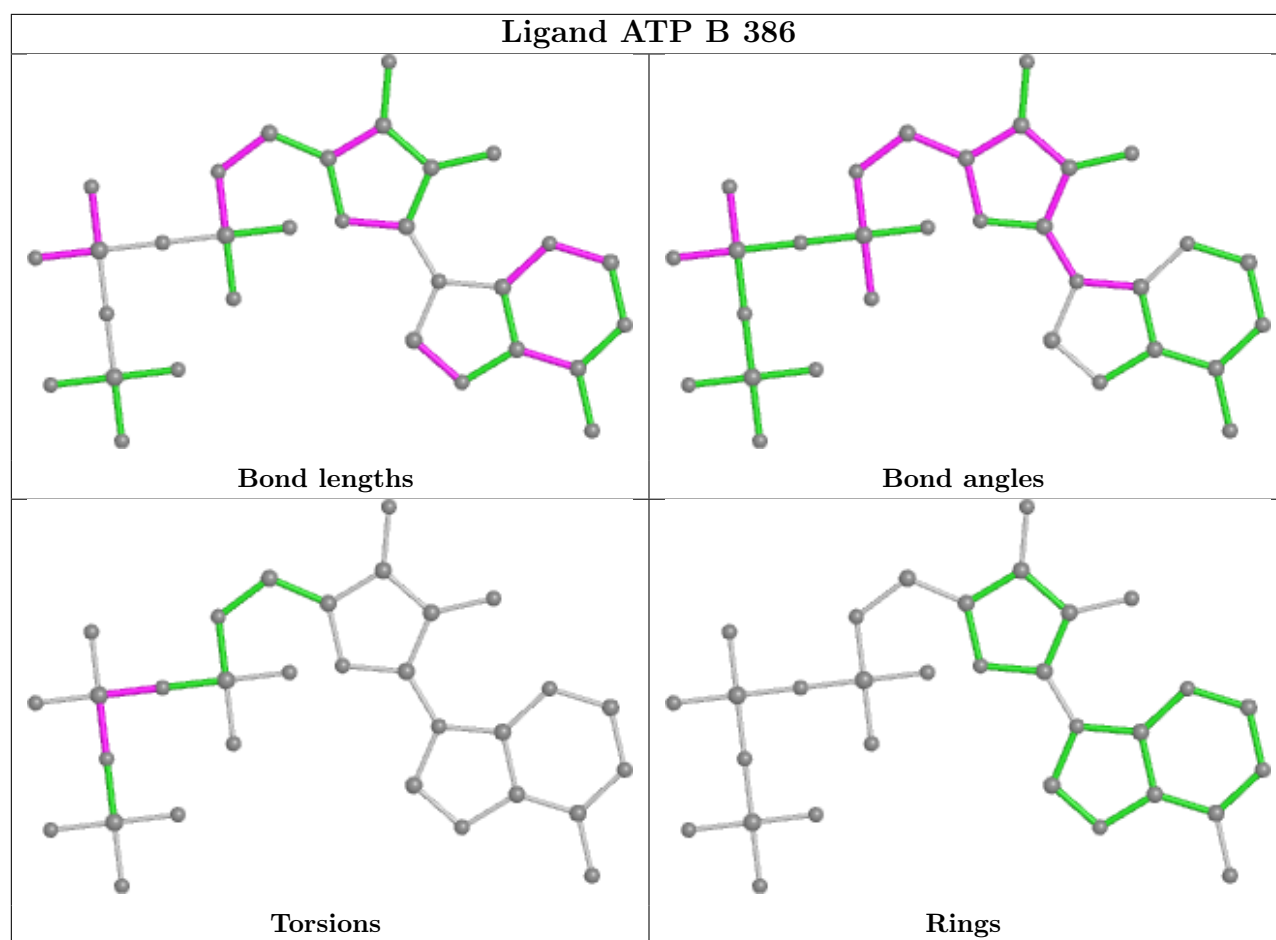| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	387	LAR	10	0
3	A	376	ATP	9	0
4	A	377	LAR	2	0
3	B	386	ATP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

Ligand LAR B 387

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 376

Bond lengths

Bond angles

Torsions

Rings

Ligand LAR A 377

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 386

Bond lengths

Bond angles

Torsions

Rings
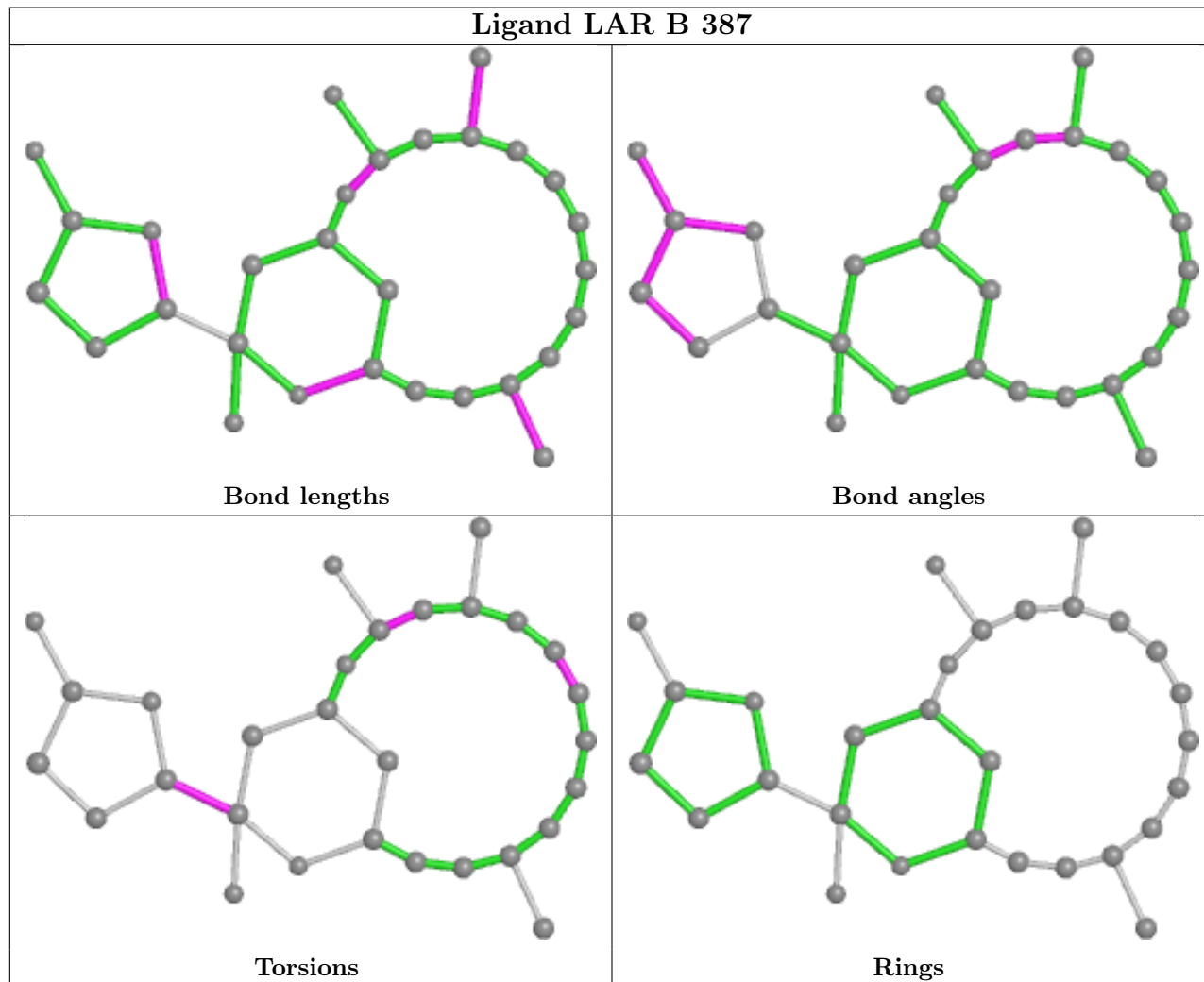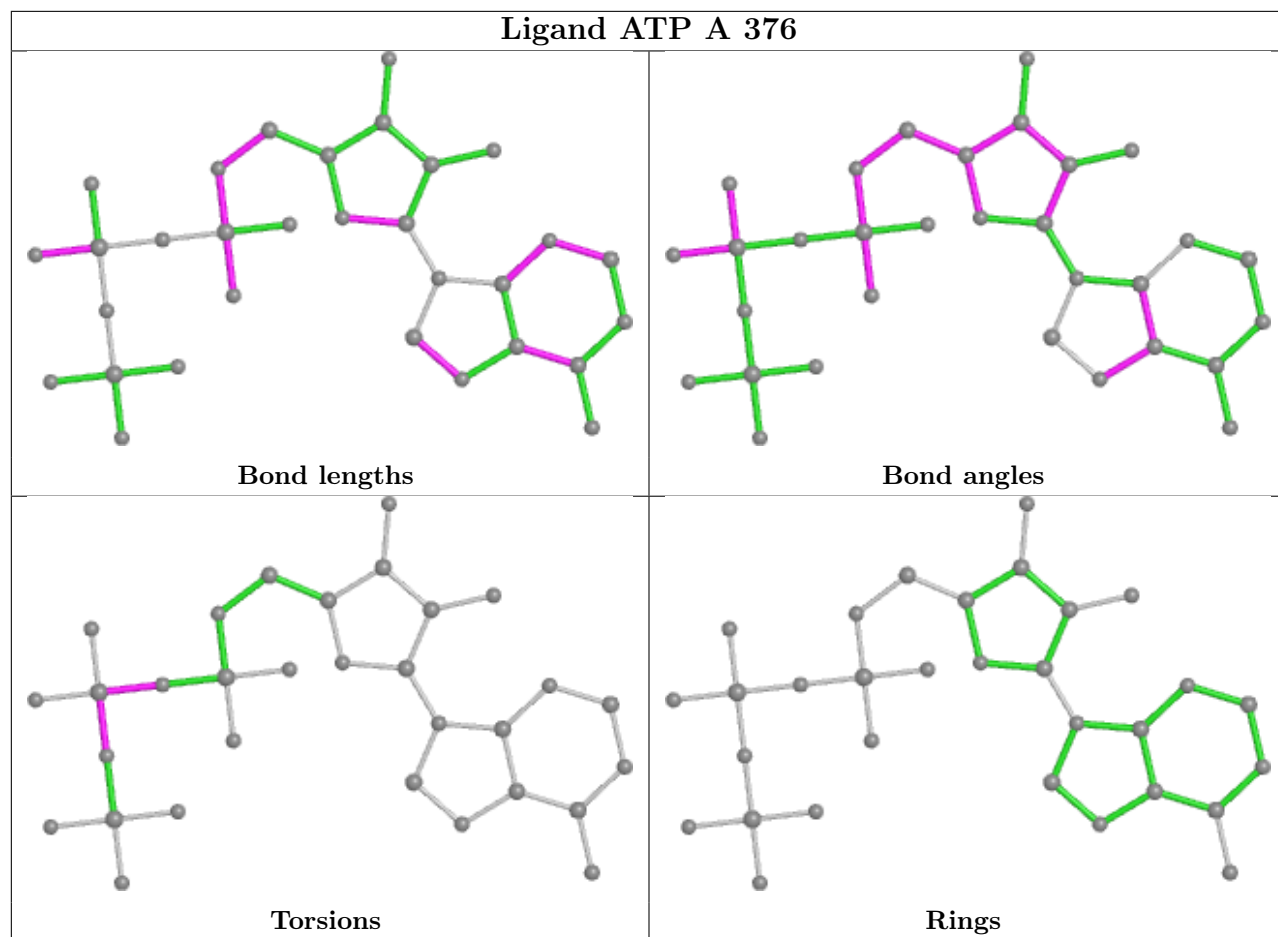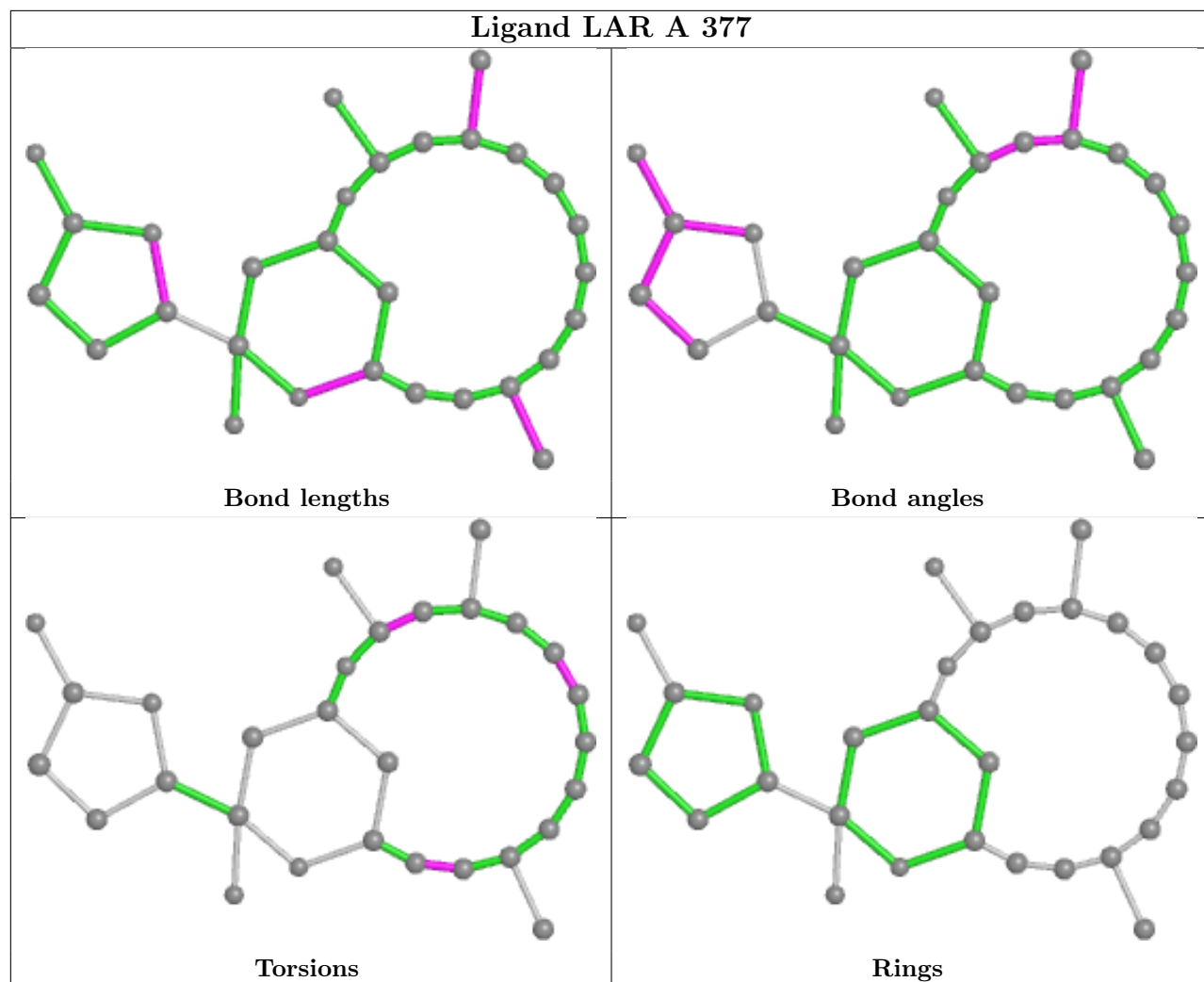
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	25:ASP	C	26:ALA	N	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	361/375 (96%)	0.05	0	100	100	38, 57, 75, 82	0
1	B	361/375 (96%)	0.22	11 (3%)	50	22	42, 68, 83, 96	0
All	All	722/750 (96%)	0.13	11 (1%)	73	46	38, 63, 80, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	ILE	3.5
1	B	33	SER	3.0
1	B	228	ALA	2.9
1	B	104	LEU	2.8
1	B	178	LEU	2.8
1	B	235	SER	2.7
1	B	152	VAL	2.5
1	B	8	LEU	2.3
1	B	61	LYS	2.1
1	B	231	ALA	2.0
1	B	222	ASP	2.0

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

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

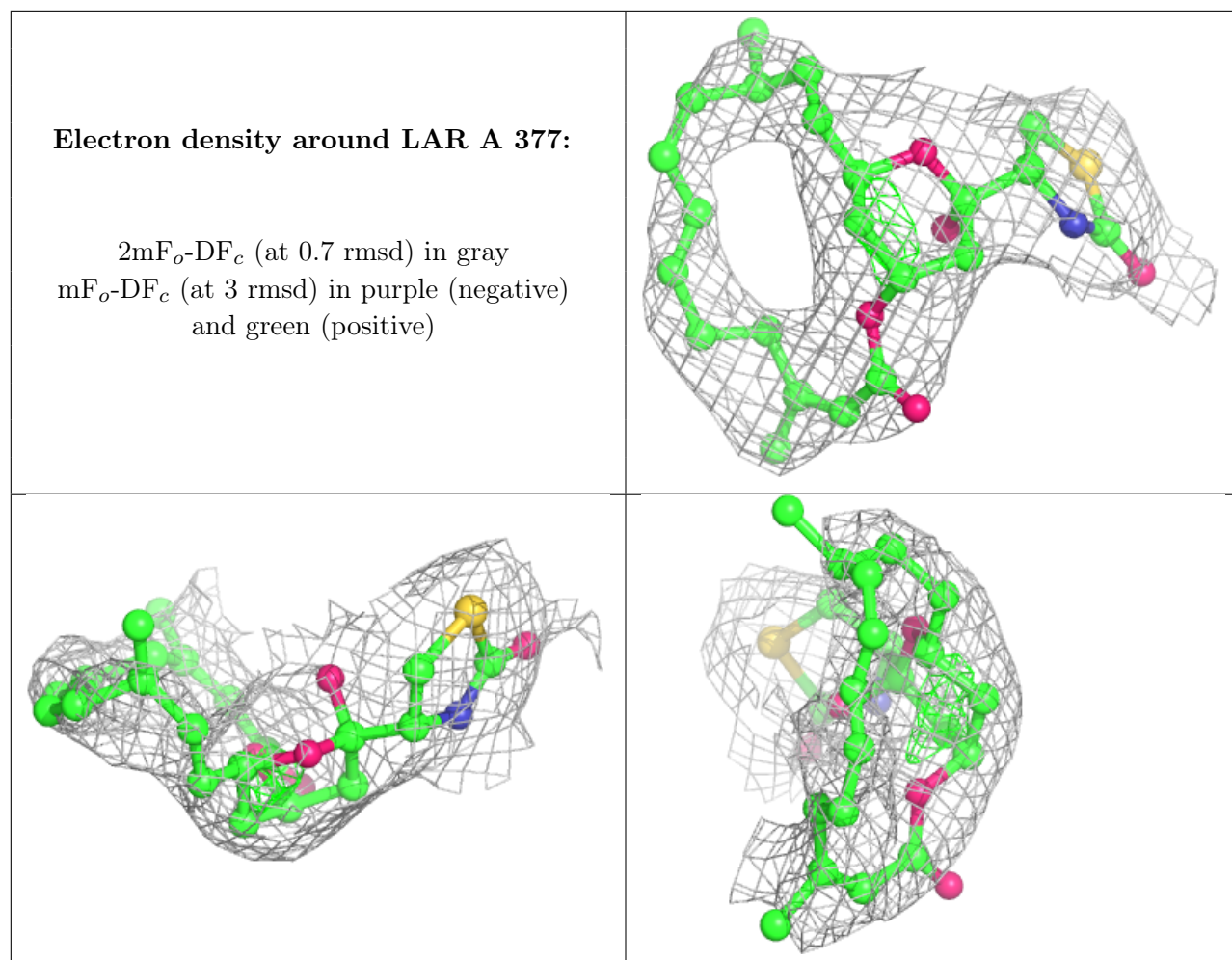## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	388	1/1	0.84	0.25	42,42,42,42	0
4	LAR	B	387	29/29	0.89	0.31	66,71,78,78	0
4	LAR	A	377	29/29	0.92	0.38	61,67,74,75	0
2	MG	A	378	1/1	0.93	0.26	36,36,36,36	0
3	ATP	B	386	31/31	0.93	0.19	53,57,61,62	0
3	ATP	A	376	31/31	0.95	0.22	37,50,55,56	0

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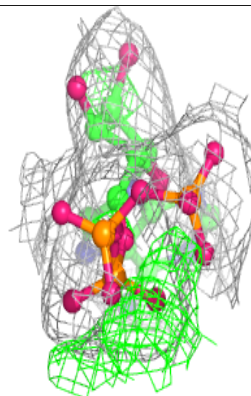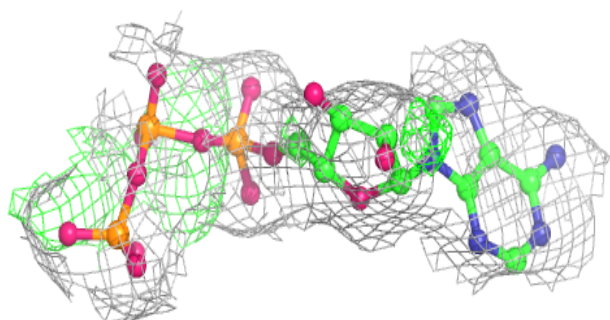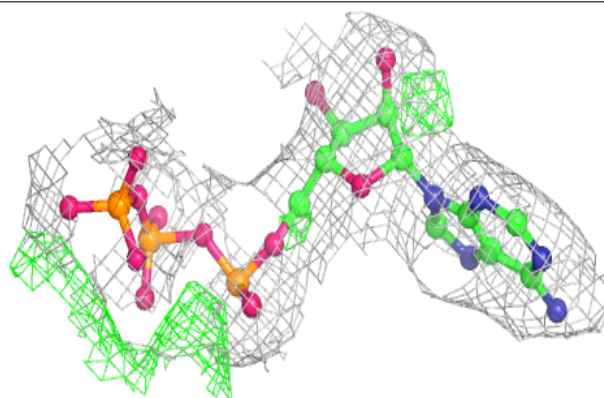

Electron density around LAR B 387:

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

Electron density around LAR A 377:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
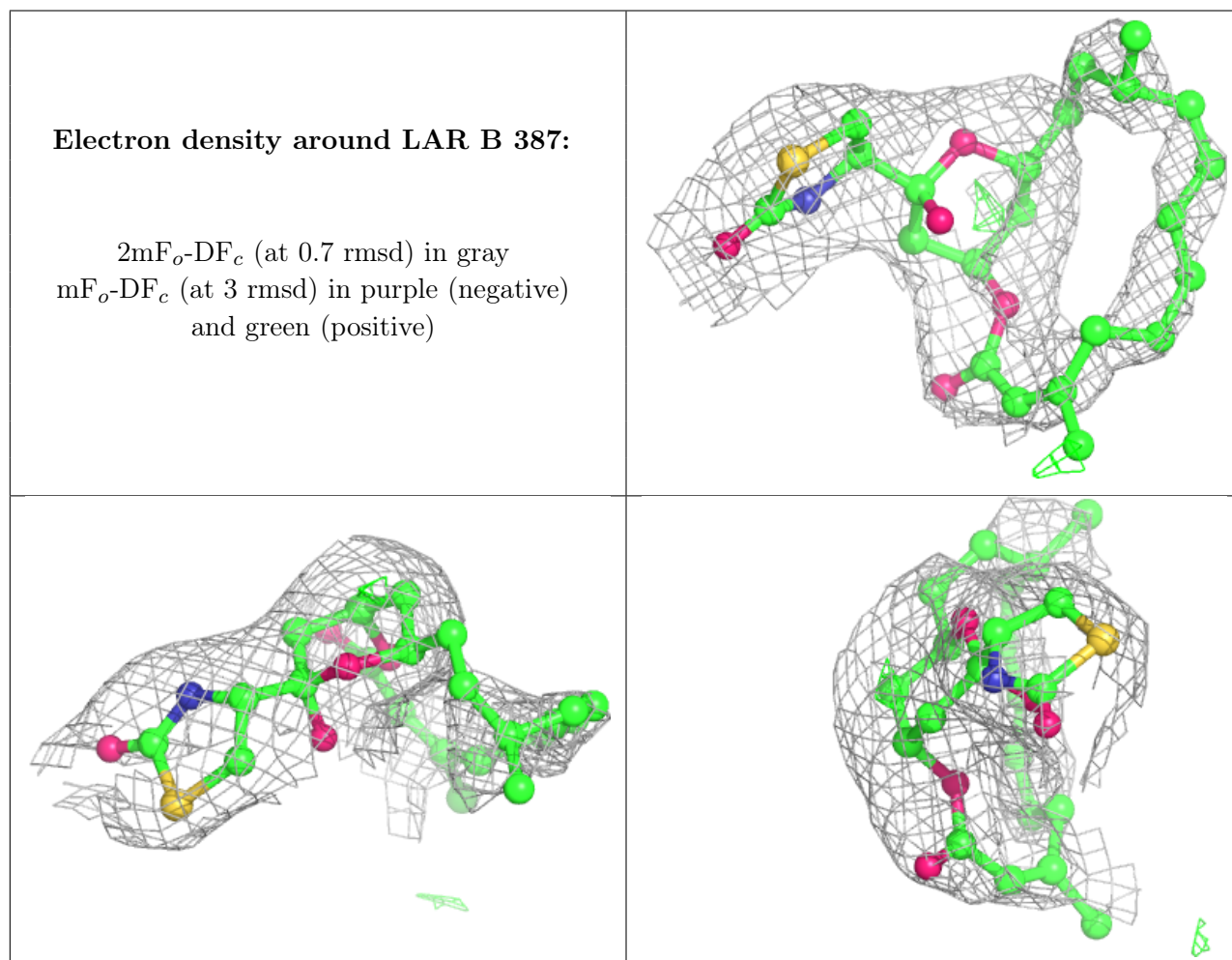
Electron density around ATP B 386:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
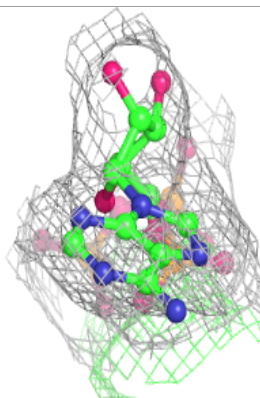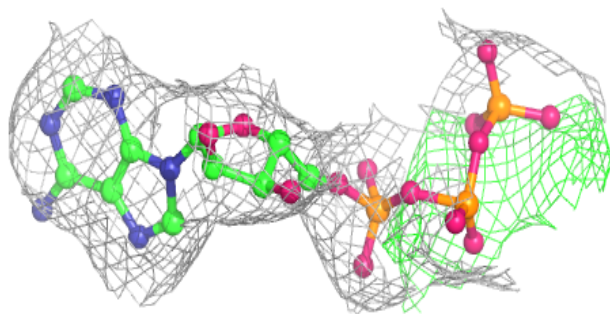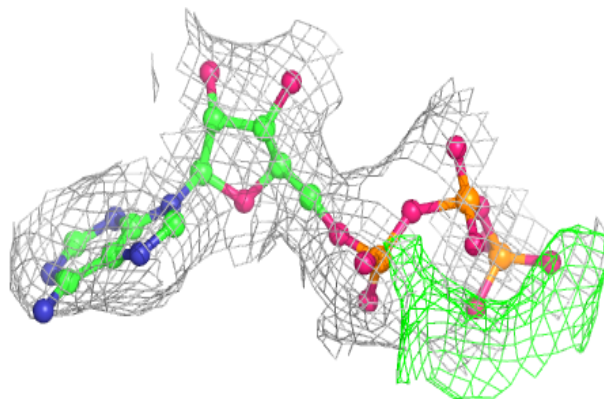
Electron density around ATP A 376:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.