



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:42 AM UTC

PDB ID : 1RFQ / pdb_00001rfq
Title : Actin Crystal Dynamics: Structural Implications for F-actin Nucleation, Polymerization and Branching Mediated by the Anti-parallel Dimer
Authors : Reutzell, 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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

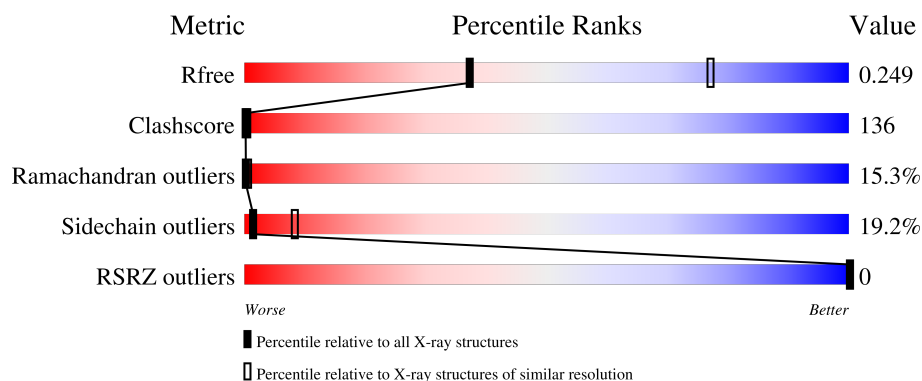
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	
1	B	375	

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 [i](#)

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.

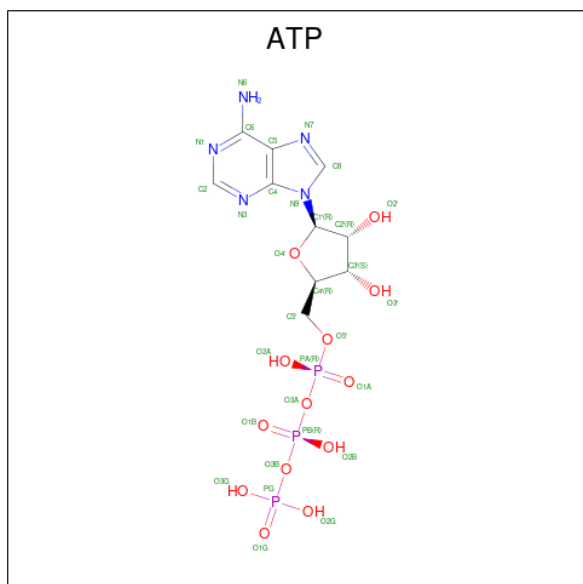
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

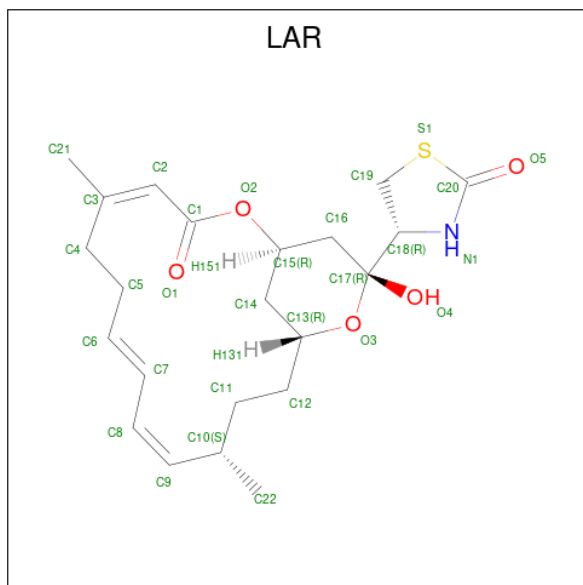
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is LATRUNCULIN A (CCD ID: LAR) (formula: $C_{22}H_{31}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
4	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

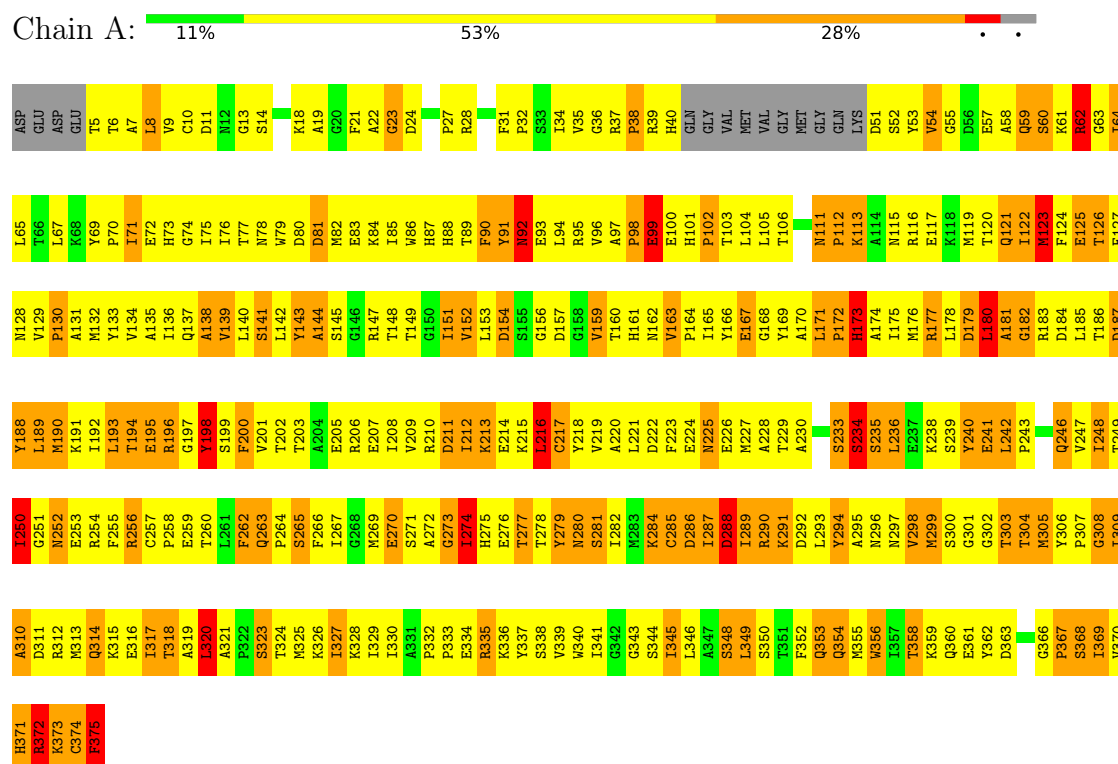
- Molecule 5 is water.

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

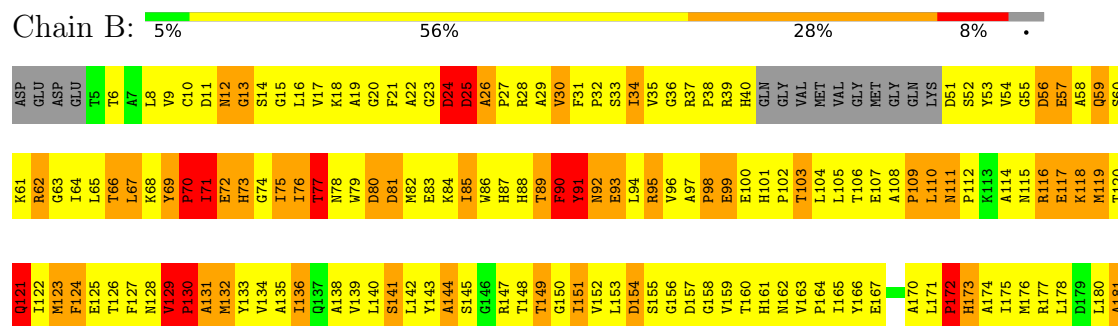
3 Residue-property plots

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



D863	T303	P243	G182
E364	T304	D244	R183
A365	M305	G245	D184
G366	Y306	Q246	L185
P367	P307	V247	T186
S368	G308	I248	D187
I369	I309	T249	Y188
V370	A310	I250	L189
H371	D311	G251	M190
K372	R312	N252	K191
K373	M313	E253	L192
G374	Q314	R254	L193
F375	K315	F255	T194
	E316	R256	E195
	I317	C257	R196
	T318	P258	G197
	A319	E259	Y198
	L320	T260	S199
	A321	L261	F200
	P322	F262	V201
	S323	Q263	T202
	T324	P264	T203
	M325	S265	A204
	K326	F266	E205
	I327	I267	R206
	K328	G268	E207
	I329	M269	I208
	I330	E270	V209
	A331	S271	R210
	P332	A272	D211
	P333	G273	I212
	E334	I274	K213
	R335	R275	E214
	K336	E276	K215
	Y337	T277	L216
	S338	T278	C217
	V339	Y279	Y218
	W340	N280	V219
	I341	S281	A220
	G342	I282	L221
	G343	M283	D222
	S344	K284	F223
	I345	C285	E224
	L346	D286	W225
	A347	I287	E226
	S348	D288	M227
	L349	I289	A228
	S350	R290	T229
	T351	K291	A230
	F352	D292	A231
	Q353	L293	S232
	Q354	Y294	S233
	M355	A295	S234
	W356	N296	S235
	I357	N297	L236
	T358	V298	E237
	K359	M299	K238
	Q360	S300	S239
	E361	G301	
	Y362	G302	L242

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 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 98.6 (50.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.261 0.205 , 0.249	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 , 205.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	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	0.96	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, LAR

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	0.87	4/2891 (0.1%)	1.49	58/3919 (1.5%)
1	B	0.92	10/2891 (0.3%)	1.48	70/3919 (1.8%)
All	All	0.89	14/5782 (0.2%)	1.48	128/7838 (1.6%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	SER	N-CA	25.57	1.79	1.46
1	B	200	PHE	N-CA	18.71	1.70	1.46
1	B	25	ASP	C-N	-9.97	1.20	1.33
1	A	298	VAL	CA-C	-8.89	1.45	1.52
1	B	26	ALA	C-N	-8.26	1.26	1.33
1	B	263	GLN	CA-C	6.76	1.61	1.52
1	A	235	SER	CA-C	-6.72	1.43	1.52
1	B	201	VAL	CA-C	6.10	1.60	1.52
1	A	356	TRP	C-N	-6.00	1.25	1.33
1	B	74	GLY	CA-C	5.94	1.59	1.51
1	B	266	PHE	C-N	5.64	1.41	1.33
1	B	23	GLY	C-N	5.21	1.41	1.33
1	B	24	ASP	C-N	5.20	1.41	1.33
1	B	93	GLU	N-CA	5.17	1.52	1.46

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	PHE	CA-CB-CG	-21.42	92.38	113.80
1	B	200	PHE	CA-CB-CG	17.30	131.10	113.80
1	A	270	GLU	N-CA-C	-12.84	89.86	109.24
1	A	272	ALA	CA-C-N	-12.80	99.61	123.03
1	A	272	ALA	C-N-CA	-12.80	99.61	123.03
1	B	230	ALA	CA-C-N	-12.53	100.45	120.63
1	B	230	ALA	C-N-CA	-12.53	100.45	120.63
1	A	234	SER	CA-C-N	-12.16	98.32	121.54
1	A	234	SER	C-N-CA	-12.16	98.32	121.54
1	A	200	PHE	CA-C-N	11.90	143.39	121.97
1	A	200	PHE	C-N-CA	11.90	143.39	121.97
1	B	57	GLU	N-CA-C	-11.68	98.53	111.14
1	A	374	CYS	CA-C-N	-10.94	102.02	121.70
1	A	374	CYS	C-N-CA	-10.94	102.02	121.70
1	A	200	PHE	CA-CB-CG	10.75	124.55	113.80
1	B	199	SER	CA-C-N	-10.58	101.33	121.54
1	B	199	SER	C-N-CA	-10.58	101.33	121.54
1	A	235	SER	N-CA-C	-10.11	89.26	110.80
1	B	263	GLN	OE1-CD-NE2	-10.03	112.57	122.60
1	B	196	ARG	N-CA-C	-9.57	101.80	113.19
1	B	73	HIS	CA-C-N	-9.54	108.53	122.46
1	B	73	HIS	C-N-CA	-9.54	108.53	122.46
1	A	372	ARG	O-C-N	9.49	133.96	123.52
1	A	198	TYR	CB-CA-C	9.26	124.90	109.99
1	A	270	GLU	N-CA-CB	9.10	127.52	111.69
1	A	372	ARG	CA-C-N	8.87	138.47	121.54
1	A	372	ARG	C-N-CA	8.87	138.47	121.54
1	B	70	PRO	O-C-N	8.71	134.40	122.64
1	A	194	THR	N-CA-C	-8.67	100.65	111.75
1	A	270	GLU	CA-C-N	-8.20	105.88	121.54
1	A	270	GLU	C-N-CA	-8.20	105.88	121.54
1	A	294	TYR	N-CA-C	8.02	120.10	111.36
1	A	374	CYS	CA-C-O	-7.72	111.21	120.32
1	B	200	PHE	CA-C-N	7.46	135.41	121.97
1	B	200	PHE	C-N-CA	7.46	135.41	121.97
1	B	270	GLU	N-CA-C	-7.44	105.08	112.97
1	B	24	ASP	CA-C-N	7.28	135.44	121.54
1	B	24	ASP	C-N-CA	7.28	135.44	121.54
1	A	279	TYR	N-CA-C	-7.18	102.50	111.11
1	B	320	LEU	N-CA-C	-7.10	105.81	114.75
1	A	320	LEU	N-CA-C	-6.82	103.93	111.36
1	B	129	VAL	N-CA-C	6.77	115.32	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	TYR	CA-CB-CG	6.72	126.00	113.90
1	B	73	HIS	CA-CB-CG	-6.71	107.09	113.80
1	B	93	GLU	N-CA-C	-6.71	96.52	110.80
1	A	234	SER	N-CA-C	-6.67	103.87	113.21
1	B	226	GLU	N-CA-C	-6.66	102.65	111.24
1	B	111	ASN	CA-C-N	6.61	126.59	119.78
1	B	111	ASN	C-N-CA	6.61	126.59	119.78
1	A	187	ASP	N-CA-C	-6.57	103.81	110.97
1	B	263	GLN	CG-CD-NE2	6.53	126.19	116.40
1	A	196	ARG	CB-CA-C	-6.47	101.27	111.17
1	A	284	LYS	N-CA-C	-6.46	102.79	112.54
1	B	371	HIS	CA-C-N	-6.44	113.11	122.44
1	B	371	HIS	C-N-CA	-6.44	113.11	122.44
1	B	200	PHE	O-C-N	6.43	131.15	122.59
1	A	216	LEU	N-CA-C	6.41	120.92	112.72
1	B	349	LEU	O-C-N	-6.40	114.08	122.59
1	B	95	ARG	N-CA-C	-6.37	103.46	110.91
1	A	356	TRP	N-CA-C	6.32	118.49	110.33
1	B	346	LEU	N-CA-C	-6.27	103.58	111.11
1	B	130	PRO	CA-N-CD	-6.26	103.23	112.00
1	A	240	TYR	N-CA-C	6.18	118.47	108.34
1	B	131	ALA	CA-C-N	-6.09	112.24	122.29
1	B	131	ALA	C-N-CA	-6.09	112.24	122.29
1	B	222	ASP	CA-C-N	-6.07	109.79	121.94
1	B	222	ASP	C-N-CA	-6.07	109.79	121.94
1	B	236	LEU	N-CA-C	6.05	119.53	107.62
1	B	70	PRO	CA-C-N	6.01	132.79	121.97
1	B	70	PRO	C-N-CA	6.01	132.79	121.97
1	B	26	ALA	O-C-N	6.00	128.24	121.94
1	A	281	SER	N-CA-C	-6.00	105.04	112.72
1	B	71	ILE	CA-C-N	5.94	130.56	122.84
1	B	71	ILE	C-N-CA	5.94	130.56	122.84
1	A	123	MET	O-C-N	-5.93	114.70	122.59
1	A	349	LEU	N-CA-C	5.91	118.83	110.14
1	A	309	ILE	N-CA-C	-5.90	103.89	110.62
1	A	111	ASN	CA-C-N	5.88	127.19	119.84
1	A	111	ASN	C-N-CA	5.88	127.19	119.84
1	B	308	GLY	N-CA-C	-5.87	107.78	115.47
1	A	171	LEU	CA-C-N	5.83	127.12	119.84
1	A	171	LEU	C-N-CA	5.83	127.12	119.84
1	A	265	SER	N-CA-C	-5.79	103.94	113.50
1	A	212	ILE	N-CA-C	-5.79	104.69	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	PHE	N-CA-C	-5.77	105.89	113.17
1	B	317	ILE	N-CA-C	5.76	121.33	109.34
1	A	122	ILE	CA-C-O	-5.69	115.49	121.41
1	B	200	PHE	N-CA-C	5.63	122.80	110.80
1	A	180	LEU	O-C-N	-5.63	115.10	122.59
1	B	71	ILE	CA-C-O	5.61	127.79	120.78
1	A	356	TRP	CA-C-N	-5.55	115.40	123.06
1	A	356	TRP	C-N-CA	-5.55	115.40	123.06
1	A	143	TYR	N-CA-C	-5.55	105.24	112.23
1	B	266	PHE	CA-C-N	-5.54	112.00	121.97
1	B	266	PHE	C-N-CA	-5.54	112.00	121.97
1	B	223	PHE	N-CA-C	-5.51	106.53	113.20
1	A	273	GLY	CA-C-N	-5.49	112.08	121.97
1	A	273	GLY	C-N-CA	-5.49	112.08	121.97
1	A	285	CYS	N-CA-C	5.46	117.75	108.02
1	B	305	MET	N-CA-C	5.46	120.07	113.41
1	B	306	TYR	CA-C-N	5.45	126.65	119.84
1	B	306	TYR	C-N-CA	5.45	126.65	119.84
1	B	309	ILE	N-CA-C	-5.45	105.92	113.00
1	B	372	ARG	CA-C-N	-5.42	113.14	123.32
1	B	372	ARG	C-N-CA	-5.42	113.14	123.32
1	B	236	LEU	CA-C-N	5.39	131.23	122.39
1	B	236	LEU	C-N-CA	5.39	131.23	122.39
1	B	121	GLN	N-CA-C	-5.36	105.35	111.14
1	A	163	VAL	N-CA-C	5.31	120.36	108.88
1	A	248	ILE	N-CA-C	5.31	116.67	108.44
1	B	8	LEU	N-CA-C	5.26	117.68	109.52
1	B	365	ALA	N-CA-C	5.25	118.51	112.57
1	A	102	PRO	N-CA-C	-5.25	102.86	111.21
1	B	103	THR	N-CA-C	5.24	117.98	109.24
1	A	250	ILE	N-CA-C	5.23	116.19	108.45
1	B	262	PHE	N-CA-C	-5.23	106.76	112.72
1	A	196	ARG	CA-C-N	5.22	131.65	121.41
1	A	196	ARG	C-N-CA	5.22	131.65	121.41
1	B	200	PHE	CB-CG-CD1	5.22	129.57	120.70
1	B	326	LYS	N-CA-C	-5.21	99.69	110.80
1	B	334	GLU	N-CA-C	-5.21	107.21	113.21
1	B	265	SER	CA-C-N	-5.18	112.81	120.38
1	B	265	SER	C-N-CA	-5.18	112.81	120.38
1	B	270	GLU	CA-C-O	5.17	126.73	119.80
1	A	167	GLU	N-CA-C	-5.14	106.09	112.47
1	B	325	MET	CA-C-N	5.08	131.25	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	MET	C-N-CA	5.08	131.25	121.54
1	B	71	ILE	N-CA-C	-5.00	98.93	109.34

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	Mainchain,Peptide
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	726	0
1	B	2829	0	2794	876	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	5674	1562	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 136.

All (1562) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:235:SER:C	1:B:236:LEU:HD23	1.48	1.38
1:B:71:ILE:CD1	1:B:82:MET:CE	2.04	1.34
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:B:71:ILE:CD1	1:B:82:MET:HE2	1.67	1.22
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	1.22
1:B:71:ILE:HD12	1:B:82:MET:CE	1.64	1.18
1:A:187:ASP:HA	1:A:190:MET:HE2	1.26	1.17
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
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: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:B:21:PHE:HB2	1:B:24:ASP:CG	1.77	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:A:123:MET:HB3	1:A:129:VAL:CG2	1.82	1.06
1:B:71:ILE:HD12	1:B:82:MET:HE1	1.33	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:B:71:ILE:CD1	1:B:82:MET:HE1	1.84	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:A:372:ARG:HG3	1:B:372:ARG:HB3	1.34	1.04
1:A:123:MET:HE3	1:A:129:VAL:HG11	1.38	1.04
1:B:91:TYR:O	1:B:95:ARG:HD2	1.58	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:SER:C	1:B:200:PHE:CA	2.33	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:325:MET:HE3	1:B:325:MET:HA	1.40	1.00
1:B:103:THR:C	1:B:356:TRP:CH2	2.39	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:234:SER:C	1:A:235:SER:CA	2.36	0.98
1:A:373:LYS:CD	1:B:373:LYS:HA	1.92	0.98
1:B:78:ASN:CG	1:B:81:ASP:HB2	1.87	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
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: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: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:252:ASN:HD21	1:B:256:ARG:HH21	1.12	0.95
1:B:230:ALA:O	1:B:231:ALA:C	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:269:MET:HE3	1:A:269:MET:HA	1.50	0.91
1:A:92:ASN:H	1:A:92:ASN:ND2	1.66	0.91
1:A:235:SER:N	1:A:235:SER:C	2.28	0.91
1:A:325:MET:HE3	1:A:326:LYS:N	1.85	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
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:299:MET:HE2	1:A:304:THR:HB	1.54	0.89
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:A:154:ASP:CG	1:A:300:SER:OG	2.17	0.87
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:235:SER:C	1:B:236:LEU:CD2	2.44	0.86
1:B:355:MET:HE1	1:B:374:CYS:SG	2.16	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:76:ILE:HG23	1:A:82:MET:HE3	1.58	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:187:ASP:HA	1:B:190:MET:HE2	1.56	0.84
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:A:227:MET:HE1	1:A:256:ARG:HD3	1.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:ARG:O	5:B:391:HOH:O	1.79	0.81
1:B:274:ILE:HD12	1:B:275:HIS:H	1.45	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:230:ALA:C	1:B:232:SER:N	2.32	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:A:98:PRO:C	1:A:100:GLU:H	1.88	0.81
1:B:334:GLU:C	1:B:336:LYS:H	1.87	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:A:176:MET:HE2	1:A:280:ASN:HB2	1.62	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:B:142:LEU:HD21	1:B:148:THR:C	2.05	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:233:SER:C	1:B:235:SER:H	1.87	0.80
1:B:372:ARG:HG3	1:B:372:ARG:O	1.81	0.80
1:A:156:GLY:HA3	3:A:376:ATP:O3G	1.81	0.80
1:B:103:THR:C	1:B:356:TRP:HH2	1.89	0.80
1:B:243:PRO:C	1:B:245:GLY:H	1.91	0.80
1:B:355:MET:HE3	1:B:375:PHE:HE1	1.45	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:A:121:GLN:CD	1:A:125:GLU:HG3	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:PHE:HA	1:A:205:GLU:CD	2.08	0.79
1:A:238:LYS:C	1:A:249:THR:HG22	2.08	0.79
1:B:72:GLU:CD	1:B:77:THR:HG21	2.07	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:71:ILE:HD12	1:B:82:MET:HE2	1.35	0.79
1:B:91:TYR:C	1:B:93:GLU:H	1.89	0.78
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:325:MET:HE3	1:A:326:LYS:H	1.46	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: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: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:B:118:LYS:HB2	1:B:118:LYS:HZ3	1.48	0.76
1:A:83:GLU:C	1:A:85:ILE:H	1.92	0.76
1:A:218:TYR:CE2	1:A:254:ARG:HB3	2.20	0.76
1:B:352:PHE:HE2	1:B:356:TRP:CZ2	2.02	0.76
1:B:319:ALA:C	1:B:320:LEU:HD12	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:195:GLU:C	1:B:197:GLY:H	1.94	0.75
1:B:140:LEU:HD22	1:B:343:GLY:HA2	1.68	0.75
1:B:269:MET:C	1:B:271:SER:H	1.91	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:B:132:MET:HE3	1:B:132:MET:O	1.85	0.75
1:A:154:ASP:OD1	1:A:300:SER:OG	2.02	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:71:ILE:HD11	1:B:82:MET:HE3	1.70	0.74
1:A:99:GLU:HA	1:A:129:VAL:HA	1.68	0.74
1:A:200:PHE:HD2	1:A:205:GLU:CD	1.94	0.74
1:A:352:PHE:O	1:A:355:MET:HB2	1.87	0.74
1:B:354:GLN:HE21	1:B:355:MET:HE1	1.52	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: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:71:ILE:HD11	1:B:82:MET:HE2	1.48	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:252:ASN:C	1:A:256:ARG:HG3	2.14	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
1:A:99:GLU:C	1:A:130:PRO:HD3	2.13	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:132:MET:C	1:B:356:TRP:CE3	2.67	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:A:263:GLN:C	1:A:265:SER:H	1.97	0.72
1:B:188:TYR:HE2	1:B:257:CYS:HA	1.54	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:222:ASP:CG	1:A:225:ASN:HB2	2.14	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: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: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:305:MET:HE2	1:B:336:LYS:HB2	1.71	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:A:287:ILE:HG23	1:A:288:ASP:N	2.05	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:346:LEU:O	1:B:349:LEU:HD21	1.91	0.70
1:B:107:GLU:HG2	1:B:135:ALA:C	2.15	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: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:355:MET:HE3	1:B:375:PHE:CE1	2.26	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:A:71:ILE:HG13	1:A:82:MET:HE1	1.74	0.69
1:B:39:ARG:HD2	1:B:64:ILE:O	1.92	0.69
1:B:91:TYR:C	1:B:93:GLU:N	2.45	0.69
1:A:76:ILE:HD12	1:A:76:ILE:N	2.08	0.69
1:A:234:SER:C	1:A:236:LEU:H	2.00	0.69
1:A:7:ALA:CB	1:A:102:PRO:HB2	2.22	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: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:B:140:LEU:HD13	1:B:343:GLY:HA3	1.75	0.68
1:B:108:ALA:HB3	1:B:111:ASN:HB2	1.73	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:143:TYR:C	1:A:145:SER:H	2.00	0.68
1:A:209:VAL:O	1:A:212:ILE:HB	1.93	0.68
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:104:LEU:C	1:A:104:LEU:HD23	2.19	0.67
1:A:238:LYS:HG3	1:A:239:SER:N	2.09	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:228:ALA:C	1:B:230:ALA:H	2.03	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:B:343:GLY:C	1:B:345:ILE:H	2.02	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:B:89:THR:O	1:B:93:GLU:HB2	1.96	0.66
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:A:198:TYR:HH	1:A:248:ILE:HG23	1.57	0.66
1:B:369:ILE:HD12	1:B:372:ARG:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:227:MET:CE	1:A:256:ARG:HD3	2.25	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:275:HIS:HA	1:B:313:MET:HE1	1.78	0.66
1:B:239:SER:HA	1:B:248:ILE:O	1.96	0.66
1:A:307:PRO:C	1:A:309:ILE:H	2.04	0.66
1:A:295:ALA:HA	1:A:328:LYS:H	1.59	0.65
1:B:132:MET:C	1:B:356:TRP:HE3	2.04	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:A:91:TYR:C	1:A:93:GLU:H	2.04	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: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:230:ALA:C	1:B:232:SER:H	2.03	0.65
1:B:349:LEU:O	1:B:350:SER:C	2.37	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:176:MET:HE2	1:A:277:THR:HA	1.79	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:260:THR:HA	1:B:266:PHE:CD1	2.32	0.65
1:B:291:LYS:HG3	1:B:325:MET:HE1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLU:C	1:B:197:GLY:N	2.53	0.65
1:B:242:LEU:HD12	1:B:244:ASP:H	1.62	0.65
1:A:83:GLU:C	1:A:85:ILE:N	2.55	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
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:143:TYR:CD1	1:A:346:LEU:HD11	2.33	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:235:SER:C	1:A:236:LEU:HD13	2.23	0.64
1:A:133:TYR:OH	1:A:375:PHE:HA	1.98	0.64
1:B:80:ASP:C	1:B:83:GLU:HG3	2.23	0.64
1:B:352:PHE:CE2	1:B:356:TRP:CE2	2.86	0.64
1:A:97:ALA:HB3	1:A:100:GLU:CD	2.21	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: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:76:ILE:HD11	1:B:119:MET:HE1	1.79	0.63
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: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:A:59:GLN:C	1:A:59:GLN:CD	2.67	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:B:202:THR:HG1	1:B:204:ALA:HB3	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:HH11	1:B:214:GLU:CD	2.07	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:289:ILE:HD12	1:B:289:ILE:C	2.23	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:B:307:PRO:C	1:B:309:ILE:H	2.05	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:A:195:GLU:OE2	1:A:195:GLU:HA	1.98	0.62
1:B:110:LEU:CD1	1:B:175:ILE:HD12	2.24	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:A:234:SER:C	1:A:236:LEU:N	2.58	0.62
1:A:247:VAL:C	1:A:248:ILE:HG13	2.25	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: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: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:A:337:TYR:O	1:A:338:SER:C	2.43	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:22:ALA:C	1:A:24:ASP:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:THR:HA	1:B:321:ALA:CB	2.25	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:A:187:ASP:O	1:A:188:TYR:C	2.44	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:A:9:VAL:HB	1:A:340:TRP:CE2	2.36	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:142:LEU:HD21	1:B:148:THR:CA	2.31	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: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: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:B:236:LEU:CD2	1:B:236:LEU:N	2.45	0.60
1:B:334:GLU:C	1:B:336:LYS:N	2.57	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: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:233:SER:C	1:B:235:SER:N	2.50	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:189:LEU:O	1:A:190:MET:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.65	0.60
1:B:252:ASN:H	1:B:252:ASN:HD22	1.50	0.60
1:A:323:SER:OG	1:A:324:THR:N	2.31	0.60
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:A:98:PRO:C	1:A:100:GLU:N	2.56	0.60
1:A:89:THR:C	1:A:93:GLU:HB3	2.26	0.59
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:143:TYR:C	1:A:145:SER:N	2.56	0.59
1:A:239:SER:HA	1:A:249:THR:HG22	1.83	0.59
1:A:373:LYS:CD	1:B:373:LYS:C	2.75	0.59
1:B:53:TYR:CB	1:B:61:LYS:HE3	2.31	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:346:LEU:O	1:B:349:LEU:HD23	2.01	0.59
1:A:269:MET:CG	1:A:270:GLU:H	1.95	0.59
1:A:289:ILE:O	1:A:290:ARG:C	2.45	0.59
1:B:59:GLN:HG3	1:B:60:SER:N	2.17	0.59
1:B:247:VAL:C	1:B:248:ILE:HD12	2.27	0.59
1:B:325:MET:HA	1:B:325:MET:CE	2.23	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:76:ILE:HG23	1:A:82:MET:CE	2.30	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:B:337:TYR:C	1:B:341:ILE:HG13	2.28	0.59
1:A:98:PRO:HG2	1:A:99:GLU:H	1.67	0.59
1:A:122:ILE:O	1:A:123:MET:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LYS:O	1:B:217:CYS:HB2	2.02	0.59
1:B:362:TYR:C	1:B:364:GLU:H	2.10	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: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:176:MET:HE2	1:A:280:ASN:CB	2.34	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
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: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: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:B:207:GLU:CD	4:B:387:LAR:HO4	2.11	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:373:LYS:HG3	1:B:372:ARG:HB2	1.84	0.58
1:A:71:ILE:HG13	1:A:82:MET:HE3	1.85	0.58
1:B:268:GLY:O	1:B:269:MET:C	2.43	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: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:234:SER:C	1:A:236:LEU:HD22	2.30	0.57
1:B:318:THR:C	1:B:320:LEU:H	2.12	0.57
1:A:93:GLU:HG3	1:A:94:LEU:CD1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:132:MET:C	1:B:356:TRP:CZ3	2.82	0.57
1:A:61:LYS:HB2	1:A:65:LEU:HD22	1.87	0.57
1:A:85:ILE:O	1:A:86:TRP:C	2.47	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
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:12:ASN:O	1:B:13:GLY:C	2.45	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:91:TYR:C	1:A:93:GLU:N	2.63	0.57
1:A:183:ARG:NH1	1:A:183:ARG:CB	2.68	0.57
1:B:98:PRO:C	1:B:100:GLU:H	2.12	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:B:207:GLU:CD	1:B:210:ARG:HH21	2.12	0.57
1:A:185:LEU:H	1:A:185:LEU:CD1	2.13	0.57
1:B:79:TRP:CE3	1:B:118:LYS:HG2	2.39	0.57
1:B:79:TRP:O	1:B:80:ASP:C	2.48	0.57
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:223:PHE:HB2	1:A:259:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:136:ILE:O	1:A:137:GLN:C	2.48	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
1:A:263:GLN:C	1:A:265:SER:N	2.61	0.56
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:89:THR:O	1:B:90:PHE:C	2.48	0.56
1:A:121:GLN:OE1	1:A:125:GLU:HG3	2.04	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:A:252:ASN:CG	1:A:256:ARG:HE	2.14	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:7:ALA:C	1:A:8:LEU:HG	2.30	0.56
1:A:209:VAL:CA	1:A:212:ILE:HD12	2.35	0.56
1:B:76:ILE:CD1	1:B:119:MET:HE1	2.36	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:166:TYR:C	1:A:168:GLY:N	2.63	0.55
1:A:250:ILE:N	1:A:250:ILE:CD1	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:116:ARG:C	1:B:118:LYS:H	2.14	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:A:152:VAL:HG12	1:A:153:LEU:N	2.22	0.55
1:B:329:ILE:O	1:B:330:ILE:C	2.48	0.55
1:B:334:GLU:O	1:B:336:LYS:N	2.37	0.55
1:A:216:LEU:N	1:A:216:LEU:HD22	2.20	0.55
1:B:111:ASN:HD21	1:B:115:ASN:HB2	1.72	0.55
1:B:172:PRO:O	1:B:173:HIS:C	2.49	0.55
1:B:182:GLY:C	1:B:184:ASP:H	2.14	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: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:B:21:PHE:HE2	1:B:28:ARG:CZ	2.20	0.55
1:A:205:GLU:HA	1:A:208:ILE:CD1	2.37	0.54
1:B:283:MET:C	1:B:285:CYS:H	2.15	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:307:PRO:C	1:B:309:ILE:N	2.64	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:B:301:GLY:C	1:B:304:THR:HG23	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:LEU:HD11	1:B:244:ASP:HB2	1.89	0.54
1:B:299:MET:HE1	1:B:329:ILE:HG21	1.88	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: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
1:B:138:ALA:O	1:B:152:VAL:HG21	2.08	0.54
1:B:193:LEU:C	1:B:195:GLU:H	2.14	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:A:282:ILE:C	1:A:284:LYS:H	2.15	0.54
1:A:373:LYS:HD3	1:B:373:LYS:C	2.33	0.54
1:A:180:LEU:C	1:A:180:LEU:HD12	2.33	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: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:17:VAL:C	1:B:18:LYS:HD3	2.33	0.54
1:B:39:ARG:NE	1:B:66:THR:HG23	2.23	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:79:TRP:O	1:A:80:ASP:C	2.50	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:A:185:LEU:HB3	1:A:257:CYS:HG	1.72	0.53
1:A:290:ARG:O	1:A:291:LYS:C	2.50	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:79:TRP:H	1:B:79:TRP:CD1	2.24	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:240:TYR:O	1:A:242:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:HG2	1:B:367:PRO:C	2.33	0.53
1:A:156:GLY:HA2	3:A:376:ATP:O1A	2.09	0.53
1:A:193:LEU:C	1:A:195:GLU:N	2.61	0.53
1:A:317:ILE:O	1:A:317:ILE:HD12	2.08	0.53
1:B:243:PRO:O	1:B:245:GLY:N	2.40	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:314:GLN:NE2	1:B:318:THR:OG1	2.41	0.53
1:B:315:LYS:O	1:B:316:GLU:C	2.52	0.53
1:A:226:GLU:HG2	1:A:255:PHE:CD1	2.42	0.53
1:B:188:TYR:O	1:B:189:LEU:C	2.51	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: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
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:B:333:PRO:C	1:B:335:ARG:H	2.16	0.53
1:A:22:ALA:O	1:A:24:ASP:N	2.41	0.53
1:A:93:GLU:C	1:A:93:GLU:OE1	2.52	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:59:GLN:C	1:A:61:LYS:H	2.17	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:193:LEU:C	1:B:195:GLU:N	2.66	0.53
1:B:212:ILE:O	1:B:213:LYS:C	2.52	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:23:GLY:O	1:A:24:ASP:C	2.52	0.52
1:A:151:ILE:HG22	1:A:151:ILE:O	2.09	0.52
1:B:132:MET:CA	1:B:356:TRP:CE3	2.92	0.52
1:B:313:MET:O	1:B:314:GLN:C	2.52	0.52
1:A:313:MET:O	1:A:314:GLN:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:VAL:O	1:B:212:ILE:N	2.41	0.52
1:B:232:SER:O	1:B:233:SER:C	2.53	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:243:PRO:C	1:B:245:GLY:N	2.59	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:229:THR:C	1:B:232:SER:HB2	2.35	0.52
1:A:116:ARG:NH1	1:A:116:ARG:CB	2.72	0.52
1:A:303:THR:C	1:A:305:MET:N	2.68	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: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
1:A:123:MET:C	1:A:129:VAL:HG22	2.34	0.52
1:A:133:TYR:CE1	1:A:375:PHE:HA	2.44	0.52
1:B:132:MET:HE3	1:B:132:MET:C	2.34	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:B:105:LEU:HD11	1:B:123:MET:HE3	1.91	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:A:269:MET:HA	1:A:269:MET:CE	2.33	0.52
1:A:352:PHE:O	1:A:353:GLN:C	2.53	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:307:PRO:C	1:A:309:ILE:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HB2	1:A:216:LEU:HD22	1.92	0.52
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:A:279:TYR:C	1:A:281:SER:H	2.18	0.51
1:A:285:CYS:O	1:A:286:ASP:C	2.53	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:B:362:TYR:C	1:B:364:GLU:N	2.68	0.51
1:A:350:SER:CA	1:A:353:GLN:HE21	2.23	0.51
1:B:11:ASP:C	1:B:13:GLY:H	2.18	0.51
1:B:186:THR:C	1:B:188:TYR:N	2.65	0.51
1:A:6:THR:O	1:A:102:PRO:HD2	2.11	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:315:LYS:O	1:A:316:GLU:C	2.54	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
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:151:ILE:HD13	1:B:163:VAL:C	2.36	0.51
1:B:227:MET:HG2	1:B:255:PHE:HE1	1.76	0.51
1:A:317:ILE:C	1:A:319:ALA:N	2.66	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:166:TYR:C	1:A:168:GLY:H	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:CD2	1:B:165:ILE:HG21	2.41	0.51
1:B:203:THR:O	1:B:204:ALA:C	2.52	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:B:343:GLY:C	1:B:345:ILE:N	2.67	0.51
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:170:ALA:C	1:B:172:PRO:HD3	2.36	0.50
1:A:64:ILE:HG13	1:A:65:LEU:CD1	2.41	0.50
1:B:21:PHE:O	1:B:22:ALA:C	2.55	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:188:TYR:CE2	1:B:257:CYS:HA	2.40	0.50
1:B:338:SER:N	1:B:341:ILE:HD12	2.27	0.50
1:B:349:LEU:HD12	1:B:351:THR:C	2.35	0.50
1:A:218:TYR:HE2	1:A:254:ARG:CB	2.21	0.50
1:B:79:TRP:C	1:B:81:ASP:N	2.69	0.50
1:B:116:ARG:C	1:B:118:LYS:N	2.70	0.50
1:B:147:ARG:NH2	1:B:330:ILE:HG21	2.26	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:13:GLY:O	1:B:14:SER:C	2.53	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
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:B:61:LYS:C	1:B:63:GLY:N	2.69	0.50
1:B:92:ASN:N	1:B:92:ASN:ND2	2.56	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:A:276:GLU:C	1:A:278:THR:N	2.69	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:305:MET:HE2	1:A:336:LYS:N	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:MET:CE	1:B:374:CYS:SG	2.97	0.50
1:A:73:HIS:O	1:A:159:VAL:HG11	2.12	0.49
1:A:87:HIS:ND1	1:A:87:HIS:C	2.70	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:286:ASP:O	1:A:287:ILE:C	2.55	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:346:LEU:C	1:B:348:SER:H	2.18	0.49
1:B:151:ILE:HD11	1:B:164:PRO:HG3	1.94	0.49
1:B:337:TYR:O	1:B:338:SER:C	2.55	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:B:79:TRP:CZ3	1:B:118:LYS:HG2	2.47	0.49
1:B:91:TYR:O	1:B:92:ASN:C	2.55	0.49
1:B:142:LEU:CD2	1:B:148:THR:HA	2.43	0.49
1:B:335:ARG:HG2	1:B:335:ARG:NH2	2.26	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:122:ILE:O	1:B:123:MET:C	2.55	0.49
1:B:144:ALA:HB2	1:B:342:GLY:HA3	1.94	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: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:133:TYR:HH	1:A:375:PHE:N	2.10	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:A:338:SER:O	1:A:339:VAL:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:CE2	1:B:316:GLU:HG3	2.43	0.49
1:A:79:TRP:CZ2	1:A:115:ASN:OD1	2.66	0.49
1:A:200:PHE:CD2	1:A:205:GLU:CD	2.84	0.49
1:A:314:GLN:O	1:A:317:ILE:HG23	2.12	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:285:CYS:HB3	1:A:289:ILE:HD11	1.95	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:123:MET:O	1:B:124:PHE:C	2.55	0.48
1:B:132:MET:CA	1:B:356:TRP:CZ3	2.95	0.48
1:B:210:ARG:HB2	4:B:387:LAR:C20	2.43	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:B:91:TYR:O	1:B:95:ARG:CD	2.47	0.48
1:B:359:LYS:NZ	1:B:363:ASP:OD1	2.36	0.48
1:A:51:ASP:CG	1:A:52:SER:H	2.19	0.48
1:A:248:ILE:HG22	1:A:249:THR:N	2.28	0.48
1:B:187:ASP:CG	1:B:206:ARG:NH2	2.71	0.48
1:A:287:ILE:O	1:A:289:ILE:N	2.47	0.48
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: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:317:ILE:O	1:A:318:THR:C	2.56	0.48
1:B:162:ASN:ND2	1:B:278:THR:OG1	2.47	0.48
1:A:79:TRP:HA	1:A:82:MET:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:THR:HG21	4:A:377:LAR:S1	2.54	0.48
1:B:143:TYR:C	1:B:145:SER:H	2.22	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: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:120:THR:O	1:A:121:GLN:C	2.57	0.47
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:A:234:SER:O	1:A:236:LEU:N	2.40	0.47
1:A:303:THR:O	1:A:304:THR:C	2.57	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: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: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:280:ASN:N	1:A:280:ASN:ND2	2.52	0.47
1:A:9:VAL:HG12	1:A:340:TRP:CD1	2.50	0.47
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:CG	1:A:94:LEU:HD12	2.41	0.47
1:A:121:GLN:NE2	1:A:121:GLN:C	2.73	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:262:PHE:C	1:A:264:PRO:HD3	2.39	0.47
1:A:287:ILE:O	1:A:288:ASP:C	2.56	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLU:C	1:B:255:PHE:N	2.73	0.47
1:B:322:PRO:O	1:B:323:SER:C	2.58	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:A:354:GLN:CD	1:A:355:MET:HE2	2.40	0.47
1:B:92:ASN:ND2	1:B:92:ASN:H	2.12	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:A:358:THR:HG23	1:A:361:GLU:CD	2.39	0.47
1:B:121:GLN:O	1:B:122:ILE:C	2.57	0.47
1:B:222:ASP:C	1:B:224:GLU:H	2.22	0.47
1:B:283:MET:C	1:B:285:CYS:N	2.72	0.47
1:B:328:LYS:C	1:B:329:ILE:HD13	2.39	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: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:149:THR:HG1	1:A:167:GLU:N	2.13	0.47
1:A:189:LEU:O	1:A:191:LYS:N	2.48	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
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:B:24:ASP:C	1:B:26:ALA:H	2.20	0.46
1:B:164:PRO:HG2	1:B:174:ALA:O	2.15	0.46
1:B:186:THR:O	1:B:187:ASP:C	2.57	0.46
1:A:11:ASP:HA	1:A:106:THR:HG21	1.97	0.46
1:A:276:GLU:C	1:A:278:THR:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD11	1:B:244:ASP:CB	2.45	0.46
1:B:274:ILE:O	1:B:275:HIS:C	2.58	0.46
1:A:290:ARG:O	1:A:293:LEU:N	2.47	0.46
1:A:326:LYS:HZ1	1:A:328:LYS:HB2	1.80	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:359:LYS:O	1:A:360:GLN:C	2.57	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: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:350:SER:C	1:A:352:PHE:N	2.73	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:296:ASN:C	1:B:297:ASN:CG	2.84	0.46
1:B:337:TYR:O	1:B:340:TRP:N	2.49	0.46
1:A:276:GLU:O	1:A:279:TYR:N	2.48	0.46
1:B:53:TYR:CG	1:B:61:LYS:HE3	2.51	0.46
1:A:22:ALA:C	1:A:24:ASP:N	2.73	0.46
1:A:309:ILE:HG23	1:A:310:ALA:N	2.30	0.46
1:B:132:MET:HE3	1:B:357:ILE:HD12	1.98	0.46
1:B:259:GLU:C	1:B:261:LEU:N	2.73	0.46
1:B:314:GLN:HE22	1:B:318:THR:CG2	2.28	0.46
1:A:64:ILE:C	1:A:65:LEU:HD12	2.40	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:A:113:LYS:CA	1:A:116:ARG:HH12	2.23	0.45
1:B:228:ALA:C	1:B:230:ALA:N	2.72	0.45
1:B:306:TYR:CE1	3:B:386:ATP:H2	2.34	0.45
1:B:308:GLY:C	1:B:310:ALA:H	2.22	0.45
1:B:308:GLY:C	1:B:310:ALA:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:C	1:A:341:ILE:HG13	2.41	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:191:LYS:C	1:A:193:LEU:H	2.24	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: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:A:303:THR:C	1:A:305:MET:H	2.23	0.45
1:A:329:ILE:C	1:A:330:ILE:HD12	2.42	0.45
1:A:373:LYS:HD2	1:B:373:LYS:C	2.40	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
1:B:193:LEU:N	1:B:193:LEU:HD12	2.32	0.45
1:B:354:GLN:NE2	1:B:355:MET:HE1	2.26	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: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:193:LEU:O	1:A:194:THR:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:235:SER:CA	1:A:236:LEU:HD13	2.43	0.45
1:A:252:ASN:OD1	1:A:253:GLU:CD	2.60	0.45
1:A:264:PRO:CG	1:A:273:GLY:HA2	2.33	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:263:GLN:C	1:B:266:PHE:CD1	2.89	0.45
1:B:283:MET:O	1:B:285:CYS:N	2.50	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:299:MET:HE1	1:B:329:ILE:CG2	2.47	0.45
1:A:240:TYR:O	1:A:247:VAL:HA	2.16	0.45
1:B:299:MET:HG3	1:B:331:ALA:CB	2.47	0.45
1:B:312:ARG:O	1:B:313:MET:C	2.60	0.45
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: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:A:350:SER:C	1:A:352:PHE:H	2.24	0.44
1:B:69:TYR:CD1	1:B:69:TYR:N	2.81	0.44
1:B:216:LEU:O	1:B:217:CYS:C	2.61	0.44
1:B:222:ASP:C	1:B:224:GLU:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ALA:O	1:A:139:VAL:C	2.59	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:228:ALA:O	1:A:229:THR:C	2.60	0.44
1:B:262:PHE:C	1:B:263:GLN:HG2	2.40	0.44
1:A:274:ILE:O	1:A:275:HIS:C	2.61	0.44
1:A:352:PHE:HA	1:A:355:MET:CG	2.46	0.44
1:B:31:PHE:CD1	1:B:31:PHE:C	2.96	0.44
1:B:109:PRO:HB2	1:B:161:HIS:ND1	2.33	0.44
1:B:210:ARG:HG2	1:B:214:GLU:CD	2.43	0.44
1:B:298:VAL:HA	1:B:330:ILE:O	2.17	0.44
1:B:318:THR:C	1:B:320:LEU:N	2.75	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:51:ASP:CG	1:A:52:SER:N	2.76	0.44
1:A:74:GLY:O	1:A:75:ILE:HG12	2.18	0.44
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:B:273:GLY:O	1:B:274:ILE:C	2.60	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:251:GLY:O	1:A:252:ASN:C	2.61	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:6:THR:C	1:B:102:PRO:HD2	2.42	0.43
1:B:9:VAL:HB	1:B:340:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:PRO:C	1:B:100:GLU:N	2.74	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: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:A:72:GLU:O	1:A:73:HIS:HB2	2.17	0.43
1:A:104:LEU:C	1:A:104:LEU:CD2	2.88	0.43
1:A:226:GLU:HG3	1:A:255:PHE:CE2	2.51	0.43
1:A:343:GLY:O	1:A:344:SER:C	2.62	0.43
1:B:9:VAL:HB	1:B:340:TRP:NE1	2.33	0.43
1:B:105:LEU:CD1	1:B:123:MET:HE3	2.49	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:B:244:ASP:C	1:B:246:GLN:H	2.22	0.43
1:B:303:THR:C	1:B:305:MET:H	2.25	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: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:A:220:ALA:O	1:A:221:LEU:C	2.61	0.43
1:B:70:PRO:HB2	1:B:71:ILE:H	1.29	0.43
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:123:MET:O	1:A:124:PHE:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:275:HIS:CA	1:B:313:MET:HE1	2.47	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:B:52:SER:OG	1:B:84:LYS:NZ	2.49	0.42
1:A:153:LEU:H	1:A:299:MET:HA	1.84	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:253:GLU:C	1:B:255:PHE:H	2.25	0.42
1:B:288:ASP:OD1	1:B:288:ASP:C	2.61	0.42
1:B:310:ALA:C	1:B:312:ARG:N	2.77	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:119:MET:HE3	1:A:119:MET:HB2	1.83	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:104:LEU:N	1:B:356:TRP:HH2	2.14	0.42
1:B:188:TYR:O	1:B:191:LYS:HB3	2.19	0.42
1:B:226:GLU:C	1:B:228:ALA:H	2.28	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:HA	1:A:307:PRO:HD2	2.01	0.42
1:A:222:ASP:OD2	1:A:222:ASP:C	2.62	0.42
1:A:226:GLU:HG2	1:A:255:PHE:CG	2.55	0.42
1:B:78:ASN:O	1:B:81:ASP:CB	2.68	0.42
1:B:89:THR:HG22	1:B:90:PHE:N	2.33	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:360:GLN:C	1:B:362:TYR:H	2.27	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:74:GLY:C	1:A:75:ILE:HG12	2.44	0.42
1:A:117:GLU:OE1	1:A:367:PRO:HB2	2.19	0.42
1:A:132:MET:HE3	1:A:132:MET:HB2	1.90	0.42
1:A:306:TYR:CZ	3:A:376:ATP:H2	2.37	0.42
1:B:190:MET:SD	1:B:206:ARG:HG3	2.59	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:310:ALA:O	1:A:311:ASP:C	2.61	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:311:ASP:OD1	1:B:311:ASP:N	2.47	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
1:B:18:LYS:N	1:B:18:LYS:CD	2.82	0.42
1:B:29:ALA:C	1:B:30:VAL:HG23	2.45	0.42
1:B:56:ASP:HA	1:B:59:GLN:HB3	2.01	0.42
1:B:86:TRP:O	1:B:87:HIS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:171:LEU:O	1:B:172:PRO:C	2.61	0.42
1:B:172:PRO:HD2	1:B:173:HIS:HE1	1.84	0.42
1:B:189:LEU:C	1:B:191:LYS:H	2.26	0.42
1:B:317:ILE:H	1:B:317:ILE:HG13	1.71	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:308:GLY:O	1:A:309:ILE:C	2.63	0.42
1:A:91:TYR:HB3	1:A:92:ASN:HD22	1.85	0.41
1:A:253:GLU:CD	1:A:253:GLU:H	2.28	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: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: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:198:TYR:HH	1:A:248:ILE:CG2	2.17	0.41
1:A:301:GLY:O	1:A:302:GLY:C	2.62	0.41
1:A:354:GLN:OE1	1:A:372:ARG:NH1	2.49	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:B:141:SER:CA	1:B:338:SER:OG	2.67	0.41
1:B:189:LEU:C	1:B:191:LYS:N	2.78	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:THR:HG23	1:B:132:MET:CE	2.50	0.41
1:B:175:ILE:HG22	1:B:176:MET:N	2.35	0.41
1:B:181:ALA:O	1:B:182:GLY:C	2.63	0.41
1:B:209:VAL:O	1:B:210:ARG:C	2.62	0.41
1:B:269:MET:HB3	1:B:271:SER:HB3	2.02	0.41
1:B:277:THR:O	1:B:278:THR:C	2.64	0.41
1:A:159:VAL:HG22	3:A:376:ATP:O2G	2.19	0.41
1:A:188:TYR:O	1:A:189:LEU:C	2.64	0.41
1:A:210:ARG:CZ	1:A:210:ARG:HB3	2.50	0.41
1:A:279:TYR:C	1:A:281:SER:N	2.78	0.41
1:A:312:ARG:O	1:A:316:GLU:HG2	2.21	0.41
1:B:21:PHE:C	1:B:22:ALA:O	2.62	0.41
1:B:59:GLN:NE2	4:B:387:LAR:H223	2.33	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:365:ALA:C	1:B:366:GLY:O	2.63	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:B:16:LEU:HD11	4:B:387:LAR:O1	2.20	0.41
1:B:57:GLU:C	1:B:61:LYS:HE2	2.45	0.41
1:B:124:PHE:O	1:B:125:GLU:C	2.63	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:A:14:SER:HA	1:A:71:ILE:HG21	2.02	0.41
1:A:79:TRP:CD1	1:A:79:TRP:H	2.37	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:172:PRO:C	1:A:174:ALA:N	2.79	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:253:GLU:O	1:A:254:ARG:C	2.64	0.41
1:A:320:LEU:HG	1:A:320:LEU:H	1.52	0.41
1:B:20:GLY:HA3	1:B:27:PRO:HA	2.01	0.41
1:B:93:GLU:HB3	1:B:94:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:MET:HG2	1:B:281:SER:HB2	2.03	0.41
1:B:264:PRO:C	1:B:266:PHE:N	2.77	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:218:TYR:OH	1:A:226:GLU:CD	2.64	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:B:286:ASP:C	1:B:288:ASP:N	2.79	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:117:GLU:HG2	1:A:371:HIS:CE1	2.56	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:345:ILE:O	1:A:346:LEU:C	2.63	0.40
1:B:56:ASP:C	1:B:59:GLN:HB3	2.46	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:B:224:GLU:C	1:B:226:GLU:N	2.77	0.40
1:B:263:GLN:C	1:B:266:PHE:HD1	2.18	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:61:LYS:O	1:B:62:ARG:C	2.64	0.40
1:B:242:LEU:CG	1:B:244:ASP:HB3	2.51	0.40
1:B:37:ARG:O	1:B:65:LEU:HA	2.22	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:358:THR:O	1:B:359:LYS:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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	0

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
1	A	310	ALA
1	A	348	SER
1	B	25	ASP
1	B	70	PRO
1	B	116	ARG

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Mol	Chain	Res	Type
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
1	A	190	MET
1	A	241	GLU
1	A	286	ASP
1	A	353	GLN
1	B	12	ASN

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Mol	Chain	Res	Type
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
1	A	233	SER
1	A	291	LYS
1	A	299	MET
1	B	311	ASP
1	B	315	LYS

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Mol	Chain	Res	Type
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/318 (96%)	257 (84%)	50 (16%)	2	12
1	B	307/318 (96%)	239 (78%)	68 (22%)	1	5
All	All	614/636 (96%)	496 (81%)	118 (19%)	1	8

All (118) 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	77	THR
1	A	81	ASP
1	A	90	PHE
1	A	92	ASN
1	A	99	GLU
1	A	112	PRO
1	A	113	LYS

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Mol	Chain	Res	Type
1	A	121	GLN
1	A	126	THR
1	A	141	SER
1	A	151	ILE
1	A	152	VAL
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	242	LEU
1	A	246	GLN
1	A	250	ILE
1	A	256	ARG
1	A	263	GLN
1	A	271	SER
1	A	274	ILE
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	354	GLN
1	A	358	THR
1	A	369	ILE
1	A	375	PHE
1	B	25	ASP
1	B	34	ILE
1	B	56	ASP
1	B	59	GLN
1	B	66	THR

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Mol	Chain	Res	Type
1	B	67	LEU
1	B	69	TYR
1	B	71	ILE
1	B	72	GLU
1	B	75	ILE
1	B	76	ILE
1	B	77	THR
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	129	VAL
1	B	130	PRO
1	B	132	MET
1	B	136	ILE
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	200	PHE
1	B	202	THR
1	B	212	ILE
1	B	215	LYS
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	248	ILE
1	B	250	ILE
1	B	252	ASN
1	B	262	PHE
1	B	263	GLN
1	B	264	PRO

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Mol	Chain	Res	Type
1	B	267	ILE
1	B	270	GLU
1	B	274	ILE
1	B	275	HIS
1	B	288	ASP
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	313	MET
1	B	318	THR
1	B	324	THR
1	B	326	LYS
1	B	329	ILE
1	B	330	ILE
1	B	349	LEU
1	B	364	GLU
1	B	372	ARG
1	B	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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

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Mol	Chain	Res	Type
1	B	115	ASN
1	B	121	GLN
1	B	128	ASN
1	B	162	ASN
1	B	252	ASN
1	B	280	ASN
1	B	314	GLN
1	B	354	GLN
1	B	360	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	1.29	5 (16%)	32,43,43	1.47	3 (9%)
4	LAR	A	377	-	30,31,31	1.33	4 (13%)	32,43,43	1.56	3 (9%)
3	ATP	B	386	2	32,33,33	2.44	9 (28%)	48,52,52	3.01	14 (29%)
3	ATP	A	376	2	32,33,33	2.19	11 (34%)	48,52,52	2.91	14 (29%)

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
4	LAR	A	377	-	-	3/23/51/51	0/2/3/3
3	ATP	B	386	2	-	3/22/38/38	0/3/3/3
3	ATP	A	376	2	-	2/22/38/38	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	386	ATP	PB-O3A	8.78	1.69	1.59
3	A	376	ATP	PB-O3A	5.74	1.65	1.59
3	B	386	ATP	O5'-C5'	-4.85	1.26	1.44
3	A	376	ATP	O5'-C5'	-4.72	1.26	1.44
3	B	386	ATP	C5-C6	4.03	1.52	1.41
4	A	377	LAR	C18-N1	4.00	1.51	1.46
4	B	387	LAR	C18-N1	3.71	1.51	1.46
3	A	376	ATP	C5-C6	3.67	1.51	1.41
3	B	386	ATP	C4-N3	3.55	1.41	1.34
3	A	376	ATP	C4-N3	3.47	1.40	1.34
3	A	376	ATP	PA-O5'	-3.06	1.47	1.59
3	B	386	ATP	PA-O5'	-2.99	1.47	1.59
3	A	376	ATP	O4'-C1'	2.94	1.48	1.42
3	A	376	ATP	PB-O1B	-2.90	1.40	1.50
3	B	386	ATP	C3'-C4'	-2.63	1.46	1.53
4	B	387	LAR	O3-C13	2.52	1.50	1.44
3	B	386	ATP	O4'-C1'	2.50	1.47	1.42
3	B	386	ATP	PB-O1B	-2.49	1.42	1.50
3	A	376	ATP	PA-O3A	-2.44	1.56	1.59
4	A	377	LAR	C21-C3	2.36	1.56	1.50
4	B	387	LAR	C22-C10	2.29	1.61	1.53
4	A	377	LAR	C22-C10	2.23	1.61	1.53
4	A	377	LAR	O3-C13	2.19	1.49	1.44
3	B	386	ATP	PB-O2B	-2.14	1.45	1.55
3	A	376	ATP	PA-O1A	-2.13	1.43	1.50
4	B	387	LAR	C21-C3	2.12	1.55	1.50
3	A	376	ATP	C4-N9	-2.06	1.33	1.37
3	A	376	ATP	C8-N9	2.06	1.41	1.37
4	B	387	LAR	O2-C1	2.05	1.38	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	386	ATP	O5'-C5'-C4'	12.25	150.71	108.99
3	A	376	ATP	O5'-C5'-C4'	11.25	147.30	108.99
3	A	376	ATP	O3A-PB-O1B	-7.40	88.44	110.70
3	B	386	ATP	O3A-PB-O1B	-7.28	88.80	110.70
3	B	386	ATP	O5'-PA-O1A	-7.11	80.74	108.94
3	A	376	ATP	O5'-PA-O1A	-7.00	81.21	108.94
3	A	376	ATP	PA-O5'-C5'	6.09	156.26	121.35
3	B	386	ATP	PA-O5'-C5'	5.64	153.66	121.35
3	B	386	ATP	C5'-C4'-C3'	-5.08	96.93	115.21
4	A	377	LAR	C19-S1-C20	5.05	94.96	92.04
3	A	376	ATP	O2B-PB-O3B	4.84	120.36	107.27
3	B	386	ATP	O2B-PB-O3B	4.84	120.35	107.27
4	B	387	LAR	C19-S1-C20	4.81	94.83	92.04
3	A	376	ATP	C5'-C4'-C3'	-4.32	99.64	115.21
3	A	376	ATP	O2A-PA-O3A	4.23	118.71	107.27
3	B	386	ATP	O2A-PA-O3A	3.97	118.01	107.27
4	A	377	LAR	C3-C2-C1	3.83	136.50	127.36
3	B	386	ATP	O2B-PB-O3A	-3.60	97.55	107.27
4	B	387	LAR	C3-C2-C1	3.58	135.90	127.36
3	A	376	ATP	O2B-PB-O3A	-3.53	97.73	107.27
3	B	386	ATP	O4'-C4'-C3'	3.33	111.76	105.15
3	B	386	ATP	O3A-PA-O1A	3.01	119.75	110.70
3	A	376	ATP	O3A-PA-O1A	2.73	118.91	110.70
3	A	376	ATP	O4'-C4'-C3'	2.66	110.43	105.15
3	B	386	ATP	C6-C5-C4	-2.45	113.83	117.18
3	A	376	ATP	C6-C5-C4	-2.38	113.93	117.18
4	A	377	LAR	C21-C3-C2	-2.16	116.54	122.90
3	B	386	ATP	O2B-PB-O1B	2.11	122.28	112.44
3	A	376	ATP	O2B-PB-O1B	2.11	122.25	112.44
3	A	376	ATP	O2A-PA-O1A	2.08	122.11	112.44
3	A	376	ATP	C1'-N9-C8	2.06	131.67	127.09
3	B	386	ATP	O2A-PA-O1A	2.05	122.00	112.44
4	B	387	LAR	C21-C3-C2	-2.03	116.91	122.90
3	B	386	ATP	O3B-PB-O1B	2.01	116.76	110.70

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	387	LAR	O3-C17-C18-C19
3	A	376	ATP	PG-O3B-PB-O2B

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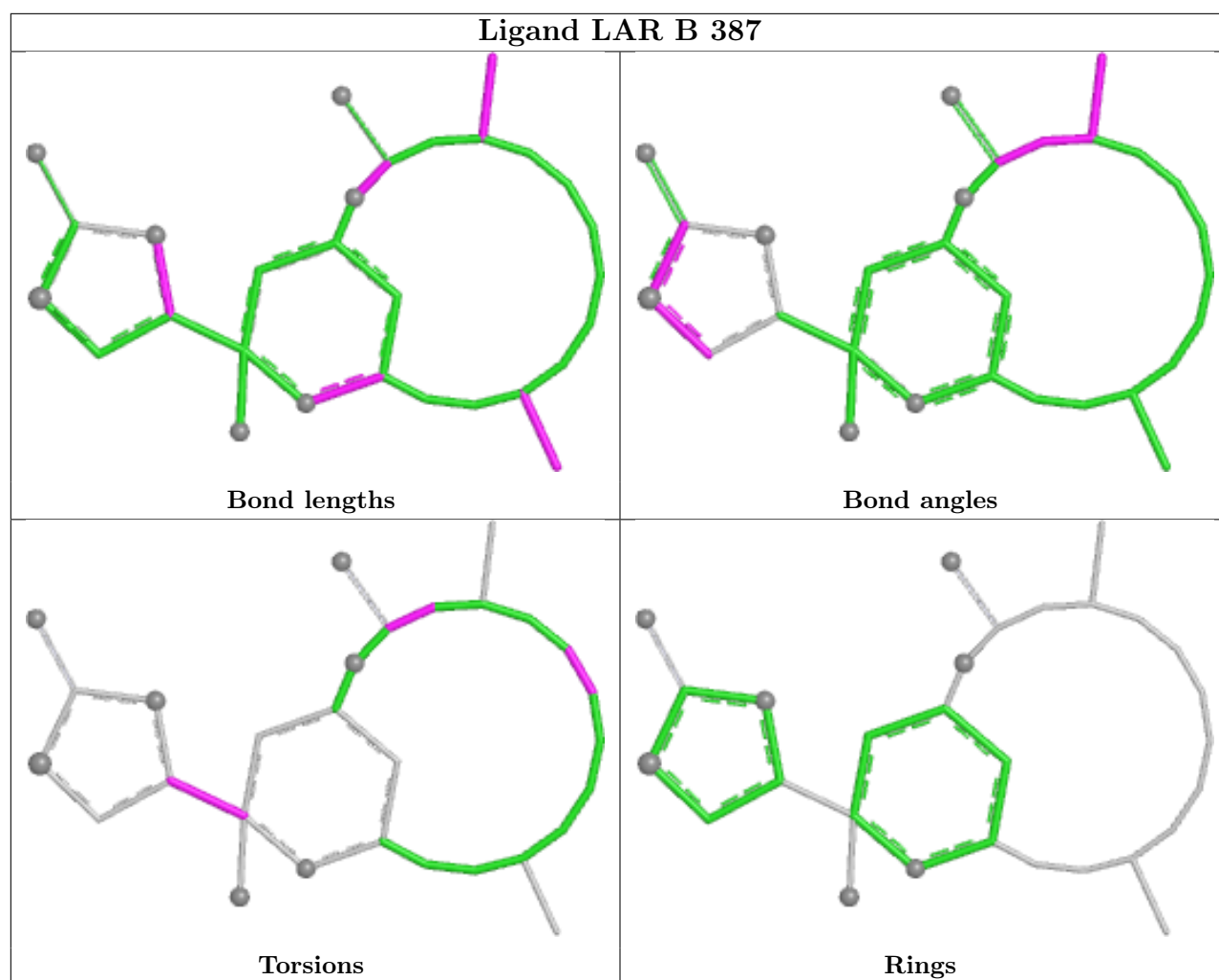
Mol	Chain	Res	Type	Atoms
3	B	386	ATP	PG-O3B-PB-O2B
4	B	387	LAR	O2-C1-C2-C3
3	B	386	ATP	PA-O3A-PB-O2B
4	B	387	LAR	O1-C1-C2-C3
3	A	376	ATP	PA-O3A-PB-O2B
4	A	377	LAR	O2-C1-C2-C3
4	A	377	LAR	C10-C11-C12-C13
4	A	377	LAR	C4-C5-C6-C7
4	B	387	LAR	C4-C5-C6-C7
3	B	386	ATP	PA-O3A-PB-O1B

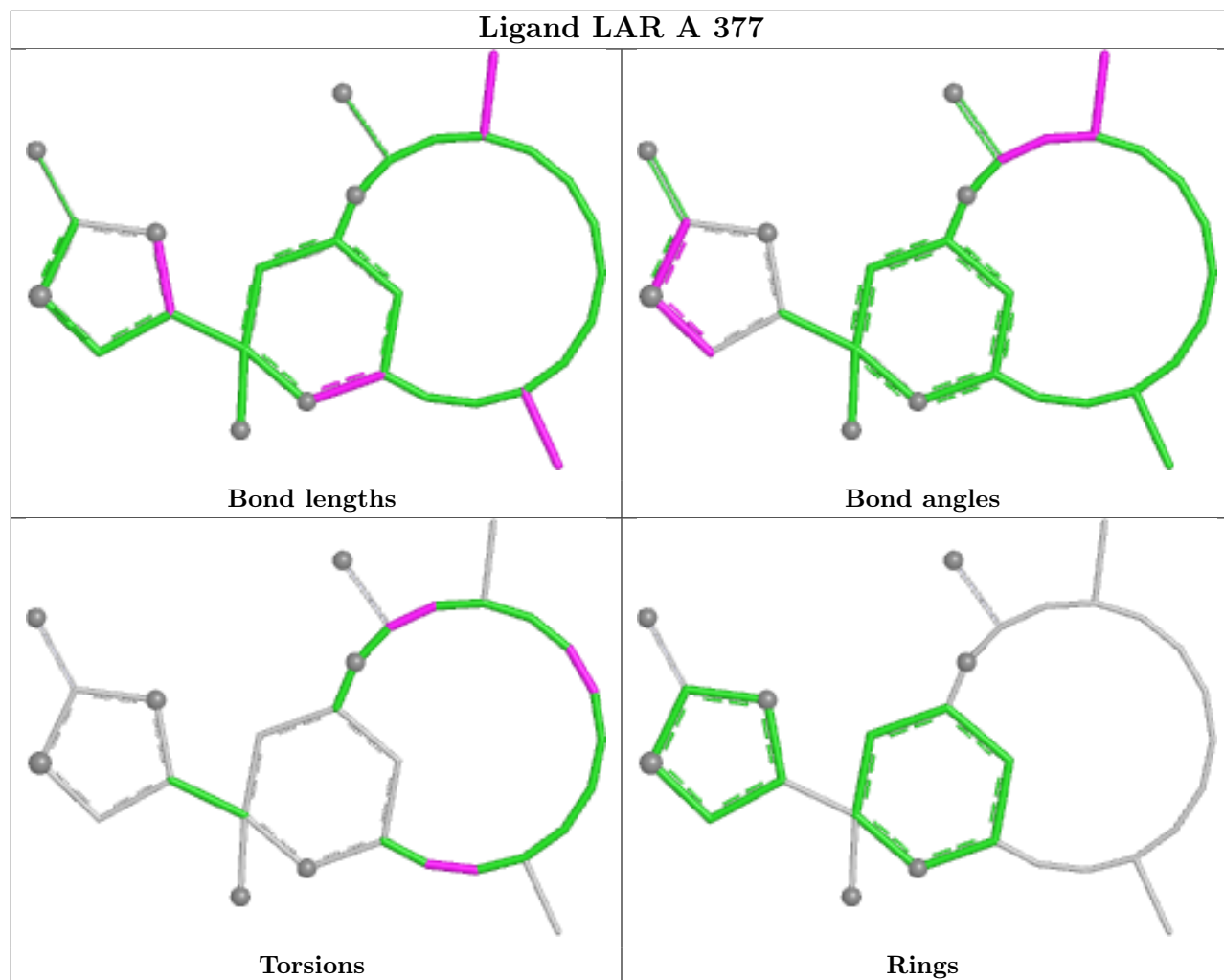
There are no ring outliers.

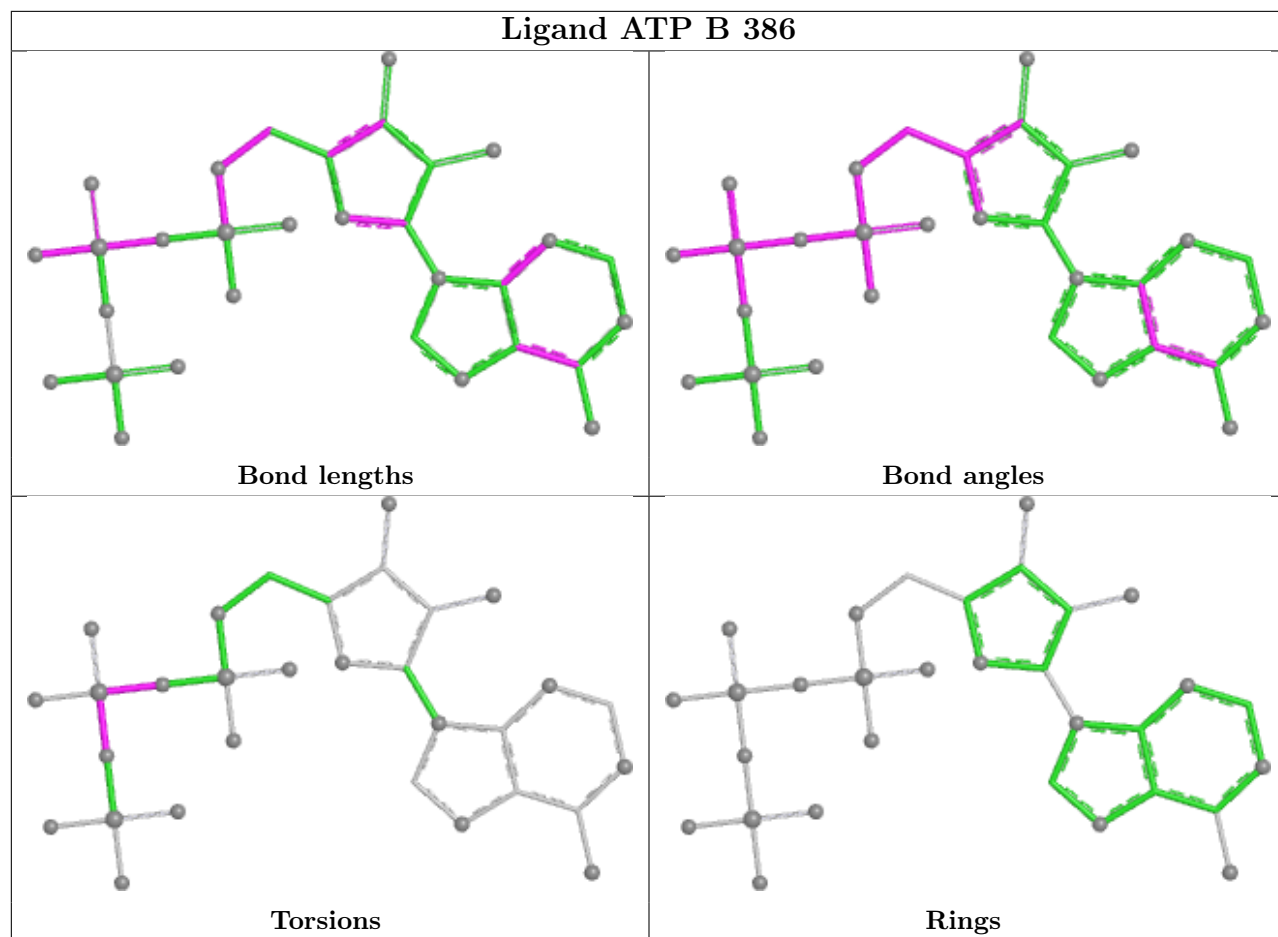
4 monomers are involved in 31 short contacts:

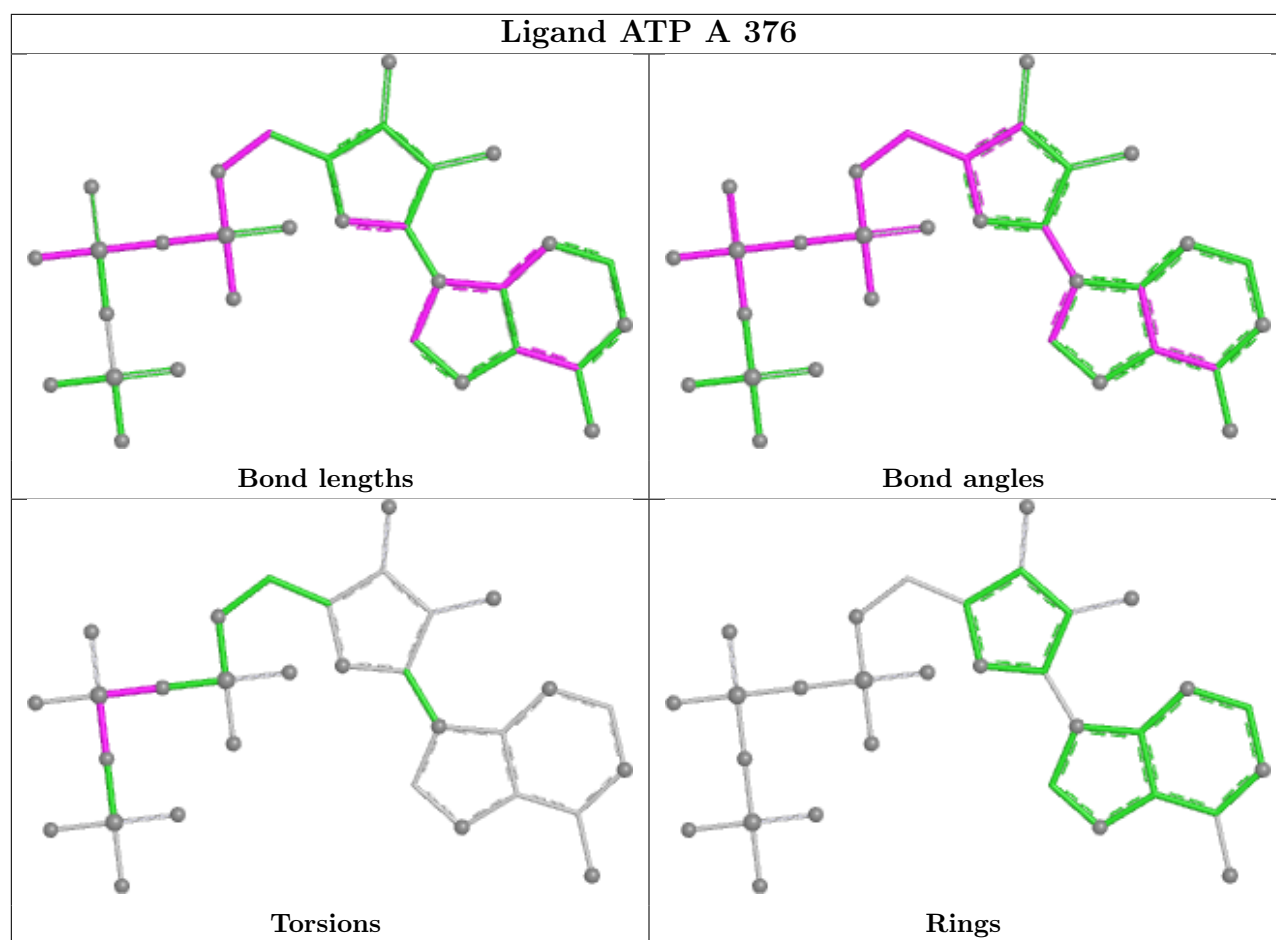
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	387	LAR	10	0
4	A	377	LAR	2	0
3	B	386	ATP	10	0
3	A	376	ATP	9	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	361/375 (96%)	-1.26	0 100 100	38, 57, 75, 82	0
1	B	361/375 (96%)	-1.12	0 100 100	42, 68, 83, 96	0
All	All	722/750 (96%)	-1.19	0 100 100	38, 63, 80, 96	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

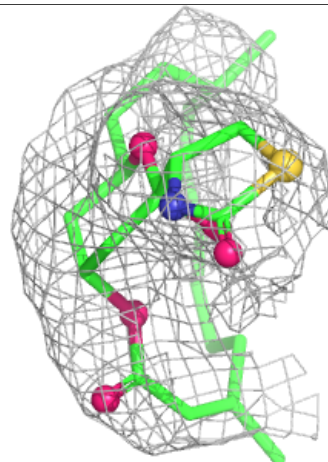
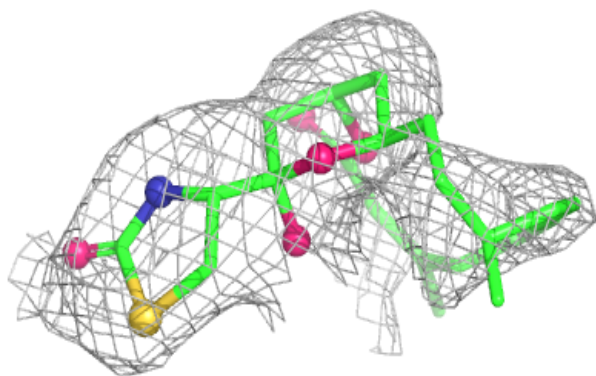
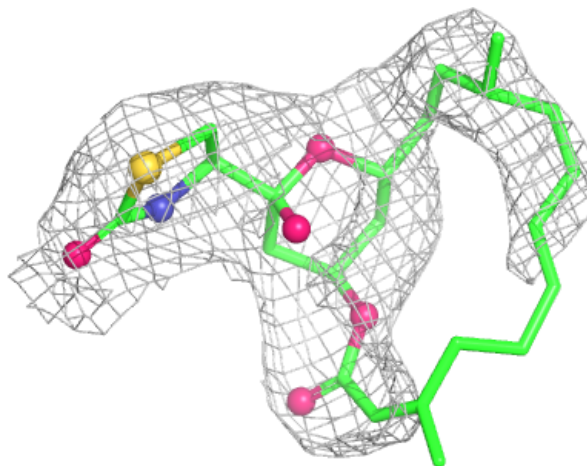
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LAR	B	387	29/29	0.98	0.07	66,71,78,78	0
2	MG	B	388	1/1	0.99	0.04	42,42,42,42	0
3	ATP	A	376	31/31	0.99	0.03	37,50,55,56	0
3	ATP	B	386	31/31	0.99	0.03	53,57,61,62	0
4	LAR	A	377	29/29	0.99	0.05	61,67,74,75	0
2	MG	A	378	1/1	0.99	0.05	36,36,36,36	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.

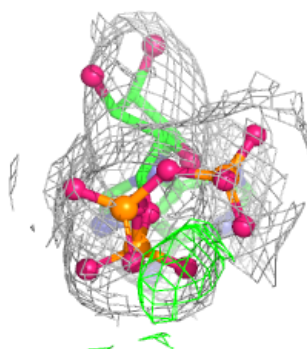
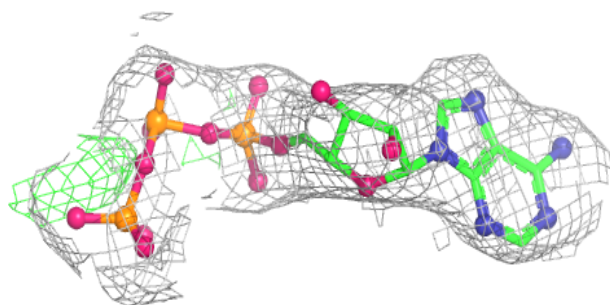
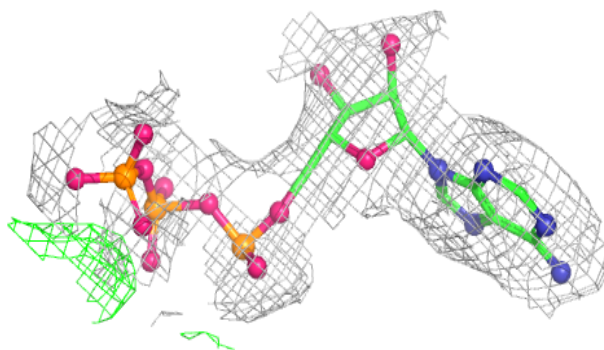
Electron density around LAR B 387:

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

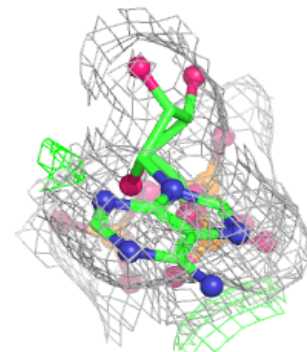
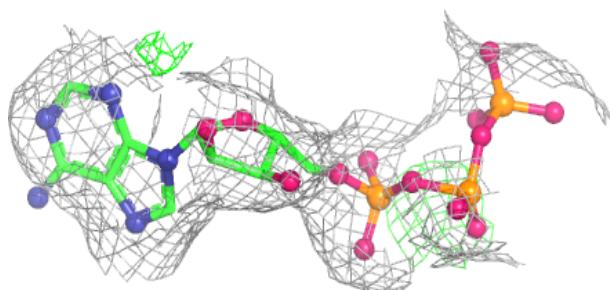
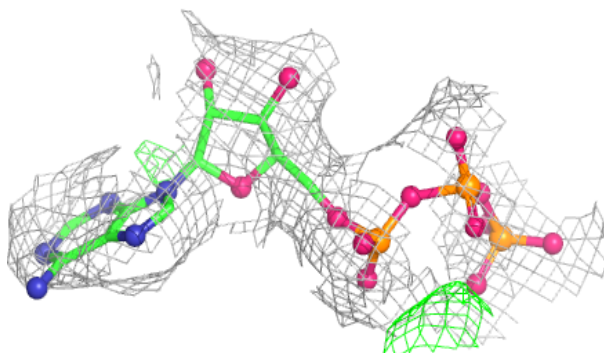


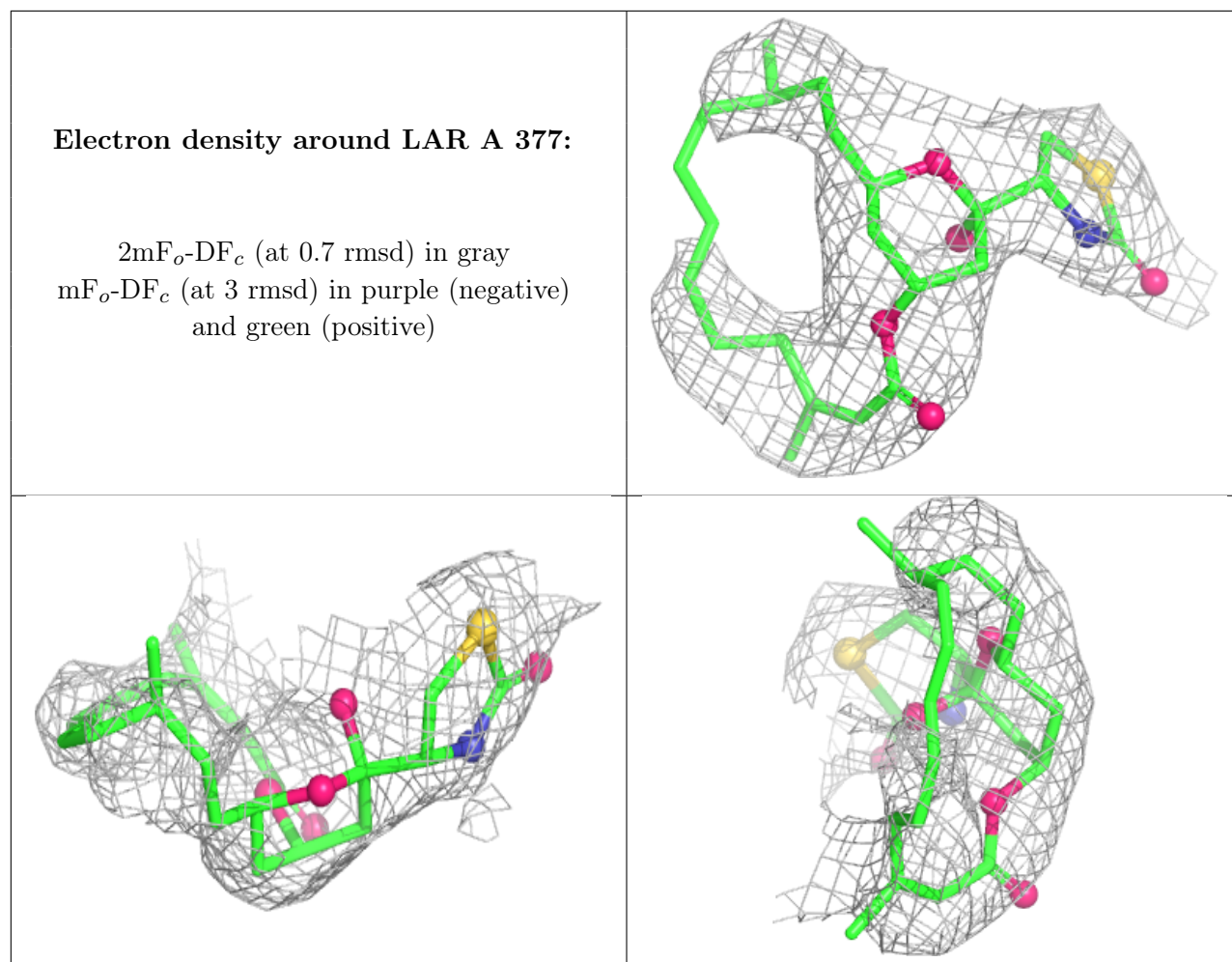
Electron density around ATP A 376:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.