



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:16 AM UTC

PDB ID : 2QUI / pdb_00002qui
Title : Crystal structures of human tryptophanyl-tRNA synthetase in complex with
Tryptophanamide and ATP
Authors : Shen, N.; Ding, J.P.
Deposited on : 2007-08-05
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

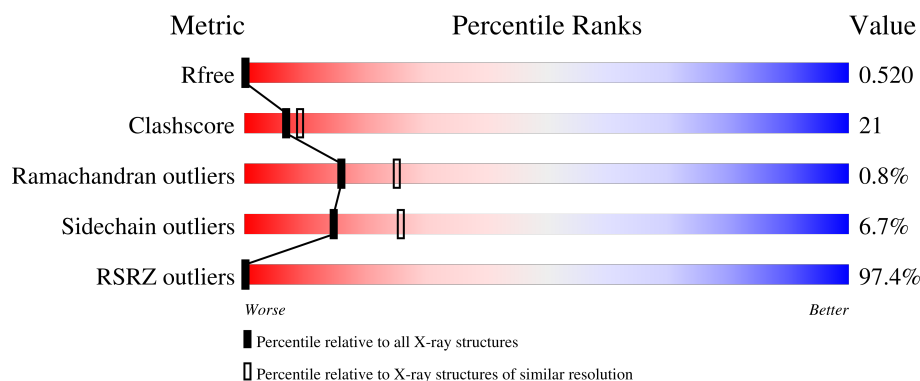
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	477	79% 19% 56% 7% 18%
1	B	477	78% 27% 46% 6% 21%

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	LTN	A	501	-	X	X	-
3	LTN	B	478	-	X	-	-
4	ATP	A	502	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6469 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3127	2005	525	582	15			
1	B	379	Total	C	N	O	S	0	0	0
			3054	1960	519	560	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	472	HIS	-	expression tag	UNP P23381
A	473	HIS	-	expression tag	UNP P23381
A	474	HIS	-	expression tag	UNP P23381
A	475	HIS	-	expression tag	UNP P23381
A	476	HIS	-	expression tag	UNP P23381
A	477	HIS	-	expression tag	UNP P23381
B	472	HIS	-	expression tag	UNP P23381
B	473	HIS	-	expression tag	UNP P23381
B	474	HIS	-	expression tag	UNP P23381
B	475	HIS	-	expression tag	UNP P23381
B	476	HIS	-	expression tag	UNP P23381
B	477	HIS	-	expression tag	UNP P23381

- 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		

- Molecule 3 is L-TRYPTOPHANAMIDE (CCD ID: LTN) (formula: C₁₁H₁₃N₃O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total 120	O 120	0	0
5	B	106	Total 106	O 106	0	0

T421	L361	T301	W241	K181	E121	ASP
S422	T362	D302	G242	W182	R122	CYS
G423	D363	I303	M243	L183	A123	PRO
A424	T364	Q304	S244	Q184	T124	PRO
N425	A365	C305	G245	D185	G125	GLY
L426	K366	L306	G246	V186	Q126	ASN
T427	Q367	I307	F247	F187	F127	PRO
G428	I368	F308	Y248	N188	P128	ALA
E429	K369	C309	K249	V189	H129	PRO
L430	T370	A310	N250	P190	H130	PRO
K431	K371	I311	V251	L191	F131	THR
K432	V372	D312	V252	V192	L132	ASN
N433	N373	Q313	K253	I193	R133	HIS
L434	K374	D314	I254	Q194	R134	GLY
L435	H375	F315	Q255	M195	G135	PRO
E436	A376	Y316	K256	T196	I136	ASP
V437	F377	R317	H257	D197	F137	ALA
L438	S378	R318	V258	D198	F138	THR
Q439	G379	M319	T259	E199	S139	GLU
P440	G380	T320	F260	K200	H140	ALA
L441	R381	R321	N261	Y201	R141	GLU
L442	D382	D322	Q262	L202	D142	GLU
A443	T383	V323	V263	M203	M143	ASP
E444	I384	A324	K264	K204	N144	PHE
H445	F385	P325	G265	D205	Q145	VAL
Q446	E386	R326	I266	L206	V146	ASP
A447	H387	I327	F267	T207	L147	PRO
R448	R388	G328	G268	L208	D148	TRP
R449	Q389	Y329	F269	D209	A149	THR
K450	F390	P330	T270	Q210	Y150	VAL
E451	G391	K331	D271	A211	E151	GLN
V452	G392	P332	S272	Y212	N152	THR
T453	N393	A333	D273	S213	K153	SER
D454	C394	L334	C274	Y214	K154	SER
E455	D395	L335	I275	A215	P155	ALA
L456	V396	H336	G276	V216	F156	ALA
V457	D397	S337	K277	E217	Y157	LYS
K458	V398	T338	I278	N218	L158	I98
E459	S399	F339	I279	A219	Y159	D99
F460	F400	P340	F280	K220	T160	Y100
M461	M401	A341	P281	D221	G161	D101
T462	Y402	A342	A282	I222	R162	K102
P463	L403	L343	I283	I223	G163	L103
R464	T404	Q344	Q284	A224	P164	L104
K465	F405	G345	A285	C225	S165	V105
L466	F406	A346	A286	G226	S166	F106
S467	L407	Q347	P287	F227	E167	F107
F468	E408	T348	S288	D228	A168	G108
D469	D409	K349	F289	I229	M169	S109
F470	D410	M350	S290	N230	H170	S110
Q471	D411	S351	N291	K231	V171	K111
H472	K412	A352	S292	T232	G172	I112
H473	L413	S353	F293	F233	H173	D113
H474	E414	D354	P294	I234	L174	K114
H475	Q415	P355	Q295	F235	I175	E115
HIS	T416	N356	I296	S236	P176	E116
HIS	R417	S357	F297	D237	F177	I117
HIS	K418	S358	R298	L238	I178	M118
HIS	D419	I359	D299	D239	F179	M119
HIS	Y420	F360	R300	Y240	T180	I120

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.70Å 79.70Å 383.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.40) 95.2 (50.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.238 0.508 , 0.520	Depositor DCC
R_{free} test set	2417 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.54 , 497.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.48	EDS
Total number of atoms	6469	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: LTN, ATP, MG

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	0.42	0/3204	0.95	11/4331 (0.3%)
1	B	0.44	0/3132	0.94	12/4230 (0.3%)
All	All	0.43	0/6336	0.95	23/8561 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	ARG	N-CA-C	-10.11	100.34	111.36
1	A	318	ARG	N-CA-C	-10.07	100.38	111.36
1	B	292	SER	N-CA-C	-8.50	102.91	113.28
1	B	375	HIS	N-CA-C	6.06	121.72	113.97
1	B	438	LEU	N-CA-C	5.98	117.59	111.14
1	B	186	VAL	N-CA-C	5.97	116.71	110.62
1	A	290	SER	N-CA-C	5.83	118.39	111.33
1	B	346	ALA	N-CA-C	-5.72	106.15	113.01
1	A	430	LEU	N-CA-C	-5.71	104.96	111.07
1	B	352	ALA	N-CA-C	-5.54	106.60	113.19
1	A	382	ASP	N-CA-C	5.50	117.28	111.28
1	B	340	PHE	N-CA-C	-5.44	102.80	109.65
1	A	137	PHE	N-CA-C	-5.40	97.70	107.75
1	A	292	SER	N-CA-C	-5.39	106.21	112.89
1	A	340	PHE	N-CA-C	-5.30	101.57	109.42
1	B	406	PHE	N-CA-C	5.26	121.43	114.12
1	A	358	SER	N-CA-C	5.20	117.59	109.52
1	B	293	PHE	CA-C-N	5.11	125.15	119.32
1	B	293	PHE	C-N-CA	5.11	125.15	119.32
1	B	196	THR	N-CA-C	5.06	118.54	110.70
1	A	189	VAL	N-CA-C	5.05	113.45	107.84
1	A	235	PHE	N-CA-C	5.05	117.47	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	PRO	N-CA-C	5.01	118.92	111.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3127	0	3049	131	2188
1	B	3054	0	2978	135	1612
2	A	1	0	0	0	0
3	A	15	0	11	1	7
3	B	15	0	11	1	0
4	A	31	0	12	10	77
5	A	120	0	0	8	109
5	B	106	0	0	4	88
All	All	6469	0	6061	261	3584

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 21.

All (261) 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:B:250:ASN:HD21	1:B:291:ASN:ND2	1.59	0.98
1:A:207:THR:HG22	1:A:210:GLN:H	1.35	0.90
1:A:165:SER:HB2	4:A:502:ATP:O3G	1.73	0.88
1:B:457:VAL:HG12	1:B:461:MET:HE2	1.56	0.88
1:A:250:ASN:HD21	1:A:291:ASN:ND2	1.73	0.87
1:A:344:GLN:HE22	1:A:357:SER:HA	1.40	0.87
1:A:98:ILE:HD11	1:A:103:LEU:HD22	1.61	0.83
1:B:398:VAL:HA	1:B:401:MET:HE3	1.62	0.82
1:B:250:ASN:HD21	1:B:291:ASN:HD21	1.27	0.80
1:A:227:PHE:HB3	1:A:232:THR:HG21	1.64	0.79
1:A:251:VAL:O	1:A:255:GLN:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:PHE:HE1	1:B:278:ILE:HD12	1.47	0.79
1:B:227:PHE:HB3	1:B:232:THR:HG21	1.65	0.78
1:A:352:ALA:C	1:A:354:ASP:H	1.91	0.78
1:A:250:ASN:HD21	1:A:291:ASN:HD21	1.30	0.78
1:B:409:ASP:OD2	1:B:412:LYS:HB2	1.85	0.77
1:B:293:PHE:HB3	1:B:296:ILE:HG23	1.65	0.77
1:B:129:HIS:HD2	1:B:131:PHE:H	1.30	0.77
1:A:141:ARG:HD2	1:A:334:LEU:HD12	1.65	0.76
1:A:92:THR:HG21	1:A:98:ILE:HA	1.67	0.76
1:B:372:VAL:HG12	1:B:431:LYS:HG3	1.66	0.76
1:B:293:PHE:HA	1:B:295:GLN:HE22	1.52	0.73
1:A:159:TYR:CZ	1:A:287:PRO:HG2	2.24	0.72
1:B:129:HIS:CD2	1:B:131:PHE:H	2.07	0.72
1:B:140:HIS:HD2	1:B:143:MET:H	1.35	0.72
1:B:455:GLU:CD	1:B:455:GLU:H	1.96	0.71
1:A:307:ILE:HB	1:A:334:LEU:HD23	1.72	0.71
1:B:159:TYR:CZ	1:B:287:PRO:HG2	2.25	0.71
1:B:228:ASP:O	1:B:232:THR:HG23	1.91	0.70
1:B:393:ASN:HD22	1:B:393:ASN:C	1.97	0.70
1:A:364:THR:OG1	1:A:367:GLN:HG3	1.92	0.70
1:A:137:PHE:CZ	1:A:337:SER:HB3	2.27	0.69
1:A:228:ASP:O	1:A:232:THR:HG23	1.92	0.69
1:A:427:THR:HG21	5:A:597:HOH:O	1.92	0.69
1:A:95:ALA:HA	1:A:347:GLN:HE21	1.56	0.69
1:A:253:LYS:O	1:A:257:HIS:HD2	1.78	0.66
1:A:376:ALA:HB3	1:A:431:LYS:HE2	1.78	0.66
1:B:324:ALA:HB3	1:B:325:PRO:HD3	1.77	0.66
1:B:169:MET:HE1	1:B:221:ASP:HB2	1.78	0.65
1:B:307:ILE:HB	1:B:334:LEU:HD23	1.79	0.65
1:A:164:PRO:HG2	5:A:619:HOH:O	1.96	0.65
1:A:258:VAL:HG11	1:A:319:MET:HE2	1.78	0.65
1:A:140:HIS:HD2	1:A:143:MET:H	1.45	0.65
1:A:271:ASP:HB3	1:B:261:ASN:ND2	2.12	0.64
1:B:137:PHE:CZ	1:B:337:SER:HB3	2.32	0.64
1:A:466:LEU:O	1:A:468:PHE:N	2.30	0.64
1:A:202:LEU:HA	1:B:256:LYS:HD3	1.80	0.64
1:B:140:HIS:CD2	1:B:143:MET:H	2.15	0.64
1:A:344:GLN:HE22	1:A:357:SER:CA	2.11	0.63
1:B:234:ILE:O	1:B:461:MET:HA	1.98	0.63
1:A:350:MET:HE2	1:A:358:SER:HA	1.79	0.63
1:B:253:LYS:O	1:B:257:HIS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ALA:HB3	1:B:431:LYS:HE2	1.81	0.62
1:B:259:THR:OG1	1:B:262:GLN:HG3	1.99	0.62
1:B:442:ILE:O	1:B:446:GLN:HG3	1.99	0.62
1:B:294:PRO:HD2	1:B:295:GLN:NE2	2.15	0.62
1:A:207:THR:CG2	1:A:210:GLN:H	2.11	0.61
1:A:207:THR:HG22	1:A:210:GLN:HG3	1.81	0.61
1:B:295:GLN:NE2	1:B:295:GLN:H	1.99	0.60
1:A:303:ILE:HD12	1:A:303:ILE:N	2.16	0.60
1:A:340:PHE:HB3	4:A:502:ATP:HN62	1.67	0.60
1:B:260:PHE:CE1	1:B:278:ILE:HD12	2.32	0.60
1:A:350:MET:HG3	1:A:358:SER:HB3	1.83	0.59
1:B:393:ASN:ND2	1:B:395:ASP:H	2.01	0.59
1:A:350:MET:CG	1:A:358:SER:HB3	2.32	0.59
1:B:359:ILE:HD12	1:B:359:ILE:N	2.18	0.59
1:A:372:VAL:HG12	1:A:431:LYS:HG3	1.85	0.58
1:A:86:ASP:HB2	1:A:87:PRO:HD2	1.85	0.58
1:B:350:MET:O	1:B:351:SER:HB2	2.04	0.58
1:B:124:THR:CG2	1:B:186:VAL:HG13	2.34	0.58
1:B:393:ASN:C	1:B:393:ASN:ND2	2.62	0.57
1:A:139:SER:HB3	1:A:336:HIS:HB2	1.86	0.57
1:B:174:LEU:HD11	1:B:361:LEU:HD11	1.86	0.57
1:B:311:ILE:HG23	1:B:336:HIS:HB3	1.86	0.57
1:B:281:PRO:CB	1:B:319:MET:HE1	2.34	0.57
1:A:259:THR:HG23	1:A:262:GLN:HE21	1.69	0.57
1:B:170:HIS:HD2	1:B:172:GLY:H	1.53	0.56
1:B:294:PRO:HD2	1:B:295:GLN:HE21	1.70	0.56
1:A:341:PRO:HA	5:A:551:HOH:O	2.05	0.55
1:B:398:VAL:CA	1:B:401:MET:HE3	2.33	0.55
1:B:121:GLU:HG3	1:B:126:GLN:O	2.06	0.55
1:B:169:MET:CE	1:B:218:ASN:HA	2.37	0.55
1:A:90:VAL:HG21	1:A:349:LYS:HD3	1.89	0.54
1:A:162:ARG:O	1:A:164:PRO:HD3	2.08	0.54
1:A:352:ALA:C	1:A:354:ASP:N	2.60	0.54
1:A:442:ILE:O	1:A:446:GLN:HG3	2.06	0.54
1:B:124:THR:HG21	1:B:186:VAL:CG1	2.37	0.54
1:B:169:MET:HE2	1:B:218:ASN:HA	1.90	0.54
1:A:207:THR:HG23	1:A:209:ASP:H	1.74	0.53
1:B:199:GLU:HB2	1:B:280:PHE:CE1	2.43	0.53
1:A:366:LYS:HB2	5:A:546:HOH:O	2.08	0.53
1:B:293:PHE:HB3	1:B:296:ILE:CG2	2.35	0.53
1:A:98:ILE:CD1	1:A:103:LEU:HD22	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:HB3	4:A:502:ATP:HN61	1.74	0.52
1:A:453:THR:O	1:A:457:VAL:HG23	2.08	0.52
1:B:171:VAL:HG22	1:B:406:PHE:CZ	2.44	0.52
1:A:401:MET:O	1:A:404:THR:HB	2.09	0.52
1:B:221:ASP:OD2	1:B:445:HIS:HE1	1.92	0.52
1:B:259:THR:H	1:B:262:GLN:NE2	2.08	0.52
1:B:139:SER:HB3	1:B:336:HIS:HB2	1.92	0.52
1:A:95:ALA:HA	1:A:347:GLN:NE2	2.24	0.52
1:B:251:VAL:O	1:B:255:GLN:HG3	2.09	0.52
1:B:343:LEU:HG	1:B:358:SER:HA	1.91	0.52
1:B:219:ALA:O	1:B:223:ILE:HG13	2.10	0.52
1:B:393:ASN:HD22	1:B:394:CYS:N	2.07	0.52
1:B:340:PHE:O	1:B:350:MET:HE2	2.10	0.51
1:A:136:ILE:HD11	1:A:404:THR:HG22	1.91	0.51
1:A:259:THR:H	1:A:262:GLN:NE2	2.09	0.51
1:A:234:ILE:O	1:A:461:MET:HA	2.10	0.51
1:B:170:HIS:HD2	1:B:172:GLY:N	2.08	0.51
1:A:228:ASP:O	1:A:232:THR:CG2	2.59	0.51
1:A:349:LYS:HA	5:A:551:HOH:O	2.11	0.51
1:A:90:VAL:HG21	1:A:339:PHE:CE1	2.45	0.50
4:A:502:ATP:H5'1	5:A:622:HOH:O	2.12	0.50
1:A:170:HIS:HD2	1:A:172:GLY:N	2.10	0.50
1:A:192:VAL:HG13	1:A:235:PHE:HE1	1.77	0.50
1:A:303:ILE:HD12	1:A:303:ILE:H	1.76	0.50
1:B:260:PHE:CE2	1:B:264:LYS:HD2	2.47	0.50
1:A:393:ASN:ND2	1:A:395:ASP:H	2.10	0.50
1:A:441:LEU:C	1:A:441:LEU:HD23	2.37	0.50
3:A:501:LTN:N	4:A:502:ATP:H4'	2.27	0.49
1:A:350:MET:HB3	4:A:502:ATP:N6	2.27	0.49
1:A:344:GLN:NE2	1:A:357:SER:HB2	2.26	0.49
1:A:87:PRO:HG3	1:A:315:PRO:HG2	1.94	0.49
1:A:393:ASN:C	1:A:393:ASN:HD22	2.19	0.49
1:A:452:VAL:O	1:A:452:VAL:CG2	2.60	0.49
1:B:355:PRO:HA	1:B:360:PHE:CE2	2.47	0.49
1:A:86:ASP:HB2	1:A:87:PRO:CD	2.43	0.49
1:B:364:THR:OG1	1:B:367:GLN:HG3	2.13	0.49
1:B:354:ASP:OD2	1:B:357:SER:HB2	2.13	0.49
1:A:92:THR:HG21	1:A:98:ILE:CA	2.38	0.49
1:A:259:THR:HA	1:B:274:CYS:HA	1.93	0.49
1:B:296:ILE:HD12	1:B:296:ILE:O	2.13	0.49
1:B:139:SER:OG	1:B:336:HIS:HD2	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:HB	1:A:199:GLU:HB2	1.94	0.48
1:B:342:ALA:HA	1:B:350:MET:HG2	1.94	0.48
1:B:369:LYS:HA	1:B:435:ILE:HD13	1.94	0.48
1:B:267:PHE:HE1	1:B:319:MET:HE3	1.77	0.48
1:B:358:SER:HB3	5:B:480:HOH:O	2.13	0.48
1:B:102:LYS:O	1:B:105:VAL:HG12	2.14	0.48
1:B:124:THR:HG21	1:B:186:VAL:HG13	1.96	0.48
1:B:464:ARG:NH1	5:B:509:HOH:O	2.46	0.48
1:A:86:ASP:OD2	1:A:86:ASP:N	2.46	0.48
1:B:281:PRO:HB2	1:B:319:MET:HE1	1.95	0.48
1:B:250:ASN:ND2	1:B:291:ASN:HD21	2.03	0.47
1:A:221:ASP:OD1	1:A:445:HIS:HE1	1.97	0.47
1:A:324:ALA:N	1:A:325:PRO:HD2	2.29	0.47
1:B:455:GLU:CD	1:B:455:GLU:N	2.70	0.47
1:A:87:PRO:HG2	1:A:267:PHE:HD2	1.80	0.47
1:B:344:GLN:CD	1:B:344:GLN:H	2.23	0.47
1:A:198:ASP:O	1:A:202:LEU:HD22	2.14	0.47
1:A:100:TYR:O	1:A:104:ILE:HG13	2.14	0.47
1:B:351:SER:C	1:B:353:SER:H	2.23	0.46
1:A:87:PRO:HD3	1:A:315:PRO:HG3	1.98	0.46
1:A:312:ASP:OD2	4:A:502:ATP:O2'	2.31	0.46
1:B:441:LEU:HD22	1:B:442:ILE:HD12	1.97	0.46
1:A:137:PHE:CE2	1:A:337:SER:HB3	2.51	0.46
1:A:144:ASN:HB3	5:A:506:HOH:O	2.15	0.46
1:A:207:THR:CG2	1:A:210:GLN:HG3	2.46	0.46
1:B:255:GLN:HE21	1:B:279:SER:HB2	1.80	0.46
1:B:448:ARG:HA	1:B:451:GLU:OE2	2.16	0.46
1:A:141:ARG:HB2	1:A:334:LEU:HB2	1.96	0.46
1:A:344:GLN:NE2	1:A:357:SER:CB	2.79	0.45
1:B:330:PRO:HD2	5:B:515:HOH:O	2.16	0.45
1:B:391:GLY:HA3	1:B:421:THR:O	2.16	0.45
1:B:384:ILE:O	1:B:388:ARG:HG2	2.16	0.45
1:B:384:ILE:HG13	5:B:567:HOH:O	2.17	0.45
1:B:170:HIS:CD2	1:B:172:GLY:H	2.34	0.45
1:B:292:SER:C	1:B:294:PRO:HD3	2.41	0.45
1:A:294:PRO:HG2	1:A:295:GLN:NE2	2.31	0.45
1:B:174:LEU:CD1	1:B:361:LEU:HD11	2.45	0.45
1:B:293:PHE:N	1:B:294:PRO:HD3	2.31	0.45
1:B:394:CYS:HB3	1:B:400:PHE:CD2	2.51	0.45
1:A:233:PHE:CZ	1:A:235:PHE:HB3	2.52	0.45
1:B:393:ASN:HD21	1:B:395:ASP:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:THR:HG23	1:A:209:ASP:N	2.30	0.45
1:A:352:ALA:O	1:A:354:ASP:N	2.49	0.45
1:B:250:ASN:ND2	1:B:291:ASN:ND2	2.44	0.45
1:B:281:PRO:HB3	1:B:319:MET:HE1	1.97	0.45
1:A:260:PHE:HA	1:A:263:VAL:HG22	1.99	0.44
1:B:453:THR:OG1	1:B:455:GLU:HG2	2.18	0.44
1:A:274:CYS:HA	1:B:259:THR:HA	1.99	0.44
1:B:199:GLU:HB2	1:B:280:PHE:CZ	2.53	0.44
1:B:295:GLN:H	1:B:295:GLN:CD	2.23	0.44
1:B:141:ARG:HD2	1:B:334:LEU:HD12	1.99	0.44
1:B:453:THR:H	1:B:456:ILE:HD12	1.83	0.44
1:A:100:TYR:HB3	1:A:138:PHE:CE2	2.52	0.44
1:A:126:GLN:HG2	5:A:514:HOH:O	2.17	0.44
1:A:466:LEU:O	1:A:467:SER:C	2.61	0.44
1:A:311:ILE:HD13	1:A:311:ILE:O	2.17	0.44
1:A:140:HIS:CD2	1:A:143:MET:H	2.29	0.44
1:A:344:GLN:H	1:A:344:GLN:CD	2.25	0.44
1:B:359:ILE:N	1:B:359:ILE:CD1	2.81	0.44
1:A:200:LYS:HD3	1:A:200:LYS:HA	1.77	0.43
1:A:275:ILE:HG22	1:B:278:ILE:HG22	2.00	0.43
1:A:159:TYR:CD1	1:A:159:TYR:C	2.94	0.43
1:A:347:GLN:CD	1:A:347:GLN:H	2.26	0.43
1:B:124:THR:HB	1:B:186:VAL:HG13	1.99	0.43
1:B:169:MET:CE	1:B:221:ASP:HB2	2.47	0.43
1:B:298:ARG:HD2	1:B:470:PHE:O	2.18	0.43
1:A:141:ARG:NH1	1:A:314:ASP:OD2	2.51	0.43
1:A:348:THR:HG22	1:A:349:LYS:N	2.33	0.43
1:A:420:TYR:HE1	1:A:427:THR:HA	1.83	0.43
1:B:294:PRO:CD	1:B:295:GLN:NE2	2.82	0.43
1:B:453:THR:OG1	1:B:456:ILE:HG13	2.18	0.43
1:B:159:TYR:CD1	1:B:159:TYR:C	2.97	0.43
1:A:92:THR:HG22	1:A:93:SER:N	2.34	0.43
1:B:100:TYR:O	1:B:104:ILE:HG13	2.19	0.43
1:B:344:GLN:CD	1:B:344:GLN:N	2.77	0.43
1:A:159:TYR:O	1:A:307:ILE:HG23	2.19	0.43
1:B:441:LEU:HD23	1:B:441:LEU:C	2.45	0.42
1:A:129:HIS:HB2	1:A:182:TRP:CD2	2.54	0.42
1:B:169:MET:HE2	1:B:218:ASN:ND2	2.34	0.42
1:B:175:ILE:HB	1:B:176:PRO:CD	2.49	0.42
1:B:229:ILE:HD11	1:B:459:GLU:HB3	2.00	0.42
1:A:83:ASP:OD2	1:A:99:ASP:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ASN:ND2	1:A:393:ASN:C	2.76	0.42
1:B:159:TYR:CZ	3:B:478:LTN:HZ2	2.55	0.42
1:B:323:VAL:HG12	1:B:326:ARG:NH2	2.34	0.42
1:B:373:ASN:HD22	1:B:431:LYS:HG2	1.83	0.42
1:B:441:LEU:CD2	1:B:442:ILE:HD12	2.48	0.42
1:A:139:SER:OG	1:A:336:HIS:HD2	2.03	0.42
1:B:130:HIS:HB3	1:B:133:ARG:NH2	2.35	0.42
1:A:259:THR:OG1	1:A:262:GLN:HG3	2.20	0.42
1:A:348:THR:HG22	1:A:349:LYS:O	2.20	0.42
1:B:159:TYR:CE2	1:B:287:PRO:HG2	2.54	0.42
1:B:396:VAL:C	1:B:401:MET:HE2	2.44	0.42
1:A:196:THR:HB	1:A:199:GLU:CB	2.49	0.42
1:A:291:ASN:C	1:A:291:ASN:HD22	2.28	0.42
1:B:348:THR:OG1	1:B:349:LYS:N	2.53	0.42
1:B:126:GLN:HG3	1:B:186:VAL:HG22	2.01	0.42
1:A:137:PHE:CE1	1:A:337:SER:HB3	2.54	0.42
1:A:191:LEU:HD21	1:A:193:ILE:HD11	2.01	0.41
1:A:334:LEU:HD13	1:A:336:HIS:HE1	1.85	0.41
1:A:271:ASP:HB3	1:B:261:ASN:HD21	1.85	0.41
1:A:162:ARG:NH1	4:A:502:ATP:O1G	2.50	0.41
1:A:344:GLN:HE21	1:A:357:SER:HB2	1.85	0.41
1:B:186:VAL:HG12	1:B:187:PHE:CD1	2.55	0.41
1:A:198:ASP:OD2	1:A:237:ASP:HB3	2.19	0.41
1:B:221:ASP:CG	1:B:449:ARG:HE	2.28	0.41
1:A:240:TYR:CZ	1:A:244:SER:HB2	2.56	0.41
1:A:340:PHE:HB3	4:A:502:ATP:N6	2.34	0.41
1:B:182:TRP:CZ2	1:B:186:VAL:HG21	2.55	0.41
1:B:280:PHE:N	1:B:281:PRO:CD	2.83	0.41
1:B:417:ARG:HH11	1:B:417:ARG:HG2	1.86	0.41
1:A:278:ILE:CD1	1:B:260:PHE:HB2	2.50	0.41
1:A:344:GLN:CD	1:A:344:GLN:N	2.79	0.41
1:A:369:LYS:HG3	1:A:435:ILE:HD13	2.03	0.41
1:B:230:ASN:HB3	1:B:467:SER:OG	2.20	0.41
1:B:259:THR:HG23	1:B:262:GLN:HE21	1.84	0.41
1:A:136:ILE:HD13	1:A:405:PHE:CD2	2.56	0.41
1:A:173:HIS:CE1	4:A:502:ATP:O2G	2.74	0.41
1:A:189:VAL:HB	1:A:190:PRO:HD2	2.02	0.41
1:A:156:PHE:HB2	1:A:304:GLN:HB3	2.03	0.40
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.95	0.40
1:A:409:ASP:CG	1:A:412:LYS:HB2	2.47	0.40
1:B:301:THR:O	1:B:301:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:NE2	1:A:357:SER:HA	2.22	0.40
1:B:162:ARG:O	1:B:164:PRO:HD3	2.21	0.40
1:B:229:ILE:HA	1:B:460:PHE:CE1	2.57	0.40
1:B:129:HIS:HB2	1:B:182:TRP:CD2	2.56	0.40

All (3584) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ARG:N	1:A:442:ILE:CG2[3_365]	0.14	2.06
1:A:322:ASP:N	1:A:443:ALA:O[3_365]	0.19	2.01
1:A:138:PHE:CA	1:A:431:LYS:CG[3_365]	0.20	2.00
1:A:140:HIS:O	1:A:435:ILE:C[3_365]	0.20	2.00
1:A:164:PRO:O	1:A:273:ASP:CG[4_435]	0.20	2.00
1:B:430:LEU:CD1	1:B:432:LYS:NZ[2_355]	0.20	2.00
1:B:381:ARG:CG	1:B:404:THR:C[4_445]	0.25	1.95
1:A:322:ASP:O	1:A:447:ALA:CB[3_365]	0.26	1.94
1:A:302:ASP:OD2	1:A:303:ILE:CA[2_345]	0.27	1.93
1:A:328:GLY:CA	1:A:469:ASP:CA[2_345]	0.27	1.93
1:A:457:VAL:CG2	1:B:273:ASP:C[4_435]	0.28	1.92
1:B:372:VAL:CG1	1:B:431:LYS:CE[3_465]	0.28	1.92
1:B:430:LEU:CA	1:B:433:ALA:N[4_445]	0.28	1.92
1:A:339:PHE:CE2	1:A:343:LEU:N[3_365]	0.31	1.89
1:A:84:PHE:CE2	1:A:356:ASN:ND2[2_245]	0.34	1.86
1:A:103:LEU:N	1:A:402:TYR:N[3_365]	0.34	1.86
1:A:328:GLY:C	1:A:469:ASP:C[2_345]	0.36	1.84
1:A:327:ILE:C	1:A:469:ASP:CG[2_345]	0.37	1.83
1:A:84:PHE:CZ	4:A:502:ATP:C5[3_365]	0.38	1.82
1:B:105:VAL:CG1	1:B:465:LYS:CG[3_365]	0.38	1.82
1:B:380:GLY:N	5:B:537:HOH:O[2_355]	0.38	1.82
1:B:426:LEU:N	1:B:436:GLU:CD[2_355]	0.38	1.82
1:A:89:THR:N	1:A:351:SER:C[3_365]	0.39	1.81
1:B:430:LEU:N	1:B:432:LYS:CB[2_355]	0.39	1.81
1:A:110:SER:CA	1:A:433:ALA:O[3_365]	0.40	1.80
1:A:84:PHE:CD1	4:A:502:ATP:N1[3_365]	0.42	1.78
1:A:218:ASN:ND2	1:A:269:PHE:CD2[4_435]	0.42	1.78
1:A:328:GLY:N	1:A:469:ASP:CB[2_345]	0.42	1.78
1:B:98:ILE:CG2	5:B:513:HOH:O[4_445]	0.42	1.78
1:B:375:HIS:CG	1:B:375:HIS:CD2[4_445]	0.42	1.78
1:A:114:LYS:N	1:A:429:GLU:CG[3_365]	0.43	1.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ILE:O	1:A:359:ILE:CG1[3_365]	0.44	1.76
1:A:85:VAL:CG2	1:A:341:PRO:O[3_365]	0.45	1.75
1:A:454:ASP:CB	1:B:277:LYS:CD[4_435]	0.46	1.74
1:A:457:VAL:CA	1:B:273:ASP:N[4_435]	0.46	1.74
1:B:99:ASP:CG	1:B:448:ARG:O[4_445]	0.46	1.74
1:B:365:ALA:O	1:B:402:TYR:CD1[3_465]	0.46	1.74
1:A:101:ASP:CA	1:A:400:PHE:CA[3_365]	0.47	1.73
1:A:218:ASN:OD1	1:A:269:PHE:CB[4_435]	0.48	1.72
1:A:356:ASN:N	4:A:502:ATP:C2'[4_435]	0.48	1.72
1:B:372:VAL:C	1:B:373:ASN:N[4_445]	0.48	1.72
1:B:401:MET:N	1:B:439:GLN:CB[4_445]	0.48	1.72
1:A:321:ARG:CB	1:A:443:ALA:CB[3_365]	0.50	1.70
1:B:426:LEU:CA	1:B:436:GLU:CG[2_355]	0.51	1.69
1:A:105:VAL:CB	1:A:403:LEU:C[3_365]	0.53	1.67
1:A:83:ASP:CB	1:A:341:PRO:CG[3_365]	0.54	1.66
1:A:89:THR:OG1	1:A:351:SER:OG[3_365]	0.54	1.66
1:A:100:TYR:CA	1:A:398:VAL:C[3_365]	0.54	1.66
1:A:111:LYS:CE	1:A:430:LEU:CB[3_365]	0.54	1.66
1:A:266:ILE:CG2	1:A:361:LEU:CD1[3_365]	0.54	1.66
1:A:94:SER:N	1:A:94:SER:O[3_365]	0.55	1.65
1:A:140:HIS:CA	1:A:435:ILE:CB[3_365]	0.55	1.65
1:B:373:ASN:N	1:B:373:ASN:CA[4_445]	0.55	1.65
1:B:429:GLU:N	1:B:430:LEU:CA[4_445]	0.55	1.65
1:A:312:ASP:CB	1:A:358:SER:CA[3_365]	0.56	1.64
1:B:359:ILE:CG1	1:B:377:PHE:CB[3_465]	0.56	1.64
1:A:84:PHE:C	1:A:340:PHE:O[3_365]	0.57	1.63
1:A:89:THR:O	1:A:351:SER:N[3_365]	0.57	1.63
1:A:101:ASP:CB	1:A:400:PHE:CB[3_365]	0.57	1.63
1:A:257:HIS:O	1:A:450:LYS:N[3_365]	0.57	1.63
1:A:338:THR:CG2	1:A:376:ALA:C[3_365]	0.57	1.63
1:B:395:ASP:CA	1:B:441:LEU:CA[4_445]	0.57	1.63
1:A:307:ILE:C	1:A:366:LYS:C[3_365]	0.58	1.62
1:A:313:GLN:CG	1:A:371:LYS:NZ[3_365]	0.58	1.62
1:B:102:LYS:CB	1:B:451:GLU:C[4_445]	0.58	1.62
1:B:387:HIS:C	1:B:413:LEU:CD2[4_445]	0.59	1.61
1:A:318:ARG:O	1:A:442:ILE:O[3_365]	0.60	1.60
1:A:82:GLU:OE2	1:A:100:TYR:CE2[3_365]	0.61	1.59
1:A:92:THR:CG2	1:A:346:ALA:CA[3_365]	0.61	1.59
1:A:138:PHE:O	1:A:431:LYS:CA[3_365]	0.61	1.59
1:A:171:VAL:CG1	1:A:318:ARG:NH2[4_435]	0.61	1.59
1:B:395:ASP:O	1:B:441:LEU:C[4_445]	0.61	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ASP:O	1:B:422:SER:O[3_465]	0.61	1.59
1:A:162:ARG:NE	1:A:269:PHE:N[4_435]	0.62	1.58
1:A:209:ASP:C	1:B:258:VAL:C[4_435]	0.62	1.58
1:A:308:PRO:CB	1:A:370:THR:OG1[3_365]	0.62	1.58
1:B:407:LEU:CG	1:B:420:TYR:O[3_465]	0.62	1.58
1:B:141:ARG:CG	1:B:472:HIS:CA[3_365]	0.63	1.57
1:A:317:PHE:CG	1:A:363:ASP:C[3_365]	0.64	1.56
1:A:320:THR:N	1:A:446:GLN:CG[3_365]	0.64	1.56
1:A:210:GLN:C	1:A:274:CYS:CA[4_435]	0.65	1.55
1:A:355:PRO:CG	4:A:502:ATP:C5'[4_435]	0.65	1.55
1:B:389:GLN:O	1:B:410:ASP:OD1[4_445]	0.65	1.55
1:A:110:SER:C	1:A:433:ALA:C[3_365]	0.66	1.54
1:A:302:ASP:CB	1:A:303:ILE:CG1[2_345]	0.66	1.54
1:B:109:SER:C	1:B:470:PHE:C[3_365]	0.66	1.54
1:B:366:LYS:C	1:B:402:TYR:CZ[3_465]	0.66	1.54
1:B:372:VAL:O	1:B:373:ASN:CA[2_355]	0.66	1.54
1:B:372:VAL:CA	1:B:373:ASN:O[2_355]	0.66	1.54
1:A:82:GLU:O	1:A:344:GLN:O[2_245]	0.67	1.53
1:A:94:SER:C	1:A:95:ALA:N[3_365]	0.67	1.53
1:A:101:ASP:C	1:A:400:PHE:C[3_365]	0.67	1.53
1:A:141:ARG:NE	1:A:438:LEU:C[3_365]	0.67	1.53
1:A:335:LEU:C	1:A:369:LYS:C[3_365]	0.67	1.53
1:B:104:ILE:CA	1:B:298:ARG:NH2[3_365]	0.67	1.53
1:B:371:LYS:O	1:B:374:LYS:CA[2_355]	0.67	1.53
1:B:380:GLY:C	1:B:402:TYR:O[4_445]	0.67	1.53
1:B:429:GLU:N	1:B:433:ALA:N[2_355]	0.67	1.53
1:B:430:LEU:O	1:B:432:LYS:CA[4_445]	0.67	1.53
1:A:219:ALA:C	1:A:260:PHE:C[4_435]	0.68	1.52
1:A:220:LYS:CE	1:B:275:ILE:N[4_435]	0.68	1.52
1:B:321:ARG:NE	1:B:472:HIS:CE1[3_365]	0.68	1.52
1:B:375:HIS:ND1	1:B:375:HIS:NE2[2_355]	0.68	1.52
1:B:381:ARG:C	1:B:401:MET:O[4_445]	0.68	1.52
1:B:455:GLU:CD	1:B:464:ARG:N[2_345]	0.68	1.52
1:A:89:THR:CB	1:A:351:SER:CB[3_365]	0.69	1.51
1:A:107:PHE:N	1:A:406:PHE:CD2[3_365]	0.69	1.51
1:A:209:ASP:C	1:B:258:VAL:O[4_435]	0.69	1.51
1:B:366:LYS:CD	1:B:377:PHE:CZ[2_355]	0.69	1.51
1:B:375:HIS:CE1	1:B:375:HIS:NE2[2_355]	0.69	1.51
1:B:388:ARG:NH2	1:B:417:ARG:N[4_445]	0.69	1.51
1:A:105:VAL:CB	1:A:403:LEU:O[3_365]	0.70	1.50
1:A:167:GLU:CB	1:A:277:LYS:O[4_435]	0.70	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASP:C	1:A:272:SER:CB[4_435]	0.70	1.50
1:A:209:ASP:CB	1:B:258:VAL:CA[4_435]	0.70	1.50
1:A:212:TYR:CA	1:B:260:PHE:N[4_435]	0.70	1.50
1:A:213:SER:OG	1:A:275:ILE:CB[4_435]	0.70	1.50
1:A:220:LYS:CA	1:A:259:THR:C[4_435]	0.70	1.50
1:A:306:LEU:O	1:A:366:LYS:CG[3_365]	0.70	1.50
1:A:322:ASP:CG	1:A:444:GLU:O[3_365]	0.70	1.50
1:B:171:VAL:CG1	1:B:366:LYS:CD[4_445]	0.70	1.50
1:B:416:ILE:CD1	1:B:425:MET:C[3_465]	0.70	1.50
1:A:91:GLN:C	1:A:348:THR:O[3_365]	0.71	1.49
1:A:91:GLN:CA	1:A:349:LYS:N[3_365]	0.71	1.49
1:A:102:LYS:N	1:A:400:PHE:C[3_365]	0.71	1.49
1:A:138:PHE:CB	1:A:431:LYS:CD[3_365]	0.71	1.49
1:A:212:TYR:CD1	1:B:260:PHE:C[4_435]	0.71	1.49
1:A:219:ALA:C	1:A:261:ASN:N[4_435]	0.71	1.49
1:A:322:ASP:CG	1:A:444:GLU:C[3_365]	0.71	1.49
1:B:426:LEU:CB	1:B:436:GLU:CB[2_355]	0.71	1.49
1:A:82:GLU:CB	1:A:377:PHE:CB[2_245]	0.72	1.48
1:A:164:PRO:C	1:A:273:ASP:OD2[4_435]	0.72	1.48
1:A:327:ILE:CA	1:A:469:ASP:OD2[2_345]	0.72	1.48
1:B:372:VAL:C	1:B:372:VAL:O[3_465]	0.72	1.48
1:A:88:TRP:C	1:A:351:SER:O[3_365]	0.73	1.47
1:A:102:LYS:C	1:A:401:MET:C[3_365]	0.73	1.47
1:A:165:SER:CA	5:A:620:HOH:O[4_435]	0.73	1.47
1:A:219:ALA:O	1:A:261:ASN:N[4_435]	0.73	1.47
1:B:341:PRO:CA	1:B:364:THR:N[4_445]	0.73	1.47
1:B:371:LYS:C	1:B:376:ALA:N[3_465]	0.73	1.47
1:A:155:PRO:CG	5:A:618:HOH:O[2_345]	0.74	1.46
1:A:166:SER:OG	1:A:203:TRP:CZ2[4_435]	0.74	1.46
1:A:346:ALA:O	1:A:347:GLN:OE1[3_365]	0.74	1.46
1:B:380:GLY:C	1:B:402:TYR:C[4_445]	0.74	1.46
1:B:386:GLU:OE1	5:B:533:HOH:O[4_445]	0.74	1.46
1:A:91:GLN:CA	1:A:348:THR:C[3_365]	0.75	1.45
1:A:367:GLN:NE2	3:A:501:LTN:CZ2[4_435]	0.75	1.45
1:B:384:ILE:CD1	1:B:394:CYS:CB[4_445]	0.75	1.45
1:B:431:LYS:N	1:B:431:LYS:C[4_445]	0.75	1.45
1:A:139:SER:C	1:A:435:ILE:CG1[3_365]	0.76	1.44
1:A:162:ARG:NE	1:A:268:GLY:C[4_435]	0.76	1.44
1:B:381:ARG:O	1:B:401:MET:C[4_445]	0.76	1.44
1:B:420:TYR:CD2	1:B:437:VAL:CG2[4_445]	0.76	1.44
1:A:93:SER:OG	1:A:98:ILE:N[3_365]	0.77	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:C	1:A:402:TYR:CB[3_365]	0.77	1.43
1:A:167:GLU:OE2	1:A:276:GLY:O[4_435]	0.77	1.43
1:B:98:ILE:O	1:B:446:GLN:C[4_445]	0.77	1.43
1:A:138:PHE:CD2	1:A:399:SER:OG[3_365]	0.78	1.42
1:B:375:HIS:CE1	1:B:375:HIS:CE1[3_465]	0.78	1.42
1:A:141:ARG:CZ	1:A:438:LEU:C[3_365]	0.79	1.41
1:A:236:SER:CA	1:A:271:ASP:OD2[4_435]	0.79	1.41
1:A:319:MET:O	1:A:446:GLN:CB[3_365]	0.79	1.41
1:A:335:LEU:CG	1:A:369:LYS:CG[3_365]	0.79	1.41
1:B:359:ILE:CD1	1:B:377:PHE:CA[3_465]	0.79	1.41
1:B:432:LYS:CG	1:B:433:ALA:N[3_465]	0.79	1.41
1:A:94:SER:OG	1:A:95:ALA:C[3_365]	0.80	1.40
1:A:106:ARG:CD	1:A:405:PHE:CD2[3_365]	0.80	1.40
1:A:319:MET:C	1:A:446:GLN:CG[3_365]	0.80	1.40
1:A:355:PRO:C	4:A:502:ATP:C3'[4_435]	0.80	1.40
1:B:110:SER:O	1:B:471:GLN:CD[3_365]	0.80	1.40
1:B:262:GLN:O	5:B:553:HOH:O[3_365]	0.80	1.40
1:A:97:GLY:CA	5:A:599:HOH:O[3_365]	0.81	1.39
1:A:111:LYS:O	1:A:433:ALA:N[3_365]	0.81	1.39
1:A:212:TYR:CD1	1:B:260:PHE:O[4_435]	0.81	1.39
1:A:300:ARG:CA	1:A:300:ARG:O[2_345]	0.81	1.39
1:A:338:THR:CA	1:A:376:ALA:N[3_365]	0.81	1.39
1:B:109:SER:C	1:B:470:PHE:O[3_365]	0.81	1.39
1:B:400:PHE:N	1:B:435:ILE:O[4_445]	0.81	1.39
1:A:88:TRP:CB	1:A:352:ALA:CA[3_365]	0.82	1.38
1:A:94:SER:CB	1:A:96:LYS:N[3_365]	0.82	1.38
1:A:137:PHE:CE1	1:A:374:LYS:CG[3_365]	0.82	1.38
1:A:141:ARG:CD	1:A:439:GLN:N[3_365]	0.82	1.38
1:A:148:ASP:CB	1:A:152:ASN:ND2[2_345]	0.82	1.38
1:A:169:MET:SD	1:A:263:VAL:O[4_435]	0.82	1.38
1:A:335:LEU:CA	1:A:369:LYS:CA[3_365]	0.82	1.38
1:A:349:LYS:NZ	1:A:354:ASP:CG[3_365]	0.82	1.38
1:B:381:ARG:O	1:B:401:MET:O[4_445]	0.82	1.38
1:A:101:ASP:N	1:A:400:PHE:N[3_365]	0.83	1.37
1:A:258:VAL:CG1	1:A:449:ARG:CG[3_365]	0.83	1.37
1:A:338:THR:CA	1:A:375:HIS:C[3_365]	0.83	1.37
1:B:106:ARG:CB	5:B:581:HOH:O[3_365]	0.83	1.37
1:B:341:PRO:C	1:B:364:THR:N[4_445]	0.83	1.37
1:B:345:GLY:N	1:B:363:ASP:OD2[4_445]	0.83	1.37
1:B:369:LYS:NZ	1:B:397:ASP:CG[2_355]	0.83	1.37
1:B:392:GLY:N	1:B:407:LEU:CA[4_445]	0.83	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:CA	1:B:432:LYS:CG[2_355]	0.83	1.37
1:A:103:LEU:CG	1:A:402:TYR:CD1[3_365]	0.84	1.36
1:A:103:LEU:CD2	1:A:402:TYR:CZ[3_365]	0.84	1.36
1:A:213:SER:CB	1:A:275:ILE:CA[4_435]	0.84	1.36
1:A:273:ASP:N	5:A:619:HOH:O[3_365]	0.84	1.36
1:A:328:GLY:O	1:A:470:PHE:N[2_345]	0.84	1.36
1:A:336:HIS:O	1:A:373:ASN:N[3_365]	0.84	1.36
1:A:440:PRO:CD	5:A:589:HOH:O[4_435]	0.84	1.36
1:B:397:ASP:CA	1:B:438:LEU:CB[4_445]	0.84	1.36
1:B:429:GLU:C	1:B:429:GLU:O[4_445]	0.84	1.36
1:A:94:SER:CA	1:A:94:SER:C[3_365]	0.85	1.35
1:A:221:ASP:C	1:A:262:GLN:CA[4_435]	0.85	1.35
1:A:221:ASP:CA	1:A:262:GLN:C[4_435]	0.85	1.35
1:B:274:CYS:CB	5:A:573:HOH:O[3_365]	0.85	1.35
1:B:109:SER:O	1:B:470:PHE:C[3_365]	0.85	1.35
1:B:340:PHE:O	1:B:364:THR:CG2[4_445]	0.85	1.35
1:B:368:ILE:CB	1:B:398:VAL:CG1[3_465]	0.85	1.35
1:A:212:TYR:O	1:B:260:PHE:CB[4_435]	0.86	1.34
1:A:307:ILE:CD1	1:A:364:THR:CB[3_365]	0.86	1.34
1:A:338:THR:N	1:A:376:ALA:N[3_365]	0.86	1.34
1:A:356:ASN:CB	4:A:502:ATP:N9[4_435]	0.86	1.34
1:B:459:GLU:CB	1:B:459:GLU:CG[2_345]	0.86	1.34
1:A:92:THR:C	1:A:347:GLN:OE1[2_245]	0.87	1.33
1:A:93:SER:CB	1:A:346:ALA:N[2_245]	0.87	1.33
1:A:323:VAL:CG1	1:A:446:GLN:O[3_365]	0.87	1.33
1:A:461:MET:CG	1:B:271:ASP:N[4_435]	0.87	1.33
1:B:307:ILE:CG2	1:B:475:HIS:CD2[3_365]	0.87	1.33
1:B:389:GLN:CA	5:B:502:HOH:O[4_445]	0.87	1.33
1:B:391:GLY:CA	1:B:407:LEU:O[4_445]	0.87	1.33
1:B:412:LYS:O	1:B:424:ALA:CA[3_465]	0.87	1.33
1:B:432:LYS:CD	1:B:433:ALA:CA[3_465]	0.87	1.33
1:A:87:PRO:CD	1:A:170:HIS:CB[3_365]	0.88	1.32
1:A:93:SER:O	1:A:97:GLY:O[3_365]	0.88	1.32
1:B:429:GLU:N	1:B:432:LYS:C[2_355]	0.88	1.32
1:B:430:LEU:C	1:B:432:LYS:CA[4_445]	0.88	1.32
1:A:83:ASP:O	1:A:341:PRO:N[3_365]	0.89	1.31
1:A:86:ASP:N	1:A:350:MET:CG[3_365]	0.89	1.31
1:A:90:VAL:CG2	1:A:357:SER:OG[3_365]	0.89	1.31
1:A:100:TYR:O	1:A:399:SER:C[3_365]	0.89	1.31
1:A:102:LYS:N	1:A:401:MET:N[3_365]	0.89	1.31
1:A:141:ARG:C	1:A:439:GLN:OE1[3_365]	0.89	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:CD	1:A:439:GLN:CA[3_365]	0.89	1.31
1:A:309:CYS:O	1:A:371:LYS:CA[3_365]	0.89	1.31
1:B:102:LYS:CD	1:B:452:VAL:CA[4_445]	0.89	1.31
1:B:141:ARG:CG	1:B:472:HIS:C[3_365]	0.89	1.31
1:B:372:VAL:O	1:B:373:ASN:N[4_445]	0.89	1.31
1:A:93:SER:CA	1:A:347:GLN:NE2[2_245]	0.90	1.30
1:A:236:SER:OG	1:B:261:ASN:ND2[4_435]	0.90	1.30
1:A:307:ILE:O	1:A:366:LYS:O[3_365]	0.90	1.30
1:A:317:PHE:CD2	1:A:363:ASP:C[3_365]	0.90	1.30
1:A:336:HIS:CB	1:A:372:VAL:CG2[3_365]	0.90	1.30
1:B:99:ASP:O	1:B:450:LYS:N[4_445]	0.90	1.30
1:B:102:LYS:N	1:B:451:GLU:CA[4_445]	0.90	1.30
1:B:341:PRO:N	1:B:364:THR:CA[4_445]	0.90	1.30
1:B:412:LYS:C	1:B:424:ALA:N[3_465]	0.90	1.30
1:A:94:SER:OG	1:A:95:ALA:O[3_365]	0.91	1.29
1:A:209:ASP:CA	1:B:258:VAL:C[4_435]	0.91	1.29
1:A:212:TYR:CE1	1:B:260:PHE:O[4_435]	0.91	1.29
1:A:297:PHE:O	1:A:301:THR:CG2[2_345]	0.91	1.29
1:A:299:ASP:CA	1:A:299:ASP:CA[2_345]	0.91	1.29
1:A:320:THR:CA	1:A:446:GLN:OE1[3_365]	0.91	1.29
1:A:334:LEU:N	1:A:439:GLN:NE2[3_365]	0.91	1.29
1:A:335:LEU:CG	1:A:369:LYS:CD[3_365]	0.91	1.29
1:A:338:THR:C	1:A:375:HIS:O[3_365]	0.91	1.29
1:B:372:VAL:N	1:B:373:ASN:O[2_355]	0.91	1.29
1:B:428:GLY:C	1:B:430:LEU:C[4_445]	0.91	1.29
1:B:453:THR:CB	1:B:465:LYS:N[2_345]	0.91	1.29
1:A:88:TRP:CA	1:A:352:ALA:CA[3_365]	0.92	1.28
1:A:103:LEU:C	1:A:402:TYR:CA[3_365]	0.92	1.28
1:A:105:VAL:CG1	1:A:403:LEU:O[3_365]	0.92	1.28
1:A:310:ALA:N	1:A:371:LYS:CG[3_365]	0.92	1.28
1:A:335:LEU:O	1:A:370:THR:N[3_365]	0.92	1.28
1:A:338:THR:CG2	1:A:376:ALA:O[3_365]	0.92	1.28
1:B:141:ARG:NE	1:B:472:HIS:CB[3_365]	0.92	1.28
1:B:459:GLU:CB	1:B:459:GLU:CB[2_345]	0.92	1.28
1:A:140:HIS:N	1:A:435:ILE:CB[3_365]	0.93	1.27
1:A:220:LYS:CE	1:B:274:CYS:C[4_435]	0.93	1.27
1:A:316:TYR:CD1	1:A:360:PHE:CB[3_365]	0.93	1.27
1:A:320:THR:N	1:A:446:GLN:CD[3_365]	0.93	1.27
1:B:340:PHE:CD1	5:B:524:HOH:O[4_445]	0.93	1.27
1:B:383:THR:CG2	1:B:443:ALA:CB[2_355]	0.93	1.27
1:A:91:GLN:CB	1:A:349:LYS:N[3_365]	0.94	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:C	1:A:437:VAL:CG1[3_365]	0.94	1.26
1:A:234:ILE:CD1	1:A:261:ASN:OD1[4_435]	0.94	1.26
1:A:309:CYS:O	1:A:371:LYS:N[3_365]	0.94	1.26
1:A:454:ASP:CG	1:B:277:LYS:CG[4_435]	0.94	1.26
1:B:346:ALA:C	1:B:362:THR:N[4_445]	0.94	1.26
1:B:374:LYS:O	1:B:374:LYS:CB[3_465]	0.94	1.26
1:A:141:ARG:O	1:A:439:GLN:OE1[3_365]	0.95	1.25
1:A:307:ILE:N	1:A:366:LYS:CA[3_365]	0.95	1.25
1:A:316:TYR:CA	1:A:362:THR:N[3_365]	0.95	1.25
1:A:317:PHE:CG	1:A:363:ASP:O[3_365]	0.95	1.25
1:B:110:SER:O	1:B:471:GLN:CG[3_365]	0.95	1.25
1:B:431:LYS:N	1:B:432:LYS:N[4_445]	0.95	1.25
1:A:82:GLU:CB	1:A:377:PHE:CG[2_245]	0.96	1.24
1:A:91:GLN:C	1:A:348:THR:C[3_365]	0.96	1.24
1:A:94:SER:CA	1:A:94:SER:O[3_365]	0.96	1.24
1:A:209:ASP:O	1:B:258:VAL:O[4_435]	0.96	1.24
1:A:307:ILE:C	1:A:366:LYS:O[3_365]	0.96	1.24
1:A:346:ALA:C	1:A:347:GLN:OE1[3_365]	0.96	1.24
1:A:356:ASN:CG	4:A:502:ATP:N9[4_435]	0.96	1.24
1:B:134:ARG:NE	1:B:390:PHE:N[3_465]	0.96	1.24
1:A:84:PHE:CD1	4:A:502:ATP:C6[3_365]	0.97	1.23
1:A:89:THR:CA	1:A:351:SER:CB[3_365]	0.97	1.23
1:A:89:THR:C	1:A:351:SER:N[3_365]	0.97	1.23
1:A:103:LEU:CB	1:A:402:TYR:CD1[3_365]	0.97	1.23
1:A:140:HIS:CA	1:A:435:ILE:CG2[3_365]	0.97	1.23
1:A:209:ASP:CB	1:B:258:VAL:CB[4_435]	0.97	1.23
1:A:215:ALA:O	1:A:260:PHE:CZ[4_435]	0.97	1.23
1:A:220:LYS:CA	1:A:259:THR:O[4_435]	0.97	1.23
1:A:257:HIS:CA	1:A:450:LYS:C[3_365]	0.97	1.23
1:A:300:ARG:C	1:A:300:ARG:CB[2_345]	0.97	1.23
1:A:318:ARG:CA	1:A:442:ILE:CB[3_365]	0.97	1.23
1:A:319:MET:SD	5:A:532:HOH:O[3_365]	0.97	1.23
1:A:322:ASP:OD1	1:A:444:GLU:C[3_365]	0.97	1.23
1:A:334:LEU:CD1	1:A:368:ILE:CD1[3_365]	0.97	1.23
1:A:338:THR:O	1:A:375:HIS:CA[3_365]	0.97	1.23
1:A:356:ASN:CB	4:A:502:ATP:C4[4_435]	0.97	1.23
1:B:110:SER:OG	5:B:494:HOH:O[3_365]	0.97	1.23
1:B:140:HIS:CA	1:B:473:HIS:CE1[3_365]	0.97	1.23
1:B:340:PHE:CE1	5:B:524:HOH:O[4_445]	0.97	1.23
1:B:370:THR:O	1:B:374:LYS:CA[4_445]	0.97	1.23
1:B:416:ILE:CD1	1:B:425:MET:CA[3_465]	0.97	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LYS:CB	1:B:431:LYS:CB[3_465]	0.97	1.23
1:B:431:LYS:O	5:B:501:HOH:O[4_445]	0.97	1.23
1:A:111:LYS:N	1:A:433:ALA:C[3_365]	0.98	1.22
1:A:139:SER:O	1:A:435:ILE:CD1[3_365]	0.98	1.22
1:A:216:VAL:CG2	1:B:260:PHE:CE1[4_435]	0.98	1.22
1:A:266:ILE:CD1	1:A:445:HIS:NE2[3_365]	0.98	1.22
1:A:312:ASP:C	1:A:359:ILE:N[3_365]	0.98	1.22
1:A:328:GLY:O	1:A:469:ASP:C[2_345]	0.98	1.22
1:B:99:ASP:O	1:B:450:LYS:CA[4_445]	0.98	1.22
1:B:110:SER:N	1:B:471:GLN:N[3_365]	0.98	1.22
1:B:395:ASP:O	1:B:442:ILE:N[4_445]	0.98	1.22
1:A:86:ASP:CB	1:A:170:HIS:NE2[3_365]	0.99	1.21
1:A:164:PRO:CD	1:A:270:THR:CB[4_435]	0.99	1.21
1:A:216:VAL:CG2	1:B:260:PHE:CD1[4_435]	0.99	1.21
1:A:221:ASP:OD2	1:A:263:VAL:CG1[4_435]	0.99	1.21
1:A:312:ASP:CA	1:A:358:SER:C[3_365]	0.99	1.21
1:A:326:ARG:NH1	1:A:451:GLU:CG[3_365]	0.99	1.21
1:A:327:ILE:C	1:A:469:ASP:OD2[2_345]	0.99	1.21
1:A:338:THR:C	1:A:375:HIS:C[3_365]	0.99	1.21
1:B:141:ARG:NH2	1:B:298:ARG:O[3_365]	0.99	1.21
1:B:384:ILE:CG1	1:B:440:PRO:CG[2_355]	0.99	1.21
1:B:416:ILE:CB	1:B:436:GLU:OE1[4_445]	0.99	1.21
1:A:92:THR:C	1:A:346:ALA:O[3_365]	1.00	1.20
1:A:101:ASP:CA	1:A:400:PHE:N[3_365]	1.00	1.20
1:A:166:SER:CB	1:A:203:TRP:CZ2[4_435]	1.00	1.20
1:A:210:GLN:CB	1:A:274:CYS:CB[4_435]	1.00	1.20
1:A:319:MET:O	1:A:446:GLN:CA[3_365]	1.00	1.20
1:A:321:ARG:NE	1:A:439:GLN:O[3_365]	1.00	1.20
1:B:402:TYR:CA	1:B:439:GLN:NE2[4_445]	1.00	1.20
1:B:430:LEU:CB	1:B:432:LYS:CG[2_355]	1.00	1.20
1:A:137:PHE:CB	1:A:373:ASN:CB[3_365]	1.01	1.19
1:A:211:ALA:C	1:A:273:ASP:O[4_435]	1.01	1.19
1:A:307:ILE:CA	1:A:366:LYS:CA[3_365]	1.01	1.19
1:A:315:PRO:O	1:A:361:LEU:CA[3_365]	1.01	1.19
1:A:336:HIS:CE1	1:A:368:ILE:CG2[3_365]	1.01	1.19
1:B:99:ASP:CA	1:B:449:ARG:N[4_445]	1.01	1.19
1:B:103:LEU:N	1:B:450:LYS:O[4_445]	1.01	1.19
1:B:346:ALA:O	1:B:362:THR:N[4_445]	1.01	1.19
1:B:359:ILE:CD1	1:B:370:THR:OG1[4_445]	1.01	1.19
1:B:372:VAL:C	1:B:373:ASN:C[2_355]	1.01	1.19
1:B:401:MET:CA	1:B:439:GLN:CB[4_445]	1.01	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:C	1:B:432:LYS:C[4_445]	1.01	1.19
1:A:88:TRP:O	1:A:351:SER:O[3_365]	1.02	1.18
1:A:93:SER:C	1:A:347:GLN:NE2[2_245]	1.02	1.18
1:A:100:TYR:CB	1:A:399:SER:N[3_365]	1.02	1.18
1:A:116:LEU:CD2	1:A:432:LYS:CG[3_365]	1.02	1.18
1:A:220:LYS:CB	1:A:259:THR:C[4_435]	1.02	1.18
1:A:335:LEU:O	1:A:369:LYS:C[3_365]	1.02	1.18
1:A:336:HIS:O	1:A:372:VAL:C[3_365]	1.02	1.18
1:A:347:GLN:CA	1:A:347:GLN:CB[3_365]	1.02	1.18
1:B:369:LYS:CB	1:B:378:SER:CB[2_355]	1.02	1.18
1:B:372:VAL:C	1:B:373:ASN:CA[2_355]	1.02	1.18
1:A:83:ASP:C	1:A:341:PRO:N[3_365]	1.03	1.17
1:A:97:GLY:C	5:A:518:HOH:O[3_365]	1.03	1.17
1:A:100:TYR:CA	1:A:399:SER:N[3_365]	1.03	1.17
1:A:105:VAL:N	1:A:403:LEU:CA[3_365]	1.03	1.17
1:A:312:ASP:C	1:A:358:SER:C[3_365]	1.03	1.17
1:B:334:LEU:CA	1:B:473:HIS:CB[3_365]	1.03	1.17
1:B:344:GLN:N	1:B:371:LYS:CE[4_445]	1.03	1.17
1:B:366:LYS:C	1:B:402:TYR:OH[3_465]	1.03	1.17
1:B:368:ILE:CA	1:B:398:VAL:CG1[3_465]	1.03	1.17
1:B:384:ILE:CA	1:B:400:PHE:CE2[4_445]	1.03	1.17
1:B:426:LEU:N	1:B:436:GLU:OE2[2_355]	1.03	1.17
1:A:111:LYS:CG	1:A:430:LEU:C[3_365]	1.04	1.16
1:A:212:TYR:CG	1:B:260:PHE:C[4_435]	1.04	1.16
1:A:215:ALA:O	1:A:260:PHE:CE1[4_435]	1.04	1.16
1:A:258:VAL:N	1:A:449:ARG:O[3_365]	1.04	1.16
1:A:307:ILE:O	1:A:366:LYS:C[3_365]	1.04	1.16
1:A:318:ARG:C	1:A:442:ILE:O[3_365]	1.04	1.16
1:A:318:ARG:O	1:A:442:ILE:C[3_365]	1.04	1.16
1:A:458:LYS:O	1:B:270:THR:CG2[4_435]	1.04	1.16
1:B:130:HIS:NE2	1:B:381:ARG:NH2[3_465]	1.04	1.16
1:B:171:VAL:CG1	1:B:377:PHE:CZ[3_465]	1.04	1.16
1:B:262:GLN:C	5:B:553:HOH:O[3_365]	1.04	1.16
1:B:346:ALA:C	1:B:361:LEU:C[4_445]	1.04	1.16
1:B:392:GLY:O	1:B:406:PHE:O[4_445]	1.04	1.16
1:B:458:LYS:CB	1:B:462:THR:OG1[2_345]	1.04	1.16
1:A:83:ASP:O	1:A:341:PRO:CD[3_365]	1.05	1.15
1:A:88:TRP:CG	1:A:352:ALA:CB[3_365]	1.05	1.15
1:A:90:VAL:CG1	1:A:342:ALA:CB[3_365]	1.05	1.15
1:A:111:LYS:CG	1:A:430:LEU:CA[3_365]	1.05	1.15
1:A:111:LYS:C	1:A:433:ALA:N[3_365]	1.05	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:N	1:A:432:LYS:N[3_365]	1.05	1.15
1:A:169:MET:CB	1:A:267:PHE:CB[4_435]	1.05	1.15
1:A:213:SER:OG	1:A:275:ILE:CG2[4_435]	1.05	1.15
1:A:318:ARG:CD	1:A:441:LEU:CD2[3_365]	1.05	1.15
1:B:375:HIS:ND1	1:B:375:HIS:CD2[4_445]	1.05	1.15
1:A:106:ARG:CB	1:A:405:PHE:CB[3_365]	1.06	1.14
1:A:137:PHE:N	1:A:373:ASN:O[3_365]	1.06	1.14
1:A:162:ARG:CZ	1:A:268:GLY:C[4_435]	1.06	1.14
1:A:210:GLN:O	1:A:274:CYS:C[4_435]	1.06	1.14
1:A:221:ASP:C	1:A:262:GLN:C[4_435]	1.06	1.14
1:B:104:ILE:CG2	1:B:469:ASP:OD2[3_365]	1.06	1.14
1:B:105:VAL:CG2	5:B:492:HOH:O[3_365]	1.06	1.14
1:B:366:LYS:CG	1:B:377:PHE:CZ[2_355]	1.06	1.14
1:B:372:VAL:N	1:B:376:ALA:N[3_465]	1.06	1.14
1:A:86:ASP:CB	1:A:170:HIS:CD2[3_365]	1.07	1.13
1:A:103:LEU:CA	1:A:402:TYR:CA[3_365]	1.07	1.13
1:A:210:GLN:O	1:A:274:CYS:CA[4_435]	1.07	1.13
1:A:212:TYR:CE2	1:B:263:VAL:CG2[4_435]	1.07	1.13
1:A:216:VAL:CG1	1:B:278:ILE:CD1[4_435]	1.07	1.13
1:A:257:HIS:O	1:A:449:ARG:C[3_365]	1.07	1.13
1:A:335:LEU:N	1:A:369:LYS:CB[3_365]	1.07	1.13
1:B:371:LYS:CA	1:B:374:LYS:O[2_355]	1.07	1.13
1:B:374:LYS:C	1:B:375:HIS:CA[4_445]	1.07	1.13
1:B:416:ILE:CG2	1:B:436:GLU:OE1[4_445]	1.07	1.13
1:B:430:LEU:CA	1:B:432:LYS:C[4_445]	1.07	1.13
1:A:164:PRO:O	1:A:273:ASP:OD1[4_435]	1.08	1.12
1:A:166:SER:O	1:A:269:PHE:CE1[4_435]	1.08	1.12
1:A:197:ASP:CA	1:A:272:SER:N[4_435]	1.08	1.12
1:A:337:SER:N	1:A:371:LYS:C[3_365]	1.08	1.12
1:A:347:GLN:CB	1:A:347:GLN:CB[3_365]	1.08	1.12
1:B:107:PHE:C	1:B:298:ARG:CA[3_365]	1.08	1.12
1:B:375:HIS:NE2	1:B:375:HIS:NE2[4_445]	1.08	1.12
1:B:383:THR:O	1:B:404:THR:CG2[4_445]	1.08	1.12
1:A:84:PHE:CA	1:A:340:PHE:O[3_365]	1.09	1.11
1:A:103:LEU:N	1:A:401:MET:C[3_365]	1.09	1.11
1:A:105:VAL:O	1:A:406:PHE:CA[3_365]	1.09	1.11
1:A:106:ARG:NH1	1:A:340:PHE:CD1[3_365]	1.09	1.11
1:A:110:SER:C	1:A:434:LEU:N[3_365]	1.09	1.11
1:A:206:LEU:CD2	5:A:587:HOH:O[4_435]	1.09	1.11
1:A:209:ASP:CA	1:B:258:VAL:CA[4_435]	1.09	1.11
1:A:222:ILE:CA	1:A:261:ASN:O[4_435]	1.09	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ARG:CA	1:A:442:ILE:CA[3_365]	1.09	1.11
1:A:329:TYR:CD1	1:A:470:PHE:C[2_345]	1.09	1.11
1:A:339:PHE:O	5:A:547:HOH:O[3_365]	1.09	1.11
1:B:458:LYS:CG	1:B:462:THR:OG1[2_345]	1.09	1.11
1:A:86:ASP:CG	1:A:170:HIS:CE1[3_365]	1.10	1.10
1:A:107:PHE:CA	1:A:406:PHE:CD2[3_365]	1.10	1.10
1:A:167:GLU:CG	1:A:277:LYS:C[4_435]	1.10	1.10
1:A:197:ASP:CB	1:A:272:SER:N[4_435]	1.10	1.10
1:A:211:ALA:O	1:A:273:ASP:O[4_435]	1.10	1.10
1:A:314:ASP:CB	1:A:359:ILE:CG2[3_365]	1.10	1.10
1:A:315:PRO:CD	1:A:359:ILE:O[3_365]	1.10	1.10
1:A:316:TYR:N	1:A:360:PHE:C[3_365]	1.10	1.10
1:A:317:PHE:CB	1:A:363:ASP:O[3_365]	1.10	1.10
1:A:326:ARG:CZ	1:A:451:GLU:CG[3_365]	1.10	1.10
1:B:274:CYS:SG	5:A:573:HOH:O[3_365]	1.10	1.10
1:B:109:SER:O	1:B:470:PHE:CA[3_365]	1.10	1.10
1:A:100:TYR:OH	1:A:343:LEU:O[3_365]	1.11	1.09
1:A:139:SER:O	1:A:435:ILE:CG1[3_365]	1.11	1.09
1:A:141:ARG:NE	1:A:438:LEU:O[3_365]	1.11	1.09
1:A:164:PRO:CD	1:A:270:THR:OG1[4_435]	1.11	1.09
1:A:300:ARG:O	1:A:300:ARG:CB[2_345]	1.11	1.09
1:A:312:ASP:CG	1:A:358:SER:N[3_365]	1.11	1.09
1:A:320:THR:CA	1:A:446:GLN:CD[3_365]	1.11	1.09
1:A:322:ASP:OD2	1:A:444:GLU:O[3_365]	1.11	1.09
1:A:440:PRO:CG	5:A:589:HOH:O[4_435]	1.11	1.09
1:A:457:VAL:CB	1:B:273:ASP:N[4_435]	1.11	1.09
1:B:102:LYS:CB	1:B:452:VAL:N[4_445]	1.11	1.09
1:B:107:PHE:O	1:B:298:ARG:CA[3_365]	1.11	1.09
1:B:392:GLY:N	1:B:407:LEU:CB[4_445]	1.11	1.09
1:B:407:LEU:CD2	1:B:420:TYR:O[3_465]	1.11	1.09
1:B:430:LEU:CB	1:B:433:ALA:C[4_445]	1.11	1.09
1:B:453:THR:CG2	1:B:465:LYS:CA[2_345]	1.11	1.09
1:A:89:THR:CA	1:A:351:SER:CA[3_365]	1.12	1.08
1:A:91:GLN:O	1:A:348:THR:O[3_365]	1.12	1.08
1:A:113:ASP:CA	1:A:429:GLU:CB[3_365]	1.12	1.08
1:A:113:ASP:C	1:A:429:GLU:CG[3_365]	1.12	1.08
1:A:197:ASP:O	1:A:272:SER:CB[4_435]	1.12	1.08
1:A:212:TYR:CB	1:B:259:THR:C[4_435]	1.12	1.08
1:A:300:ARG:CA	1:A:300:ARG:C[2_345]	1.12	1.08
1:A:307:ILE:N	1:A:366:LYS:CB[3_365]	1.12	1.08
1:A:316:TYR:N	1:A:360:PHE:O[3_365]	1.12	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:TYR:CD2	1:A:362:THR:OG1[3_365]	1.12	1.08
1:A:335:LEU:N	1:A:369:LYS:CA[3_365]	1.12	1.08
1:A:355:PRO:O	4:A:502:ATP:O3'[4_435]	1.12	1.08
1:B:108:GLY:CA	1:B:298:ARG:N[3_365]	1.12	1.08
1:B:334:LEU:O	1:B:473:HIS:CG[3_365]	1.12	1.08
1:B:369:LYS:CE	1:B:397:ASP:OD2[2_355]	1.12	1.08
1:B:392:GLY:CA	1:B:407:LEU:N[4_445]	1.12	1.08
1:B:402:TYR:N	1:B:439:GLN:NE2[4_445]	1.12	1.08
1:B:428:GLY:O	1:B:431:LYS:N[4_445]	1.12	1.08
1:A:257:HIS:CA	1:A:450:LYS:O[3_365]	1.13	1.07
1:A:314:ASP:CA	1:A:359:ILE:CG2[3_365]	1.13	1.07
1:A:338:THR:O	1:A:375:HIS:CB[3_365]	1.13	1.07
1:A:457:VAL:CB	1:B:273:ASP:CA[4_435]	1.13	1.07
1:B:171:VAL:N	1:B:366:LYS:NZ[4_445]	1.13	1.07
1:B:359:ILE:CB	1:B:377:PHE:CB[3_465]	1.13	1.07
1:B:369:LYS:NZ	1:B:397:ASP:OD2[2_355]	1.13	1.07
1:B:388:ARG:N	1:B:413:LEU:CD2[4_445]	1.13	1.07
1:B:426:LEU:CA	1:B:436:GLU:CD[2_355]	1.13	1.07
1:A:88:TRP:C	1:A:351:SER:C[3_365]	1.14	1.06
1:A:93:SER:N	1:A:347:GLN:OE1[2_245]	1.14	1.06
1:A:94:SER:CA	1:A:95:ALA:N[2_245]	1.14	1.06
1:A:113:ASP:CA	1:A:429:GLU:CA[3_365]	1.14	1.06
1:A:197:ASP:CA	1:A:272:SER:CA[4_435]	1.14	1.06
1:A:221:ASP:OD2	1:A:263:VAL:CB[4_435]	1.14	1.06
1:A:337:SER:N	1:A:372:VAL:N[3_365]	1.14	1.06
1:A:457:VAL:CA	1:B:272:SER:C[4_435]	1.14	1.06
1:B:103:LEU:CB	1:B:450:LYS:CG[4_445]	1.14	1.06
1:B:307:ILE:CD1	1:B:475:HIS:N[3_365]	1.14	1.06
1:B:334:LEU:CG	1:B:474:HIS:N[3_365]	1.14	1.06
1:B:346:ALA:N	1:B:360:PHE:O[4_445]	1.14	1.06
1:B:366:LYS:O	1:B:402:TYR:CZ[3_465]	1.14	1.06
1:B:384:ILE:N	1:B:440:PRO:CB[2_355]	1.14	1.06
1:B:400:PHE:CD1	1:B:436:GLU:O[4_445]	1.14	1.06
1:B:406:PHE:CE1	5:B:562:HOH:O[3_465]	1.14	1.06
1:B:412:LYS:NZ	1:B:419:ASP:CB[3_465]	1.14	1.06
1:B:428:GLY:C	1:B:430:LEU:CA[4_445]	1.14	1.06
1:A:84:PHE:CE1	4:A:502:ATP:C6[3_365]	1.15	1.05
1:A:88:TRP:CB	1:A:352:ALA:C[3_365]	1.15	1.05
1:A:97:GLY:N	5:A:599:HOH:O[3_365]	1.15	1.05
1:A:112:ILE:CA	1:A:432:LYS:N[3_365]	1.15	1.05
1:A:137:PHE:CA	1:A:373:ASN:CA[3_365]	1.15	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:CD	1:A:276:GLY:O[4_435]	1.15	1.05
1:A:219:ALA:O	1:A:261:ASN:CA[4_435]	1.15	1.05
1:A:335:LEU:CB	1:A:369:LYS:CG[3_365]	1.15	1.05
1:B:107:PHE:O	1:B:298:ARG:C[3_365]	1.15	1.05
1:B:341:PRO:CG	1:B:364:THR:C[4_445]	1.15	1.05
1:B:359:ILE:CB	1:B:377:PHE:CG[3_465]	1.15	1.05
1:B:371:LYS:CB	1:B:375:HIS:O[3_465]	1.15	1.05
1:B:381:ARG:CG	1:B:404:THR:O[4_445]	1.15	1.05
1:B:392:GLY:C	1:B:406:PHE:O[4_445]	1.15	1.05
1:B:392:GLY:C	1:B:406:PHE:C[4_445]	1.15	1.05
1:B:394:CYS:CA	1:B:437:VAL:O[4_445]	1.15	1.05
1:B:402:TYR:N	1:B:439:GLN:CD[4_445]	1.15	1.05
1:B:440:PRO:C	5:B:567:HOH:O[2_355]	1.15	1.05
1:A:84:PHE:CZ	4:A:502:ATP:C4[3_365]	1.16	1.04
1:A:102:LYS:C	1:A:401:MET:O[3_365]	1.16	1.04
1:A:102:LYS:O	1:A:401:MET:O[3_365]	1.16	1.04
1:A:106:ARG:O	1:A:406:PHE:CD1[3_365]	1.16	1.04
1:A:140:HIS:N	1:A:435:ILE:CG1[3_365]	1.16	1.04
1:A:222:ILE:N	1:A:261:ASN:O[4_435]	1.16	1.04
1:A:307:ILE:CA	1:A:366:LYS:CB[3_365]	1.16	1.04
1:A:327:ILE:O	1:A:469:ASP:OD1[2_345]	1.16	1.04
1:A:356:ASN:OD1	4:A:502:ATP:C8[4_435]	1.16	1.04
1:B:370:THR:O	1:B:371:LYS:O[3_465]	1.16	1.04
1:B:379:GLY:C	5:B:537:HOH:O[2_355]	1.16	1.04
1:B:395:ASP:C	1:B:441:LEU:CA[4_445]	1.16	1.04
1:B:397:ASP:O	1:B:439:GLN:N[4_445]	1.16	1.04
1:B:400:PHE:CG	1:B:436:GLU:O[4_445]	1.16	1.04
1:B:425:MET:CE	1:B:429:GLU:OE1[3_465]	1.16	1.04
1:B:455:GLU:OE2	1:B:464:ARG:N[2_345]	1.16	1.04
1:A:85:VAL:CA	1:A:350:MET:CB[3_365]	1.17	1.03
1:A:91:GLN:CG	5:A:531:HOH:O[2_245]	1.17	1.03
1:A:91:GLN:CB	5:A:531:HOH:O[2_245]	1.17	1.03
1:A:93:SER:N	1:A:346:ALA:O[3_365]	1.17	1.03
1:A:94:SER:CB	1:A:95:ALA:C[3_365]	1.17	1.03
1:A:95:ALA:N	1:A:95:ALA:N[4_435]	1.17	1.03
1:A:141:ARG:NH1	1:A:438:LEU:CB[3_365]	1.17	1.03
1:A:141:ARG:CZ	1:A:438:LEU:O[3_365]	1.17	1.03
1:A:217:GLU:CB	1:A:278:ILE:CG2[4_435]	1.17	1.03
1:A:279:SER:CA	5:A:555:HOH:O[3_365]	1.17	1.03
1:A:454:ASP:O	1:B:273:ASP:OD1[4_435]	1.17	1.03
1:A:454:ASP:CB	1:B:277:LYS:CE[4_435]	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASP:CB	1:B:448:ARG:C[4_445]	1.17	1.03
1:B:341:PRO:CA	1:B:364:THR:CA[4_445]	1.17	1.03
1:B:345:GLY:C	1:B:360:PHE:O[4_445]	1.17	1.03
1:B:374:LYS:CA	1:B:375:HIS:N[4_445]	1.17	1.03
1:B:388:ARG:C	5:B:535:HOH:O[4_445]	1.17	1.03
1:B:412:LYS:CB	1:B:422:SER:OG[3_465]	1.17	1.03
1:A:141:ARG:NE	1:A:439:GLN:N[3_365]	1.18	1.02
1:A:141:ARG:CB	1:A:439:GLN:CB[3_365]	1.18	1.02
1:A:211:ALA:CB	1:A:272:SER:O[4_435]	1.18	1.02
1:A:259:THR:CG2	1:A:452:VAL:CB[3_365]	1.18	1.02
1:A:266:ILE:CD1	1:A:445:HIS:CE1[3_365]	1.18	1.02
1:A:320:THR:CB	1:A:446:GLN:OE1[3_365]	1.18	1.02
1:A:336:HIS:C	1:A:372:VAL:N[3_365]	1.18	1.02
5:A:606:HOH:O	5:A:611:HOH:O[2_345]	1.18	1.02
1:B:98:ILE:O	1:B:446:GLN:O[4_445]	1.18	1.02
1:B:105:VAL:CG1	1:B:465:LYS:CB[3_365]	1.18	1.02
1:B:368:ILE:CB	1:B:398:VAL:CB[3_465]	1.18	1.02
1:B:409:ASP:O	1:B:422:SER:C[3_465]	1.18	1.02
1:B:413:LEU:N	1:B:423:GLY:C[3_465]	1.18	1.02
1:A:84:PHE:CE1	4:A:502:ATP:C5[3_365]	1.19	1.01
1:A:92:THR:O	1:A:347:GLN:C[3_365]	1.19	1.01
1:A:111:LYS:N	1:A:434:LEU:N[3_365]	1.19	1.01
1:A:169:MET:CG	1:A:267:PHE:CB[4_435]	1.19	1.01
1:A:195:MET:CB	1:A:271:ASP:OD1[4_435]	1.19	1.01
1:A:218:ASN:OD1	1:A:269:PHE:CG[4_435]	1.19	1.01
1:A:219:ALA:CA	1:A:260:PHE:C[4_435]	1.19	1.01
1:A:220:LYS:N	1:A:260:PHE:CA[4_435]	1.19	1.01
1:A:322:ASP:N	1:A:443:ALA:C[3_365]	1.19	1.01
1:A:339:PHE:N	1:A:375:HIS:O[3_365]	1.19	1.01
1:B:344:GLN:N	1:B:371:LYS:CD[4_445]	1.19	1.01
1:B:389:GLN:CB	5:B:502:HOH:O[4_445]	1.19	1.01
1:B:399:SER:OG	1:B:435:ILE:CG1[4_445]	1.19	1.01
1:B:400:PHE:CD2	1:B:440:PRO:CD[4_445]	1.19	1.01
1:B:413:LEU:CA	1:B:423:GLY:O[3_465]	1.19	1.01
1:B:429:GLU:O	1:B:429:GLU:O[3_465]	1.19	1.01
1:A:84:PHE:CZ	4:A:502:ATP:N7[3_365]	1.20	1.00
1:A:110:SER:OG	1:A:436:GLU:CB[3_365]	1.20	1.00
1:A:169:MET:CB	1:A:267:PHE:CG[4_435]	1.20	1.00
1:A:356:ASN:CG	4:A:502:ATP:C8[4_435]	1.20	1.00
1:B:159:TYR:O	1:B:475:HIS:CE1[3_365]	1.20	1.00
1:B:359:ILE:CG1	1:B:377:PHE:CA[3_465]	1.20	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:N	5:B:567:HOH:O[2_355]	1.20	1.00
1:A:92:THR:CB	1:A:346:ALA:C[3_365]	1.21	0.99
1:A:218:ASN:CG	1:A:269:PHE:CB[4_435]	1.21	0.99
1:A:317:PHE:C	1:A:442:ILE:CG2[3_365]	1.21	0.99
1:A:335:LEU:CA	1:A:369:LYS:CB[3_365]	1.21	0.99
1:A:336:HIS:C	1:A:372:VAL:CA[3_365]	1.21	0.99
1:B:100:TYR:N	1:B:447:ALA:O[4_445]	1.21	0.99
1:B:102:LYS:CD	1:B:452:VAL:C[4_445]	1.21	0.99
1:B:395:ASP:C	1:B:441:LEU:C[4_445]	1.21	0.99
1:B:399:SER:CB	1:B:435:ILE:CG1[4_445]	1.21	0.99
1:B:399:SER:CB	1:B:435:ILE:CB[4_445]	1.21	0.99
1:B:420:TYR:CD2	1:B:437:VAL:CB[4_445]	1.21	0.99
1:A:103:LEU:CG	1:A:402:TYR:CG[3_365]	1.22	0.98
1:A:321:ARG:CB	1:A:443:ALA:CA[3_365]	1.22	0.98
1:B:371:LYS:O	1:B:375:HIS:N[3_465]	1.22	0.98
1:B:375:HIS:CD2	1:B:375:HIS:NE2[4_445]	1.22	0.98
1:B:380:GLY:CA	1:B:402:TYR:C[4_445]	1.22	0.98
1:B:396:VAL:CG1	1:B:441:LEU:CD2[4_445]	1.22	0.98
1:B:400:PHE:CA	1:B:435:ILE:O[4_445]	1.22	0.98
1:A:175:ILE:O	1:A:374:LYS:CE[3_365]	1.23	0.97
1:A:175:ILE:O	1:A:374:LYS:NZ[3_365]	1.23	0.97
1:A:216:VAL:CG1	1:B:278:ILE:CG1[4_435]	1.23	0.97
1:A:302:ASP:N	1:A:303:ILE:CD1[2_345]	1.23	0.97
1:B:99:ASP:CB	1:B:448:ARG:O[4_445]	1.23	0.97
1:B:141:ARG:NE	1:B:472:HIS:CG[3_365]	1.23	0.97
1:B:346:ALA:O	1:B:361:LEU:C[4_445]	1.23	0.97
1:B:372:VAL:CA	1:B:373:ASN:C[2_355]	1.23	0.97
1:B:373:ASN:N	1:B:373:ASN:C[4_445]	1.23	0.97
1:B:387:HIS:C	1:B:413:LEU:CG[4_445]	1.23	0.97
1:A:86:ASP:CG	1:A:170:HIS:NE2[3_365]	1.24	0.96
1:A:97:GLY:O	5:A:518:HOH:O[3_365]	1.24	0.96
1:A:100:TYR:N	1:A:398:VAL:CA[3_365]	1.24	0.96
1:A:164:PRO:CA	1:A:273:ASP:OD2[4_435]	1.24	0.96
1:A:258:VAL:CG1	1:A:449:ARG:CD[3_365]	1.24	0.96
1:A:266:ILE:CG2	1:A:361:LEU:CG[3_365]	1.24	0.96
1:A:299:ASP:CB	5:A:601:HOH:O[2_345]	1.24	0.96
1:A:302:ASP:CG	1:A:303:ILE:CB[2_345]	1.24	0.96
1:A:306:LEU:C	1:A:366:LYS:CG[3_365]	1.24	0.96
1:A:315:PRO:C	1:A:361:LEU:CA[3_365]	1.24	0.96
1:A:329:TYR:CD1	1:A:470:PHE:O[2_345]	1.24	0.96
1:B:141:ARG:CB	1:B:473:HIS:N[3_365]	1.24	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ARG:CZ	1:B:417:ARG:N[4_445]	1.24	0.96
1:B:429:GLU:CA	1:B:429:GLU:O[4_445]	1.24	0.96
1:A:103:LEU:CG	1:A:402:TYR:CE1[3_365]	1.25	0.95
1:A:116:LEU:CB	1:A:432:LYS:CE[3_365]	1.25	0.95
1:A:141:ARG:CZ	1:A:438:LEU:CA[3_365]	1.25	0.95
1:A:145:GLN:CG	1:A:152:ASN:O[2_345]	1.25	0.95
1:A:155:PRO:CD	5:A:618:HOH:O[2_345]	1.25	0.95
1:A:220:LYS:NZ	1:B:275:ILE:N[4_435]	1.25	0.95
1:A:220:LYS:NZ	1:B:275:ILE:CA[4_435]	1.25	0.95
1:A:302:ASP:CG	1:A:303:ILE:CA[2_345]	1.25	0.95
1:A:328:GLY:N	1:A:469:ASP:CG[2_345]	1.25	0.95
1:A:329:TYR:CD2	1:A:471:GLN:CB[2_345]	1.25	0.95
1:B:110:SER:N	1:B:471:GLN:CA[3_365]	1.25	0.95
1:B:368:ILE:CG2	1:B:398:VAL:CA[3_465]	1.25	0.95
1:B:374:LYS:O	1:B:375:HIS:CB[4_445]	1.25	0.95
1:B:396:VAL:N	1:B:441:LEU:CB[4_445]	1.25	0.95
1:B:427:THR:OG1	1:B:435:ILE:CG2[2_355]	1.25	0.95
1:B:430:LEU:N	1:B:433:ALA:N[4_445]	1.25	0.95
1:A:101:ASP:C	1:A:400:PHE:CA[3_365]	1.26	0.94
1:A:101:ASP:C	1:A:400:PHE:O[3_365]	1.26	0.94
1:A:106:ARG:N	1:A:402:TYR:O[3_365]	1.26	0.94
1:A:212:TYR:C	1:B:260:PHE:N[4_435]	1.26	0.94
1:A:312:ASP:CA	1:A:359:ILE:N[3_365]	1.26	0.94
1:A:338:THR:CB	1:A:376:ALA:C[3_365]	1.26	0.94
1:B:99:ASP:CG	1:B:448:ARG:C[4_445]	1.26	0.94
1:B:99:ASP:C	1:B:450:LYS:N[4_445]	1.26	0.94
1:B:369:LYS:NZ	1:B:438:LEU:CG[3_465]	1.26	0.94
1:B:371:LYS:O	1:B:374:LYS:C[2_355]	1.26	0.94
1:B:375:HIS:ND1	1:B:375:HIS:CE1[3_465]	1.26	0.94
1:B:389:GLN:N	5:B:502:HOH:O[4_445]	1.26	0.94
1:B:403:LEU:CD2	1:B:420:TYR:CE1[3_465]	1.26	0.94
1:B:409:ASP:CB	1:B:422:SER:CA[3_465]	1.26	0.94
1:B:426:LEU:N	1:B:436:GLU:OE1[2_355]	1.26	0.94
1:B:432:LYS:CD	1:B:433:ALA:N[3_465]	1.26	0.94
1:A:86:ASP:O	1:A:358:SER:CB[3_365]	1.27	0.93
1:A:167:GLU:CA	1:A:277:LYS:O[4_435]	1.27	0.93
1:A:208:LEU:O	1:B:259:THR:CB[4_435]	1.27	0.93
1:A:328:GLY:CA	1:A:469:ASP:CB[2_345]	1.27	0.93
1:B:99:ASP:OD2	1:B:448:ARG:O[4_445]	1.27	0.93
1:B:101:ASP:O	1:B:465:LYS:NZ[3_365]	1.27	0.93
1:B:346:ALA:O	1:B:362:THR:CA[4_445]	1.27	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:C	1:B:375:HIS:N[4_445]	1.27	0.93
1:B:381:ARG:CB	1:B:404:THR:CA[4_445]	1.27	0.93
1:B:420:TYR:CG	1:B:437:VAL:CG2[4_445]	1.27	0.93
1:A:85:VAL:CG1	1:A:350:MET:CE[3_365]	1.28	0.92
1:A:114:LYS:N	1:A:429:GLU:CD[3_365]	1.28	0.92
1:A:213:SER:CB	1:A:275:ILE:CB[4_435]	1.28	0.92
1:A:220:LYS:N	1:A:260:PHE:C[4_435]	1.28	0.92
1:A:258:VAL:CA	1:A:449:ARG:O[3_365]	1.28	0.92
1:A:266:ILE:CB	1:A:361:LEU:CD1[3_365]	1.28	0.92
1:A:312:ASP:CB	1:A:358:SER:N[3_365]	1.28	0.92
1:A:321:ARG:C	1:A:443:ALA:O[3_365]	1.28	0.92
1:A:321:ARG:CD	1:A:439:GLN:O[3_365]	1.28	0.92
1:A:335:LEU:C	1:A:369:LYS:CA[3_365]	1.28	0.92
1:B:102:LYS:CE	1:B:453:THR:N[4_445]	1.28	0.92
1:B:366:LYS:CA	1:B:402:TYR:CZ[3_465]	1.28	0.92
1:B:388:ARG:NH2	1:B:416:ILE:C[4_445]	1.28	0.92
1:B:389:GLN:C	1:B:410:ASP:OD1[4_445]	1.28	0.92
1:B:397:ASP:C	1:B:438:LEU:CB[4_445]	1.28	0.92
1:B:399:SER:O	1:B:427:THR:CG2[3_465]	1.28	0.92
1:B:428:GLY:O	1:B:431:LYS:C[2_355]	1.28	0.92
1:B:453:THR:CG2	1:B:465:LYS:CB[2_345]	1.28	0.92
1:A:87:PRO:CB	1:A:360:PHE:CE2[3_365]	1.29	0.91
1:A:94:SER:CA	1:A:95:ALA:CA[2_245]	1.29	0.91
1:A:100:TYR:O	1:A:399:SER:CA[3_365]	1.29	0.91
1:A:140:HIS:O	1:A:435:ILE:O[3_365]	1.29	0.91
1:A:141:ARG:CG	1:A:439:GLN:N[3_365]	1.29	0.91
1:A:164:PRO:C	1:A:273:ASP:CG[4_435]	1.29	0.91
1:A:179:PHE:CE2	5:A:572:HOH:O[3_365]	1.29	0.91
1:A:197:ASP:CB	1:A:271:ASP:C[4_435]	1.29	0.91
1:A:219:ALA:N	1:A:260:PHE:O[4_435]	1.29	0.91
1:A:221:ASP:CA	1:A:263:VAL:N[4_435]	1.29	0.91
1:A:329:TYR:CE1	1:A:470:PHE:O[2_345]	1.29	0.91
1:A:355:PRO:C	4:A:502:ATP:O3'[4_435]	1.29	0.91
1:A:357:SER:N	4:A:502:ATP:O2'[4_435]	1.29	0.91
1:A:457:VAL:CG2	1:B:273:ASP:CA[4_435]	1.29	0.91
1:B:99:ASP:CB	1:B:449:ARG:N[4_445]	1.29	0.91
1:B:105:VAL:CB	1:B:465:LYS:CG[3_365]	1.29	0.91
1:B:381:ARG:CD	1:B:404:THR:O[4_445]	1.29	0.91
1:B:388:ARG:O	5:B:535:HOH:O[4_445]	1.29	0.91
1:B:412:LYS:C	1:B:424:ALA:CA[3_465]	1.29	0.91
1:A:82:GLU:OE2	1:A:100:TYR:CZ[3_365]	1.30	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:CB	1:A:346:ALA:CA[3_365]	1.30	0.90
1:A:101:ASP:O	1:A:400:PHE:O[3_365]	1.30	0.90
1:A:103:LEU:CA	1:A:402:TYR:N[3_365]	1.30	0.90
1:A:106:ARG:CD	1:A:405:PHE:CG[3_365]	1.30	0.90
1:A:111:LYS:CB	1:A:430:LEU:O[3_365]	1.30	0.90
1:A:141:ARG:CB	1:A:439:GLN:CG[3_365]	1.30	0.90
1:A:221:ASP:CB	1:A:263:VAL:N[4_435]	1.30	0.90
1:B:101:ASP:CB	1:B:451:GLU:CG[4_445]	1.30	0.90
1:B:110:SER:C	1:B:471:GLN:CG[3_365]	1.30	0.90
1:B:229:ILE:CD1	1:B:459:GLU:OE2[2_345]	1.30	0.90
1:B:334:LEU:CB	1:B:473:HIS:CA[3_365]	1.30	0.90
1:B:372:VAL:CB	1:B:373:ASN:CG[4_445]	1.30	0.90
1:B:372:VAL:CG1	1:B:431:LYS:NZ[3_465]	1.30	0.90
1:B:428:GLY:O	1:B:432:LYS:N[2_355]	1.30	0.90
1:B:428:GLY:C	1:B:431:LYS:N[4_445]	1.30	0.90
1:B:432:LYS:CG	1:B:433:ALA:CA[3_465]	1.30	0.90
1:B:455:GLU:OE2	1:B:464:ARG:CA[2_345]	1.30	0.90
1:A:93:SER:N	1:A:347:GLN:CD[2_245]	1.31	0.89
1:A:164:PRO:O	1:A:273:ASP:OD2[4_435]	1.31	0.89
1:A:167:GLU:CG	1:A:277:LYS:O[4_435]	1.31	0.89
1:A:218:ASN:CG	1:A:269:PHE:CG[4_435]	1.31	0.89
1:A:220:LYS:CD	1:B:275:ILE:N[4_435]	1.31	0.89
1:A:234:ILE:CD1	1:A:261:ASN:CG[4_435]	1.31	0.89
1:A:307:ILE:CD1	1:A:364:THR:CA[3_365]	1.31	0.89
1:A:316:TYR:CA	1:A:361:LEU:C[3_365]	1.31	0.89
1:A:317:PHE:CZ	1:A:367:GLN:OE1[3_365]	1.31	0.89
1:A:349:LYS:NZ	1:A:354:ASP:OD2[3_365]	1.31	0.89
1:A:455:GLU:N	1:B:277:LYS:NZ[4_435]	1.31	0.89
1:B:106:ARG:CA	5:B:581:HOH:O[3_365]	1.31	0.89
1:B:334:LEU:N	1:B:473:HIS:CB[3_365]	1.31	0.89
1:B:341:PRO:CA	1:B:363:ASP:C[4_445]	1.31	0.89
1:B:369:LYS:NZ	1:B:397:ASP:CB[2_355]	1.31	0.89
1:B:380:GLY:O	1:B:402:TYR:O[4_445]	1.31	0.89
1:B:387:HIS:CE1	1:B:403:LEU:CB[4_445]	1.31	0.89
1:B:427:THR:OG1	1:B:435:ILE:CB[2_355]	1.31	0.89
1:B:428:GLY:C	1:B:432:LYS:C[2_355]	1.31	0.89
1:A:105:VAL:O	1:A:406:PHE:N[3_365]	1.32	0.88
1:A:327:ILE:O	1:A:469:ASP:CG[2_345]	1.32	0.88
1:A:355:PRO:CA	4:A:502:ATP:C3'[4_435]	1.32	0.88
1:A:356:ASN:N	4:A:502:ATP:C1'[4_435]	1.32	0.88
1:B:202:LEU:O	5:A:523:HOH:O[3_365]	1.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:SER:O	1:B:470:PHE:O[3_365]	1.32	0.88
1:B:140:HIS:CB	1:B:473:HIS:CE1[3_365]	1.32	0.88
1:B:373:ASN:ND2	1:B:431:LYS:CG[2_355]	1.32	0.88
1:B:397:ASP:CB	1:B:438:LEU:CA[4_445]	1.32	0.88
1:B:428:GLY:C	1:B:433:ALA:N[2_355]	1.32	0.88
1:A:89:THR:CB	1:A:351:SER:OG[3_365]	1.33	0.87
1:A:92:THR:CA	1:A:346:ALA:O[3_365]	1.33	0.87
1:A:92:THR:CG2	1:A:346:ALA:C[3_365]	1.33	0.87
1:A:95:ALA:CB	1:A:96:LYS:N[4_435]	1.33	0.87
1:A:103:LEU:CD2	1:A:402:TYR:CE1[3_365]	1.33	0.87
1:A:136:ILE:C	1:A:373:ASN:O[3_365]	1.33	0.87
1:A:197:ASP:OD1	1:B:261:ASN:OD1[4_435]	1.33	0.87
1:A:212:TYR:CB	1:B:260:PHE:N[4_435]	1.33	0.87
1:A:217:GLU:CA	1:A:278:ILE:CG2[4_435]	1.33	0.87
1:A:218:ASN:C	1:A:260:PHE:O[4_435]	1.33	0.87
1:A:220:LYS:C	1:A:259:THR:O[4_435]	1.33	0.87
1:A:257:HIS:C	1:A:450:LYS:CA[3_365]	1.33	0.87
1:A:300:ARG:CB	1:A:301:THR:N[2_345]	1.33	0.87
1:A:310:ALA:O	1:A:371:LYS:CD[3_365]	1.33	0.87
1:A:333:ALA:O	1:A:365:ALA:C[3_365]	1.33	0.87
1:A:335:LEU:C	1:A:369:LYS:O[3_365]	1.33	0.87
1:B:130:HIS:CA	1:B:390:PHE:CD2[3_465]	1.33	0.87
1:B:140:HIS:CA	1:B:473:HIS:NE2[3_365]	1.33	0.87
1:B:340:PHE:C	1:B:364:THR:CG2[4_445]	1.33	0.87
1:B:374:LYS:C	1:B:374:LYS:CB[3_465]	1.33	0.87
1:B:401:MET:N	1:B:439:GLN:CG[4_445]	1.33	0.87
1:B:420:TYR:OH	1:B:434:LEU:CD1[4_445]	1.33	0.87
1:B:428:GLY:N	1:B:432:LYS:O[2_355]	1.33	0.87
1:A:86:ASP:CB	1:A:170:HIS:CE1[3_365]	1.34	0.86
1:A:99:ASP:CB	1:A:401:MET:CG[3_365]	1.34	0.86
1:A:207:THR:CG2	1:B:257:HIS:C[4_435]	1.34	0.86
1:A:214:TYR:CE1	1:A:277:LYS:N[4_435]	1.34	0.86
1:A:309:CYS:SG	1:A:367:GLN:O[3_365]	1.34	0.86
1:A:319:MET:C	1:A:446:GLN:CB[3_365]	1.34	0.86
1:A:322:ASP:CA	1:A:443:ALA:O[3_365]	1.34	0.86
1:A:322:ASP:C	1:A:447:ALA:CB[3_365]	1.34	0.86
1:B:171:VAL:CB	1:B:366:LYS:CE[4_445]	1.34	0.86
1:B:334:LEU:O	1:B:473:HIS:ND1[3_365]	1.34	0.86
1:B:368:ILE:CG1	1:B:398:VAL:CB[3_465]	1.34	0.86
1:B:428:GLY:C	1:B:432:LYS:CG[3_465]	1.34	0.86
1:B:430:LEU:CG	1:B:432:LYS:NZ[2_355]	1.34	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LYS:N	1:B:431:LYS:O[4_445]	1.34	0.86
1:A:89:THR:N	1:A:351:SER:CA[3_365]	1.35	0.85
1:A:94:SER:C	1:A:94:SER:C[4_435]	1.35	0.85
1:A:106:ARG:C	1:A:406:PHE:CD2[3_365]	1.35	0.85
1:A:165:SER:C	5:A:620:HOH:O[4_435]	1.35	0.85
1:A:222:ILE:N	1:A:261:ASN:C[4_435]	1.35	0.85
1:A:222:ILE:CB	1:A:261:ASN:O[4_435]	1.35	0.85
1:A:322:ASP:CB	1:A:444:GLU:O[3_365]	1.35	0.85
1:A:328:GLY:C	1:A:469:ASP:O[2_345]	1.35	0.85
1:A:457:VAL:CG2	1:B:273:ASP:O[4_435]	1.35	0.85
1:B:108:GLY:N	1:B:298:ARG:CA[3_365]	1.35	0.85
1:B:347:GLN:N	1:B:361:LEU:N[4_445]	1.35	0.85
1:B:374:LYS:CA	1:B:375:HIS:CA[4_445]	1.35	0.85
1:B:402:TYR:CB	1:B:439:GLN:NE2[4_445]	1.35	0.85
1:B:407:LEU:CD2	1:B:420:TYR:C[3_465]	1.35	0.85
1:B:431:LYS:CA	1:B:431:LYS:C[4_445]	1.35	0.85
1:A:82:GLU:CG	1:A:377:PHE:CG[2_245]	1.36	0.84
1:A:83:ASP:N	5:A:547:HOH:O[2_245]	1.36	0.84
1:A:84:PHE:CE2	4:A:502:ATP:C5[3_365]	1.36	0.84
1:A:92:THR:O	1:A:347:GLN:CA[3_365]	1.36	0.84
1:A:94:SER:CB	1:A:95:ALA:CB[2_245]	1.36	0.84
1:A:100:TYR:C	1:A:399:SER:C[3_365]	1.36	0.84
1:A:100:TYR:N	1:A:398:VAL:N[3_365]	1.36	0.84
1:A:162:ARG:CG	1:A:269:PHE:O[4_435]	1.36	0.84
1:A:165:SER:CB	5:A:620:HOH:O[4_435]	1.36	0.84
1:A:210:GLN:CD	1:B:256:LYS:O[4_435]	1.36	0.84
1:A:220:LYS:CB	1:A:259:THR:O[4_435]	1.36	0.84
1:A:257:HIS:CB	1:A:450:LYS:CB[3_365]	1.36	0.84
1:A:307:ILE:CG2	1:A:367:GLN:N[3_365]	1.36	0.84
1:A:315:PRO:CG	1:A:359:ILE:O[3_365]	1.36	0.84
1:A:316:TYR:O	1:A:361:LEU:O[3_365]	1.36	0.84
1:A:317:PHE:CD2	1:A:364:THR:N[3_365]	1.36	0.84
1:A:323:VAL:N	1:A:447:ALA:N[3_365]	1.36	0.84
1:B:97:GLY:O	1:B:445:HIS:ND1[4_445]	1.36	0.84
1:B:134:ARG:NH2	1:B:391:GLY:N[3_465]	1.36	0.84
1:B:134:ARG:CZ	1:B:390:PHE:CA[3_465]	1.36	0.84
1:B:372:VAL:O	1:B:373:ASN:C[3_465]	1.36	0.84
1:B:387:HIS:O	1:B:413:LEU:CD2[4_445]	1.36	0.84
1:B:392:GLY:N	1:B:407:LEU:N[4_445]	1.36	0.84
1:B:430:LEU:CA	1:B:432:LYS:CD[2_355]	1.36	0.84
1:A:84:PHE:CA	1:A:340:PHE:C[3_365]	1.37	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASP:OD2	5:A:603:HOH:O[3_365]	1.37	0.83
1:A:102:LYS:N	1:A:400:PHE:O[3_365]	1.37	0.83
1:A:137:PHE:CG	1:A:373:ASN:CB[3_365]	1.37	0.83
1:A:140:HIS:O	1:A:436:GLU:N[3_365]	1.37	0.83
1:A:166:SER:CB	1:A:203:TRP:CE2[4_435]	1.37	0.83
1:A:209:ASP:CA	1:B:259:THR:N[4_435]	1.37	0.83
1:A:302:ASP:OD2	1:A:303:ILE:N[2_345]	1.37	0.83
1:A:308:PRO:CA	1:A:370:THR:OG1[3_365]	1.37	0.83
1:A:308:PRO:CD	1:A:366:LYS:CD[3_365]	1.37	0.83
1:A:316:TYR:N	1:A:361:LEU:N[3_365]	1.37	0.83
1:A:318:ARG:C	1:A:442:ILE:C[3_365]	1.37	0.83
1:B:366:LYS:CG	1:B:377:PHE:CE1[2_355]	1.37	0.83
1:B:371:LYS:O	1:B:374:LYS:N[2_355]	1.37	0.83
1:B:395:ASP:C	1:B:441:LEU:CB[4_445]	1.37	0.83
1:B:397:ASP:O	1:B:438:LEU:C[4_445]	1.37	0.83
1:B:410:ASP:O	5:B:538:HOH:O[3_465]	1.37	0.83
1:B:429:GLU:N	1:B:430:LEU:C[4_445]	1.37	0.83
1:A:88:TRP:CD1	1:A:352:ALA:CB[3_365]	1.38	0.82
1:A:88:TRP:CB	1:A:352:ALA:CB[3_365]	1.38	0.82
1:A:91:GLN:N	1:A:349:LYS:O[3_365]	1.38	0.82
1:A:101:ASP:CB	1:A:400:PHE:CA[3_365]	1.38	0.82
1:A:111:LYS:CD	1:A:430:LEU:CB[3_365]	1.38	0.82
1:A:111:LYS:CA	1:A:430:LEU:O[3_365]	1.38	0.82
1:A:137:PHE:CE2	1:A:370:THR:O[3_365]	1.38	0.82
1:A:210:GLN:CA	1:A:274:CYS:CB[4_435]	1.38	0.82
1:A:221:ASP:CB	1:A:263:VAL:CA[4_435]	1.38	0.82
1:A:319:MET:CE	5:A:519:HOH:O[3_365]	1.38	0.82
1:A:319:MET:CG	5:A:532:HOH:O[3_365]	1.38	0.82
1:A:347:GLN:CA	1:A:347:GLN:CG[3_365]	1.38	0.82
1:B:134:ARG:N	1:B:390:PHE:CE1[3_465]	1.38	0.82
1:B:134:ARG:CD	1:B:386:GLU:O[3_465]	1.38	0.82
1:B:134:ARG:NH2	1:B:390:PHE:C[3_465]	1.38	0.82
1:B:366:LYS:C	1:B:402:TYR:CE1[3_465]	1.38	0.82
1:B:429:GLU:N	1:B:432:LYS:CG[3_465]	1.38	0.82
1:A:82:GLU:CG	1:A:377:PHE:CB[2_245]	1.39	0.81
1:A:84:PHE:CG	4:A:502:ATP:N1[3_365]	1.39	0.81
1:A:110:SER:CB	1:A:433:ALA:O[3_365]	1.39	0.81
1:A:114:LYS:NZ	1:A:388:ARG:NH1[3_365]	1.39	0.81
1:A:164:PRO:CB	1:A:270:THR:N[4_435]	1.39	0.81
1:A:206:LEU:CD1	5:A:529:HOH:O[4_435]	1.39	0.81
1:A:218:ASN:O	1:A:264:LYS:N[4_435]	1.39	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:N	1:A:260:PHE:N[4_435]	1.39	0.81
1:A:221:ASP:N	1:A:263:VAL:N[4_435]	1.39	0.81
1:A:318:ARG:CB	1:A:442:ILE:CG1[3_365]	1.39	0.81
1:A:326:ARG:CB	5:A:610:HOH:O[3_365]	1.39	0.81
1:A:328:GLY:C	1:A:470:PHE:N[2_345]	1.39	0.81
1:B:104:ILE:N	1:B:298:ARG:NH2[3_365]	1.39	0.81
1:B:307:ILE:CD1	1:B:475:HIS:CA[3_365]	1.39	0.81
1:B:384:ILE:CD1	1:B:394:CYS:SG[4_445]	1.39	0.81
1:B:397:ASP:CB	1:B:438:LEU:CB[4_445]	1.39	0.81
1:B:409:ASP:OD2	1:B:422:SER:CB[3_465]	1.39	0.81
1:A:102:LYS:C	1:A:402:TYR:N[3_365]	1.40	0.80
1:A:105:VAL:N	1:A:403:LEU:N[3_365]	1.40	0.80
1:A:106:ARG:O	1:A:406:PHE:CG[3_365]	1.40	0.80
1:A:109:SER:CB	1:A:434:LEU:O[3_365]	1.40	0.80
1:A:109:SER:O	1:A:437:VAL:CB[3_365]	1.40	0.80
1:A:110:SER:C	1:A:433:ALA:O[3_365]	1.40	0.80
1:A:111:LYS:CE	1:A:430:LEU:CG[3_365]	1.40	0.80
1:A:111:LYS:N	1:A:433:ALA:CA[3_365]	1.40	0.80
1:A:148:ASP:CG	1:A:152:ASN:ND2[2_345]	1.40	0.80
1:A:220:LYS:NZ	1:B:275:ILE:C[4_435]	1.40	0.80
1:A:307:ILE:CA	1:A:366:LYS:C[3_365]	1.40	0.80
1:A:317:PHE:CD1	1:A:363:ASP:CB[3_365]	1.40	0.80
1:A:322:ASP:CB	1:A:444:GLU:C[3_365]	1.40	0.80
1:A:339:PHE:CB	1:A:344:GLN:CD[3_365]	1.40	0.80
1:A:356:ASN:N	4:A:502:ATP:C3'[4_435]	1.40	0.80
1:A:356:ASN:N	4:A:502:ATP:O2'[4_435]	1.40	0.80
1:B:275:ILE:CG1	5:A:520:HOH:O[3_365]	1.40	0.80
1:B:171:VAL:CA	1:B:366:LYS:NZ[4_445]	1.40	0.80
1:B:369:LYS:CE	1:B:397:ASP:CG[2_355]	1.40	0.80
1:B:371:LYS:C	1:B:375:HIS:C[3_465]	1.40	0.80
1:B:381:ARG:CB	1:B:404:THR:C[4_445]	1.40	0.80
1:B:382:ASP:OD2	1:B:405:PHE:CZ[4_445]	1.40	0.80
1:A:89:THR:N	1:A:351:SER:O[3_365]	1.41	0.79
1:A:90:VAL:CG2	1:A:357:SER:CB[3_365]	1.41	0.79
1:A:98:ILE:CG1	1:A:398:VAL:CG2[3_365]	1.41	0.79
1:A:103:LEU:CB	1:A:402:TYR:CG[3_365]	1.41	0.79
1:A:106:ARG:C	1:A:406:PHE:CG[3_365]	1.41	0.79
1:A:111:LYS:NZ	1:A:430:LEU:CB[3_365]	1.41	0.79
1:A:138:PHE:CE1	1:A:376:ALA:CB[3_365]	1.41	0.79
1:A:166:SER:O	1:A:269:PHE:CD1[4_435]	1.41	0.79
1:A:169:MET:O	1:A:267:PHE:CD2[4_435]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:CA	1:A:267:PHE:CG[4_435]	1.41	0.79
1:A:197:ASP:CB	1:A:272:SER:CA[4_435]	1.41	0.79
1:A:209:ASP:OD2	1:B:258:VAL:CG2[4_435]	1.41	0.79
1:A:313:GLN:CB	1:A:363:ASP:OD2[3_365]	1.41	0.79
1:A:336:HIS:CB	1:A:372:VAL:CB[3_365]	1.41	0.79
1:A:355:PRO:CD	4:A:502:ATP:C5'[4_435]	1.41	0.79
1:A:386:GLU:OE2	1:A:417:ARG:NE[4_435]	1.41	0.79
1:B:140:HIS:N	1:B:471:GLN:NE2[3_365]	1.41	0.79
1:B:169:MET:O	1:B:347:GLN:CB[3_465]	1.41	0.79
1:B:317:PHE:CE1	1:B:475:HIS:C[3_365]	1.41	0.79
1:B:366:LYS:O	1:B:402:TYR:OH[3_465]	1.41	0.79
1:B:368:ILE:CG2	1:B:398:VAL:C[3_465]	1.41	0.79
1:B:381:ARG:CD	1:B:404:THR:C[4_445]	1.41	0.79
1:B:430:LEU:CB	1:B:433:ALA:CA[4_445]	1.41	0.79
1:B:430:LEU:CD1	1:B:432:LYS:CE[2_355]	1.41	0.79
1:B:453:THR:CG2	1:B:465:LYS:N[2_345]	1.41	0.79
1:A:84:PHE:CZ	1:A:356:ASN:ND2[2_245]	1.42	0.78
1:A:86:ASP:CB	1:A:170:HIS:CG[3_365]	1.42	0.78
1:A:96:LYS:O	1:A:377:PHE:CE2[3_365]	1.42	0.78
1:A:103:LEU:CD1	1:A:402:TYR:CE1[3_365]	1.42	0.78
1:A:111:LYS:CD	1:A:430:LEU:CA[3_365]	1.42	0.78
1:A:138:PHE:N	1:A:431:LYS:CG[3_365]	1.42	0.78
1:A:140:HIS:C	1:A:435:ILE:C[3_365]	1.42	0.78
1:A:162:ARG:CD	1:A:268:GLY:C[4_435]	1.42	0.78
1:A:169:MET:N	1:A:267:PHE:CD2[4_435]	1.42	0.78
1:A:169:MET:CB	1:A:267:PHE:CA[4_435]	1.42	0.78
1:A:210:GLN:N	1:B:258:VAL:O[4_435]	1.42	0.78
1:A:257:HIS:CA	1:A:450:LYS:CA[3_365]	1.42	0.78
1:A:312:ASP:OD2	1:A:358:SER:N[3_365]	1.42	0.78
1:A:314:ASP:N	1:A:359:ILE:CG2[3_365]	1.42	0.78
1:B:102:LYS:CA	1:B:451:GLU:CA[4_445]	1.42	0.78
1:B:341:PRO:CB	1:B:363:ASP:O[4_445]	1.42	0.78
1:B:344:GLN:CB	1:B:355:PRO:O[4_445]	1.42	0.78
1:B:365:ALA:C	1:B:402:TYR:CD1[3_465]	1.42	0.78
1:B:367:GLN:CG	5:B:480:HOH:O[3_465]	1.42	0.78
1:B:373:ASN:CB	1:B:431:LYS:NZ[4_445]	1.42	0.78
1:B:374:LYS:CB	1:B:375:HIS:CB[2_355]	1.42	0.78
1:B:374:LYS:O	1:B:375:HIS:CA[4_445]	1.42	0.78
1:B:375:HIS:CD2	1:B:375:HIS:CD2[4_445]	1.42	0.78
1:B:382:ASP:OD1	1:B:405:PHE:CE1[4_445]	1.42	0.78
1:B:429:GLU:CA	1:B:429:GLU:C[4_445]	1.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:GLU:C	1:B:432:LYS:CB[2_355]	1.42	0.78
1:A:169:MET:CA	1:A:267:PHE:CB[4_435]	1.43	0.77
1:A:210:GLN:OE1	1:B:256:LYS:O[4_435]	1.43	0.77
1:A:215:ALA:C	1:A:260:PHE:CE1[4_435]	1.43	0.77
1:A:218:ASN:O	1:A:260:PHE:O[4_435]	1.43	0.77
1:A:322:ASP:OD1	1:A:444:GLU:CA[3_365]	1.43	0.77
1:A:334:LEU:CA	1:A:365:ALA:O[3_365]	1.43	0.77
1:A:356:ASN:C	4:A:502:ATP:O2'[4_435]	1.43	0.77
1:B:264:LYS:CE	5:A:560:HOH:O[3_365]	1.43	0.77
1:B:134:ARG:CZ	1:B:390:PHE:N[3_465]	1.43	0.77
1:B:171:VAL:CB	1:B:366:LYS:CD[4_445]	1.43	0.77
1:B:372:VAL:O	1:B:373:ASN:O[3_465]	1.43	0.77
1:B:444:GLU:N	5:B:552:HOH:O[3_465]	1.43	0.77
1:A:84:PHE:CB	1:A:344:GLN:OE1[2_245]	1.44	0.76
1:A:85:VAL:CG2	1:A:341:PRO:C[3_365]	1.44	0.76
1:A:89:THR:O	1:A:350:MET:C[3_365]	1.44	0.76
1:A:89:THR:N	1:A:352:ALA:N[3_365]	1.44	0.76
1:A:90:VAL:C	1:A:349:LYS:O[3_365]	1.44	0.76
1:A:93:SER:CB	1:A:345:GLY:C[2_245]	1.44	0.76
1:A:99:ASP:O	1:A:401:MET:CB[3_365]	1.44	0.76
1:A:100:TYR:O	1:A:399:SER:O[3_365]	1.44	0.76
1:A:105:VAL:CG2	1:A:403:LEU:C[3_365]	1.44	0.76
1:A:107:PHE:CE1	1:A:340:PHE:CZ[3_365]	1.44	0.76
1:A:197:ASP:CA	1:A:272:SER:CB[4_435]	1.44	0.76
1:A:212:TYR:C	1:B:260:PHE:CA[4_435]	1.44	0.76
1:A:234:ILE:O	5:B:573:HOH:O[4_435]	1.44	0.76
1:A:302:ASP:CG	1:A:303:ILE:N[2_345]	1.44	0.76
1:A:302:ASP:OD2	1:A:303:ILE:C[2_345]	1.44	0.76
1:A:335:LEU:N	1:A:369:LYS:N[3_365]	1.44	0.76
1:A:337:SER:O	1:A:371:LYS:O[3_365]	1.44	0.76
1:B:368:ILE:CG1	1:B:398:VAL:CG2[3_465]	1.44	0.76
1:B:375:HIS:CG	1:B:375:HIS:ND1[3_465]	1.44	0.76
1:B:380:GLY:CA	1:B:403:LEU:N[4_445]	1.44	0.76
1:B:397:ASP:CA	1:B:438:LEU:CA[4_445]	1.44	0.76
1:A:112:ILE:O	1:A:428:GLY:C[3_365]	1.45	0.75
1:A:112:ILE:O	1:A:429:GLU:N[3_365]	1.45	0.75
1:A:169:MET:O	1:A:267:PHE:CE2[4_435]	1.45	0.75
1:A:212:TYR:CD1	1:B:261:ASN:N[4_435]	1.45	0.75
1:A:214:TYR:CA	1:A:278:ILE:CG1[4_435]	1.45	0.75
1:A:214:TYR:C	1:A:278:ILE:CG1[4_435]	1.45	0.75
1:A:215:ALA:C	1:A:260:PHE:CZ[4_435]	1.45	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:HIS:CB	1:A:450:LYS:CA[3_365]	1.45	0.75
1:A:289:PHE:CD1	1:A:471:GLN:C[2_345]	1.45	0.75
1:A:306:LEU:C	1:A:366:LYS:CB[3_365]	1.45	0.75
1:A:311:ILE:O	1:A:359:ILE:CD1[3_365]	1.45	0.75
1:A:316:TYR:CE1	1:A:360:PHE:CG[3_365]	1.45	0.75
1:A:321:ARG:NE	1:A:439:GLN:C[3_365]	1.45	0.75
1:A:367:GLN:CD	3:A:501:LTN:CZ2[4_435]	1.45	0.75
1:B:98:ILE:CB	5:B:513:HOH:O[4_445]	1.45	0.75
1:B:102:LYS:C	1:B:450:LYS:O[4_445]	1.45	0.75
1:B:110:SER:N	1:B:470:PHE:C[3_365]	1.45	0.75
1:B:371:LYS:CA	1:B:375:HIS:C[3_465]	1.45	0.75
1:B:372:VAL:N	1:B:376:ALA:CA[3_465]	1.45	0.75
1:B:381:ARG:CG	1:B:404:THR:CA[4_445]	1.45	0.75
1:B:428:GLY:CA	1:B:431:LYS:O[2_355]	1.45	0.75
1:B:430:LEU:N	1:B:432:LYS:CG[2_355]	1.45	0.75
1:A:94:SER:C	1:A:95:ALA:CA[3_365]	1.46	0.74
1:A:104:ILE:N	1:A:402:TYR:CB[3_365]	1.46	0.74
1:A:112:ILE:CG2	5:A:569:HOH:O[3_365]	1.46	0.74
1:A:162:ARG:O	1:A:270:THR:CG2[4_435]	1.46	0.74
1:A:169:MET:CA	1:A:267:PHE:CD2[4_435]	1.46	0.74
1:A:215:ALA:O	1:A:260:PHE:CE2[4_435]	1.46	0.74
1:A:217:GLU:N	1:A:278:ILE:CG2[4_435]	1.46	0.74
1:A:217:GLU:O	1:A:263:VAL:CG2[4_435]	1.46	0.74
1:A:218:ASN:ND2	1:A:269:PHE:CG[4_435]	1.46	0.74
1:A:219:ALA:CA	1:A:260:PHE:O[4_435]	1.46	0.74
1:A:299:ASP:C	1:A:299:ASP:C[2_345]	1.46	0.74
1:A:320:THR:C	1:A:446:GLN:OE1[3_365]	1.46	0.74
1:A:326:ARG:NH2	1:A:451:GLU:N[3_365]	1.46	0.74
1:A:335:LEU:CD1	1:A:369:LYS:CE[3_365]	1.46	0.74
1:A:336:HIS:CA	1:A:372:VAL:N[3_365]	1.46	0.74
1:A:338:THR:CA	1:A:375:HIS:O[3_365]	1.46	0.74
1:A:356:ASN:CA	4:A:502:ATP:C1'[4_435]	1.46	0.74
1:A:444:GLU:OE1	5:A:617:HOH:O[4_435]	1.46	0.74
1:B:334:LEU:C	1:B:473:HIS:CG[3_365]	1.46	0.74
1:B:384:ILE:CB	1:B:400:PHE:CE2[4_445]	1.46	0.74
1:B:399:SER:C	1:B:435:ILE:CG2[4_445]	1.46	0.74
1:B:409:ASP:CB	1:B:422:SER:CB[3_465]	1.46	0.74
1:B:431:LYS:CA	1:B:431:LYS:CB[3_465]	1.46	0.74
1:B:440:PRO:CA	5:B:567:HOH:O[2_355]	1.46	0.74
1:B:458:LYS:CB	1:B:462:THR:CB[2_345]	1.46	0.74
1:A:83:ASP:OD2	1:A:401:MET:SD[3_365]	1.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:CD2	1:A:402:TYR:CE2[3_365]	1.47	0.73
1:A:111:LYS:CG	1:A:430:LEU:O[3_365]	1.47	0.73
1:A:113:ASP:N	1:A:429:GLU:CA[3_365]	1.47	0.73
1:A:140:HIS:O	1:A:435:ILE:CA[3_365]	1.47	0.73
1:A:169:MET:C	1:A:267:PHE:CD2[4_435]	1.47	0.73
1:A:212:TYR:CB	1:B:259:THR:O[4_435]	1.47	0.73
1:A:218:ASN:OD1	1:A:269:PHE:CA[4_435]	1.47	0.73
1:A:220:LYS:O	1:A:262:GLN:CB[4_435]	1.47	0.73
1:A:221:ASP:CB	1:A:262:GLN:C[4_435]	1.47	0.73
1:A:257:HIS:C	1:A:449:ARG:O[3_365]	1.47	0.73
1:A:309:CYS:C	1:A:371:LYS:CG[3_365]	1.47	0.73
1:A:312:ASP:C	1:A:358:SER:O[3_365]	1.47	0.73
1:A:318:ARG:CA	1:A:442:ILE:CG2[3_365]	1.47	0.73
1:A:327:ILE:C	1:A:469:ASP:OD1[2_345]	1.47	0.73
1:A:336:HIS:CG	1:A:372:VAL:CG2[3_365]	1.47	0.73
1:A:456:ILE:O	1:B:272:SER:OG[4_435]	1.47	0.73
1:B:102:LYS:CG	1:B:452:VAL:C[4_445]	1.47	0.73
1:B:108:GLY:CA	1:B:297:PHE:C[3_365]	1.47	0.73
1:B:109:SER:C	1:B:471:GLN:N[3_365]	1.47	0.73
1:B:343:LEU:CD2	1:B:367:GLN:O[4_445]	1.47	0.73
1:B:348:THR:O	1:B:362:THR:OG1[4_445]	1.47	0.73
1:B:370:THR:O	1:B:371:LYS:C[3_465]	1.47	0.73
1:B:378:SER:O	1:B:402:TYR:CD2[4_445]	1.47	0.73
1:B:387:HIS:ND1	1:B:403:LEU:C[4_445]	1.47	0.73
1:B:388:ARG:NH1	1:B:416:ILE:N[4_445]	1.47	0.73
1:B:395:ASP:O	1:B:441:LEU:O[4_445]	1.47	0.73
1:B:426:LEU:CB	1:B:436:GLU:CG[2_355]	1.47	0.73
1:B:428:GLY:O	1:B:432:LYS:CA[3_465]	1.47	0.73
1:B:430:LEU:O	1:B:432:LYS:C[4_445]	1.47	0.73
1:B:431:LYS:CA	5:B:501:HOH:O[2_355]	1.47	0.73
1:B:432:LYS:CB	1:B:433:ALA:N[3_465]	1.47	0.73
1:B:455:GLU:OE1	5:B:563:HOH:O[2_345]	1.47	0.73
1:A:82:GLU:OE1	1:A:398:VAL:CG2[2_245]	1.48	0.72
1:A:83:ASP:O	1:A:340:PHE:C[3_365]	1.48	0.72
1:A:92:THR:CG2	1:A:346:ALA:CB[3_365]	1.48	0.72
1:A:92:THR:CA	1:A:346:ALA:C[3_365]	1.48	0.72
1:A:93:SER:OG	1:A:345:GLY:CA[2_245]	1.48	0.72
1:A:114:LYS:CG	1:A:429:GLU:OE1[3_365]	1.48	0.72
1:A:140:HIS:ND1	1:A:432:LYS:O[3_365]	1.48	0.72
1:A:141:ARG:CA	1:A:439:GLN:OE1[3_365]	1.48	0.72
1:A:207:THR:CG2	1:B:257:HIS:CA[4_435]	1.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:CD2	1:A:363:ASP:O[3_365]	1.48	0.72
1:A:355:PRO:CD	4:A:502:ATP:O5'[4_435]	1.48	0.72
1:A:356:ASN:ND2	4:A:502:ATP:C5[4_435]	1.48	0.72
1:A:356:ASN:CG	4:A:502:ATP:C4[4_435]	1.48	0.72
1:A:454:ASP:OD1	1:B:277:LYS:CG[4_435]	1.48	0.72
1:B:99:ASP:OD2	5:B:583:HOH:O[4_445]	1.48	0.72
1:B:109:SER:CA	1:B:470:PHE:O[3_365]	1.48	0.72
1:B:141:ARG:CD	1:B:472:HIS:CB[3_365]	1.48	0.72
1:B:171:VAL:CG1	1:B:366:LYS:CG[4_445]	1.48	0.72
1:B:343:LEU:C	1:B:371:LYS:CD[4_445]	1.48	0.72
1:B:347:GLN:N	1:B:361:LEU:CA[4_445]	1.48	0.72
1:B:372:VAL:CB	1:B:373:ASN:CB[4_445]	1.48	0.72
1:B:375:HIS:CG	1:B:375:HIS:NE2[4_445]	1.48	0.72
1:B:381:ARG:CD	1:B:405:PHE:N[4_445]	1.48	0.72
1:B:384:ILE:CB	1:B:440:PRO:CG[2_355]	1.48	0.72
1:B:388:ARG:CD	1:B:413:LEU:O[4_445]	1.48	0.72
1:B:409:ASP:CG	1:B:422:SER:CB[3_465]	1.48	0.72
1:B:430:LEU:C	1:B:432:LYS:N[4_445]	1.48	0.72
1:B:431:LYS:N	5:B:501:HOH:O[2_355]	1.48	0.72
1:A:82:GLU:OE1	1:A:98:ILE:O[3_365]	1.49	0.71
1:A:91:GLN:N	1:A:349:LYS:C[3_365]	1.49	0.71
1:A:110:SER:CA	1:A:433:ALA:C[3_365]	1.49	0.71
1:A:208:LEU:O	1:B:259:THR:CA[4_435]	1.49	0.71
1:A:217:GLU:OE1	1:B:275:ILE:CB[4_435]	1.49	0.71
1:A:257:HIS:CB	1:A:450:LYS:C[3_365]	1.49	0.71
1:A:258:VAL:CB	1:A:449:ARG:CG[3_365]	1.49	0.71
1:A:279:SER:C	5:A:555:HOH:O[3_365]	1.49	0.71
1:A:308:PRO:N	1:A:366:LYS:O[3_365]	1.49	0.71
1:A:312:ASP:O	1:A:359:ILE:N[3_365]	1.49	0.71
1:A:328:GLY:C	1:A:469:ASP:CA[2_345]	1.49	0.71
1:A:337:SER:C	1:A:371:LYS:O[3_365]	1.49	0.71
1:A:337:SER:CA	1:A:371:LYS:O[3_365]	1.49	0.71
1:A:339:PHE:CD2	1:A:344:GLN:N[3_365]	1.49	0.71
1:B:110:SER:O	1:B:471:GLN:OE1[3_365]	1.49	0.71
1:B:340:PHE:CG	5:B:524:HOH:O[4_445]	1.49	0.71
1:B:368:ILE:CG2	1:B:398:VAL:CB[3_465]	1.49	0.71
1:B:388:ARG:N	1:B:413:LEU:CG[4_445]	1.49	0.71
1:B:430:LEU:CD2	1:B:434:LEU:C[4_445]	1.49	0.71
1:A:82:GLU:CA	1:A:377:PHE:CB[2_245]	1.50	0.70
1:A:90:VAL:O	1:A:348:THR:CG2[3_365]	1.50	0.70
1:A:90:VAL:CG1	1:A:91:GLN:OE1[4_435]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:O	1:A:95:ALA:CA[3_365]	1.50	0.70
1:A:310:ALA:C	1:A:371:LYS:CB[3_365]	1.50	0.70
1:A:312:ASP:CB	1:A:358:SER:C[3_365]	1.50	0.70
1:A:320:THR:OG1	1:A:446:GLN:NE2[3_365]	1.50	0.70
1:A:339:PHE:CE2	1:A:343:LEU:CA[3_365]	1.50	0.70
1:A:355:PRO:C	4:A:502:ATP:C2'[4_435]	1.50	0.70
1:A:454:ASP:CB	1:B:277:LYS:CG[4_435]	1.50	0.70
1:A:457:VAL:O	1:B:270:THR:OG1[4_435]	1.50	0.70
1:B:102:LYS:CB	1:B:451:GLU:O[4_445]	1.50	0.70
1:B:133:ARG:CB	1:B:390:PHE:CZ[3_465]	1.50	0.70
1:B:346:ALA:O	1:B:361:LEU:O[4_445]	1.50	0.70
1:B:347:GLN:N	1:B:362:THR:N[4_445]	1.50	0.70
1:B:380:GLY:CA	1:B:402:TYR:O[4_445]	1.50	0.70
1:B:382:ASP:O	1:B:401:MET:CG[4_445]	1.50	0.70
1:B:382:ASP:CG	1:B:405:PHE:CE1[4_445]	1.50	0.70
1:B:412:LYS:NZ	1:B:419:ASP:CA[3_465]	1.50	0.70
1:B:430:LEU:CB	1:B:434:LEU:N[4_445]	1.50	0.70
1:A:84:PHE:O	1:A:350:MET:N[3_365]	1.51	0.69
1:A:90:VAL:CB	1:A:91:GLN:OE1[4_435]	1.51	0.69
1:A:212:TYR:CG	1:B:260:PHE:O[4_435]	1.51	0.69
1:A:257:HIS:O	1:A:450:LYS:CA[3_365]	1.51	0.69
1:A:313:GLN:C	1:A:363:ASP:OD2[3_365]	1.51	0.69
1:A:335:LEU:CD1	1:A:369:LYS:CD[3_365]	1.51	0.69
1:A:338:THR:N	1:A:375:HIS:C[3_365]	1.51	0.69
1:A:339:PHE:CD2	1:A:343:LEU:N[3_365]	1.51	0.69
1:A:457:VAL:CG2	1:B:274:CYS:N[4_435]	1.51	0.69
1:B:140:HIS:O	1:B:471:GLN:CB[3_365]	1.51	0.69
1:B:317:PHE:C	1:B:474:HIS:CE1[3_365]	1.51	0.69
1:B:317:PHE:CB	1:B:474:HIS:CD2[3_365]	1.51	0.69
1:B:344:GLN:CG	1:B:355:PRO:O[4_445]	1.51	0.69
1:B:366:LYS:CE	1:B:377:PHE:CZ[2_355]	1.51	0.69
1:B:381:ARG:CD	1:B:405:PHE:CA[4_445]	1.51	0.69
1:B:382:ASP:O	1:B:439:GLN:O[2_355]	1.51	0.69
1:B:395:ASP:CA	1:B:441:LEU:CB[4_445]	1.51	0.69
1:B:397:ASP:CB	1:B:438:LEU:N[4_445]	1.51	0.69
1:B:403:LEU:CD1	1:B:427:THR:N[3_465]	1.51	0.69
1:B:409:ASP:C	1:B:422:SER:O[3_465]	1.51	0.69
1:A:92:THR:CG2	1:A:346:ALA:N[3_365]	1.52	0.68
1:A:102:LYS:CB	1:A:401:MET:CA[3_365]	1.52	0.68
1:A:111:LYS:CD	1:A:430:LEU:CG[3_365]	1.52	0.68
1:A:141:ARG:NH1	1:A:438:LEU:CA[3_365]	1.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:O	1:A:272:SER:OG[4_435]	1.52	0.68
1:A:211:ALA:CA	1:A:273:ASP:C[4_435]	1.52	0.68
1:A:307:ILE:CG1	1:A:364:THR:OG1[3_365]	1.52	0.68
1:A:309:CYS:O	1:A:371:LYS:CB[3_365]	1.52	0.68
1:A:318:ARG:N	1:A:442:ILE:CB[3_365]	1.52	0.68
1:A:329:TYR:CE2	1:A:471:GLN:CB[2_345]	1.52	0.68
1:A:337:SER:N	1:A:371:LYS:O[3_365]	1.52	0.68
1:A:339:PHE:CB	1:A:344:GLN:OE1[3_365]	1.52	0.68
1:A:339:PHE:CD2	1:A:343:LEU:CA[3_365]	1.52	0.68
1:B:429:GLU:N	1:B:432:LYS:CD[3_465]	1.52	0.68
1:A:86:ASP:CB	1:A:170:HIS:ND1[3_365]	1.53	0.67
1:A:93:SER:OG	1:A:97:GLY:C[3_365]	1.53	0.67
1:A:102:LYS:CA	1:A:401:MET:CA[3_365]	1.53	0.67
1:A:137:PHE:CZ	1:A:370:THR:O[3_365]	1.53	0.67
1:A:138:PHE:CA	1:A:431:LYS:CD[3_365]	1.53	0.67
1:A:140:HIS:C	1:A:435:ILE:CG2[3_365]	1.53	0.67
1:A:213:SER:OG	1:A:275:ILE:CG1[4_435]	1.53	0.67
1:A:213:SER:CB	1:A:275:ILE:N[4_435]	1.53	0.67
1:A:234:ILE:C	1:B:271:ASP:OD2[4_435]	1.53	0.67
1:A:236:SER:N	1:A:271:ASP:OD2[4_435]	1.53	0.67
1:A:336:HIS:NE2	1:A:368:ILE:CG2[3_365]	1.53	0.67
1:A:338:THR:CG2	1:A:376:ALA:CA[3_365]	1.53	0.67
1:A:382:ASP:OD1	1:A:400:PHE:CZ[4_435]	1.53	0.67
1:A:454:ASP:CA	1:B:277:LYS:CD[4_435]	1.53	0.67
1:B:97:GLY:N	1:B:445:HIS:CB[4_445]	1.53	0.67
1:B:98:ILE:C	1:B:446:GLN:O[4_445]	1.53	0.67
1:B:99:ASP:N	1:B:449:ARG:CB[4_445]	1.53	0.67
1:B:134:ARG:CZ	1:B:390:PHE:C[3_465]	1.53	0.67
1:B:340:PHE:CZ	5:B:524:HOH:O[4_445]	1.53	0.67
1:B:344:GLN:OE1	1:B:356:ASN:ND2[4_445]	1.53	0.67
1:B:344:GLN:CB	1:B:371:LYS:NZ[4_445]	1.53	0.67
1:B:370:THR:O	1:B:375:HIS:C[2_355]	1.53	0.67
1:B:378:SER:C	1:B:402:TYR:CD2[4_445]	1.53	0.67
1:B:381:ARG:CB	1:B:404:THR:CB[4_445]	1.53	0.67
1:B:412:LYS:O	1:B:424:ALA:C[3_465]	1.53	0.67
1:B:426:LEU:CG	1:B:436:GLU:CB[2_355]	1.53	0.67
1:B:431:LYS:CA	1:B:432:LYS:N[4_445]	1.53	0.67
1:B:455:GLU:N	1:B:463:PRO:O[2_345]	1.53	0.67
1:B:455:GLU:CB	1:B:462:THR:O[2_345]	1.53	0.67
1:A:84:PHE:CG	4:A:502:ATP:C6[3_365]	1.54	0.66
1:A:86:ASP:OD2	1:A:350:MET:O[3_365]	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:C	1:A:400:PHE:N[3_365]	1.54	0.66
1:A:107:PHE:CZ	1:A:171:VAL:CG2[3_365]	1.54	0.66
1:A:138:PHE:CA	1:A:431:LYS:CB[3_365]	1.54	0.66
1:A:140:HIS:NE2	1:A:436:GLU:CG[3_365]	1.54	0.66
1:A:140:HIS:N	1:A:435:ILE:CA[3_365]	1.54	0.66
1:A:208:LEU:O	1:B:259:THR:N[4_435]	1.54	0.66
1:A:222:ILE:N	1:A:262:GLN:N[4_435]	1.54	0.66
1:A:257:HIS:C	1:A:450:LYS:N[3_365]	1.54	0.66
1:A:317:PHE:CD1	1:A:363:ASP:C[3_365]	1.54	0.66
1:A:335:LEU:CA	1:A:369:LYS:C[3_365]	1.54	0.66
1:A:339:PHE:CE2	1:A:342:ALA:C[3_365]	1.54	0.66
1:A:349:LYS:NZ	1:A:354:ASP:OD1[3_365]	1.54	0.66
1:B:99:ASP:CB	1:B:449:ARG:CA[4_445]	1.54	0.66
1:B:109:SER:N	1:B:298:ARG:CB[3_365]	1.54	0.66
1:B:307:ILE:CD1	1:B:475:HIS:CB[3_365]	1.54	0.66
1:B:321:ARG:NH2	5:B:519:HOH:O[3_365]	1.54	0.66
1:B:344:GLN:CA	1:B:371:LYS:NZ[4_445]	1.54	0.66
1:B:347:GLN:CB	1:B:361:LEU:N[4_445]	1.54	0.66
1:B:359:ILE:CD1	1:B:377:PHE:CB[3_465]	1.54	0.66
1:B:369:LYS:CG	1:B:434:LEU:CD2[3_465]	1.54	0.66
1:B:371:LYS:CA	1:B:374:LYS:CB[4_445]	1.54	0.66
1:B:372:VAL:CB	1:B:431:LYS:CE[3_465]	1.54	0.66
1:B:381:ARG:CG	1:B:405:PHE:N[4_445]	1.54	0.66
1:B:391:GLY:C	1:B:407:LEU:O[4_445]	1.54	0.66
1:B:400:PHE:CD2	1:B:440:PRO:CG[4_445]	1.54	0.66
1:B:413:LEU:CA	1:B:423:GLY:C[3_465]	1.54	0.66
1:B:416:ILE:CG1	1:B:425:MET:CA[3_465]	1.54	0.66
1:A:84:PHE:N	1:A:340:PHE:C[3_365]	1.55	0.65
1:A:93:SER:N	1:A:347:GLN:NE2[2_245]	1.55	0.65
1:A:100:TYR:CD2	1:A:377:PHE:O[3_365]	1.55	0.65
1:A:100:TYR:C	1:A:399:SER:N[3_365]	1.55	0.65
1:A:103:LEU:CD1	1:A:402:TYR:CD1[3_365]	1.55	0.65
1:A:105:VAL:CA	1:A:403:LEU:CA[3_365]	1.55	0.65
1:A:108:GLY:O	1:A:437:VAL:CG1[3_365]	1.55	0.65
1:A:138:PHE:O	1:A:431:LYS:C[3_365]	1.55	0.65
1:A:144:ASN:O	1:A:152:ASN:OD1[2_345]	1.55	0.65
1:A:145:GLN:NE2	1:A:153:LYS:CB[2_345]	1.55	0.65
1:A:165:SER:O	1:A:277:LYS:NZ[4_435]	1.55	0.65
1:A:215:ALA:O	1:A:260:PHE:CD1[4_435]	1.55	0.65
1:A:221:ASP:CA	1:A:262:GLN:CA[4_435]	1.55	0.65
1:A:289:PHE:CD1	1:A:471:GLN:O[2_345]	1.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ILE:C	1:A:359:ILE:CG1[3_365]	1.55	0.65
1:A:312:ASP:C	1:A:359:ILE:CA[3_365]	1.55	0.65
1:A:315:PRO:C	1:A:361:LEU:N[3_365]	1.55	0.65
1:A:321:ARG:CA	1:A:443:ALA:CA[3_365]	1.55	0.65
1:A:327:ILE:CG2	1:A:450:LYS:NZ[3_365]	1.55	0.65
1:A:339:PHE:CZ	1:A:357:SER:O[3_365]	1.55	0.65
1:A:458:LYS:C	1:B:270:THR:OG1[4_435]	1.55	0.65
1:A:458:LYS:CG	5:B:578:HOH:O[4_435]	1.55	0.65
1:B:102:LYS:CA	1:B:451:GLU:C[4_445]	1.55	0.65
1:B:108:GLY:N	1:B:298:ARG:CB[3_365]	1.55	0.65
1:B:341:PRO:CG	1:B:365:ALA:N[4_445]	1.55	0.65
1:B:347:GLN:N	1:B:361:LEU:C[4_445]	1.55	0.65
1:B:372:VAL:CG1	1:B:431:LYS:CD[3_465]	1.55	0.65
1:B:374:LYS:O	1:B:375:HIS:C[4_445]	1.55	0.65
1:B:396:VAL:CB	1:B:441:LEU:CD2[4_445]	1.55	0.65
1:B:425:MET:C	1:B:436:GLU:OE2[2_355]	1.55	0.65
1:B:430:LEU:CD2	1:B:433:ALA:O[4_445]	1.55	0.65
1:A:87:PRO:CB	1:A:360:PHE:CD2[3_365]	1.56	0.64
1:A:103:LEU:O	1:A:402:TYR:CB[3_365]	1.56	0.64
1:A:105:VAL:C	1:A:406:PHE:N[3_365]	1.56	0.64
1:A:210:GLN:NE2	1:B:256:LYS:CA[4_435]	1.56	0.64
1:A:212:TYR:O	1:B:260:PHE:CA[4_435]	1.56	0.64
1:A:218:ASN:CG	1:A:269:PHE:CD2[4_435]	1.56	0.64
1:A:302:ASP:OD2	1:A:303:ILE:CB[2_345]	1.56	0.64
1:A:311:ILE:CG2	1:A:343:LEU:CG[3_365]	1.56	0.64
1:A:311:ILE:O	1:A:359:ILE:CB[3_365]	1.56	0.64
1:A:321:ARG:C	1:A:443:ALA:C[3_365]	1.56	0.64
1:A:336:HIS:C	1:A:372:VAL:C[3_365]	1.56	0.64
1:A:457:VAL:N	1:B:272:SER:O[4_435]	1.56	0.64
1:A:461:MET:CB	1:B:270:THR:CA[4_435]	1.56	0.64
1:B:99:ASP:N	1:B:449:ARG:CA[4_445]	1.56	0.64
1:B:359:ILE:N	1:B:377:PHE:CD1[3_465]	1.56	0.64
1:B:370:THR:O	1:B:376:ALA:N[2_355]	1.56	0.64
1:B:371:LYS:O	1:B:375:HIS:CA[3_465]	1.56	0.64
1:B:373:ASN:OD1	1:B:399:SER:OG[2_355]	1.56	0.64
1:B:381:ARG:CB	1:B:404:THR:OG1[4_445]	1.56	0.64
1:B:387:HIS:O	1:B:413:LEU:CG[4_445]	1.56	0.64
1:B:399:SER:CA	1:B:435:ILE:CG2[4_445]	1.56	0.64
1:B:401:MET:CG	1:B:439:GLN:O[4_445]	1.56	0.64
1:B:403:LEU:N	1:B:439:GLN:OE1[4_445]	1.56	0.64
1:B:431:LYS:C	5:B:501:HOH:O[4_445]	1.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:CA	1:A:341:PRO:CG[3_365]	1.57	0.63
1:A:84:PHE:CZ	1:A:356:ASN:CG[2_245]	1.57	0.63
1:A:84:PHE:O	1:A:340:PHE:O[3_365]	1.57	0.63
1:A:100:TYR:N	1:A:397:ASP:C[3_365]	1.57	0.63
1:A:106:ARG:O	1:A:406:PHE:CE1[3_365]	1.57	0.63
1:A:109:SER:CA	1:A:438:LEU:N[3_365]	1.57	0.63
1:A:109:SER:C	1:A:437:VAL:CB[3_365]	1.57	0.63
1:A:112:ILE:O	1:A:428:GLY:O[3_365]	1.57	0.63
1:A:137:PHE:CA	1:A:373:ASN:C[3_365]	1.57	0.63
1:A:162:ARG:CZ	1:A:269:PHE:N[4_435]	1.57	0.63
1:A:164:PRO:CD	1:A:270:THR:CA[4_435]	1.57	0.63
1:A:216:VAL:O	1:A:260:PHE:CB[4_435]	1.57	0.63
1:A:273:ASP:CA	5:A:619:HOH:O[3_365]	1.57	0.63
1:A:320:THR:CB	1:A:446:GLN:CD[3_365]	1.57	0.63
1:A:356:ASN:CA	4:A:502:ATP:O2'[4_435]	1.57	0.63
1:B:108:GLY:N	1:B:298:ARG:N[3_365]	1.57	0.63
1:B:136:ILE:CG1	1:B:386:GLU:OE2[3_465]	1.57	0.63
1:B:341:PRO:CD	1:B:365:ALA:N[4_445]	1.57	0.63
1:B:368:ILE:CG1	1:B:398:VAL:CG1[3_465]	1.57	0.63
1:B:372:VAL:CA	1:B:372:VAL:O[3_465]	1.57	0.63
1:B:384:ILE:CG1	1:B:400:PHE:CD2[4_445]	1.57	0.63
1:B:387:HIS:CG	1:B:413:LEU:CD1[4_445]	1.57	0.63
1:B:395:ASP:N	1:B:441:LEU:CB[4_445]	1.57	0.63
1:A:110:SER:OG	1:A:436:GLU:CA[3_365]	1.58	0.62
1:A:138:PHE:CB	1:A:431:LYS:CG[3_365]	1.58	0.62
1:A:208:LEU:O	1:B:259:THR:CG2[4_435]	1.58	0.62
1:A:234:ILE:CB	1:B:271:ASP:OD2[4_435]	1.58	0.62
1:A:307:ILE:CB	1:A:367:GLN:N[3_365]	1.58	0.62
1:A:309:CYS:SG	1:A:367:GLN:C[3_365]	1.58	0.62
1:A:317:PHE:CE2	1:A:364:THR:N[3_365]	1.58	0.62
1:A:328:GLY:CA	1:A:469:ASP:N[2_345]	1.58	0.62
1:A:329:TYR:N	1:A:469:ASP:O[2_345]	1.58	0.62
1:A:335:LEU:CD2	1:A:369:LYS:CG[3_365]	1.58	0.62
1:A:349:LYS:CG	5:A:531:HOH:O[3_365]	1.58	0.62
1:A:356:ASN:CB	4:A:502:ATP:C1'[4_435]	1.58	0.62
1:A:383:THR:CG2	5:A:559:HOH:O[4_435]	1.58	0.62
1:B:105:VAL:O	1:B:295:GLN:O[3_365]	1.58	0.62
1:B:130:HIS:CD2	1:B:381:ARG:NH2[3_465]	1.58	0.62
1:B:340:PHE:C	1:B:364:THR:CB[4_445]	1.58	0.62
1:B:343:LEU:CA	1:B:367:GLN:O[4_445]	1.58	0.62
1:B:347:GLN:CA	1:B:361:LEU:N[4_445]	1.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLY:O	1:B:402:TYR:C[4_445]	1.58	0.62
1:B:382:ASP:CG	1:B:405:PHE:CZ[4_445]	1.58	0.62
1:B:416:ILE:CG1	1:B:436:GLU:OE1[4_445]	1.58	0.62
1:B:420:TYR:CE2	1:B:437:VAL:CB[4_445]	1.58	0.62
1:B:455:GLU:CG	1:B:464:ARG:N[2_345]	1.58	0.62
1:A:88:TRP:CA	1:A:352:ALA:C[3_365]	1.59	0.61
1:A:93:SER:C	1:A:94:SER:O[3_365]	1.59	0.61
1:A:112:ILE:N	1:A:431:LYS:C[3_365]	1.59	0.61
1:A:135:GLY:O	1:A:431:LYS:NZ[3_365]	1.59	0.61
1:A:169:MET:N	1:A:267:PHE:CG[4_435]	1.59	0.61
1:A:220:LYS:NZ	1:B:276:GLY:N[4_435]	1.59	0.61
1:A:222:ILE:CD1	1:A:264:LYS:CB[4_435]	1.59	0.61
1:A:259:THR:CG2	1:A:452:VAL:CG2[3_365]	1.59	0.61
1:A:313:GLN:CA	1:A:363:ASP:OD2[3_365]	1.59	0.61
1:A:322:ASP:OD1	1:A:445:HIS:N[3_365]	1.59	0.61
1:A:329:TYR:CG	1:A:471:GLN:N[2_345]	1.59	0.61
1:A:329:TYR:N	1:A:469:ASP:C[2_345]	1.59	0.61
1:A:347:GLN:O	1:A:348:THR:N[3_365]	1.59	0.61
1:B:334:LEU:CB	1:B:473:HIS:CB[3_365]	1.59	0.61
1:B:343:LEU:CD1	1:B:370:THR:CB[4_445]	1.59	0.61
1:B:373:ASN:N	1:B:373:ASN:N[4_445]	1.59	0.61
1:B:406:PHE:CZ	5:B:562:HOH:O[3_465]	1.59	0.61
1:B:408:GLU:N	5:B:580:HOH:O[3_465]	1.59	0.61
1:B:412:LYS:CE	1:B:419:ASP:CB[3_465]	1.59	0.61
1:B:430:LEU:CB	1:B:433:ALA:N[4_445]	1.59	0.61
1:B:455:GLU:C	1:B:464:ARG:CD[2_345]	1.59	0.61
1:A:85:VAL:C	1:A:350:MET:CB[3_365]	1.60	0.60
1:A:91:GLN:N	1:A:349:LYS:N[3_365]	1.60	0.60
1:A:92:THR:O	1:A:347:GLN:O[3_365]	1.60	0.60
1:A:137:PHE:CB	1:A:373:ASN:CA[3_365]	1.60	0.60
1:A:138:PHE:CE2	1:A:399:SER:OG[3_365]	1.60	0.60
1:A:145:GLN:CD	1:A:152:ASN:O[2_345]	1.60	0.60
1:A:162:ARG:CZ	1:A:268:GLY:O[4_435]	1.60	0.60
1:A:166:SER:OG	1:A:203:TRP:CE2[4_435]	1.60	0.60
1:A:212:TYR:CZ	1:B:260:PHE:O[4_435]	1.60	0.60
1:A:213:SER:O	1:A:278:ILE:CD1[4_435]	1.60	0.60
1:A:217:GLU:OE2	1:B:275:ILE:O[4_435]	1.60	0.60
1:A:239:ASP:OD1	1:B:265:GLY:N[4_435]	1.60	0.60
1:A:311:ILE:CB	1:A:343:LEU:CD2[3_365]	1.60	0.60
1:A:311:ILE:C	1:A:359:ILE:CD1[3_365]	1.60	0.60
1:A:316:TYR:CB	1:A:362:THR:N[3_365]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLY:CA	1:A:469:ASP:C[2_345]	1.60	0.60
1:A:329:TYR:CD1	1:A:471:GLN:N[2_345]	1.60	0.60
1:A:334:LEU:CD1	1:A:368:ILE:CG1[3_365]	1.60	0.60
1:A:338:THR:CA	1:A:376:ALA:CA[3_365]	1.60	0.60
1:A:339:PHE:CD2	1:A:343:LEU:C[3_365]	1.60	0.60
1:A:356:ASN:OD1	4:A:502:ATP:N9[4_435]	1.60	0.60
1:A:386:GLU:OE2	1:A:417:ARG:CZ[4_435]	1.60	0.60
1:B:326:ARG:NH1	5:A:511:HOH:O[3_365]	1.60	0.60
1:B:104:ILE:CA	1:B:298:ARG:CZ[3_365]	1.60	0.60
1:B:131:PHE:CE1	1:B:381:ARG:NH1[3_465]	1.60	0.60
1:B:371:LYS:CB	1:B:375:HIS:C[3_465]	1.60	0.60
1:B:389:GLN:O	1:B:410:ASP:CG[4_445]	1.60	0.60
1:B:394:CYS:O	1:B:441:LEU:N[4_445]	1.60	0.60
1:B:399:SER:O	1:B:435:ILE:CG2[4_445]	1.60	0.60
1:B:400:PHE:C	1:B:439:GLN:CB[4_445]	1.60	0.60
1:B:412:LYS:C	1:B:423:GLY:C[3_465]	1.60	0.60
1:B:412:LYS:O	1:B:424:ALA:N[3_465]	1.60	0.60
1:B:413:LEU:N	1:B:424:ALA:N[3_465]	1.60	0.60
1:B:455:GLU:CA	1:B:462:THR:O[2_345]	1.60	0.60
1:A:83:ASP:C	1:A:341:PRO:CD[3_365]	1.61	0.59
1:A:83:ASP:C	1:A:340:PHE:C[3_365]	1.61	0.59
1:A:85:VAL:N	1:A:340:PHE:O[3_365]	1.61	0.59
1:A:86:ASP:OD1	1:A:170:HIS:NE2[3_365]	1.61	0.59
1:A:92:THR:C	1:A:346:ALA:C[3_365]	1.61	0.59
1:A:100:TYR:N	1:A:397:ASP:O[3_365]	1.61	0.59
1:A:100:TYR:C	1:A:399:SER:CA[3_365]	1.61	0.59
1:A:100:TYR:CD1	1:A:398:VAL:CG1[3_365]	1.61	0.59
1:A:102:LYS:CA	1:A:400:PHE:O[3_365]	1.61	0.59
1:A:102:LYS:CA	1:A:401:MET:C[3_365]	1.61	0.59
1:A:105:VAL:CA	1:A:403:LEU:C[3_365]	1.61	0.59
1:A:107:PHE:CB	1:A:438:LEU:CD2[3_365]	1.61	0.59
1:A:112:ILE:CG2	1:A:428:GLY:O[3_365]	1.61	0.59
1:A:138:PHE:C	1:A:431:LYS:CB[3_365]	1.61	0.59
1:A:197:ASP:CB	1:A:271:ASP:O[4_435]	1.61	0.59
1:A:209:ASP:O	1:B:258:VAL:C[4_435]	1.61	0.59
1:A:221:ASP:O	1:A:262:GLN:CA[4_435]	1.61	0.59
1:A:234:ILE:CG2	1:B:271:ASP:OD2[4_435]	1.61	0.59
1:A:257:HIS:C	1:A:449:ARG:C[3_365]	1.61	0.59
1:A:299:ASP:CG	5:A:601:HOH:O[2_345]	1.61	0.59
1:A:302:ASP:CB	1:A:303:ILE:CB[2_345]	1.61	0.59
1:A:311:ILE:CG2	1:A:343:LEU:CD2[3_365]	1.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:CA	1:A:443:ALA:CB[3_365]	1.61	0.59
1:A:322:ASP:C	1:A:447:ALA:N[3_365]	1.61	0.59
1:A:349:LYS:CB	5:A:531:HOH:O[3_365]	1.61	0.59
1:A:440:PRO:N	5:A:589:HOH:O[4_435]	1.61	0.59
1:A:458:LYS:O	1:B:270:THR:CB[4_435]	1.61	0.59
1:B:141:ARG:CD	1:B:472:HIS:C[3_365]	1.61	0.59
1:B:141:ARG:CB	1:B:472:HIS:C[3_365]	1.61	0.59
1:B:321:ARG:CD	1:B:472:HIS:CE1[3_365]	1.61	0.59
1:B:344:GLN:CG	1:B:371:LYS:NZ[4_445]	1.61	0.59
1:B:366:LYS:CE	1:B:377:PHE:CE2[2_355]	1.61	0.59
1:B:371:LYS:C	1:B:374:LYS:C[2_355]	1.61	0.59
1:B:372:VAL:C	1:B:373:ASN:O[2_355]	1.61	0.59
1:B:375:HIS:N	1:B:375:HIS:N[3_465]	1.61	0.59
1:B:378:SER:OG	1:B:402:TYR:CB[4_445]	1.61	0.59
1:B:381:ARG:O	1:B:401:MET:CA[4_445]	1.61	0.59
1:B:384:ILE:N	1:B:440:PRO:CA[2_355]	1.61	0.59
1:B:396:VAL:O	1:B:442:ILE:CD1[4_445]	1.61	0.59
1:B:416:ILE:CG2	1:B:426:LEU:CG[3_465]	1.61	0.59
1:B:416:ILE:CG2	1:B:436:GLU:CD[4_445]	1.61	0.59
1:B:427:THR:O	1:B:430:LEU:O[4_445]	1.61	0.59
1:B:430:LEU:CA	1:B:433:ALA:CA[4_445]	1.61	0.59
1:B:430:LEU:O	1:B:432:LYS:CB[4_445]	1.61	0.59
1:A:86:ASP:OD1	1:A:170:HIS:CE1[3_365]	1.62	0.58
1:A:87:PRO:O	1:A:360:PHE:CZ[3_365]	1.62	0.58
1:A:100:TYR:CA	1:A:398:VAL:O[3_365]	1.62	0.58
1:A:109:SER:O	1:A:437:VAL:CG2[3_365]	1.62	0.58
1:A:159:TYR:CB	5:A:585:HOH:O[3_365]	1.62	0.58
1:A:159:TYR:CE2	1:A:364:THR:CG2[3_365]	1.62	0.58
1:A:164:PRO:CG	1:A:270:THR:C[4_435]	1.62	0.58
1:A:167:GLU:OE1	1:A:279:SER:N[4_435]	1.62	0.58
1:A:300:ARG:CD	1:A:301:THR:CA[2_345]	1.62	0.58
1:A:302:ASP:CG	1:A:303:ILE:CG1[2_345]	1.62	0.58
1:A:339:PHE:CZ	1:A:343:LEU:N[3_365]	1.62	0.58
1:A:457:VAL:N	1:B:272:SER:C[4_435]	1.62	0.58
1:B:134:ARG:CZ	1:B:391:GLY:N[3_465]	1.62	0.58
1:B:141:ARG:CD	1:B:472:HIS:CG[3_365]	1.62	0.58
1:B:342:ALA:N	1:B:367:GLN:OE1[4_445]	1.62	0.58
1:B:371:LYS:CA	1:B:376:ALA:N[3_465]	1.62	0.58
1:B:393:ASN:N	1:B:406:PHE:O[4_445]	1.62	0.58
1:B:396:VAL:N	1:B:441:LEU:CG[4_445]	1.62	0.58
1:B:397:ASP:CA	1:B:438:LEU:CG[4_445]	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:MET:N	1:B:439:GLN:CA[4_445]	1.62	0.58
1:B:416:ILE:CD1	1:B:425:MET:O[3_465]	1.62	0.58
1:B:428:GLY:O	1:B:432:LYS:CB[3_465]	1.62	0.58
1:B:454:ASP:C	1:B:463:PRO:O[2_345]	1.62	0.58
1:A:84:PHE:CE2	1:A:356:ASN:CG[2_245]	1.63	0.57
1:A:92:THR:C	1:A:347:GLN:CD[2_245]	1.63	0.57
1:A:98:ILE:N	5:A:518:HOH:O[3_365]	1.63	0.57
1:A:100:TYR:CZ	1:A:343:LEU:O[3_365]	1.63	0.57
1:A:110:SER:O	1:A:434:LEU:N[3_365]	1.63	0.57
1:A:162:ARG:NH1	1:A:268:GLY:C[4_435]	1.63	0.57
1:A:214:TYR:CD1	1:A:274:CYS:O[4_435]	1.63	0.57
1:A:220:LYS:CA	1:A:260:PHE:N[4_435]	1.63	0.57
1:A:221:ASP:CB	1:A:262:GLN:O[4_435]	1.63	0.57
1:A:222:ILE:N	1:A:262:GLN:CA[4_435]	1.63	0.57
1:A:317:PHE:CD1	1:A:363:ASP:CA[3_365]	1.63	0.57
1:A:322:ASP:C	1:A:447:ALA:CA[3_365]	1.63	0.57
1:A:335:LEU:CB	1:A:369:LYS:CB[3_365]	1.63	0.57
1:A:461:MET:CE	1:B:260:PHE:CE2[4_435]	1.63	0.57
1:A:461:MET:CG	1:B:270:THR:C[4_435]	1.63	0.57
1:B:110:SER:CA	1:B:471:GLN:N[3_365]	1.63	0.57
1:B:134:ARG:NH2	1:B:390:PHE:CA[3_465]	1.63	0.57
1:B:134:ARG:CG	1:B:390:PHE:CD1[3_465]	1.63	0.57
1:B:141:ARG:N	1:B:473:HIS:ND1[3_365]	1.63	0.57
1:B:229:ILE:CD1	1:B:459:GLU:CD[2_345]	1.63	0.57
1:B:342:ALA:CA	1:B:367:GLN:CD[4_445]	1.63	0.57
1:B:348:THR:C	1:B:362:THR:OG1[4_445]	1.63	0.57
1:B:375:HIS:CD2	1:B:375:HIS:CE1[2_355]	1.63	0.57
1:B:380:GLY:CA	5:B:537:HOH:O[2_355]	1.63	0.57
1:B:430:LEU:CA	1:B:432:LYS:CB[2_355]	1.63	0.57
1:A:84:PHE:CD1	4:A:502:ATP:C2[3_365]	1.64	0.56
1:A:84:PHE:CE1	4:A:502:ATP:N1[3_365]	1.64	0.56
1:A:89:THR:CG2	1:A:354:ASP:OD1[2_245]	1.64	0.56
1:A:92:THR:CA	1:A:347:GLN:OE1[2_245]	1.64	0.56
1:A:106:ARG:CG	1:A:405:PHE:CB[3_365]	1.64	0.56
1:A:138:PHE:CB	1:A:431:LYS:CE[3_365]	1.64	0.56
1:A:138:PHE:C	1:A:431:LYS:CA[3_365]	1.64	0.56
1:A:209:ASP:CG	1:B:258:VAL:CG2[4_435]	1.64	0.56
1:A:209:ASP:C	1:B:259:THR:N[4_435]	1.64	0.56
1:A:221:ASP:C	1:A:262:GLN:O[4_435]	1.64	0.56
1:A:238:LEU:CB	1:B:261:ASN:CB[4_435]	1.64	0.56
1:A:257:HIS:CB	1:A:450:LYS:CG[3_365]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:CYS:C	1:A:371:LYS:CB[3_365]	1.64	0.56
1:A:336:HIS:N	1:A:369:LYS:O[3_365]	1.64	0.56
1:A:355:PRO:CG	4:A:502:ATP:C4'[4_435]	1.64	0.56
1:A:458:LYS:N	1:B:273:ASP:CG[4_435]	1.64	0.56
1:B:99:ASP:N	1:B:449:ARG:N[4_445]	1.64	0.56
1:B:334:LEU:CG	1:B:473:HIS:C[3_365]	1.64	0.56
1:B:341:PRO:CD	1:B:364:THR:CA[4_445]	1.64	0.56
1:B:342:ALA:CA	1:B:367:GLN:OE1[4_445]	1.64	0.56
1:B:345:GLY:O	1:B:363:ASP:CG[4_445]	1.64	0.56
1:B:367:GLN:N	1:B:402:TYR:OH[3_465]	1.64	0.56
1:B:367:GLN:CB	5:B:480:HOH:O[3_465]	1.64	0.56
1:B:372:VAL:CB	1:B:373:ASN:OD1[4_445]	1.64	0.56
1:B:415:GLN:NE2	5:B:536:HOH:O[3_465]	1.64	0.56
1:B:425:MET:C	1:B:436:GLU:CD[2_355]	1.64	0.56
1:B:429:GLU:N	1:B:430:LEU:N[4_445]	1.64	0.56
1:A:100:TYR:CA	1:A:398:VAL:CA[3_365]	1.65	0.55
1:A:100:TYR:N	1:A:398:VAL:C[3_365]	1.65	0.55
1:A:112:ILE:CB	1:A:432:LYS:N[3_365]	1.65	0.55
1:A:154:LYS:CE	1:A:304:GLN:CG[2_345]	1.65	0.55
1:A:210:GLN:CA	1:A:274:CYS:CA[4_435]	1.65	0.55
1:A:217:GLU:OE2	1:B:275:ILE:CA[4_435]	1.65	0.55
1:A:302:ASP:OD1	1:A:303:ILE:CD1[2_345]	1.65	0.55
1:A:309:CYS:CB	1:A:367:GLN:O[3_365]	1.65	0.55
1:A:317:PHE:CG	1:A:364:THR:N[3_365]	1.65	0.55
1:A:326:ARG:NE	1:A:447:ALA:O[3_365]	1.65	0.55
1:A:338:THR:O	1:A:375:HIS:C[3_365]	1.65	0.55
1:A:347:GLN:N	1:A:347:GLN:OE1[3_365]	1.65	0.55
1:B:99:ASP:OD1	1:B:448:ARG:O[4_445]	1.65	0.55
1:B:317:PHE:O	1:B:474:HIS:ND1[3_365]	1.65	0.55
1:B:341:PRO:O	1:B:364:THR:OG1[4_445]	1.65	0.55
1:B:344:GLN:O	1:B:360:PHE:N[4_445]	1.65	0.55
1:B:344:GLN:CA	1:B:371:LYS:CD[4_445]	1.65	0.55
1:B:347:GLN:N	1:B:360:PHE:C[4_445]	1.65	0.55
1:B:365:ALA:O	1:B:402:TYR:CG[3_465]	1.65	0.55
1:B:368:ILE:O	1:B:376:ALA:CB[3_465]	1.65	0.55
1:B:372:VAL:C	1:B:372:VAL:C[3_465]	1.65	0.55
1:B:387:HIS:ND1	1:B:403:LEU:CB[4_445]	1.65	0.55
1:B:391:GLY:C	1:B:407:LEU:CA[4_445]	1.65	0.55
1:B:429:GLU:CA	1:B:430:LEU:N[4_445]	1.65	0.55
1:A:84:PHE:CD2	1:A:356:ASN:ND2[2_245]	1.66	0.54
1:A:88:TRP:N	1:A:352:ALA:CA[3_365]	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:THR:C	1:A:351:SER:CA[3_365]	1.66	0.54
1:A:93:SER:CA	1:A:347:GLN:CD[2_245]	1.66	0.54
1:A:94:SER:N	1:A:347:GLN:NE2[2_245]	1.66	0.54
1:A:99:ASP:N	1:A:401:MET:SD[3_365]	1.66	0.54
1:A:107:PHE:N	1:A:406:PHE:CG[3_365]	1.66	0.54
1:A:111:LYS:NZ	1:A:430:LEU:CD1[3_365]	1.66	0.54
1:A:112:ILE:CD1	5:A:569:HOH:O[3_365]	1.66	0.54
1:A:159:TYR:CG	5:A:585:HOH:O[3_365]	1.66	0.54
1:A:164:PRO:O	1:A:273:ASP:CB[4_435]	1.66	0.54
1:A:214:TYR:C	1:A:278:ILE:CD1[4_435]	1.66	0.54
1:A:220:LYS:O	1:A:262:GLN:CG[4_435]	1.66	0.54
1:A:307:ILE:CD1	1:A:364:THR:OG1[3_365]	1.66	0.54
1:A:313:GLN:N	1:A:358:SER:O[3_365]	1.66	0.54
1:A:316:TYR:C	1:A:361:LEU:C[3_365]	1.66	0.54
1:A:323:VAL:N	1:A:447:ALA:CA[3_365]	1.66	0.54
1:A:327:ILE:CA	1:A:469:ASP:CG[2_345]	1.66	0.54
1:A:332:PRO:C	1:A:365:ALA:CB[3_365]	1.66	0.54
1:B:99:ASP:CA	1:B:448:ARG:C[4_445]	1.66	0.54
1:B:321:ARG:NE	1:B:472:HIS:ND1[3_365]	1.66	0.54
1:B:391:GLY:C	1:B:407:LEU:C[4_445]	1.66	0.54
1:B:397:ASP:CB	1:B:438:LEU:CG[4_445]	1.66	0.54
1:B:469:ASP:O	5:B:577:HOH:O[4_435]	1.66	0.54
1:A:82:GLU:CD	1:A:100:TYR:CE2[3_365]	1.67	0.53
1:A:105:VAL:CB	1:A:404:THR:N[3_365]	1.67	0.53
1:A:106:ARG:CZ	1:A:340:PHE:CD1[3_365]	1.67	0.53
1:A:138:PHE:C	1:A:431:LYS:CG[3_365]	1.67	0.53
1:A:167:GLU:C	1:A:269:PHE:CZ[4_435]	1.67	0.53
1:A:171:VAL:CB	1:A:318:ARG:NH2[4_435]	1.67	0.53
1:A:208:LEU:CB	1:B:262:GLN:NE2[4_435]	1.67	0.53
1:A:210:GLN:NE2	1:B:256:LYS:CB[4_435]	1.67	0.53
1:A:212:TYR:CG	1:B:260:PHE:CA[4_435]	1.67	0.53
1:A:291:ASN:CB	1:A:298:ARG:O[2_345]	1.67	0.53
1:A:300:ARG:N	1:A:300:ARG:N[2_345]	1.67	0.53
1:A:306:LEU:O	1:A:366:LYS:CB[3_365]	1.67	0.53
1:A:308:PRO:C	1:A:370:THR:CB[3_365]	1.67	0.53
1:A:313:GLN:CG	1:A:371:LYS:CE[3_365]	1.67	0.53
1:A:318:ARG:CB	1:A:442:ILE:CB[3_365]	1.67	0.53
1:A:327:ILE:C	1:A:469:ASP:CB[2_345]	1.67	0.53
1:B:102:LYS:CD	1:B:453:THR:N[4_445]	1.67	0.53
1:B:111:LYS:CB	1:B:469:ASP:OD1[3_365]	1.67	0.53
1:B:134:ARG:NH1	1:B:391:GLY:N[3_465]	1.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:C	1:B:375:HIS:CB[4_445]	1.67	0.53
1:B:392:GLY:C	1:B:407:LEU:N[4_445]	1.67	0.53
1:B:394:CYS:O	5:B:567:HOH:O[3_465]	1.67	0.53
1:A:87:PRO:CD	1:A:170:HIS:CG[3_365]	1.68	0.52
1:A:90:VAL:CA	1:A:349:LYS:O[3_365]	1.68	0.52
1:A:92:THR:N	1:A:348:THR:O[3_365]	1.68	0.52
1:A:93:SER:O	1:A:97:GLY:C[3_365]	1.68	0.52
1:A:103:LEU:CA	1:A:402:TYR:CB[3_365]	1.68	0.52
1:A:105:VAL:CA	1:A:403:LEU:O[3_365]	1.68	0.52
1:A:109:SER:N	1:A:437:VAL:CG1[3_365]	1.68	0.52
1:A:110:SER:O	1:A:435:ILE:N[3_365]	1.68	0.52
1:A:111:LYS:CD	1:A:430:LEU:CD2[3_365]	1.68	0.52
1:A:197:ASP:C	1:A:272:SER:CA[4_435]	1.68	0.52
1:A:218:ASN:CA	1:A:263:VAL:CG2[4_435]	1.68	0.52
1:A:236:SER:N	1:B:264:LYS:NZ[4_435]	1.68	0.52
1:A:254:ILE:O	5:A:515:HOH:O[3_365]	1.68	0.52
1:A:302:ASP:OD1	1:A:303:ILE:N[2_345]	1.68	0.52
1:A:307:ILE:C	1:A:367:GLN:N[3_365]	1.68	0.52
1:A:309:CYS:C	1:A:371:LYS:CA[3_365]	1.68	0.52
1:A:313:GLN:N	1:A:359:ILE:CA[3_365]	1.68	0.52
1:A:314:ASP:O	1:A:442:ILE:CD1[3_365]	1.68	0.52
1:A:317:PHE:CE1	1:A:363:ASP:CA[3_365]	1.68	0.52
1:A:319:MET:O	1:A:446:GLN:N[3_365]	1.68	0.52
1:B:99:ASP:O	1:B:450:LYS:C[4_445]	1.68	0.52
1:B:105:VAL:CG1	1:B:465:LYS:CD[3_365]	1.68	0.52
1:B:106:ARG:O	1:B:294:PRO:O[3_365]	1.68	0.52
1:B:108:GLY:CA	1:B:298:ARG:CA[3_365]	1.68	0.52
1:B:133:ARG:CA	1:B:390:PHE:CZ[3_465]	1.68	0.52
1:B:141:ARG:CD	1:B:472:HIS:CA[3_365]	1.68	0.52
1:B:341:PRO:CB	1:B:363:ASP:C[4_445]	1.68	0.52
1:B:341:PRO:N	1:B:364:THR:CB[4_445]	1.68	0.52
1:B:365:ALA:O	1:B:402:TYR:CE1[3_465]	1.68	0.52
1:B:367:GLN:CA	5:B:480:HOH:O[3_465]	1.68	0.52
1:B:369:LYS:CE	1:B:438:LEU:CD1[3_465]	1.68	0.52
1:B:372:VAL:N	1:B:376:ALA:CB[3_465]	1.68	0.52
1:B:412:LYS:CD	1:B:419:ASP:O[3_465]	1.68	0.52
1:B:429:GLU:CA	1:B:433:ALA:N[2_355]	1.68	0.52
1:B:432:LYS:O	1:B:432:LYS:NZ[4_445]	1.68	0.52
1:B:458:LYS:CB	1:B:462:THR:CG2[2_345]	1.68	0.52
1:A:82:GLU:OE2	1:A:100:TYR:CD2[3_365]	1.69	0.51
1:A:91:GLN:O	5:A:551:HOH:O[3_365]	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:N	1:A:94:SER:C[3_365]	1.69	0.51
1:A:107:PHE:CE1	1:A:340:PHE:CE2[3_365]	1.69	0.51
1:A:112:ILE:C	1:A:429:GLU:C[3_365]	1.69	0.51
1:A:141:ARG:O	1:A:439:GLN:CD[3_365]	1.69	0.51
1:A:162:ARG:NE	1:A:268:GLY:O[4_435]	1.69	0.51
1:A:162:ARG:NH1	1:A:268:GLY:CA[4_435]	1.69	0.51
1:A:164:PRO:CG	1:A:270:THR:O[4_435]	1.69	0.51
1:A:169:MET:CG	1:A:267:PHE:CA[4_435]	1.69	0.51
1:A:197:ASP:OD2	1:B:261:ASN:CG[4_435]	1.69	0.51
1:A:220:LYS:CB	1:A:259:THR:CA[4_435]	1.69	0.51
1:A:299:ASP:C	1:A:300:ARG:N[2_345]	1.69	0.51
1:A:312:ASP:OD1	1:A:358:SER:O[3_365]	1.69	0.51
1:A:316:TYR:CB	1:A:363:ASP:N[3_365]	1.69	0.51
1:A:316:TYR:CE1	1:A:360:PHE:CB[3_365]	1.69	0.51
1:A:322:ASP:CG	1:A:445:HIS:N[3_365]	1.69	0.51
1:A:339:PHE:CD1	1:A:344:GLN:NE2[3_365]	1.69	0.51
1:A:339:PHE:CE1	1:A:357:SER:CA[3_365]	1.69	0.51
1:A:386:GLU:OE1	1:A:414:GLU:OE1[4_435]	1.69	0.51
1:A:457:VAL:CA	1:B:273:ASP:CA[4_435]	1.69	0.51
1:A:458:LYS:CD	5:B:578:HOH:O[4_435]	1.69	0.51
5:A:583:HOH:O	5:A:583:HOH:O[2_345]	1.69	0.51
1:B:107:PHE:C	1:B:298:ARG:CB[3_365]	1.69	0.51
1:B:307:ILE:CG1	1:B:475:HIS:CG[3_365]	1.69	0.51
1:B:370:THR:OG1	1:B:377:PHE:CA[2_355]	1.69	0.51
1:B:372:VAL:O	1:B:373:ASN:CB[2_355]	1.69	0.51
1:B:392:GLY:CA	1:B:407:LEU:CA[4_445]	1.69	0.51
1:B:393:ASN:N	1:B:406:PHE:C[4_445]	1.69	0.51
1:B:395:ASP:CA	1:B:441:LEU:N[4_445]	1.69	0.51
1:B:412:LYS:CA	1:B:424:ALA:N[3_465]	1.69	0.51
1:A:89:THR:CG2	1:A:351:SER:CB[3_365]	1.70	0.50
1:A:100:TYR:CG	1:A:398:VAL:CB[3_365]	1.70	0.50
1:A:112:ILE:O	1:A:429:GLU:CA[3_365]	1.70	0.50
1:A:145:GLN:CG	1:A:152:ASN:C[2_345]	1.70	0.50
1:A:148:ASP:OD2	1:A:152:ASN:CG[2_345]	1.70	0.50
1:A:208:LEU:C	1:B:262:GLN:NE2[4_435]	1.70	0.50
1:A:210:GLN:C	1:A:274:CYS:N[4_435]	1.70	0.50
1:A:214:TYR:OH	1:A:274:CYS:SG[4_435]	1.70	0.50
1:A:220:LYS:NZ	1:B:274:CYS:C[4_435]	1.70	0.50
1:A:302:ASP:CA	1:A:303:ILE:CD1[2_345]	1.70	0.50
1:A:322:ASP:O	1:A:447:ALA:CA[3_365]	1.70	0.50
1:A:328:GLY:N	1:A:469:ASP:CA[2_345]	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASN:ND2	4:A:502:ATP:N7[4_435]	1.70	0.50
1:A:440:PRO:O	5:A:613:HOH:O[4_435]	1.70	0.50
1:A:457:VAL:CB	1:B:273:ASP:C[4_435]	1.70	0.50
1:B:102:LYS:CG	1:B:453:THR:N[4_445]	1.70	0.50
1:B:102:LYS:CG	1:B:452:VAL:CA[4_445]	1.70	0.50
1:B:300:ARG:CD	5:B:548:HOH:O[4_435]	1.70	0.50
1:B:368:ILE:N	1:B:398:VAL:CG1[3_465]	1.70	0.50
1:B:370:THR:CG2	1:B:375:HIS:O[2_355]	1.70	0.50
1:B:370:THR:O	1:B:374:LYS:N[4_445]	1.70	0.50
1:B:374:LYS:CB	1:B:375:HIS:N[4_445]	1.70	0.50
1:B:381:ARG:CA	1:B:401:MET:O[4_445]	1.70	0.50
1:A:88:TRP:CA	1:A:352:ALA:N[3_365]	1.71	0.49
1:A:92:THR:N	1:A:348:THR:N[3_365]	1.71	0.49
1:A:111:LYS:O	1:A:432:LYS:C[3_365]	1.71	0.49
1:A:209:ASP:CG	1:B:258:VAL:CB[4_435]	1.71	0.49
1:A:210:GLN:CG	1:B:256:LYS:C[4_435]	1.71	0.49
1:A:212:TYR:CA	1:B:260:PHE:CA[4_435]	1.71	0.49
1:A:224:ALA:N	1:A:262:GLN:CG[4_435]	1.71	0.49
1:A:312:ASP:CG	1:A:358:SER:CA[3_365]	1.71	0.49
1:A:313:GLN:C	1:A:360:PHE:N[3_365]	1.71	0.49
1:A:316:TYR:N	1:A:361:LEU:CA[3_365]	1.71	0.49
1:A:317:PHE:CE1	1:A:363:ASP:CB[3_365]	1.71	0.49
1:A:318:ARG:CB	1:A:442:ILE:CA[3_365]	1.71	0.49
1:A:356:ASN:CB	4:A:502:ATP:N3[4_435]	1.71	0.49
1:A:367:GLN:CD	3:A:501:LTN:CH2[4_435]	1.71	0.49
1:A:382:ASP:OD1	1:A:400:PHE:CE2[4_435]	1.71	0.49
1:B:141:ARG:CG	1:B:472:HIS:N[3_365]	1.71	0.49
1:B:159:TYR:O	1:B:475:HIS:NE2[3_365]	1.71	0.49
1:B:334:LEU:CD2	1:B:474:HIS:O[3_365]	1.71	0.49
1:B:343:LEU:CB	1:B:367:GLN:O[4_445]	1.71	0.49
1:B:344:GLN:N	1:B:371:LYS:NZ[4_445]	1.71	0.49
1:B:371:LYS:C	1:B:374:LYS:CA[2_355]	1.71	0.49
1:B:372:VAL:CA	1:B:373:ASN:CB[4_445]	1.71	0.49
1:B:373:ASN:O	1:B:373:ASN:CB[3_465]	1.71	0.49
1:B:377:PHE:O	1:B:438:LEU:CD1[4_445]	1.71	0.49
1:B:378:SER:CA	1:B:402:TYR:CD2[4_445]	1.71	0.49
1:B:381:ARG:N	1:B:402:TYR:O[4_445]	1.71	0.49
1:B:391:GLY:C	1:B:407:LEU:N[4_445]	1.71	0.49
1:B:396:VAL:CA	1:B:441:LEU:CD2[4_445]	1.71	0.49
1:B:412:LYS:NZ	1:B:419:ASP:C[3_465]	1.71	0.49
1:B:428:GLY:O	1:B:430:LEU:C[4_445]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:CD1	1:B:432:LYS:O[4_445]	1.71	0.49
1:A:84:PHE:CE1	4:A:502:ATP:C4[3_365]	1.72	0.48
1:A:84:PHE:CE2	4:A:502:ATP:N7[3_365]	1.72	0.48
1:A:89:THR:CB	1:A:351:SER:CA[3_365]	1.72	0.48
1:A:91:GLN:CD	5:A:531:HOH:O[2_245]	1.72	0.48
1:A:92:THR:N	1:A:348:THR:C[3_365]	1.72	0.48
1:A:103:LEU:CG	1:A:402:TYR:CD2[3_365]	1.72	0.48
1:A:141:ARG:NH1	1:A:438:LEU:C[3_365]	1.72	0.48
1:A:143:MET:CE	1:A:369:LYS:NZ[3_365]	1.72	0.48
1:A:212:TYR:CZ	1:B:264:LYS:N[4_435]	1.72	0.48
1:A:213:SER:C	1:A:278:ILE:CD1[4_435]	1.72	0.48
1:A:214:TYR:CZ	1:A:274:CYS:SG[4_435]	1.72	0.48
1:A:220:LYS:N	1:A:259:THR:C[4_435]	1.72	0.48
1:A:234:ILE:CA	1:B:271:ASP:OD2[4_435]	1.72	0.48
1:A:329:TYR:CG	1:A:471:GLN:CB[2_345]	1.72	0.48
1:A:334:LEU:CD2	1:A:364:THR:O[3_365]	1.72	0.48
1:A:336:HIS:C	1:A:373:ASN:N[3_365]	1.72	0.48
1:A:336:HIS:O	1:A:372:VAL:CA[3_365]	1.72	0.48
1:A:338:THR:C	1:A:375:HIS:CA[3_365]	1.72	0.48
1:B:98:ILE:O	1:B:447:ALA:N[4_445]	1.72	0.48
1:B:340:PHE:CD2	1:B:364:THR:OG1[4_445]	1.72	0.48
1:B:342:ALA:O	1:B:363:ASP:CB[4_445]	1.72	0.48
1:B:343:LEU:CG	1:B:367:GLN:O[4_445]	1.72	0.48
1:B:366:LYS:CD	1:B:377:PHE:CE1[2_355]	1.72	0.48
1:B:379:GLY:O	1:B:406:PHE:CB[4_445]	1.72	0.48
1:B:384:ILE:CA	1:B:440:PRO:CB[2_355]	1.72	0.48
1:B:386:GLU:CD	5:B:533:HOH:O[4_445]	1.72	0.48
1:B:388:ARG:NH2	1:B:417:ARG:CA[4_445]	1.72	0.48
1:B:400:PHE:N	1:B:435:ILE:C[4_445]	1.72	0.48
1:B:432:LYS:CE	1:B:433:ALA:CA[3_465]	1.72	0.48
1:B:455:GLU:OE1	1:B:464:ARG:N[2_345]	1.72	0.48
1:A:82:GLU:CG	1:A:377:PHE:CD2[2_245]	1.73	0.47
1:A:84:PHE:CB	1:A:344:GLN:CD[2_245]	1.73	0.47
1:A:89:THR:OG1	1:A:351:SER:CB[3_365]	1.73	0.47
1:A:102:LYS:N	1:A:401:MET:CA[3_365]	1.73	0.47
1:A:103:LEU:N	1:A:402:TYR:CA[3_365]	1.73	0.47
1:A:105:VAL:O	1:A:406:PHE:C[3_365]	1.73	0.47
1:A:106:ARG:NE	1:A:405:PHE:CD2[3_365]	1.73	0.47
1:A:108:GLY:CA	1:A:437:VAL:CG1[3_365]	1.73	0.47
1:A:112:ILE:C	1:A:429:GLU:CA[3_365]	1.73	0.47
1:A:113:ASP:C	1:A:429:GLU:CB[3_365]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:HIS:CB	1:A:435:ILE:CG2[3_365]	1.73	0.47
1:A:140:HIS:C	1:A:435:ILE:CA[3_365]	1.73	0.47
1:A:164:PRO:CG	1:A:270:THR:CA[4_435]	1.73	0.47
1:A:210:GLN:CG	1:B:256:LYS:O[4_435]	1.73	0.47
1:A:210:GLN:O	1:A:274:CYS:N[4_435]	1.73	0.47
1:A:211:ALA:C	1:A:273:ASP:C[4_435]	1.73	0.47
1:A:300:ARG:N	1:A:300:ARG:O[2_345]	1.73	0.47
1:A:300:ARG:CG	1:A:301:THR:CA[2_345]	1.73	0.47
1:A:307:ILE:N	1:A:366:LYS:N[3_365]	1.73	0.47
1:A:312:ASP:CA	1:A:358:SER:CA[3_365]	1.73	0.47
1:A:313:GLN:CD	1:A:371:LYS:NZ[3_365]	1.73	0.47
1:A:321:ARG:CG	1:A:443:ALA:CB[3_365]	1.73	0.47
1:A:328:GLY:O	1:A:469:ASP:O[2_345]	1.73	0.47
1:A:333:ALA:N	1:A:365:ALA:CB[3_365]	1.73	0.47
1:A:338:THR:CB	1:A:376:ALA:CA[3_365]	1.73	0.47
1:B:101:ASP:O	1:B:465:LYS:CE[3_365]	1.73	0.47
1:B:108:GLY:C	1:B:298:ARG:CB[3_365]	1.73	0.47
1:B:109:SER:CB	5:B:508:HOH:O[3_365]	1.73	0.47
1:B:171:VAL:CB	1:B:377:PHE:CZ[3_465]	1.73	0.47
1:B:334:LEU:C	1:B:473:HIS:CB[3_365]	1.73	0.47
1:B:341:PRO:CD	1:B:364:THR:C[4_445]	1.73	0.47
1:B:371:LYS:C	1:B:374:LYS:N[4_445]	1.73	0.47
1:B:375:HIS:CG	1:B:375:HIS:CG[3_465]	1.73	0.47
1:B:379:GLY:O	1:B:406:PHE:CD1[4_445]	1.73	0.47
1:B:387:HIS:CD2	1:B:413:LEU:CD1[4_445]	1.73	0.47
1:B:391:GLY:N	1:B:407:LEU:O[4_445]	1.73	0.47
1:B:393:ASN:N	1:B:406:PHE:CB[4_445]	1.73	0.47
1:B:428:GLY:C	1:B:432:LYS:CB[3_465]	1.73	0.47
1:B:430:LEU:CB	1:B:432:LYS:CD[2_355]	1.73	0.47
1:B:430:LEU:CG	1:B:433:ALA:C[4_445]	1.73	0.47
1:B:432:LYS:CE	1:B:433:ALA:O[3_465]	1.73	0.47
1:B:432:LYS:C	1:B:432:LYS:CG[4_445]	1.73	0.47
1:A:82:GLU:CB	1:A:377:PHE:CA[2_245]	1.74	0.46
1:A:86:ASP:CA	1:A:170:HIS:CG[3_365]	1.74	0.46
1:A:88:TRP:C	1:A:352:ALA:N[3_365]	1.74	0.46
1:A:89:THR:CA	1:A:351:SER:C[3_365]	1.74	0.46
1:A:94:SER:OG	1:A:96:LYS:N[3_365]	1.74	0.46
1:A:99:ASP:C	1:A:397:ASP:O[3_365]	1.74	0.46
1:A:100:TYR:CD1	1:A:398:VAL:CB[3_365]	1.74	0.46
1:A:100:TYR:CB	1:A:398:VAL:C[3_365]	1.74	0.46
1:A:106:ARG:CA	1:A:405:PHE:CB[3_365]	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LYS:CA	1:A:429:GLU:CD[3_365]	1.74	0.46
1:A:140:HIS:C	1:A:435:ILE:CB[3_365]	1.74	0.46
1:A:141:ARG:NH2	1:A:438:LEU:CA[3_365]	1.74	0.46
1:A:163:GLY:CA	1:A:270:THR:CG2[4_435]	1.74	0.46
1:A:209:ASP:N	1:B:259:THR:N[4_435]	1.74	0.46
1:A:210:GLN:N	1:B:258:VAL:C[4_435]	1.74	0.46
1:A:212:TYR:C	1:B:260:PHE:CB[4_435]	1.74	0.46
1:A:218:ASN:ND2	1:A:269:PHE:CE2[4_435]	1.74	0.46
1:A:219:ALA:C	1:A:260:PHE:O[4_435]	1.74	0.46
1:A:221:ASP:CG	1:A:263:VAL:CA[4_435]	1.74	0.46
1:A:222:ILE:CA	1:A:261:ASN:C[4_435]	1.74	0.46
1:A:258:VAL:CG1	1:A:449:ARG:NE[3_365]	1.74	0.46
1:A:272:SER:C	5:A:619:HOH:O[3_365]	1.74	0.46
1:A:297:PHE:C	1:A:301:THR:CG2[2_345]	1.74	0.46
1:A:299:ASP:CA	1:A:299:ASP:C[2_345]	1.74	0.46
1:A:307:ILE:CD1	1:A:364:THR:C[3_365]	1.74	0.46
1:A:309:CYS:C	1:A:371:LYS:N[3_365]	1.74	0.46
1:A:310:ALA:CA	1:A:371:LYS:CB[3_365]	1.74	0.46
1:A:310:ALA:N	1:A:371:LYS:CB[3_365]	1.74	0.46
1:A:315:PRO:O	1:A:361:LEU:CB[3_365]	1.74	0.46
1:A:317:PHE:CA	1:A:363:ASP:O[3_365]	1.74	0.46
1:A:333:ALA:O	1:A:366:LYS:N[3_365]	1.74	0.46
1:B:102:LYS:CE	1:B:452:VAL:C[4_445]	1.74	0.46
1:B:108:GLY:O	1:B:297:PHE:O[3_365]	1.74	0.46
1:B:134:ARG:NE	1:B:390:PHE:CA[3_465]	1.74	0.46
1:B:134:ARG:NH1	1:B:390:PHE:C[3_465]	1.74	0.46
1:B:139:SER:OG	1:B:471:GLN:NE2[3_365]	1.74	0.46
1:B:317:PHE:CB	1:B:474:HIS:NE2[3_365]	1.74	0.46
1:B:342:ALA:N	1:B:364:THR:N[4_445]	1.74	0.46
1:B:344:GLN:CD	1:B:371:LYS:CE[4_445]	1.74	0.46
1:B:367:GLN:N	5:B:480:HOH:O[3_465]	1.74	0.46
1:B:368:ILE:CB	1:B:398:VAL:CA[3_465]	1.74	0.46
1:B:373:ASN:CB	1:B:376:ALA:CB[2_355]	1.74	0.46
1:B:373:ASN:ND2	1:B:431:LYS:CD[2_355]	1.74	0.46
1:B:381:ARG:N	1:B:402:TYR:C[4_445]	1.74	0.46
1:B:396:VAL:N	1:B:441:LEU:CD2[4_445]	1.74	0.46
1:B:400:PHE:CD1	1:B:436:GLU:C[4_445]	1.74	0.46
1:B:407:LEU:CD2	1:B:421:THR:N[3_465]	1.74	0.46
1:B:409:ASP:N	1:B:421:THR:O[3_465]	1.74	0.46
1:B:431:LYS:N	1:B:432:LYS:CA[4_445]	1.74	0.46
1:A:84:PHE:C	1:A:340:PHE:C[3_365]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASP:N	1:A:350:MET:SD[3_365]	1.75	0.45
1:A:86:ASP:N	1:A:350:MET:CB[3_365]	1.75	0.45
1:A:86:ASP:OD1	4:A:502:ATP:N7[3_365]	1.75	0.45
1:A:101:ASP:CA	1:A:400:PHE:CB[3_365]	1.75	0.45
1:A:105:VAL:O	1:A:406:PHE:CB[3_365]	1.75	0.45
1:A:108:GLY:N	1:A:406:PHE:CB[3_365]	1.75	0.45
1:A:110:SER:N	1:A:434:LEU:O[3_365]	1.75	0.45
1:A:138:PHE:O	1:A:431:LYS:CB[3_365]	1.75	0.45
1:A:140:HIS:CB	1:A:435:ILE:CB[3_365]	1.75	0.45
1:A:171:VAL:CG1	1:A:318:ARG:CZ[4_435]	1.75	0.45
1:A:214:TYR:O	1:A:278:ILE:CG1[4_435]	1.75	0.45
1:A:219:ALA:CB	1:A:260:PHE:CD2[4_435]	1.75	0.45
1:A:220:LYS:CE	1:B:275:ILE:CA[4_435]	1.75	0.45
1:A:257:HIS:C	1:A:450:LYS:C[3_365]	1.75	0.45
1:A:300:ARG:O	1:A:300:ARG:CG[2_345]	1.75	0.45
1:A:300:ARG:CA	1:A:300:ARG:CA[2_345]	1.75	0.45
1:A:302:ASP:CB	1:A:303:ILE:CD1[2_345]	1.75	0.45
1:A:307:ILE:C	1:A:366:LYS:CA[3_365]	1.75	0.45
1:A:312:ASP:O	1:A:358:SER:C[3_365]	1.75	0.45
1:A:316:TYR:C	1:A:361:LEU:O[3_365]	1.75	0.45
1:A:316:TYR:O	1:A:446:GLN:NE2[3_365]	1.75	0.45
1:A:322:ASP:OD1	1:A:444:GLU:CB[3_365]	1.75	0.45
1:A:337:SER:N	1:A:372:VAL:CA[3_365]	1.75	0.45
1:A:367:GLN:NE2	3:A:501:LTN:CH2[4_435]	1.75	0.45
1:A:457:VAL:C	1:B:273:ASP:N[4_435]	1.75	0.45
1:A:457:VAL:N	1:B:273:ASP:N[4_435]	1.75	0.45
1:B:109:SER:OG	1:B:298:ARG:NH1[3_365]	1.75	0.45
1:B:109:SER:OG	1:B:298:ARG:CD[3_365]	1.75	0.45
1:B:130:HIS:CB	1:B:390:PHE:CD2[3_465]	1.75	0.45
1:B:141:ARG:CB	1:B:472:HIS:CA[3_365]	1.75	0.45
1:B:262:GLN:CA	5:B:553:HOH:O[3_365]	1.75	0.45
1:B:307:ILE:CG2	1:B:475:HIS:NE2[3_365]	1.75	0.45
1:B:343:LEU:N	1:B:367:GLN:CB[4_445]	1.75	0.45
1:B:381:ARG:CA	1:B:405:PHE:N[4_445]	1.75	0.45
1:B:387:HIS:CB	1:B:413:LEU:CD1[4_445]	1.75	0.45
1:B:393:ASN:CG	1:B:441:LEU:CD1[4_445]	1.75	0.45
1:B:428:GLY:CA	5:B:501:HOH:O[3_465]	1.75	0.45
1:B:428:GLY:C	1:B:432:LYS:N[2_355]	1.75	0.45
1:B:430:LEU:C	1:B:433:ALA:N[4_445]	1.75	0.45
1:A:82:GLU:O	1:A:344:GLN:C[2_245]	1.76	0.44
1:A:84:PHE:CZ	4:A:502:ATP:C6[3_365]	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:N	5:A:571:HOH:O[2_245]	1.76	0.44
1:A:103:LEU:CG	1:A:402:TYR:CZ[3_365]	1.76	0.44
1:A:103:LEU:C	1:A:402:TYR:C[3_365]	1.76	0.44
1:A:115:GLU:N	1:A:429:GLU:OE2[3_365]	1.76	0.44
1:A:137:PHE:CA	1:A:373:ASN:O[3_365]	1.76	0.44
1:A:140:HIS:C	1:A:435:ILE:O[3_365]	1.76	0.44
1:A:212:TYR:CA	1:B:259:THR:C[4_435]	1.76	0.44
1:A:213:SER:CB	1:A:275:ILE:CG2[4_435]	1.76	0.44
1:A:217:GLU:OE2	1:B:275:ILE:C[4_435]	1.76	0.44
1:A:234:ILE:CD1	1:A:261:ASN:ND2[4_435]	1.76	0.44
1:A:257:HIS:N	1:A:450:LYS:O[3_365]	1.76	0.44
1:A:311:ILE:CA	1:A:359:ILE:CD1[3_365]	1.76	0.44
1:A:313:GLN:CB	1:A:371:LYS:NZ[3_365]	1.76	0.44
1:A:328:GLY:O	1:A:470:PHE:CA[2_345]	1.76	0.44
1:A:329:TYR:CB	1:A:471:GLN:N[2_345]	1.76	0.44
1:A:356:ASN:CG	4:A:502:ATP:N7[4_435]	1.76	0.44
1:A:460:PHE:N	1:B:272:SER:OG[4_435]	1.76	0.44
1:B:142:ASP:N	5:B:565:HOH:O[3_365]	1.76	0.44
1:B:171:VAL:CB	1:B:366:LYS:NZ[4_445]	1.76	0.44
1:B:372:VAL:CG2	1:B:373:ASN:OD1[4_445]	1.76	0.44
1:B:380:GLY:O	1:B:402:TYR:CA[4_445]	1.76	0.44
1:B:381:ARG:CZ	1:B:405:PHE:O[4_445]	1.76	0.44
1:B:399:SER:CB	1:B:435:ILE:CA[4_445]	1.76	0.44
1:B:401:MET:CG	1:B:439:GLN:CA[4_445]	1.76	0.44
1:B:453:THR:OG1	1:B:464:ARG:CB[2_345]	1.76	0.44
1:B:459:GLU:CA	1:B:459:GLU:CA[2_345]	1.76	0.44
1:A:93:SER:OG	1:A:98:ILE:CA[3_365]	1.77	0.43
1:A:101:ASP:O	1:A:400:PHE:C[3_365]	1.77	0.43
1:A:109:SER:OG	1:A:434:LEU:O[3_365]	1.77	0.43
1:A:112:ILE:CA	1:A:432:LYS:CA[3_365]	1.77	0.43
1:A:137:PHE:CE2	1:A:370:THR:C[3_365]	1.77	0.43
1:A:141:ARG:CD	1:A:438:LEU:C[3_365]	1.77	0.43
1:A:141:ARG:NH2	1:A:438:LEU:O[3_365]	1.77	0.43
1:A:162:ARG:NH1	1:A:268:GLY:O[4_435]	1.77	0.43
1:A:162:ARG:NE	1:A:269:PHE:CA[4_435]	1.77	0.43
1:A:168:ALA:CB	1:A:316:TYR:OH[4_435]	1.77	0.43
1:A:208:LEU:O	1:B:259:THR:OG1[4_435]	1.77	0.43
1:A:210:GLN:CD	1:B:256:LYS:C[4_435]	1.77	0.43
1:A:211:ALA:N	1:A:274:CYS:N[4_435]	1.77	0.43
1:A:211:ALA:N	1:A:274:CYS:CA[4_435]	1.77	0.43
1:A:219:ALA:CA	1:A:261:ASN:N[4_435]	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:O	1:A:363:ASP:OD2[3_365]	1.77	0.43
1:A:334:LEU:CA	1:A:439:GLN:NE2[3_365]	1.77	0.43
1:A:339:PHE:CA	1:A:344:GLN:OE1[3_365]	1.77	0.43
1:A:356:ASN:CA	4:A:502:ATP:C2'[4_435]	1.77	0.43
1:A:461:MET:CE	1:B:260:PHE:CZ[4_435]	1.77	0.43
1:B:98:ILE:O	1:B:446:GLN:CA[4_445]	1.77	0.43
1:B:134:ARG:NH2	1:B:390:PHE:N[3_465]	1.77	0.43
1:B:299:ASP:CB	1:B:318:ARG:CD[4_435]	1.77	0.43
1:B:345:GLY:CA	1:B:360:PHE:N[4_445]	1.77	0.43
1:B:366:LYS:CA	1:B:402:TYR:CE1[3_465]	1.77	0.43
1:B:368:ILE:CG2	1:B:399:SER:N[3_465]	1.77	0.43
1:B:426:LEU:C	1:B:436:GLU:CG[2_355]	1.77	0.43
1:B:428:GLY:C	1:B:432:LYS:CA[2_355]	1.77	0.43
1:B:428:GLY:CA	1:B:430:LEU:CB[4_445]	1.77	0.43
1:B:456:ILE:N	1:B:464:ARG:CD[2_345]	1.77	0.43
1:B:459:GLU:CG	1:B:459:GLU:CG[2_345]	1.77	0.43
1:A:83:ASP:CB	1:A:341:PRO:CD[3_365]	1.78	0.42
1:A:85:VAL:C	1:A:350:MET:CG[3_365]	1.78	0.42
1:A:92:THR:OG1	1:A:345:GLY:O[3_365]	1.78	0.42
1:A:101:ASP:N	1:A:400:PHE:CA[3_365]	1.78	0.42
1:A:103:LEU:O	1:A:402:TYR:CA[3_365]	1.78	0.42
1:A:106:ARG:N	1:A:406:PHE:N[3_365]	1.78	0.42
1:A:112:ILE:O	1:A:429:GLU:C[3_365]	1.78	0.42
1:A:137:PHE:CD2	1:A:373:ASN:CB[3_365]	1.78	0.42
1:A:139:SER:C	1:A:435:ILE:CD1[3_365]	1.78	0.42
1:A:169:MET:CB	1:A:267:PHE:N[4_435]	1.78	0.42
1:A:212:TYR:N	1:B:260:PHE:N[4_435]	1.78	0.42
1:A:220:LYS:CE	1:B:274:CYS:O[4_435]	1.78	0.42
1:A:221:ASP:OD2	1:A:263:VAL:CA[4_435]	1.78	0.42
1:A:326:ARG:NH2	1:A:451:GLU:CB[3_365]	1.78	0.42
1:A:337:SER:CB	1:A:375:HIS:N[3_365]	1.78	0.42
1:A:339:PHE:CG	1:A:344:GLN:N[3_365]	1.78	0.42
1:A:454:ASP:CG	1:B:277:LYS:CD[4_435]	1.78	0.42
1:B:101:ASP:CA	1:B:451:GLU:CG[4_445]	1.78	0.42
1:B:140:HIS:O	1:B:471:GLN:CA[3_365]	1.78	0.42
1:B:159:TYR:O	1:B:475:HIS:ND1[3_365]	1.78	0.42
1:B:366:LYS:CA	1:B:402:TYR:CE2[3_465]	1.78	0.42
1:B:372:VAL:CA	1:B:373:ASN:N[4_445]	1.78	0.42
1:B:381:ARG:N	1:B:404:THR:N[4_445]	1.78	0.42
1:B:416:ILE:CD1	1:B:426:LEU:N[3_465]	1.78	0.42
1:B:431:LYS:CG	1:B:431:LYS:CG[3_465]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:GLU:N	1:B:463:PRO:C[2_345]	1.78	0.42
1:B:459:GLU:CA	1:B:459:GLU:CB[2_345]	1.78	0.42
1:A:82:GLU:CB	1:A:377:PHE:CD1[2_245]	1.79	0.41
1:A:82:GLU:C	1:A:344:GLN:O[2_245]	1.79	0.41
1:A:84:PHE:CA	1:A:340:PHE:N[3_365]	1.79	0.41
1:A:91:GLN:CA	1:A:348:THR:O[3_365]	1.79	0.41
1:A:92:THR:CB	1:A:347:GLN:N[3_365]	1.79	0.41
1:A:94:SER:O	1:A:95:ALA:N[3_365]	1.79	0.41
1:A:101:ASP:CB	1:A:400:PHE:CG[3_365]	1.79	0.41
1:A:102:LYS:O	1:A:401:MET:C[3_365]	1.79	0.41
1:A:104:ILE:CA	1:A:434:LEU:CD1[3_365]	1.79	0.41
1:A:106:ARG:NH2	1:A:340:PHE:CB[3_365]	1.79	0.41
1:A:108:GLY:O	1:A:437:VAL:CA[3_365]	1.79	0.41
1:A:111:LYS:NZ	1:A:430:LEU:CG[3_365]	1.79	0.41
1:A:140:HIS:CE1	1:A:432:LYS:O[3_365]	1.79	0.41
1:A:197:ASP:N	1:A:272:SER:N[4_435]	1.79	0.41
1:A:262:GLN:NE2	1:A:452:VAL:CG1[3_365]	1.79	0.41
1:A:315:PRO:CD	1:A:359:ILE:C[3_365]	1.79	0.41
1:A:319:MET:O	1:A:446:GLN:CG[3_365]	1.79	0.41
1:A:334:LEU:C	1:A:369:LYS:CB[3_365]	1.79	0.41
1:A:458:LYS:O	1:B:270:THR:OG1[4_435]	1.79	0.41
1:B:98:ILE:N	1:B:446:GLN:CA[4_445]	1.79	0.41
1:B:99:ASP:CA	1:B:449:ARG:CA[4_445]	1.79	0.41
1:B:102:LYS:N	1:B:451:GLU:N[4_445]	1.79	0.41
1:B:102:LYS:CB	1:B:451:GLU:CA[4_445]	1.79	0.41
1:B:345:GLY:CA	1:B:363:ASP:OD2[4_445]	1.79	0.41
1:B:373:ASN:O	1:B:376:ALA:N[4_445]	1.79	0.41
1:B:387:HIS:ND1	1:B:403:LEU:CA[4_445]	1.79	0.41
1:B:400:PHE:CE1	1:B:426:LEU:CD2[3_465]	1.79	0.41
1:B:408:GLU:N	1:B:421:THR:O[3_465]	1.79	0.41
1:B:412:LYS:CA	1:B:424:ALA:CB[3_465]	1.79	0.41
1:B:416:ILE:CG2	1:B:426:LEU:CB[3_465]	1.79	0.41
1:B:427:THR:C	1:B:430:LEU:O[4_445]	1.79	0.41
1:B:428:GLY:CA	1:B:430:LEU:C[4_445]	1.79	0.41
1:B:469:ASP:C	5:B:577:HOH:O[4_435]	1.79	0.41
1:A:101:ASP:CA	1:A:400:PHE:C[3_365]	1.80	0.40
1:A:110:SER:OG	1:A:436:GLU:N[3_365]	1.80	0.40
1:A:140:HIS:CA	1:A:435:ILE:CG1[3_365]	1.80	0.40
1:A:141:ARG:N	1:A:435:ILE:CG2[3_365]	1.80	0.40
1:A:164:PRO:CG	1:A:270:THR:OG1[4_435]	1.80	0.40
1:A:197:ASP:CG	1:B:261:ASN:OD1[4_435]	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:C	1:B:259:THR:N[4_435]	1.80	0.40
1:A:219:ALA:N	1:A:260:PHE:C[4_435]	1.80	0.40
1:A:302:ASP:CA	1:A:303:ILE:CG1[2_345]	1.80	0.40
1:A:317:PHE:CE2	1:A:363:ASP:C[3_365]	1.80	0.40
1:A:318:ARG:C	1:A:442:ILE:CA[3_365]	1.80	0.40
1:A:339:PHE:CG	1:A:344:GLN:NE2[3_365]	1.80	0.40
1:A:339:PHE:CB	1:A:344:GLN:N[3_365]	1.80	0.40
1:B:109:SER:O	1:B:470:PHE:N[3_365]	1.80	0.40
1:B:342:ALA:C	1:B:367:GLN:CB[4_445]	1.80	0.40
1:B:344:GLN:CA	1:B:371:LYS:CE[4_445]	1.80	0.40
1:B:369:LYS:CD	1:B:378:SER:CA[2_355]	1.80	0.40
1:B:372:VAL:CG1	1:B:373:ASN:CG[4_445]	1.80	0.40
1:B:375:HIS:CB	1:B:375:HIS:CD2[4_445]	1.80	0.40
1:B:381:ARG:CB	1:B:405:PHE:N[4_445]	1.80	0.40
1:B:388:ARG:CD	1:B:413:LEU:C[4_445]	1.80	0.40
1:B:391:GLY:O	1:B:407:LEU:N[4_445]	1.80	0.40
1:B:397:ASP:CG	1:B:438:LEU:CG[4_445]	1.80	0.40
1:B:407:LEU:CG	1:B:420:TYR:C[3_465]	1.80	0.40
1:B:416:ILE:CD1	1:B:425:MET:N[3_465]	1.80	0.40
1:B:426:LEU:CA	1:B:436:GLU:CB[2_355]	1.80	0.40
1:B:427:THR:O	1:B:432:LYS:CA[2_355]	1.80	0.40
1:B:428:GLY:N	1:B:430:LEU:CG[4_445]	1.80	0.40
1:B:455:GLU:CD	1:B:463:PRO:C[2_345]	1.80	0.40
1:B:455:GLU:CD	1:B:464:ARG:CA[2_345]	1.80	0.40
1:A:87:PRO:CD	1:A:170:HIS:CA[3_365]	1.81	0.39
1:A:98:ILE:CG2	1:A:345:GLY:C[3_365]	1.81	0.39
1:A:100:TYR:CE2	1:A:377:PHE:N[3_365]	1.81	0.39
1:A:104:ILE:CG2	1:A:403:LEU:CD2[3_365]	1.81	0.39
1:A:107:PHE:CA	1:A:406:PHE:CE2[3_365]	1.81	0.39
1:A:112:ILE:C	1:A:428:GLY:O[3_365]	1.81	0.39
1:A:113:ASP:CB	1:A:429:GLU:CB[3_365]	1.81	0.39
1:A:114:LYS:CB	1:A:429:GLU:CD[3_365]	1.81	0.39
1:A:139:SER:N	1:A:372:VAL:CG1[3_365]	1.81	0.39
1:A:163:GLY:O	1:A:268:GLY:O[4_435]	1.81	0.39
1:A:164:PRO:C	1:A:273:ASP:OD1[4_435]	1.81	0.39
1:A:212:TYR:OH	1:B:264:LYS:N[4_435]	1.81	0.39
1:A:217:GLU:CD	1:B:275:ILE:CB[4_435]	1.81	0.39
1:A:259:THR:CG2	1:A:452:VAL:CG1[3_365]	1.81	0.39
1:A:449:ARG:NH1	1:B:275:ILE:CD1[4_435]	1.81	0.39
1:A:460:PHE:CD2	1:B:272:SER:CB[4_435]	1.81	0.39
1:B:100:TYR:N	1:B:447:ALA:C[4_445]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:N	1:B:451:GLU:CB[4_445]	1.81	0.39
1:B:130:HIS:CB	1:B:390:PHE:CB[3_465]	1.81	0.39
1:B:371:LYS:O	1:B:376:ALA:N[3_465]	1.81	0.39
1:B:381:ARG:C	1:B:401:MET:C[4_445]	1.81	0.39
1:B:392:GLY:O	1:B:406:PHE:C[4_445]	1.81	0.39
1:B:395:ASP:N	1:B:441:LEU:CA[4_445]	1.81	0.39
1:B:416:ILE:CG2	1:B:426:LEU:N[3_465]	1.81	0.39
1:B:428:GLY:C	1:B:430:LEU:N[4_445]	1.81	0.39
1:B:430:LEU:CG	1:B:432:LYS:O[4_445]	1.81	0.39
1:A:82:GLU:OE1	1:A:98:ILE:N[3_365]	1.82	0.38
1:A:82:GLU:OE1	1:A:98:ILE:C[3_365]	1.82	0.38
1:A:84:PHE:CZ	4:A:502:ATP:N9[3_365]	1.82	0.38
1:A:84:PHE:CZ	4:A:502:ATP:C8[3_365]	1.82	0.38
1:A:86:ASP:OD2	1:A:350:MET:C[3_365]	1.82	0.38
1:A:87:PRO:N	1:A:170:HIS:CB[3_365]	1.82	0.38
1:A:88:TRP:O	1:A:354:ASP:N[3_365]	1.82	0.38
1:A:99:ASP:CB	1:A:401:MET:CE[3_365]	1.82	0.38
1:A:108:GLY:O	1:A:437:VAL:C[3_365]	1.82	0.38
1:A:112:ILE:CB	5:A:569:HOH:O[3_365]	1.82	0.38
1:A:167:GLU:OE1	1:A:279:SER:CA[4_435]	1.82	0.38
1:A:204:LYS:CE	5:A:607:HOH:O[4_435]	1.82	0.38
1:A:224:ALA:CB	1:A:262:GLN:OE1[4_435]	1.82	0.38
1:A:281:PRO:CB	5:A:608:HOH:O[3_365]	1.82	0.38
1:A:326:ARG:NH2	1:A:451:GLU:CG[3_365]	1.82	0.38
1:A:335:LEU:CG	1:A:369:LYS:CE[3_365]	1.82	0.38
1:A:335:LEU:CA	1:A:369:LYS:CG[3_365]	1.82	0.38
1:A:386:GLU:OE2	1:A:417:ARG:NH2[4_435]	1.82	0.38
1:A:458:LYS:CA	1:B:273:ASP:OD2[4_435]	1.82	0.38
1:B:102:LYS:CG	1:B:452:VAL:N[4_445]	1.82	0.38
1:B:107:PHE:O	1:B:298:ARG:O[3_365]	1.82	0.38
1:B:130:HIS:O	1:B:390:PHE:CD1[3_465]	1.82	0.38
1:B:317:PHE:O	1:B:474:HIS:CE1[3_365]	1.82	0.38
1:B:338:THR:OG1	5:B:556:HOH:O[3_465]	1.82	0.38
1:B:370:THR:N	1:B:376:ALA:O[2_355]	1.82	0.38
1:B:374:LYS:CA	1:B:374:LYS:C[4_445]	1.82	0.38
1:B:378:SER:CB	1:B:402:TYR:CD2[4_445]	1.82	0.38
1:B:379:GLY:C	1:B:406:PHE:CD1[4_445]	1.82	0.38
1:B:387:HIS:O	1:B:413:LEU:CB[4_445]	1.82	0.38
1:B:388:ARG:NE	1:B:413:LEU:O[4_445]	1.82	0.38
1:B:394:CYS:C	1:B:437:VAL:O[4_445]	1.82	0.38
1:B:401:MET:CG	1:B:439:GLN:C[4_445]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:N	1:A:349:LYS:CA[3_365]	1.83	0.37
1:A:100:TYR:C	1:A:398:VAL:C[3_365]	1.83	0.37
1:A:101:ASP:N	1:A:399:SER:C[3_365]	1.83	0.37
1:A:105:VAL:CG2	1:A:403:LEU:CB[3_365]	1.83	0.37
1:A:106:ARG:NE	1:A:405:PHE:CE2[3_365]	1.83	0.37
1:A:113:ASP:N	1:A:429:GLU:C[3_365]	1.83	0.37
1:A:113:ASP:N	1:A:429:GLU:O[3_365]	1.83	0.37
1:A:148:ASP:CA	1:A:152:ASN:ND2[2_345]	1.83	0.37
1:A:164:PRO:CD	1:A:270:THR:CG2[4_435]	1.83	0.37
1:A:164:PRO:CA	1:A:270:THR:N[4_435]	1.83	0.37
1:A:176:PRO:C	1:A:374:LYS:NZ[3_365]	1.83	0.37
1:A:202:LEU:CD1	5:A:553:HOH:O[3_365]	1.83	0.37
1:A:209:ASP:N	1:B:262:GLN:NE2[4_435]	1.83	0.37
1:A:211:ALA:O	1:A:273:ASP:C[4_435]	1.83	0.37
1:A:215:ALA:N	1:A:278:ILE:CD1[4_435]	1.83	0.37
1:A:219:ALA:CB	1:A:260:PHE:CG[4_435]	1.83	0.37
1:A:318:ARG:CA	1:A:442:ILE:C[3_365]	1.83	0.37
1:A:323:VAL:CA	1:A:447:ALA:CA[3_365]	1.83	0.37
1:A:344:GLN:CB	5:A:551:HOH:O[4_435]	1.83	0.37
1:A:355:PRO:CB	4:A:502:ATP:C4'[4_435]	1.83	0.37
1:B:103:LEU:N	1:B:450:LYS:C[4_445]	1.83	0.37
1:B:108:GLY:CA	1:B:298:ARG:CB[3_365]	1.83	0.37
1:B:140:HIS:C	1:B:473:HIS:CE1[3_365]	1.83	0.37
1:B:321:ARG:CZ	5:B:519:HOH:O[3_365]	1.83	0.37
1:B:340:PHE:CZ	1:B:366:LYS:N[4_445]	1.83	0.37
1:B:341:PRO:CA	1:B:363:ASP:O[4_445]	1.83	0.37
1:B:341:PRO:CG	1:B:364:THR:O[4_445]	1.83	0.37
1:B:348:THR:CG2	1:B:360:PHE:CB[4_445]	1.83	0.37
1:B:359:ILE:CB	1:B:377:PHE:CD2[3_465]	1.83	0.37
1:B:366:LYS:O	1:B:402:TYR:CE2[3_465]	1.83	0.37
1:B:369:LYS:CB	1:B:378:SER:CA[2_355]	1.83	0.37
1:B:369:LYS:O	1:B:376:ALA:O[2_355]	1.83	0.37
1:B:371:LYS:C	1:B:373:ASN:O[2_355]	1.83	0.37
1:B:373:ASN:CG	1:B:431:LYS:CE[2_355]	1.83	0.37
1:B:380:GLY:C	1:B:403:LEU:N[4_445]	1.83	0.37
1:B:388:ARG:O	1:B:410:ASP:O[4_445]	1.83	0.37
1:B:391:GLY:CA	1:B:407:LEU:C[4_445]	1.83	0.37
1:B:397:ASP:CG	1:B:434:LEU:O[4_445]	1.83	0.37
1:B:402:TYR:N	1:B:439:GLN:CG[4_445]	1.83	0.37
1:B:427:THR:CB	1:B:435:ILE:CG2[2_355]	1.83	0.37
1:A:99:ASP:N	1:A:401:MET:CE[3_365]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:N	1:A:433:ALA:O[3_365]	1.84	0.36
1:A:145:GLN:CA	1:A:152:ASN:CB[2_345]	1.84	0.36
1:A:145:GLN:CB	1:A:152:ASN:O[2_345]	1.84	0.36
1:A:159:TYR:O	5:A:585:HOH:O[3_365]	1.84	0.36
1:A:167:GLU:CB	1:A:277:LYS:C[4_435]	1.84	0.36
1:A:209:ASP:CB	1:B:258:VAL:N[4_435]	1.84	0.36
1:A:210:GLN:C	1:A:274:CYS:CB[4_435]	1.84	0.36
1:A:217:GLU:CB	1:A:278:ILE:C[4_435]	1.84	0.36
1:A:220:LYS:N	1:A:259:THR:O[4_435]	1.84	0.36
1:A:258:VAL:CG2	5:A:515:HOH:O[3_365]	1.84	0.36
1:A:267:PHE:CZ	5:A:542:HOH:O[3_365]	1.84	0.36
1:A:300:ARG:N	1:A:300:ARG:C[2_345]	1.84	0.36
1:A:310:ALA:CA	1:A:371:LYS:CG[3_365]	1.84	0.36
1:A:317:PHE:CG	1:A:363:ASP:CA[3_365]	1.84	0.36
1:A:335:LEU:C	1:A:370:THR:N[3_365]	1.84	0.36
1:A:339:PHE:CG	1:A:344:GLN:CD[3_365]	1.84	0.36
1:A:347:GLN:CB	1:A:347:GLN:CG[3_365]	1.84	0.36
1:A:349:LYS:N	5:A:531:HOH:O[3_365]	1.84	0.36
1:A:356:ASN:ND2	4:A:502:ATP:C4[4_435]	1.84	0.36
1:A:454:ASP:OD2	1:B:277:LYS:CG[4_435]	1.84	0.36
1:B:101:ASP:CB	1:B:451:GLU:CD[4_445]	1.84	0.36
1:B:103:LEU:CG	1:B:450:LYS:CG[4_445]	1.84	0.36
1:B:229:ILE:CD1	1:B:459:GLU:OE1[2_345]	1.84	0.36
1:B:344:GLN:O	1:B:359:ILE:CA[4_445]	1.84	0.36
1:B:369:LYS:C	1:B:376:ALA:O[2_355]	1.84	0.36
1:B:369:LYS:CD	1:B:438:LEU:CD1[3_465]	1.84	0.36
1:B:370:THR:CA	1:B:376:ALA:O[2_355]	1.84	0.36
1:B:371:LYS:CA	1:B:374:LYS:C[2_355]	1.84	0.36
1:B:381:ARG:NE	1:B:404:THR:O[4_445]	1.84	0.36
1:B:384:ILE:CG1	1:B:394:CYS:CB[4_445]	1.84	0.36
1:B:384:ILE:CD1	1:B:394:CYS:CA[4_445]	1.84	0.36
1:B:392:GLY:CA	1:B:406:PHE:C[4_445]	1.84	0.36
1:B:430:LEU:CG	1:B:433:ALA:O[4_445]	1.84	0.36
1:A:91:GLN:CB	1:A:349:LYS:CA[3_365]	1.85	0.35
1:A:114:LYS:CA	1:A:429:GLU:CG[3_365]	1.85	0.35
1:A:139:SER:CA	1:A:431:LYS:O[3_365]	1.85	0.35
1:A:215:ALA:O	1:A:260:PHE:CD2[4_435]	1.85	0.35
1:A:217:GLU:C	1:A:263:VAL:CG2[4_435]	1.85	0.35
1:A:219:ALA:C	1:A:260:PHE:CA[4_435]	1.85	0.35
1:A:220:LYS:CG	1:A:259:THR:C[4_435]	1.85	0.35
1:A:221:ASP:N	1:A:259:THR:O[4_435]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:N	1:A:262:GLN:C[4_435]	1.85	0.35
1:A:257:HIS:O	1:A:449:ARG:O[3_365]	1.85	0.35
1:A:257:HIS:CB	1:A:450:LYS:O[3_365]	1.85	0.35
1:A:300:ARG:C	1:A:300:ARG:C[2_345]	1.85	0.35
1:A:308:PRO:CA	1:A:370:THR:CB[3_365]	1.85	0.35
1:A:309:CYS:N	1:A:367:GLN:O[3_365]	1.85	0.35
1:A:316:TYR:C	1:A:362:THR:N[3_365]	1.85	0.35
1:A:318:ARG:CG	1:A:442:ILE:N[3_365]	1.85	0.35
1:A:319:MET:N	1:A:442:ILE:O[3_365]	1.85	0.35
1:A:335:LEU:O	1:A:369:LYS:O[3_365]	1.85	0.35
1:A:338:THR:CB	1:A:376:ALA:N[3_365]	1.85	0.35
1:A:349:LYS:NZ	1:A:354:ASP:CB[3_365]	1.85	0.35
1:A:457:VAL:CB	1:B:273:ASP:CB[4_435]	1.85	0.35
1:B:274:CYS:CA	5:A:573:HOH:O[3_365]	1.85	0.35
1:B:102:LYS:CG	1:B:451:GLU:O[4_445]	1.85	0.35
1:B:141:ARG:CG	1:B:472:HIS:O[3_365]	1.85	0.35
1:B:340:PHE:CE2	1:B:366:LYS:CB[4_445]	1.85	0.35
1:B:341:PRO:C	1:B:364:THR:CA[4_445]	1.85	0.35
1:B:343:LEU:CD1	1:B:370:THR:CG2[4_445]	1.85	0.35
1:B:397:ASP:OD1	1:B:434:LEU:O[4_445]	1.85	0.35
1:B:413:LEU:N	1:B:423:GLY:O[3_465]	1.85	0.35
1:B:429:GLU:N	1:B:432:LYS:CB[3_465]	1.85	0.35
1:B:431:LYS:C	1:B:431:LYS:CB[3_465]	1.85	0.35
1:B:453:THR:OG1	1:B:465:LYS:N[2_345]	1.85	0.35
1:A:85:VAL:CB	1:A:341:PRO:O[3_365]	1.86	0.34
1:A:91:GLN:C	1:A:349:LYS:N[3_365]	1.86	0.34
1:A:93:SER:C	1:A:97:GLY:O[3_365]	1.86	0.34
1:A:98:ILE:CG2	1:A:345:GLY:CA[3_365]	1.86	0.34
1:A:104:ILE:N	1:A:402:TYR:CA[3_365]	1.86	0.34
1:A:106:ARG:CA	1:A:406:PHE:N[3_365]	1.86	0.34
1:A:106:ARG:CG	1:A:405:PHE:CG[3_365]	1.86	0.34
1:A:110:SER:O	1:A:433:ALA:C[3_365]	1.86	0.34
1:A:112:ILE:CB	1:A:428:GLY:O[3_365]	1.86	0.34
1:A:116:LEU:CD2	1:A:432:LYS:CD[3_365]	1.86	0.34
1:A:140:HIS:CA	1:A:435:ILE:CA[3_365]	1.86	0.34
1:A:145:GLN:OE1	1:A:152:ASN:O[2_345]	1.86	0.34
1:A:158:LEU:CD2	1:A:366:LYS:CE[3_365]	1.86	0.34
1:A:165:SER:O	1:A:277:LYS:CE[4_435]	1.86	0.34
1:A:210:GLN:NE2	1:B:256:LYS:CG[4_435]	1.86	0.34
1:A:307:ILE:CB	1:A:366:LYS:N[3_365]	1.86	0.34
1:A:307:ILE:CG2	1:A:364:THR:OG1[3_365]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:OE1	1:A:360:PHE:CD1[3_365]	1.86	0.34
1:A:313:GLN:O	1:A:360:PHE:N[3_365]	1.86	0.34
1:A:320:THR:CA	1:A:446:GLN:CG[3_365]	1.86	0.34
1:A:320:THR:N	1:A:446:GLN:OE1[3_365]	1.86	0.34
1:A:327:ILE:O	1:A:469:ASP:OD2[2_345]	1.86	0.34
1:A:338:THR:CB	1:A:375:HIS:O[3_365]	1.86	0.34
1:A:347:GLN:N	1:A:347:GLN:CG[3_365]	1.86	0.34
1:B:97:GLY:C	1:B:445:HIS:ND1[4_445]	1.86	0.34
1:B:98:ILE:C	1:B:446:GLN:C[4_445]	1.86	0.34
1:B:344:GLN:O	1:B:359:ILE:C[4_445]	1.86	0.34
1:B:369:LYS:CD	1:B:397:ASP:OD2[2_355]	1.86	0.34
1:B:371:LYS:O	1:B:375:HIS:C[3_465]	1.86	0.34
1:B:375:HIS:CG	1:B:375:HIS:CE1[3_465]	1.86	0.34
1:B:382:ASP:O	1:B:401:MET:CB[4_445]	1.86	0.34
1:B:388:ARG:CD	1:B:414:GLU:CA[4_445]	1.86	0.34
1:B:395:ASP:C	1:B:442:ILE:N[4_445]	1.86	0.34
1:B:399:SER:CB	1:B:435:ILE:CG2[4_445]	1.86	0.34
1:B:400:PHE:CG	1:B:436:GLU:C[4_445]	1.86	0.34
1:B:403:LEU:CD1	1:B:426:LEU:C[3_465]	1.86	0.34
1:B:412:LYS:CA	1:B:424:ALA:CA[3_465]	1.86	0.34
1:B:426:LEU:CB	1:B:430:LEU:CD1[4_445]	1.86	0.34
1:B:426:LEU:N	1:B:436:GLU:CG[2_355]	1.86	0.34
1:A:86:ASP:C	1:A:358:SER:CB[3_365]	1.87	0.33
1:A:99:ASP:CB	1:A:401:MET:SD[3_365]	1.87	0.33
1:A:105:VAL:CB	1:A:403:LEU:CA[3_365]	1.87	0.33
1:A:108:GLY:O	1:A:437:VAL:O[3_365]	1.87	0.33
1:A:109:SER:C	1:A:434:LEU:O[3_365]	1.87	0.33
1:A:114:LYS:NZ	1:A:423:GLY:O[3_365]	1.87	0.33
1:A:138:PHE:CG	1:A:399:SER:OG[3_365]	1.87	0.33
1:A:141:ARG:CG	1:A:439:GLN:CA[3_365]	1.87	0.33
1:A:164:PRO:N	1:A:270:THR:N[4_435]	1.87	0.33
1:A:170:HIS:O	1:A:266:ILE:O[4_435]	1.87	0.33
1:A:197:ASP:CG	1:A:271:ASP:C[4_435]	1.87	0.33
1:A:210:GLN:NE2	1:B:256:LYS:CD[4_435]	1.87	0.33
1:A:221:ASP:CA	1:A:262:GLN:O[4_435]	1.87	0.33
1:A:307:ILE:O	1:A:367:GLN:N[3_365]	1.87	0.33
1:A:316:TYR:CE1	1:A:360:PHE:CD2[3_365]	1.87	0.33
1:A:326:ARG:NH2	1:A:451:GLU:CA[3_365]	1.87	0.33
1:A:338:THR:CG2	1:A:377:PHE:N[3_365]	1.87	0.33
1:A:355:PRO:O	4:A:502:ATP:C3'[4_435]	1.87	0.33
1:A:355:PRO:C	4:A:502:ATP:O2'[4_435]	1.87	0.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:CD1	5:B:560:HOH:O[3_465]	1.87	0.33
1:B:307:ILE:CG2	1:B:475:HIS:CG[3_365]	1.87	0.33
1:B:321:ARG:CZ	1:B:472:HIS:CE1[3_365]	1.87	0.33
1:B:369:LYS:CE	1:B:438:LEU:CG[3_465]	1.87	0.33
1:B:378:SER:O	1:B:402:TYR:CE2[4_445]	1.87	0.33
1:B:396:VAL:C	1:B:442:ILE:CD1[4_445]	1.87	0.33
1:B:409:ASP:CA	1:B:422:SER:CA[3_465]	1.87	0.33
1:B:426:LEU:O	1:B:436:GLU:OE2[2_355]	1.87	0.33
1:B:427:THR:CG2	1:B:435:ILE:CG2[2_355]	1.87	0.33
1:A:91:GLN:CA	1:A:348:THR:CA[3_365]	1.88	0.32
1:A:92:THR:O	1:A:347:GLN:CB[2_245]	1.88	0.32
1:A:106:ARG:O	1:A:406:PHE:CD2[3_365]	1.88	0.32
1:A:148:ASP:OD2	1:A:152:ASN:OD1[2_345]	1.88	0.32
1:A:167:GLU:OE1	1:A:280:PHE:N[4_435]	1.88	0.32
1:A:209:ASP:CB	1:B:258:VAL:CG2[4_435]	1.88	0.32
1:A:210:GLN:O	1:A:274:CYS:O[4_435]	1.88	0.32
1:A:214:TYR:CE2	1:A:277:LYS:CG[4_435]	1.88	0.32
1:A:214:TYR:CE2	1:A:277:LYS:CD[4_435]	1.88	0.32
1:A:219:ALA:CB	1:A:260:PHE:CB[4_435]	1.88	0.32
1:A:219:ALA:O	1:A:260:PHE:C[4_435]	1.88	0.32
1:A:236:SER:CA	1:A:271:ASP:CG[4_435]	1.88	0.32
1:A:266:ILE:CG1	1:A:445:HIS:NE2[3_365]	1.88	0.32
1:A:299:ASP:N	1:A:299:ASP:O[2_345]	1.88	0.32
1:A:300:ARG:NH1	5:A:568:HOH:O[2_345]	1.88	0.32
1:A:323:VAL:CG1	1:A:446:GLN:C[3_365]	1.88	0.32
1:A:338:THR:CB	1:A:376:ALA:O[3_365]	1.88	0.32
1:A:456:ILE:O	1:B:272:SER:CB[4_435]	1.88	0.32
1:B:106:ARG:N	5:B:581:HOH:O[3_365]	1.88	0.32
1:B:110:SER:C	1:B:471:GLN:CD[3_365]	1.88	0.32
1:B:334:LEU:CG	1:B:473:HIS:CA[3_365]	1.88	0.32
1:B:334:LEU:O	1:B:473:HIS:CD2[3_365]	1.88	0.32
1:B:373:ASN:CG	1:B:431:LYS:NZ[4_445]	1.88	0.32
1:B:388:ARG:NH1	1:B:413:LEU:O[4_445]	1.88	0.32
1:B:400:PHE:CB	1:B:435:ILE:O[4_445]	1.88	0.32
1:B:409:ASP:OD2	1:B:422:SER:OG[3_465]	1.88	0.32
1:B:428:GLY:CA	1:B:432:LYS:C[2_355]	1.88	0.32
1:B:428:GLY:CA	1:B:431:LYS:N[4_445]	1.88	0.32
1:B:443:ALA:N	5:B:552:HOH:O[3_465]	1.88	0.32
1:B:453:THR:CB	1:B:464:ARG:C[2_345]	1.88	0.32
1:B:455:GLU:CG	1:B:464:ARG:CG[2_345]	1.88	0.32
1:A:88:TRP:CG	1:A:352:ALA:CA[3_365]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:CB	1:A:405:PHE:CG[3_365]	1.89	0.31
1:A:109:SER:CA	1:A:434:LEU:O[3_365]	1.89	0.31
1:A:111:LYS:CA	1:A:433:ALA:N[3_365]	1.89	0.31
1:A:112:ILE:CG1	5:A:569:HOH:O[3_365]	1.89	0.31
1:A:164:PRO:CG	1:A:270:THR:N[4_435]	1.89	0.31
1:A:197:ASP:OD2	1:A:271:ASP:O[4_435]	1.89	0.31
1:A:209:ASP:OD1	1:B:258:VAL:CG1[4_435]	1.89	0.31
1:A:267:PHE:CE1	5:A:542:HOH:O[3_365]	1.89	0.31
1:A:309:CYS:CA	1:A:367:GLN:O[3_365]	1.89	0.31
1:A:320:THR:CB	1:A:446:GLN:NE2[3_365]	1.89	0.31
1:A:338:THR:CB	1:A:377:PHE:N[3_365]	1.89	0.31
1:A:356:ASN:CG	4:A:502:ATP:C5[4_435]	1.89	0.31
1:A:454:ASP:C	1:B:277:LYS:NZ[4_435]	1.89	0.31
1:A:458:LYS:N	1:B:273:ASP:OD2[4_435]	1.89	0.31
1:B:110:SER:N	1:B:470:PHE:O[3_365]	1.89	0.31
1:B:141:ARG:CG	1:B:472:HIS:CB[3_365]	1.89	0.31
1:B:321:ARG:NE	1:B:472:HIS:NE2[3_365]	1.89	0.31
1:B:340:PHE:CD2	5:B:524:HOH:O[4_445]	1.89	0.31
1:B:341:PRO:O	1:B:364:THR:N[4_445]	1.89	0.31
1:B:366:LYS:CG	1:B:377:PHE:CE2[2_355]	1.89	0.31
1:B:367:GLN:N	1:B:402:TYR:CE1[3_465]	1.89	0.31
1:B:372:VAL:CG2	1:B:376:ALA:O[3_465]	1.89	0.31
1:B:379:GLY:O	1:B:406:PHE:CG[4_445]	1.89	0.31
1:B:397:ASP:N	1:B:438:LEU:CA[4_445]	1.89	0.31
1:B:425:MET:SD	5:B:490:HOH:O[3_465]	1.89	0.31
1:B:427:THR:OG1	1:B:435:ILE:CG1[2_355]	1.89	0.31
1:B:428:GLY:C	1:B:431:LYS:C[2_355]	1.89	0.31
1:B:428:GLY:O	1:B:430:LEU:N[4_445]	1.89	0.31
1:B:429:GLU:N	1:B:432:LYS:CA[2_355]	1.89	0.31
1:B:454:ASP:CB	1:B:463:PRO:O[2_345]	1.89	0.31
1:A:84:PHE:N	1:A:341:PRO:N[3_365]	1.90	0.30
1:A:96:LYS:O	1:A:377:PHE:CZ[3_365]	1.90	0.30
1:A:105:VAL:CG2	1:A:403:LEU:O[3_365]	1.90	0.30
1:A:106:ARG:CD	1:A:405:PHE:CE2[3_365]	1.90	0.30
1:A:109:SER:CA	1:A:437:VAL:C[3_365]	1.90	0.30
1:A:111:LYS:C	1:A:432:LYS:C[3_365]	1.90	0.30
1:A:111:LYS:O	1:A:433:ALA:CA[3_365]	1.90	0.30
1:A:136:ILE:O	1:A:373:ASN:O[3_365]	1.90	0.30
1:A:137:PHE:CZ	1:A:374:LYS:CG[3_365]	1.90	0.30
1:A:138:PHE:CD1	1:A:376:ALA:CB[3_365]	1.90	0.30
1:A:154:LYS:CE	1:A:304:GLN:CB[2_345]	1.90	0.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:CD	1:A:268:GLY:CA[4_435]	1.90	0.30
1:A:162:ARG:CD	1:A:269:PHE:N[4_435]	1.90	0.30
1:A:212:TYR:CD2	1:B:263:VAL:CG2[4_435]	1.90	0.30
1:A:220:LYS:CG	1:A:260:PHE:N[4_435]	1.90	0.30
1:A:234:ILE:CG2	1:B:271:ASP:CG[4_435]	1.90	0.30
1:A:258:VAL:CA	1:A:449:ARG:C[3_365]	1.90	0.30
1:A:299:ASP:OD2	5:A:574:HOH:O[2_345]	1.90	0.30
1:A:307:ILE:CG1	1:A:364:THR:CB[3_365]	1.90	0.30
1:A:319:MET:CB	5:A:532:HOH:O[3_365]	1.90	0.30
1:A:320:THR:N	1:A:446:GLN:CB[3_365]	1.90	0.30
1:A:322:ASP:OD1	1:A:444:GLU:O[3_365]	1.90	0.30
1:A:329:TYR:CG	1:A:471:GLN:CA[2_345]	1.90	0.30
1:A:454:ASP:CA	1:B:277:LYS:CE[4_435]	1.90	0.30
1:A:458:LYS:N	1:B:273:ASP:OD1[4_435]	1.90	0.30
1:A:461:MET:CA	5:B:573:HOH:O[4_435]	1.90	0.30
1:B:102:LYS:CG	1:B:451:GLU:C[4_445]	1.90	0.30
1:B:141:ARG:NE	1:B:472:HIS:CD2[3_365]	1.90	0.30
1:B:141:ARG:CD	1:B:472:HIS:O[3_365]	1.90	0.30
1:B:342:ALA:N	1:B:363:ASP:CA[4_445]	1.90	0.30
1:B:344:GLN:C	1:B:363:ASP:OD2[4_445]	1.90	0.30
1:B:345:GLY:O	1:B:363:ASP:OD1[4_445]	1.90	0.30
1:B:346:ALA:C	1:B:361:LEU:O[4_445]	1.90	0.30
1:B:347:GLN:CA	1:B:361:LEU:CA[4_445]	1.90	0.30
1:B:347:GLN:N	1:B:360:PHE:O[4_445]	1.90	0.30
1:B:350:MET:CG	1:B:367:GLN:CD[4_445]	1.90	0.30
1:B:359:ILE:CG1	1:B:377:PHE:CG[3_465]	1.90	0.30
1:B:369:LYS:CB	1:B:434:LEU:CD2[3_465]	1.90	0.30
1:B:370:THR:O	1:B:375:HIS:CA[2_355]	1.90	0.30
1:B:387:HIS:CE1	1:B:403:LEU:CA[4_445]	1.90	0.30
1:B:388:ARG:NE	1:B:417:ARG:CB[4_445]	1.90	0.30
1:B:400:PHE:CE2	1:B:440:PRO:CG[4_445]	1.90	0.30
1:B:426:LEU:CA	1:B:436:GLU:OE2[2_355]	1.90	0.30
1:B:428:GLY:C	1:B:430:LEU:CB[4_445]	1.90	0.30
1:B:428:GLY:O	1:B:430:LEU:O[2_355]	1.90	0.30
1:A:86:ASP:O	1:A:358:SER:OG[3_365]	1.91	0.29
1:A:92:THR:OG1	1:A:346:ALA:CA[3_365]	1.91	0.29
1:A:92:THR:O	1:A:347:GLN:OE1[2_245]	1.91	0.29
1:A:100:TYR:CE2	1:A:377:PHE:CB[3_365]	1.91	0.29
1:A:101:ASP:C	1:A:401:MET:N[3_365]	1.91	0.29
1:A:110:SER:N	1:A:437:VAL:N[3_365]	1.91	0.29
1:A:112:ILE:CA	1:A:432:LYS:CB[3_365]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:CG	1:A:439:GLN:CB[3_365]	1.91	0.29
1:A:164:PRO:CD	1:A:270:THR:N[4_435]	1.91	0.29
1:A:165:SER:O	5:A:620:HOH:O[4_435]	1.91	0.29
1:A:210:GLN:CD	1:B:256:LYS:CA[4_435]	1.91	0.29
1:A:212:TYR:N	1:B:259:THR:CA[4_435]	1.91	0.29
1:A:212:TYR:OH	1:B:264:LYS:CA[4_435]	1.91	0.29
1:A:214:TYR:N	1:A:278:ILE:CD1[4_435]	1.91	0.29
1:A:215:ALA:O	1:A:260:PHE:CG[4_435]	1.91	0.29
1:A:217:GLU:CB	1:A:278:ILE:CB[4_435]	1.91	0.29
1:A:257:HIS:CG	1:A:450:LYS:CG[3_365]	1.91	0.29
1:A:299:ASP:OD2	5:A:601:HOH:O[2_345]	1.91	0.29
1:A:307:ILE:CG2	1:A:367:GLN:CG[3_365]	1.91	0.29
1:A:308:PRO:CA	1:A:366:LYS:O[3_365]	1.91	0.29
1:A:308:PRO:N	1:A:366:LYS:C[3_365]	1.91	0.29
1:A:312:ASP:CA	1:A:358:SER:O[3_365]	1.91	0.29
1:A:336:HIS:N	1:A:369:LYS:C[3_365]	1.91	0.29
1:A:347:GLN:N	1:A:347:GLN:CD[3_365]	1.91	0.29
1:A:355:PRO:N	4:A:502:ATP:O5'[4_435]	1.91	0.29
1:A:458:LYS:CB	5:B:578:HOH:O[4_435]	1.91	0.29
1:B:99:ASP:OD1	1:B:451:GLU:CB[4_445]	1.91	0.29
1:B:99:ASP:CA	1:B:450:LYS:N[4_445]	1.91	0.29
1:B:140:HIS:O	1:B:471:GLN:C[3_365]	1.91	0.29
1:B:141:ARG:CG	1:B:473:HIS:N[3_365]	1.91	0.29
1:B:141:ARG:CZ	1:B:472:HIS:CB[3_365]	1.91	0.29
1:B:340:PHE:CE2	5:B:524:HOH:O[4_445]	1.91	0.29
1:B:341:PRO:CB	1:B:364:THR:N[4_445]	1.91	0.29
1:B:346:ALA:CB	1:B:442:ILE:CG2[4_445]	1.91	0.29
1:B:365:ALA:C	1:B:402:TYR:CE1[3_465]	1.91	0.29
1:B:366:LYS:CD	1:B:377:PHE:CE2[2_355]	1.91	0.29
1:B:369:LYS:O	1:B:431:LYS:NZ[2_355]	1.91	0.29
1:B:369:LYS:CE	1:B:397:ASP:OD1[2_355]	1.91	0.29
1:B:370:THR:C	1:B:374:LYS:CA[4_445]	1.91	0.29
1:B:372:VAL:O	1:B:372:VAL:O[3_465]	1.91	0.29
1:B:373:ASN:CA	1:B:431:LYS:NZ[4_445]	1.91	0.29
1:B:382:ASP:N	1:B:401:MET:O[4_445]	1.91	0.29
1:B:382:ASP:OD1	1:B:405:PHE:CZ[4_445]	1.91	0.29
1:B:387:HIS:CA	1:B:413:LEU:CD2[4_445]	1.91	0.29
1:B:428:GLY:N	1:B:432:LYS:C[2_355]	1.91	0.29
1:A:82:GLU:CD	1:A:398:VAL:CG2[2_245]	1.92	0.28
1:A:100:TYR:CE1	1:A:343:LEU:O[3_365]	1.92	0.28
1:A:105:VAL:CG2	1:A:403:LEU:CA[3_365]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:NH1	1:A:340:PHE:CG[3_365]	1.92	0.28
1:A:107:PHE:N	1:A:406:PHE:CE2[3_365]	1.92	0.28
1:A:109:SER:CB	1:A:438:LEU:N[3_365]	1.92	0.28
1:A:109:SER:CA	1:A:437:VAL:CB[3_365]	1.92	0.28
1:A:109:SER:N	1:A:437:VAL:CB[3_365]	1.92	0.28
1:A:111:LYS:CA	1:A:434:LEU:N[3_365]	1.92	0.28
1:A:111:LYS:N	1:A:433:ALA:CB[3_365]	1.92	0.28
1:A:148:ASP:CG	1:A:152:ASN:CG[2_345]	1.92	0.28
1:A:166:SER:CB	1:A:203:TRP:CH2[4_435]	1.92	0.28
1:A:198:ASP:N	1:A:272:SER:CB[4_435]	1.92	0.28
1:A:210:GLN:C	1:A:274:CYS:C[4_435]	1.92	0.28
1:A:211:ALA:CA	1:A:273:ASP:O[4_435]	1.92	0.28
1:A:212:TYR:CB	1:B:260:PHE:CA[4_435]	1.92	0.28
1:A:214:TYR:CZ	1:A:277:LYS:CG[4_435]	1.92	0.28
1:A:215:ALA:CA	1:A:260:PHE:CZ[4_435]	1.92	0.28
1:A:220:LYS:N	1:A:261:ASN:N[4_435]	1.92	0.28
1:A:224:ALA:CB	1:A:262:GLN:CG[4_435]	1.92	0.28
1:A:258:VAL:O	5:A:539:HOH:O[3_365]	1.92	0.28
1:A:317:PHE:CZ	1:A:363:ASP:CA[3_365]	1.92	0.28
1:A:337:SER:C	1:A:376:ALA:N[3_365]	1.92	0.28
1:A:338:THR:CB	1:A:375:HIS:C[3_365]	1.92	0.28
1:A:339:PHE:CB	1:A:344:GLN:CG[3_365]	1.92	0.28
1:A:457:VAL:N	1:B:273:ASP:CA[4_435]	1.92	0.28
1:A:461:MET:CG	1:B:271:ASP:CA[4_435]	1.92	0.28
1:B:109:SER:CB	1:B:298:ARG:CD[3_365]	1.92	0.28
1:B:229:ILE:CG2	5:B:572:HOH:O[2_345]	1.92	0.28
1:B:340:PHE:CZ	1:B:366:LYS:CB[4_445]	1.92	0.28
1:B:344:GLN:CG	1:B:371:LYS:CE[4_445]	1.92	0.28
1:B:366:LYS:N	1:B:402:TYR:CE1[3_465]	1.92	0.28
1:B:371:LYS:C	1:B:374:LYS:O[2_355]	1.92	0.28
1:B:373:ASN:CA	1:B:373:ASN:O[4_445]	1.92	0.28
1:B:387:HIS:C	1:B:413:LEU:CD1[4_445]	1.92	0.28
1:B:408:GLU:CA	5:B:580:HOH:O[3_465]	1.92	0.28
1:B:430:LEU:N	1:B:432:LYS:CA[2_355]	1.92	0.28
1:A:84:PHE:N	1:A:340:PHE:O[3_365]	1.93	0.27
1:A:84:PHE:CE2	4:A:502:ATP:C4[3_365]	1.93	0.27
1:A:93:SER:O	5:A:518:HOH:O[2_245]	1.93	0.27
1:A:93:SER:OG	1:A:346:ALA:N[2_245]	1.93	0.27
1:A:107:PHE:CD1	1:A:340:PHE:CZ[3_365]	1.93	0.27
1:A:109:SER:CA	1:A:437:VAL:CA[3_365]	1.93	0.27
1:A:111:LYS:CE	1:A:430:LEU:CA[3_365]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:C	1:A:429:GLU:O[3_365]	1.93	0.27
1:A:114:LYS:N	1:A:429:GLU:CB[3_365]	1.93	0.27
1:A:137:PHE:CE1	1:A:374:LYS:CB[3_365]	1.93	0.27
1:A:140:HIS:N	1:A:435:ILE:N[3_365]	1.93	0.27
1:A:141:ARG:NE	1:A:439:GLN:CA[3_365]	1.93	0.27
1:A:165:SER:N	1:A:273:ASP:OD2[4_435]	1.93	0.27
1:A:208:LEU:CA	1:B:262:GLN:NE2[4_435]	1.93	0.27
1:A:212:TYR:CG	1:B:261:ASN:N[4_435]	1.93	0.27
1:A:217:GLU:CG	1:A:278:ILE:CG2[4_435]	1.93	0.27
1:A:220:LYS:CA	1:A:259:THR:CA[4_435]	1.93	0.27
1:A:258:VAL:N	1:A:449:ARG:C[3_365]	1.93	0.27
1:A:266:ILE:CD1	1:A:445:HIS:CD2[3_365]	1.93	0.27
1:A:307:ILE:CA	1:A:367:GLN:N[3_365]	1.93	0.27
1:A:327:ILE:CB	1:A:450:LYS:NZ[3_365]	1.93	0.27
1:A:335:LEU:CD2	1:A:369:LYS:CE[3_365]	1.93	0.27
1:A:452:VAL:O	1:B:274:CYS:CB[4_435]	1.93	0.27
1:A:457:VAL:CB	1:B:273:ASP:O[4_435]	1.93	0.27
1:A:461:MET:CB	1:B:271:ASP:N[4_435]	1.93	0.27
1:B:99:ASP:CB	1:B:449:ARG:C[4_445]	1.93	0.27
1:B:105:VAL:C	1:B:295:GLN:O[3_365]	1.93	0.27
1:B:106:ARG:CA	1:B:295:GLN:O[3_365]	1.93	0.27
1:B:110:SER:CA	1:B:471:GLN:CG[3_365]	1.93	0.27
1:B:130:HIS:CB	1:B:390:PHE:CG[3_465]	1.93	0.27
1:B:134:ARG:NE	1:B:386:GLU:O[3_465]	1.93	0.27
1:B:171:VAL:CB	1:B:377:PHE:CE2[3_465]	1.93	0.27
1:B:378:SER:CB	1:B:402:TYR:CG[4_445]	1.93	0.27
1:B:384:ILE:CB	1:B:440:PRO:CB[2_355]	1.93	0.27
1:B:395:ASP:O	1:B:441:LEU:CA[4_445]	1.93	0.27
1:B:395:ASP:CB	1:B:441:LEU:CA[4_445]	1.93	0.27
1:B:397:ASP:OD2	1:B:434:LEU:CD1[4_445]	1.93	0.27
1:B:407:LEU:CB	1:B:420:TYR:O[3_465]	1.93	0.27
1:B:413:LEU:N	1:B:423:GLY:CA[3_465]	1.93	0.27
1:B:413:LEU:C	1:B:423:GLY:O[3_465]	1.93	0.27
1:B:416:ILE:CG1	1:B:424:ALA:O[3_465]	1.93	0.27
1:B:453:THR:CG2	1:B:465:LYS:C[2_345]	1.93	0.27
1:B:455:GLU:N	1:B:464:ARG:CB[2_345]	1.93	0.27
1:A:83:ASP:CG	1:A:341:PRO:CG[3_365]	1.94	0.26
1:A:84:PHE:CZ	1:A:356:ASN:CB[2_245]	1.94	0.26
1:A:84:PHE:CD1	4:A:502:ATP:N6[3_365]	1.94	0.26
1:A:89:THR:O	1:A:351:SER:CA[3_365]	1.94	0.26
1:A:91:GLN:CA	1:A:349:LYS:CA[3_365]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:O	1:A:402:TYR:C[3_365]	1.94	0.26
1:A:105:VAL:N	1:A:402:TYR:C[3_365]	1.94	0.26
1:A:137:PHE:N	1:A:373:ASN:C[3_365]	1.94	0.26
1:A:141:ARG:NH2	1:A:438:LEU:C[3_365]	1.94	0.26
1:A:165:SER:O	1:A:277:LYS:CD[4_435]	1.94	0.26
1:A:166:SER:O	1:A:269:PHE:CZ[4_435]	1.94	0.26
1:A:167:GLU:CG	1:A:277:LYS:CA[4_435]	1.94	0.26
1:A:167:GLU:OE2	1:A:276:GLY:C[4_435]	1.94	0.26
1:A:167:GLU:CD	1:A:280:PHE:N[4_435]	1.94	0.26
1:A:207:THR:CG2	1:B:258:VAL:N[4_435]	1.94	0.26
1:A:209:ASP:N	1:B:258:VAL:CA[4_435]	1.94	0.26
1:A:213:SER:OG	1:A:275:ILE:CA[4_435]	1.94	0.26
1:A:218:ASN:N	1:A:263:VAL:CG2[4_435]	1.94	0.26
1:A:299:ASP:N	1:A:299:ASP:CA[2_345]	1.94	0.26
1:A:315:PRO:C	1:A:360:PHE:C[3_365]	1.94	0.26
1:A:332:PRO:O	1:A:365:ALA:CB[3_365]	1.94	0.26
1:A:333:ALA:O	1:A:365:ALA:CB[3_365]	1.94	0.26
1:A:333:ALA:O	1:A:365:ALA:CA[3_365]	1.94	0.26
1:A:335:LEU:O	1:A:370:THR:CA[3_365]	1.94	0.26
1:A:336:HIS:ND1	1:A:368:ILE:O[3_365]	1.94	0.26
1:A:339:PHE:CB	1:A:344:GLN:CB[3_365]	1.94	0.26
1:A:347:GLN:C	1:A:347:GLN:CB[3_365]	1.94	0.26
1:A:347:GLN:CA	1:A:347:GLN:CD[3_365]	1.94	0.26
1:B:275:ILE:CD1	5:A:520:HOH:O[3_365]	1.94	0.26
1:B:99:ASP:OD2	1:B:448:ARG:C[4_445]	1.94	0.26
1:B:102:LYS:CA	1:B:451:GLU:O[4_445]	1.94	0.26
1:B:104:ILE:CB	1:B:298:ARG:NH2[3_365]	1.94	0.26
1:B:110:SER:CB	5:B:494:HOH:O[3_365]	1.94	0.26
1:B:317:PHE:CD1	1:B:475:HIS:C[3_365]	1.94	0.26
1:B:375:HIS:ND1	1:B:375:HIS:ND1[3_465]	1.94	0.26
1:B:384:ILE:CG2	1:B:400:PHE:CZ[4_445]	1.94	0.26
1:B:388:ARG:CD	1:B:414:GLU:N[4_445]	1.94	0.26
1:B:397:ASP:CG	1:B:438:LEU:CB[4_445]	1.94	0.26
1:B:399:SER:CB	1:B:427:THR:OG1[3_465]	1.94	0.26
1:B:400:PHE:CB	1:B:436:GLU:C[4_445]	1.94	0.26
1:B:429:GLU:CA	1:B:432:LYS:CB[3_465]	1.94	0.26
1:B:431:LYS:CA	1:B:431:LYS:O[4_445]	1.94	0.26
1:B:432:LYS:C	1:B:432:LYS:CD[4_445]	1.94	0.26
1:B:432:LYS:N	1:B:432:LYS:N[4_445]	1.94	0.26
1:A:82:GLU:OE1	1:A:98:ILE:CA[3_365]	1.95	0.25
1:A:87:PRO:C	1:A:358:SER:OG[3_365]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:CG2	1:A:345:GLY:N[3_365]	1.95	0.25
1:A:103:LEU:CG	1:A:402:TYR:CE2[3_365]	1.95	0.25
1:A:108:GLY:O	1:A:437:VAL:CB[3_365]	1.95	0.25
1:A:108:GLY:C	1:A:437:VAL:CB[3_365]	1.95	0.25
1:A:207:THR:CB	1:B:257:HIS:CA[4_435]	1.95	0.25
1:A:209:ASP:CG	1:B:258:VAL:CG1[4_435]	1.95	0.25
1:A:210:GLN:O	1:A:275:ILE:N[4_435]	1.95	0.25
1:A:217:GLU:CB	1:A:278:ILE:O[4_435]	1.95	0.25
1:A:219:ALA:O	1:A:261:ASN:C[4_435]	1.95	0.25
1:A:221:ASP:CA	1:A:262:GLN:CB[4_435]	1.95	0.25
1:A:221:ASP:CG	1:A:263:VAL:CG1[4_435]	1.95	0.25
1:A:221:ASP:N	1:A:262:GLN:C[4_435]	1.95	0.25
1:A:255:GLN:O	5:A:539:HOH:O[3_365]	1.95	0.25
1:A:312:ASP:CG	1:A:358:SER:O[3_365]	1.95	0.25
1:A:313:GLN:NE2	1:A:360:PHE:CE1[3_365]	1.95	0.25
1:A:316:TYR:CD1	1:A:360:PHE:CG[3_365]	1.95	0.25
1:A:355:PRO:CB	4:A:502:ATP:C3'[4_435]	1.95	0.25
1:A:461:MET:CB	1:B:270:THR:C[4_435]	1.95	0.25
1:B:109:SER:O	1:B:470:PHE:CB[3_365]	1.95	0.25
1:B:332:PRO:O	1:B:473:HIS:O[3_365]	1.95	0.25
1:B:334:LEU:CD2	1:B:474:HIS:N[3_365]	1.95	0.25
1:B:341:PRO:CG	1:B:364:THR:CA[4_445]	1.95	0.25
1:B:341:PRO:C	1:B:363:ASP:C[4_445]	1.95	0.25
1:B:345:GLY:O	1:B:363:ASP:N[4_445]	1.95	0.25
1:B:369:LYS:NZ	1:B:438:LEU:CB[3_465]	1.95	0.25
1:B:378:SER:N	1:B:402:TYR:CE2[4_445]	1.95	0.25
1:B:381:ARG:NH1	1:B:405:PHE:O[4_445]	1.95	0.25
1:B:389:GLN:N	5:B:535:HOH:O[4_445]	1.95	0.25
1:B:401:MET:CA	1:B:439:GLN:CG[4_445]	1.95	0.25
1:B:403:LEU:CD1	1:B:436:GLU:CG[4_445]	1.95	0.25
1:B:420:TYR:CB	1:B:437:VAL:CG2[4_445]	1.95	0.25
1:B:428:GLY:CA	1:B:430:LEU:CG[4_445]	1.95	0.25
1:B:429:GLU:N	1:B:432:LYS:O[2_355]	1.95	0.25
1:A:86:ASP:C	1:A:170:HIS:ND1[3_365]	1.96	0.24
1:A:88:TRP:CB	1:A:352:ALA:N[3_365]	1.96	0.24
1:A:100:TYR:CZ	1:A:377:PHE:N[3_365]	1.96	0.24
1:A:114:LYS:CB	1:A:429:GLU:OE1[3_365]	1.96	0.24
1:A:114:LYS:CA	1:A:429:GLU:OE2[3_365]	1.96	0.24
1:A:164:PRO:CB	1:A:273:ASP:OD2[4_435]	1.96	0.24
1:A:175:ILE:C	1:A:374:LYS:CE[3_365]	1.96	0.24
1:A:211:ALA:CA	1:A:274:CYS:N[4_435]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TYR:CE1	1:B:260:PHE:C[4_435]	1.96	0.24
1:A:213:SER:O	1:A:278:ILE:CB[4_435]	1.96	0.24
1:A:219:ALA:C	1:A:261:ASN:CA[4_435]	1.96	0.24
1:A:221:ASP:C	1:A:262:GLN:N[4_435]	1.96	0.24
1:A:307:ILE:CB	1:A:366:LYS:CA[3_365]	1.96	0.24
1:A:310:ALA:O	1:A:371:LYS:CG[3_365]	1.96	0.24
1:A:313:GLN:O	1:A:360:PHE:O[3_365]	1.96	0.24
1:A:320:THR:N	1:A:446:GLN:NE2[3_365]	1.96	0.24
1:A:322:ASP:OD2	1:A:444:GLU:C[3_365]	1.96	0.24
1:A:335:LEU:CD2	1:A:369:LYS:CD[3_365]	1.96	0.24
1:A:336:HIS:CA	1:A:372:VAL:CB[3_365]	1.96	0.24
1:A:337:SER:CB	1:A:374:LYS:N[3_365]	1.96	0.24
1:A:355:PRO:CB	4:A:502:ATP:C5'[4_435]	1.96	0.24
1:A:457:VAL:CG1	1:B:273:ASP:O[4_435]	1.96	0.24
1:B:99:ASP:O	1:B:450:LYS:CB[4_445]	1.96	0.24
1:B:103:LEU:CA	1:B:450:LYS:O[4_445]	1.96	0.24
1:B:307:ILE:CB	1:B:475:HIS:CD2[3_365]	1.96	0.24
1:B:334:LEU:C	1:B:473:HIS:CD2[3_365]	1.96	0.24
1:B:344:GLN:O	1:B:358:SER:O[4_445]	1.96	0.24
1:B:369:LYS:CD	1:B:434:LEU:CG[3_465]	1.96	0.24
1:B:373:ASN:CA	1:B:373:ASN:CA[4_445]	1.96	0.24
1:B:380:GLY:C	1:B:402:TYR:CA[4_445]	1.96	0.24
1:B:384:ILE:CG1	1:B:440:PRO:CD[2_355]	1.96	0.24
1:B:397:ASP:C	1:B:438:LEU:CA[4_445]	1.96	0.24
1:B:401:MET:CA	1:B:439:GLN:CA[4_445]	1.96	0.24
1:B:407:LEU:CD2	1:B:421:THR:C[3_465]	1.96	0.24
1:B:469:ASP:CB	5:B:577:HOH:O[4_435]	1.96	0.24
1:A:82:GLU:CD	1:A:377:PHE:CB[2_245]	1.97	0.23
1:A:83:ASP:CB	1:A:341:PRO:CB[3_365]	1.97	0.23
1:A:83:ASP:O	1:A:340:PHE:CA[3_365]	1.97	0.23
1:A:89:THR:CA	1:A:351:SER:N[3_365]	1.97	0.23
1:A:90:VAL:O	1:A:348:THR:CB[3_365]	1.97	0.23
1:A:91:GLN:N	1:A:348:THR:C[3_365]	1.97	0.23
1:A:92:THR:N	1:A:348:THR:CA[3_365]	1.97	0.23
1:A:95:ALA:O	1:A:97:GLY:O[4_435]	1.97	0.23
1:A:99:ASP:OD2	1:A:394:CYS:O[3_365]	1.97	0.23
1:A:100:TYR:CE2	1:A:377:PHE:CA[3_365]	1.97	0.23
1:A:107:PHE:CA	1:A:406:PHE:CG[3_365]	1.97	0.23
1:A:110:SER:N	1:A:434:LEU:C[3_365]	1.97	0.23
1:A:162:ARG:C	1:A:270:THR:CG2[4_435]	1.97	0.23
1:A:212:TYR:CG	1:B:259:THR:O[4_435]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TYR:N	1:B:259:THR:CB[4_435]	1.97	0.23
1:A:213:SER:N	1:B:260:PHE:N[4_435]	1.97	0.23
1:A:222:ILE:CG1	1:A:261:ASN:O[4_435]	1.97	0.23
1:A:234:ILE:CG1	1:A:261:ASN:OD1[4_435]	1.97	0.23
1:A:290:SER:OG	1:A:300:ARG:NE[2_345]	1.97	0.23
1:A:308:PRO:CG	1:A:370:THR:OG1[3_365]	1.97	0.23
1:A:309:CYS:N	1:A:370:THR:CB[3_365]	1.97	0.23
1:A:319:MET:C	1:A:446:GLN:CA[3_365]	1.97	0.23
1:A:326:ARG:CG	5:A:610:HOH:O[3_365]	1.97	0.23
1:A:336:HIS:CA	1:A:368:ILE:O[3_365]	1.97	0.23
1:A:339:PHE:CE1	1:A:357:SER:C[3_365]	1.97	0.23
1:B:99:ASP:O	1:B:449:ARG:C[4_445]	1.97	0.23
1:B:99:ASP:O	1:B:451:GLU:N[4_445]	1.97	0.23
1:B:105:VAL:N	1:B:465:LYS:CE[3_365]	1.97	0.23
1:B:133:ARG:N	1:B:390:PHE:CZ[3_465]	1.97	0.23
1:B:343:LEU:O	1:B:371:LYS:CD[4_445]	1.97	0.23
1:B:373:ASN:OD1	1:B:431:LYS:CE[2_355]	1.97	0.23
1:B:380:GLY:CA	1:B:403:LEU:CA[4_445]	1.97	0.23
1:B:396:VAL:CA	1:B:442:ILE:CD1[4_445]	1.97	0.23
1:B:407:LEU:CD1	1:B:420:TYR:O[3_465]	1.97	0.23
1:B:416:ILE:CG1	1:B:425:MET:C[3_465]	1.97	0.23
1:B:428:GLY:C	1:B:431:LYS:O[2_355]	1.97	0.23
1:B:430:LEU:N	1:B:430:LEU:O[4_445]	1.97	0.23
1:A:84:PHE:CA	1:A:340:PHE:CA[3_365]	1.98	0.22
1:A:85:VAL:C	1:A:350:MET:SD[3_365]	1.98	0.22
1:A:92:THR:CB	1:A:346:ALA:N[3_365]	1.98	0.22
1:A:103:LEU:CA	1:A:402:TYR:CD1[3_365]	1.98	0.22
1:A:103:LEU:CD2	1:A:402:TYR:OH[3_365]	1.98	0.22
1:A:106:ARG:CA	1:A:405:PHE:C[3_365]	1.98	0.22
1:A:137:PHE:CD1	1:A:374:LYS:CG[3_365]	1.98	0.22
1:A:137:PHE:CG	1:A:373:ASN:CA[3_365]	1.98	0.22
1:A:138:PHE:O	1:A:431:LYS:N[3_365]	1.98	0.22
1:A:141:ARG:CB	1:A:439:GLN:CD[3_365]	1.98	0.22
1:A:167:GLU:CG	1:A:278:ILE:N[4_435]	1.98	0.22
1:A:197:ASP:O	1:A:272:SER:CA[4_435]	1.98	0.22
1:A:208:LEU:C	1:B:259:THR:CG2[4_435]	1.98	0.22
1:A:212:TYR:CB	1:B:260:PHE:C[4_435]	1.98	0.22
1:A:217:GLU:OE2	1:B:275:ILE:CB[4_435]	1.98	0.22
1:A:220:LYS:NZ	1:B:274:CYS:O[4_435]	1.98	0.22
1:A:239:ASP:OD1	1:B:264:LYS:C[4_435]	1.98	0.22
1:A:289:PHE:CG	1:A:471:GLN:C[2_345]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:N	1:A:366:LYS:CG[3_365]	1.98	0.22
1:A:311:ILE:N	1:A:343:LEU:CD1[3_365]	1.98	0.22
1:A:312:ASP:O	1:A:359:ILE:C[3_365]	1.98	0.22
1:A:316:TYR:O	1:A:361:LEU:C[3_365]	1.98	0.22
1:A:319:MET:CA	1:A:446:GLN:CG[3_365]	1.98	0.22
1:A:327:ILE:CB	1:A:469:ASP:OD2[2_345]	1.98	0.22
1:A:327:ILE:N	1:A:469:ASP:OD2[2_345]	1.98	0.22
1:A:334:LEU:CD1	1:A:368:ILE:CB[3_365]	1.98	0.22
1:A:336:HIS:CA	1:A:372:VAL:CA[3_365]	1.98	0.22
1:A:454:ASP:O	1:B:273:ASP:CG[4_435]	1.98	0.22
1:A:461:MET:N	1:B:270:THR:CB[4_435]	1.98	0.22
1:B:103:LEU:CD1	1:B:450:LYS:CG[4_445]	1.98	0.22
1:B:107:PHE:O	1:B:298:ARG:CB[3_365]	1.98	0.22
1:B:130:HIS:O	1:B:390:PHE:CG[3_465]	1.98	0.22
1:B:133:ARG:NE	1:B:389:GLN:NE2[3_465]	1.98	0.22
1:B:340:PHE:C	1:B:364:THR:CA[4_445]	1.98	0.22
1:B:343:LEU:CB	1:B:371:LYS:CG[4_445]	1.98	0.22
1:B:343:LEU:C	1:B:371:LYS:CG[4_445]	1.98	0.22
1:B:346:ALA:C	1:B:362:THR:CA[4_445]	1.98	0.22
1:B:367:GLN:N	1:B:402:TYR:CZ[3_465]	1.98	0.22
1:B:370:THR:CA	1:B:376:ALA:C[2_355]	1.98	0.22
1:B:373:ASN:CA	1:B:373:ASN:C[4_445]	1.98	0.22
1:B:384:ILE:CA	1:B:440:PRO:CG[2_355]	1.98	0.22
1:B:395:ASP:CA	1:B:441:LEU:C[4_445]	1.98	0.22
1:B:397:ASP:CA	1:B:438:LEU:CD2[4_445]	1.98	0.22
1:B:397:ASP:C	1:B:438:LEU:C[4_445]	1.98	0.22
1:B:402:TYR:CA	1:B:439:GLN:CD[4_445]	1.98	0.22
1:B:412:LYS:CG	1:B:422:SER:OG[3_465]	1.98	0.22
1:B:427:THR:O	5:B:501:HOH:O[3_465]	1.98	0.22
1:B:432:LYS:NZ	1:B:436:GLU:N[3_465]	1.98	0.22
1:B:440:PRO:N	5:B:567:HOH:O[2_355]	1.98	0.22
1:B:455:GLU:CB	1:B:464:ARG:CD[2_345]	1.98	0.22
1:B:455:GLU:OE2	1:B:464:ARG:C[2_345]	1.98	0.22
1:A:82:GLU:OE2	1:A:398:VAL:CG2[2_245]	1.99	0.21
1:A:82:GLU:C	5:A:547:HOH:O[2_245]	1.99	0.21
1:A:92:THR:C	1:A:347:GLN:CA[3_365]	1.99	0.21
1:A:93:SER:CB	1:A:98:ILE:N[3_365]	1.99	0.21
1:A:93:SER:OG	1:A:345:GLY:C[2_245]	1.99	0.21
1:A:100:TYR:OH	1:A:343:LEU:C[3_365]	1.99	0.21
1:A:101:ASP:CG	1:A:400:PHE:CB[3_365]	1.99	0.21
1:A:105:VAL:C	1:A:402:TYR:O[3_365]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:C	1:A:433:ALA:CA[3_365]	1.99	0.21
1:A:112:ILE:CG1	1:A:432:LYS:N[3_365]	1.99	0.21
1:A:137:PHE:CE2	1:A:370:THR:CA[3_365]	1.99	0.21
1:A:166:SER:C	1:A:269:PHE:CE1[4_435]	1.99	0.21
1:A:166:SER:OG	1:A:203:TRP:CH2[4_435]	1.99	0.21
1:A:167:GLU:OE1	1:A:279:SER:C[4_435]	1.99	0.21
1:A:197:ASP:CA	1:A:272:SER:OG[4_435]	1.99	0.21
1:A:209:ASP:N	1:B:258:VAL:C[4_435]	1.99	0.21
1:A:209:ASP:C	1:B:258:VAL:CA[4_435]	1.99	0.21
1:A:212:TYR:CD2	1:B:260:PHE:O[4_435]	1.99	0.21
1:A:212:TYR:O	1:B:260:PHE:CG[4_435]	1.99	0.21
1:A:239:ASP:OD1	1:B:264:LYS:CB[4_435]	1.99	0.21
1:A:313:GLN:O	1:A:363:ASP:CG[3_365]	1.99	0.21
1:A:314:ASP:N	1:A:359:ILE:CA[3_365]	1.99	0.21
1:A:318:ARG:CG	1:A:441:LEU:CD2[3_365]	1.99	0.21
1:A:321:ARG:N	1:A:446:GLN:OE1[3_365]	1.99	0.21
1:A:327:ILE:CG2	1:A:450:LYS:CE[3_365]	1.99	0.21
1:A:347:GLN:CG	1:A:347:GLN:CG[3_365]	1.99	0.21
1:A:349:LYS:CE	1:A:354:ASP:CG[3_365]	1.99	0.21
1:B:100:TYR:CA	1:B:450:LYS:CB[4_445]	1.99	0.21
1:B:111:LYS:CA	1:B:469:ASP:OD1[3_365]	1.99	0.21
1:B:307:ILE:CG1	1:B:475:HIS:CB[3_365]	1.99	0.21
1:B:307:ILE:CG1	1:B:475:HIS:ND1[3_365]	1.99	0.21
1:B:341:PRO:N	1:B:364:THR:N[4_445]	1.99	0.21
1:B:359:ILE:CA	1:B:377:PHE:CB[3_465]	1.99	0.21
1:B:381:ARG:CB	1:B:404:THR:N[4_445]	1.99	0.21
1:B:392:GLY:N	1:B:407:LEU:C[4_445]	1.99	0.21
1:B:393:ASN:ND2	1:B:441:LEU:CD1[4_445]	1.99	0.21
1:B:399:SER:O	1:B:439:GLN:OE1[4_445]	1.99	0.21
1:B:429:GLU:N	1:B:433:ALA:CA[2_355]	1.99	0.21
1:B:429:GLU:C	1:B:429:GLU:C[3_465]	1.99	0.21
1:B:430:LEU:CD2	1:B:434:LEU:O[4_445]	1.99	0.21
1:B:455:GLU:OE2	1:B:463:PRO:C[2_345]	1.99	0.21
1:A:92:THR:C	1:A:347:GLN:N[3_365]	2.00	0.20
1:A:99:ASP:C	1:A:398:VAL:CA[3_365]	2.00	0.20
1:A:102:LYS:CA	1:A:401:MET:N[3_365]	2.00	0.20
1:A:135:GLY:CA	1:A:427:THR:OG1[3_365]	2.00	0.20
1:A:212:TYR:CE2	1:B:263:VAL:CB[4_435]	2.00	0.20
1:A:212:TYR:N	1:A:273:ASP:O[4_435]	2.00	0.20
1:A:221:ASP:O	1:A:262:GLN:O[4_435]	2.00	0.20
1:A:307:ILE:CG2	1:A:367:GLN:CB[3_365]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:CG2	1:A:367:GLN:CA[3_365]	2.00	0.20
1:A:307:ILE:CB	1:A:364:THR:OG1[3_365]	2.00	0.20
1:A:316:TYR:CB	1:A:362:THR:CA[3_365]	2.00	0.20
1:A:317:PHE:CZ	1:A:364:THR:N[3_365]	2.00	0.20
1:A:333:ALA:O	1:A:365:ALA:O[3_365]	2.00	0.20
1:A:354:ASP:OD2	4:A:502:ATP:O1A[4_435]	2.00	0.20
1:A:444:GLU:CD	5:A:617:HOH:O[4_435]	2.00	0.20
1:B:133:ARG:CB	1:B:390:PHE:CE2[3_465]	2.00	0.20
1:B:307:ILE:CD1	1:B:474:HIS:C[3_365]	2.00	0.20
1:B:321:ARG:CD	1:B:472:HIS:NE2[3_365]	2.00	0.20
1:B:341:PRO:CB	1:B:364:THR:CA[4_445]	2.00	0.20
1:B:342:ALA:O	1:B:363:ASP:CG[4_445]	2.00	0.20
1:B:359:ILE:CA	1:B:377:PHE:CG[3_465]	2.00	0.20
1:B:373:ASN:N	1:B:373:ASN:O[4_445]	2.00	0.20
1:B:381:ARG:N	1:B:403:LEU:C[4_445]	2.00	0.20
1:B:398:VAL:O	1:B:439:GLN:CG[4_445]	2.00	0.20
1:B:399:SER:C	1:B:435:ILE:O[4_445]	2.00	0.20
1:B:403:LEU:CD2	1:B:420:TYR:CZ[3_465]	2.00	0.20
1:B:407:LEU:CD2	1:B:421:THR:CA[3_465]	2.00	0.20
1:B:413:LEU:N	5:B:538:HOH:O[3_465]	2.00	0.20
1:B:427:THR:C	1:B:432:LYS:O[2_355]	2.00	0.20
1:B:430:LEU:CB	1:B:432:LYS:C[4_445]	2.00	0.20
1:B:430:LEU:CG	1:B:432:LYS:CE[2_355]	2.00	0.20
1:B:455:GLU:CG	1:B:464:ARG:CA[2_345]	2.00	0.20
1:B:458:LYS:CD	1:B:462:THR:OG1[2_345]	2.00	0.20
1:A:83:ASP:CA	1:A:341:PRO:CD[3_365]	2.01	0.19
1:A:93:SER:O	1:A:95:ALA:O[2_245]	2.01	0.19
1:A:98:ILE:CD1	1:A:398:VAL:CG1[3_365]	2.01	0.19
1:A:99:ASP:CA	1:A:401:MET:CE[3_365]	2.01	0.19
1:A:101:ASP:CA	1:A:399:SER:C[3_365]	2.01	0.19
1:A:102:LYS:CA	1:A:400:PHE:C[3_365]	2.01	0.19
1:A:154:LYS:CD	1:A:304:GLN:CG[2_345]	2.01	0.19
1:A:162:ARG:CZ	1:A:268:GLY:CA[4_435]	2.01	0.19
1:A:164:PRO:CB	1:A:270:THR:O[4_435]	2.01	0.19
1:A:169:MET:SD	1:A:263:VAL:C[4_435]	2.01	0.19
1:A:169:MET:CE	1:A:267:PHE:N[4_435]	2.01	0.19
1:A:197:ASP:C	1:A:272:SER:OG[4_435]	2.01	0.19
1:A:197:ASP:CG	1:A:271:ASP:O[4_435]	2.01	0.19
1:A:214:TYR:CD1	1:A:277:LYS:CB[4_435]	2.01	0.19
1:A:219:ALA:O	1:A:261:ASN:CB[4_435]	2.01	0.19
1:A:220:LYS:CB	1:A:260:PHE:N[4_435]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:CG2	1:A:361:LEU:CD2[3_365]	2.01	0.19
1:A:316:TYR:CB	1:A:362:THR:C[3_365]	2.01	0.19
1:A:316:TYR:CG	1:A:362:THR:OG1[3_365]	2.01	0.19
1:A:317:PHE:CE1	1:A:367:GLN:OE1[3_365]	2.01	0.19
1:A:318:ARG:CG	1:A:442:ILE:CA[3_365]	2.01	0.19
1:A:321:ARG:N	1:A:443:ALA:CA[3_365]	2.01	0.19
1:A:326:ARG:NH1	1:A:451:GLU:CD[3_365]	2.01	0.19
1:A:328:GLY:N	1:A:469:ASP:OD2[2_345]	2.01	0.19
1:A:333:ALA:C	1:A:365:ALA:CB[3_365]	2.01	0.19
1:A:338:THR:N	1:A:375:HIS:CA[3_365]	2.01	0.19
1:A:354:ASP:CA	4:A:502:ATP:O1A[4_435]	2.01	0.19
1:A:355:PRO:CG	4:A:502:ATP:O5'[4_435]	2.01	0.19
1:A:367:GLN:NE2	3:A:501:LTN:CE2[4_435]	2.01	0.19
1:A:456:ILE:C	1:B:272:SER:O[4_435]	2.01	0.19
1:A:471:GLN:CA	5:A:568:HOH:O[2_345]	2.01	0.19
1:B:97:GLY:O	1:B:445:HIS:O[4_445]	2.01	0.19
1:B:103:LEU:CD1	1:B:450:LYS:CE[4_445]	2.01	0.19
1:B:110:SER:OG	1:B:471:GLN:N[3_365]	2.01	0.19
1:B:359:ILE:CD1	1:B:377:PHE:N[3_465]	2.01	0.19
1:B:368:ILE:CB	1:B:398:VAL:C[3_465]	2.01	0.19
1:B:369:LYS:CG	1:B:378:SER:CA[2_355]	2.01	0.19
1:B:394:CYS:C	1:B:441:LEU:N[4_445]	2.01	0.19
1:B:395:ASP:O	1:B:442:ILE:CA[4_445]	2.01	0.19
1:B:401:MET:C	1:B:439:GLN:CD[4_445]	2.01	0.19
1:B:401:MET:CB	1:B:439:GLN:CA[4_445]	2.01	0.19
1:B:409:ASP:C	1:B:422:SER:C[3_465]	2.01	0.19
1:B:412:LYS:CG	1:B:419:ASP:O[3_465]	2.01	0.19
1:B:416:ILE:N	1:B:424:ALA:O[3_465]	2.01	0.19
1:B:425:MET:CE	5:B:490:HOH:O[3_465]	2.01	0.19
1:B:426:LEU:CB	1:B:432:LYS:NZ[3_465]	2.01	0.19
1:B:430:LEU:CD2	1:B:435:ILE:N[4_445]	2.01	0.19
1:B:431:LYS:CB	1:B:431:LYS:CG[4_445]	2.01	0.19
1:A:82:GLU:OE2	1:A:377:PHE:CB[2_245]	2.02	0.18
1:A:82:GLU:CA	1:A:377:PHE:CA[2_245]	2.02	0.18
1:A:84:PHE:CD2	4:A:502:ATP:C6[3_365]	2.02	0.18
1:A:84:PHE:N	1:A:344:GLN:CB[2_245]	2.02	0.18
1:A:88:TRP:CB	1:A:353:SER:N[3_365]	2.02	0.18
1:A:89:THR:CA	1:A:351:SER:OG[3_365]	2.02	0.18
1:A:92:THR:CB	1:A:345:GLY:O[3_365]	2.02	0.18
1:A:93:SER:CB	1:A:345:GLY:CA[2_245]	2.02	0.18
1:A:99:ASP:CA	1:A:401:MET:SD[3_365]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:O	1:A:400:PHE:N[3_365]	2.02	0.18
1:A:102:LYS:CA	1:A:401:MET:O[3_365]	2.02	0.18
1:A:102:LYS:CE	5:A:603:HOH:O[3_365]	2.02	0.18
1:A:105:VAL:CG1	1:A:403:LEU:C[3_365]	2.02	0.18
1:A:112:ILE:CD1	1:A:373:ASN:OD1[3_365]	2.02	0.18
1:A:113:ASP:CA	1:A:429:GLU:CG[3_365]	2.02	0.18
1:A:135:GLY:O	1:A:431:LYS:CE[3_365]	2.02	0.18
1:A:144:ASN:C	1:A:152:ASN:OD1[2_345]	2.02	0.18
1:A:159:TYR:C	5:A:585:HOH:O[3_365]	2.02	0.18
1:A:213:SER:CA	1:A:275:ILE:CG2[4_435]	2.02	0.18
1:A:214:TYR:CA	1:A:278:ILE:CD1[4_435]	2.02	0.18
1:A:234:ILE:O	1:B:271:ASP:OD2[4_435]	2.02	0.18
1:A:310:ALA:O	1:A:371:LYS:CB[3_365]	2.02	0.18
1:A:322:ASP:CB	1:A:445:HIS:N[3_365]	2.02	0.18
1:A:337:SER:N	1:A:372:VAL:C[3_365]	2.02	0.18
1:A:348:THR:OG1	1:A:348:THR:OG1[3_365]	2.02	0.18
1:A:349:LYS:CA	5:A:531:HOH:O[3_365]	2.02	0.18
1:B:104:ILE:C	1:B:298:ARG:NH2[3_365]	2.02	0.18
1:B:109:SER:N	1:B:470:PHE:O[3_365]	2.02	0.18
1:B:307:ILE:CB	1:B:475:HIS:CG[3_365]	2.02	0.18
1:B:345:GLY:O	1:B:363:ASP:CB[4_445]	2.02	0.18
1:B:347:GLN:O	1:B:362:THR:OG1[4_445]	2.02	0.18
1:B:368:ILE:CG1	1:B:398:VAL:CA[3_465]	2.02	0.18
1:B:381:ARG:C	1:B:404:THR:OG1[4_445]	2.02	0.18
1:B:384:ILE:CG1	1:B:400:PHE:CE2[4_445]	2.02	0.18
1:B:387:HIS:ND1	1:B:403:LEU:O[4_445]	2.02	0.18
1:B:387:HIS:NE2	1:B:403:LEU:CB[4_445]	2.02	0.18
1:B:389:GLN:CA	1:B:410:ASP:OD1[4_445]	2.02	0.18
1:B:397:ASP:O	1:B:438:LEU:CA[4_445]	2.02	0.18
1:B:401:MET:SD	1:B:442:ILE:CB[4_445]	2.02	0.18
1:B:427:THR:OG1	1:B:435:ILE:CD1[2_355]	2.02	0.18
1:B:430:LEU:CA	1:B:432:LYS:O[4_445]	2.02	0.18
1:B:430:LEU:CD2	1:B:433:ALA:C[4_445]	2.02	0.18
1:B:443:ALA:C	5:B:552:HOH:O[3_465]	2.02	0.18
1:A:82:GLU:N	1:A:377:PHE:CA[2_245]	2.03	0.17
1:A:84:PHE:CE1	4:A:502:ATP:C2[3_365]	2.03	0.17
1:A:89:THR:C	1:A:350:MET:C[3_365]	2.03	0.17
1:A:91:GLN:CB	1:A:348:THR:C[3_365]	2.03	0.17
1:A:91:GLN:OE1	5:A:531:HOH:O[2_245]	2.03	0.17
1:A:93:SER:N	1:A:346:ALA:C[3_365]	2.03	0.17
1:A:96:LYS:C	5:A:599:HOH:O[3_365]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:O	1:A:406:PHE:CZ[3_365]	2.03	0.17
1:A:110:SER:C	1:A:434:LEU:CA[3_365]	2.03	0.17
1:A:112:ILE:N	1:A:432:LYS:CA[3_365]	2.03	0.17
1:A:135:GLY:C	1:A:431:LYS:NZ[3_365]	2.03	0.17
1:A:139:SER:C	1:A:435:ILE:CB[3_365]	2.03	0.17
1:A:143:MET:SD	1:A:369:LYS:NZ[3_365]	2.03	0.17
1:A:212:TYR:CE2	1:B:260:PHE:O[4_435]	2.03	0.17
1:A:213:SER:O	1:A:278:ILE:CG1[4_435]	2.03	0.17
1:A:220:LYS:C	1:A:262:GLN:N[4_435]	2.03	0.17
1:A:220:LYS:CG	1:A:259:THR:CA[4_435]	2.03	0.17
1:A:307:ILE:CB	1:A:366:LYS:C[3_365]	2.03	0.17
1:A:314:ASP:N	1:A:359:ILE:CB[3_365]	2.03	0.17
1:A:315:PRO:O	1:A:361:LEU:C[3_365]	2.03	0.17
1:A:356:ASN:N	4:A:502:ATP:O3'[4_435]	2.03	0.17
1:A:367:GLN:CG	3:A:501:LTN:CH2[4_435]	2.03	0.17
1:B:110:SER:O	1:B:471:GLN:NE2[3_365]	2.03	0.17
1:B:130:HIS:O	1:B:390:PHE:CE1[3_465]	2.03	0.17
1:B:139:SER:C	1:B:471:GLN:NE2[3_365]	2.03	0.17
1:B:318:ARG:N	1:B:474:HIS:CE1[3_365]	2.03	0.17
1:B:343:LEU:CD2	1:B:370:THR:N[4_445]	2.03	0.17
1:B:346:ALA:CA	1:B:363:ASP:N[4_445]	2.03	0.17
1:B:350:MET:CG	1:B:367:GLN:NE2[4_445]	2.03	0.17
1:B:359:ILE:CG1	1:B:377:PHE:N[3_465]	2.03	0.17
1:B:366:LYS:C	1:B:402:TYR:CE2[3_465]	2.03	0.17
1:B:372:VAL:O	1:B:374:LYS:N[2_355]	2.03	0.17
1:B:374:LYS:N	1:B:374:LYS:C[4_445]	2.03	0.17
1:B:400:PHE:O	1:B:439:GLN:OE1[4_445]	2.03	0.17
1:B:425:MET:C	1:B:436:GLU:OE1[2_355]	2.03	0.17
1:B:430:LEU:O	1:B:432:LYS:O[4_445]	2.03	0.17
1:B:454:ASP:CA	1:B:463:PRO:O[2_345]	2.03	0.17
1:B:455:GLU:OE1	1:B:463:PRO:CA[2_345]	2.03	0.17
1:B:455:GLU:N	1:B:464:ARG:N[2_345]	2.03	0.17
1:A:82:GLU:N	5:A:547:HOH:O[2_245]	2.04	0.16
1:A:87:PRO:N	1:A:170:HIS:ND1[3_365]	2.04	0.16
1:A:88:TRP:N	1:A:352:ALA:N[3_365]	2.04	0.16
1:A:100:TYR:CE1	1:A:398:VAL:CG1[3_365]	2.04	0.16
1:A:103:LEU:CA	1:A:402:TYR:CG[3_365]	2.04	0.16
1:A:109:SER:OG	1:A:434:LEU:CD1[3_365]	2.04	0.16
1:A:110:SER:O	1:A:434:LEU:C[3_365]	2.04	0.16
1:A:114:LYS:CB	1:A:429:GLU:OE2[3_365]	2.04	0.16
1:A:114:LYS:N	1:A:429:GLU:OE2[3_365]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CD2	1:A:399:SER:CB[3_365]	2.04	0.16
1:A:141:ARG:N	1:A:439:GLN:OE1[3_365]	2.04	0.16
1:A:148:ASP:OD2	1:A:152:ASN:ND2[2_345]	2.04	0.16
1:A:159:TYR:CD2	1:A:364:THR:CG2[3_365]	2.04	0.16
1:A:167:GLU:N	1:A:277:LYS:O[4_435]	2.04	0.16
1:A:169:MET:CB	1:A:267:PHE:CD1[4_435]	2.04	0.16
1:A:209:ASP:CB	1:B:258:VAL:C[4_435]	2.04	0.16
1:A:210:GLN:CG	1:B:256:LYS:CA[4_435]	2.04	0.16
1:A:224:ALA:CB	1:A:262:GLN:CD[4_435]	2.04	0.16
1:A:238:LEU:CB	1:B:261:ASN:CG[4_435]	2.04	0.16
1:A:308:PRO:CB	1:A:370:THR:CB[3_365]	2.04	0.16
1:A:312:ASP:O	1:A:359:ILE:CA[3_365]	2.04	0.16
1:A:316:TYR:CA	1:A:361:LEU:CA[3_365]	2.04	0.16
1:A:317:PHE:CD1	1:A:364:THR:N[3_365]	2.04	0.16
1:A:317:PHE:CD2	1:A:363:ASP:CA[3_365]	2.04	0.16
1:A:322:ASP:CG	1:A:444:GLU:CA[3_365]	2.04	0.16
1:A:338:THR:O	1:A:375:HIS:O[3_365]	2.04	0.16
1:B:108:GLY:CA	1:B:297:PHE:O[3_365]	2.04	0.16
1:B:110:SER:C	1:B:471:GLN:OE1[3_365]	2.04	0.16
1:B:229:ILE:CG1	1:B:459:GLU:OE1[2_345]	2.04	0.16
1:B:345:GLY:CA	1:B:360:PHE:O[4_445]	2.04	0.16
1:B:359:ILE:CD1	1:B:377:PHE:C[3_465]	2.04	0.16
1:B:368:ILE:CA	1:B:398:VAL:CB[3_465]	2.04	0.16
1:B:371:LYS:C	1:B:375:HIS:CA[3_465]	2.04	0.16
1:B:373:ASN:N	1:B:373:ASN:CB[4_445]	2.04	0.16
1:B:379:GLY:CA	1:B:406:PHE:CD1[4_445]	2.04	0.16
1:B:388:ARG:CZ	1:B:413:LEU:O[4_445]	2.04	0.16
1:B:393:ASN:CA	1:B:406:PHE:O[4_445]	2.04	0.16
1:B:412:LYS:O	1:B:423:GLY:O[3_465]	2.04	0.16
1:B:428:GLY:CA	1:B:432:LYS:CG[3_465]	2.04	0.16
1:B:428:GLY:O	1:B:431:LYS:O[2_355]	2.04	0.16
1:A:86:ASP:CA	1:A:170:HIS:CD2[3_365]	2.05	0.15
1:A:91:GLN:O	1:A:348:THR:C[3_365]	2.05	0.15
1:A:92:THR:O	1:A:347:GLN:CD[2_245]	2.05	0.15
1:A:102:LYS:C	1:A:401:MET:CA[3_365]	2.05	0.15
1:A:103:LEU:O	1:A:402:TYR:C[3_365]	2.05	0.15
1:A:104:ILE:N	1:A:402:TYR:C[3_365]	2.05	0.15
1:A:107:PHE:O	1:A:441:LEU:CD1[3_365]	2.05	0.15
1:A:107:PHE:CE2	1:A:171:VAL:CG2[3_365]	2.05	0.15
1:A:111:LYS:CB	1:A:430:LEU:C[3_365]	2.05	0.15
1:A:136:ILE:C	1:A:431:LYS:NZ[3_365]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:CD1	1:A:374:LYS:N[3_365]	2.05	0.15
1:A:162:ARG:NE	1:A:268:GLY:CA[4_435]	2.05	0.15
1:A:162:ARG:CD	1:A:268:GLY:O[4_435]	2.05	0.15
1:A:173:HIS:ND1	1:A:267:PHE:O[4_435]	2.05	0.15
1:A:174:LEU:CD2	1:A:266:ILE:CA[4_435]	2.05	0.15
1:A:175:ILE:C	1:A:374:LYS:NZ[3_365]	2.05	0.15
1:A:209:ASP:CB	1:B:258:VAL:CG1[4_435]	2.05	0.15
1:A:214:TYR:CG	1:A:274:CYS:O[4_435]	2.05	0.15
1:A:238:LEU:N	1:B:261:ASN:OD1[4_435]	2.05	0.15
1:A:310:ALA:C	1:A:371:LYS:CG[3_365]	2.05	0.15
1:A:314:ASP:CG	1:A:442:ILE:CD1[3_365]	2.05	0.15
1:A:320:THR:OG1	1:A:446:GLN:CD[3_365]	2.05	0.15
1:A:334:LEU:N	1:A:439:GLN:CD[3_365]	2.05	0.15
1:A:336:HIS:N	1:A:368:ILE:O[3_365]	2.05	0.15
1:A:356:ASN:CA	4:A:502:ATP:N9[4_435]	2.05	0.15
1:A:458:LYS:CA	1:B:270:THR:OG1[4_435]	2.05	0.15
1:B:307:ILE:CA	1:B:475:HIS:CE1[3_365]	2.05	0.15
1:B:342:ALA:CA	1:B:367:GLN:CB[4_445]	2.05	0.15
1:B:345:GLY:O	1:B:360:PHE:O[4_445]	2.05	0.15
1:B:345:GLY:N	1:B:363:ASP:CG[4_445]	2.05	0.15
1:B:368:ILE:CG2	1:B:398:VAL:N[3_465]	2.05	0.15
1:B:378:SER:OG	1:B:434:LEU:CD2[4_445]	2.05	0.15
1:B:384:ILE:N	1:B:440:PRO:CG[2_355]	2.05	0.15
1:B:384:ILE:CA	1:B:400:PHE:CD2[4_445]	2.05	0.15
1:B:388:ARG:NE	1:B:417:ARG:N[4_445]	2.05	0.15
1:B:400:PHE:C	1:B:439:GLN:CG[4_445]	2.05	0.15
1:B:402:TYR:O	5:B:537:HOH:O[4_445]	2.05	0.15
1:B:430:LEU:CD2	1:B:434:LEU:CA[4_445]	2.05	0.15
1:B:430:LEU:C	1:B:432:LYS:CG[2_355]	2.05	0.15
1:B:430:LEU:C	1:B:432:LYS:O[4_445]	2.05	0.15
1:B:440:PRO:CB	5:B:567:HOH:O[2_355]	2.05	0.15
1:A:86:ASP:OD2	1:A:170:HIS:CE1[3_365]	2.06	0.14
1:A:86:ASP:CA	1:A:170:HIS:ND1[3_365]	2.06	0.14
1:A:87:PRO:CA	1:A:360:PHE:CE2[3_365]	2.06	0.14
1:A:88:TRP:CB	1:A:352:ALA:O[3_365]	2.06	0.14
1:A:94:SER:CB	1:A:96:LYS:CA[3_365]	2.06	0.14
1:A:98:ILE:O	1:A:396:VAL:O[3_365]	2.06	0.14
1:A:100:TYR:C	1:A:398:VAL:O[3_365]	2.06	0.14
1:A:103:LEU:CD2	1:A:402:TYR:CD1[3_365]	2.06	0.14
1:A:137:PHE:CG	1:A:373:ASN:C[3_365]	2.06	0.14
1:A:173:HIS:CE1	1:A:267:PHE:O[4_435]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:O	1:A:262:GLN:C[4_435]	2.06	0.14
1:A:236:SER:C	1:A:271:ASP:OD2[4_435]	2.06	0.14
1:A:259:THR:CA	1:A:452:VAL:CG2[3_365]	2.06	0.14
1:A:266:ILE:CD1	1:A:445:HIS:ND1[3_365]	2.06	0.14
1:A:279:SER:N	5:A:555:HOH:O[3_365]	2.06	0.14
1:A:297:PHE:CB	5:A:558:HOH:O[2_345]	2.06	0.14
1:A:307:ILE:CA	1:A:366:LYS:N[3_365]	2.06	0.14
1:A:312:ASP:CG	1:A:358:SER:C[3_365]	2.06	0.14
1:A:315:PRO:C	1:A:360:PHE:O[3_365]	2.06	0.14
1:A:321:ARG:C	1:A:443:ALA:CA[3_365]	2.06	0.14
1:A:336:HIS:CB	1:A:372:VAL:CA[3_365]	2.06	0.14
1:A:349:LYS:CD	1:A:357:SER:CB[3_365]	2.06	0.14
1:B:97:GLY:O	1:B:445:HIS:CE1[4_445]	2.06	0.14
1:B:103:LEU:CD1	1:B:450:LYS:CD[4_445]	2.06	0.14
1:B:133:ARG:C	1:B:390:PHE:CE1[3_465]	2.06	0.14
1:B:171:VAL:CG1	1:B:366:LYS:CE[4_445]	2.06	0.14
1:B:171:VAL:CG1	1:B:377:PHE:CE2[3_465]	2.06	0.14
1:B:347:GLN:CA	1:B:362:THR:N[4_445]	2.06	0.14
1:B:368:ILE:CD1	1:B:398:VAL:CA[3_465]	2.06	0.14
1:B:369:LYS:NZ	1:B:397:ASP:OD1[2_355]	2.06	0.14
1:B:381:ARG:O	1:B:402:TYR:N[4_445]	2.06	0.14
1:B:381:ARG:N	1:B:403:LEU:N[4_445]	2.06	0.14
1:B:395:ASP:N	1:B:441:LEU:N[4_445]	2.06	0.14
1:B:412:LYS:O	1:B:423:GLY:C[3_465]	2.06	0.14
1:B:412:LYS:CB	1:B:424:ALA:N[3_465]	2.06	0.14
1:B:416:ILE:CD1	1:B:436:GLU:OE2[4_445]	2.06	0.14
1:B:454:ASP:O	1:B:462:THR:CG2[2_345]	2.06	0.14
1:A:84:PHE:CE1	4:A:502:ATP:N3[3_365]	2.07	0.13
1:A:87:PRO:CA	1:A:358:SER:OG[3_365]	2.07	0.13
1:A:87:PRO:CG	1:A:360:PHE:CD2[3_365]	2.07	0.13
1:A:90:VAL:CB	1:A:357:SER:OG[3_365]	2.07	0.13
1:A:105:VAL:O	1:A:407:LEU:N[3_365]	2.07	0.13
1:A:109:SER:C	1:A:437:VAL:N[3_365]	2.07	0.13
1:A:137:PHE:CA	1:A:373:ASN:CB[3_365]	2.07	0.13
1:A:140:HIS:CE1	1:A:436:GLU:CG[3_365]	2.07	0.13
1:A:211:ALA:O	1:A:273:ASP:N[4_435]	2.07	0.13
1:A:212:TYR:CB	1:B:261:ASN:N[4_435]	2.07	0.13
1:A:222:ILE:CB	1:A:261:ASN:C[4_435]	2.07	0.13
1:A:223:ILE:N	1:A:261:ASN:CB[4_435]	2.07	0.13
1:A:236:SER:CB	1:A:271:ASP:OD2[4_435]	2.07	0.13
1:A:239:ASP:CG	1:B:264:LYS:CB[4_435]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:CB	1:A:363:ASP:C[3_365]	2.07	0.13
1:A:321:ARG:CB	1:A:443:ALA:N[3_365]	2.07	0.13
1:A:329:TYR:CG	1:A:470:PHE:C[2_345]	2.07	0.13
1:A:347:GLN:C	1:A:347:GLN:O[4_435]	2.07	0.13
1:A:349:LYS:CE	1:A:354:ASP:OD1[3_365]	2.07	0.13
1:B:99:ASP:C	1:B:447:ALA:O[4_445]	2.07	0.13
1:B:106:ARG:N	1:B:295:GLN:O[3_365]	2.07	0.13
1:B:350:MET:CG	1:B:367:GLN:OE1[4_445]	2.07	0.13
1:B:399:SER:OG	1:B:435:ILE:CD1[4_445]	2.07	0.13
1:B:430:LEU:CB	1:B:432:LYS:CE[2_355]	2.07	0.13
1:A:83:ASP:C	1:A:341:PRO:CA[3_365]	2.08	0.12
1:A:89:THR:C	1:A:351:SER:CB[3_365]	2.08	0.12
1:A:93:SER:CB	1:A:97:GLY:C[3_365]	2.08	0.12
1:A:106:ARG:CA	1:A:405:PHE:CA[3_365]	2.08	0.12
1:A:111:LYS:CG	1:A:430:LEU:CB[3_365]	2.08	0.12
1:A:114:LYS:C	1:A:429:GLU:OE2[3_365]	2.08	0.12
1:A:137:PHE:CE1	1:A:374:LYS:CD[3_365]	2.08	0.12
1:A:137:PHE:CB	1:A:373:ASN:CG[3_365]	2.08	0.12
1:A:137:PHE:CB	1:A:373:ASN:C[3_365]	2.08	0.12
1:A:141:ARG:CD	1:A:439:GLN:CB[3_365]	2.08	0.12
1:A:141:ARG:CA	1:A:439:GLN:CD[3_365]	2.08	0.12
1:A:141:ARG:N	1:A:435:ILE:O[3_365]	2.08	0.12
1:A:167:GLU:CG	1:A:276:GLY:O[4_435]	2.08	0.12
1:A:214:TYR:CE1	1:A:277:LYS:CA[4_435]	2.08	0.12
1:A:216:VAL:C	1:A:260:PHE:CD1[4_435]	2.08	0.12
1:A:216:VAL:CB	1:B:260:PHE:CD1[4_435]	2.08	0.12
1:A:259:THR:CB	1:A:452:VAL:CG2[3_365]	2.08	0.12
1:A:300:ARG:NH2	1:A:303:ILE:N[2_345]	2.08	0.12
1:A:309:CYS:SG	1:A:368:ILE:N[3_365]	2.08	0.12
1:A:317:PHE:CE2	1:A:363:ASP:CA[3_365]	2.08	0.12
1:A:318:ARG:O	1:A:443:ALA:N[3_365]	2.08	0.12
1:A:327:ILE:CG2	1:A:450:LYS:CD[3_365]	2.08	0.12
1:A:329:TYR:CZ	1:A:471:GLN:CB[2_345]	2.08	0.12
1:A:339:PHE:CE1	1:A:357:SER:O[3_365]	2.08	0.12
1:A:457:VAL:CA	1:B:272:SER:O[4_435]	2.08	0.12
1:B:104:ILE:CB	1:B:469:ASP:OD2[3_365]	2.08	0.12
1:B:317:PHE:CE1	1:B:475:HIS:O[3_365]	2.08	0.12
1:B:334:LEU:O	1:B:473:HIS:CB[3_365]	2.08	0.12
1:B:334:LEU:CA	1:B:473:HIS:CA[3_365]	2.08	0.12
1:B:341:PRO:O	1:B:364:THR:CA[4_445]	2.08	0.12
1:B:343:LEU:CD2	1:B:367:GLN:C[4_445]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLN:CB	1:B:371:LYS:CE[4_445]	2.08	0.12
1:B:366:LYS:O	1:B:402:TYR:CE1[3_465]	2.08	0.12
1:B:371:LYS:O	1:B:373:ASN:C[2_355]	2.08	0.12
1:B:372:VAL:CB	1:B:376:ALA:CB[3_465]	2.08	0.12
1:B:373:ASN:O	1:B:376:ALA:CB[4_445]	2.08	0.12
1:B:384:ILE:CD1	1:B:437:VAL:O[2_355]	2.08	0.12
1:B:388:ARG:CA	1:B:413:LEU:CG[4_445]	2.08	0.12
1:B:393:ASN:N	1:B:406:PHE:CA[4_445]	2.08	0.12
1:B:408:GLU:C	1:B:421:THR:O[3_465]	2.08	0.12
1:B:416:ILE:CG1	1:B:425:MET:N[3_465]	2.08	0.12
1:B:426:LEU:CB	1:B:436:GLU:CD[2_355]	2.08	0.12
1:B:455:GLU:CB	1:B:464:ARG:CG[2_345]	2.08	0.12
1:A:84:PHE:CG	1:A:344:GLN:OE1[2_245]	2.09	0.11
1:A:84:PHE:CB	1:A:344:GLN:CG[2_245]	2.09	0.11
1:A:86:ASP:CA	1:A:350:MET:CG[3_365]	2.09	0.11
1:A:88:TRP:C	1:A:352:ALA:CA[3_365]	2.09	0.11
1:A:91:GLN:CG	1:A:349:LYS:N[3_365]	2.09	0.11
1:A:92:THR:CB	1:A:347:GLN:OE1[2_245]	2.09	0.11
1:A:94:SER:C	1:A:94:SER:O[3_365]	2.09	0.11
1:A:110:SER:CB	5:A:600:HOH:O[3_365]	2.09	0.11
1:A:111:LYS:CA	1:A:433:ALA:CA[3_365]	2.09	0.11
1:A:148:ASP:CB	1:A:152:ASN:CG[2_345]	2.09	0.11
1:A:167:GLU:O	1:A:281:PRO:CG[4_435]	2.09	0.11
1:A:167:GLU:O	1:A:269:PHE:CZ[4_435]	2.09	0.11
1:A:209:ASP:CG	1:B:258:VAL:CA[4_435]	2.09	0.11
1:A:212:TYR:CD1	1:B:261:ASN:CA[4_435]	2.09	0.11
1:A:214:TYR:CD1	1:A:277:LYS:N[4_435]	2.09	0.11
1:A:214:TYR:CD2	1:A:277:LYS:CD[4_435]	2.09	0.11
1:A:216:VAL:CB	1:B:260:PHE:CE1[4_435]	2.09	0.11
1:A:224:ALA:CA	1:A:262:GLN:CG[4_435]	2.09	0.11
1:A:312:ASP:CB	1:A:358:SER:CB[3_365]	2.09	0.11
1:A:313:GLN:CA	1:A:360:PHE:N[3_365]	2.09	0.11
1:A:313:GLN:N	1:A:358:SER:C[3_365]	2.09	0.11
1:A:313:GLN:N	1:A:359:ILE:N[3_365]	2.09	0.11
1:A:316:TYR:O	1:A:362:THR:CA[3_365]	2.09	0.11
1:A:334:LEU:CD2	1:A:368:ILE:N[3_365]	2.09	0.11
1:A:337:SER:CA	1:A:371:LYS:C[3_365]	2.09	0.11
1:A:355:PRO:CD	4:A:502:ATP:O2A[4_435]	2.09	0.11
1:A:461:MET:CB	5:B:573:HOH:O[4_435]	2.09	0.11
1:B:99:ASP:CA	1:B:449:ARG:C[4_445]	2.09	0.11
1:B:159:TYR:CE2	1:B:475:HIS:O[3_365]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:TYR:CD2	1:B:475:HIS:CB[3_365]	2.09	0.11
1:B:346:ALA:C	1:B:361:LEU:CA[4_445]	2.09	0.11
1:B:366:LYS:CA	1:B:402:TYR:OH[3_465]	2.09	0.11
1:B:369:LYS:CG	1:B:378:SER:CB[2_355]	2.09	0.11
1:B:371:LYS:N	1:B:374:LYS:CB[4_445]	2.09	0.11
1:B:371:LYS:CB	1:B:374:LYS:O[2_355]	2.09	0.11
1:B:372:VAL:CG2	1:B:376:ALA:CB[3_465]	2.09	0.11
1:B:384:ILE:CG2	1:B:417:ARG:CG[4_445]	2.09	0.11
1:B:391:GLY:C	1:B:407:LEU:CB[4_445]	2.09	0.11
1:B:392:GLY:O	1:B:407:LEU:CA[4_445]	2.09	0.11
1:B:394:CYS:O	1:B:437:VAL:O[4_445]	2.09	0.11
1:B:397:ASP:OD2	1:B:434:LEU:O[4_445]	2.09	0.11
1:B:397:ASP:OD2	1:B:438:LEU:CG[4_445]	2.09	0.11
1:B:401:MET:CE	1:B:442:ILE:CB[4_445]	2.09	0.11
1:B:412:LYS:CD	1:B:425:MET:N[3_465]	2.09	0.11
1:B:430:LEU:N	1:B:433:ALA:CA[4_445]	2.09	0.11
1:A:84:PHE:CD1	4:A:502:ATP:C5[3_365]	2.10	0.10
1:A:101:ASP:OD1	1:A:430:LEU:CD2[3_365]	2.10	0.10
1:A:104:ILE:CG1	1:A:434:LEU:CB[3_365]	2.10	0.10
1:A:113:ASP:C	1:A:429:GLU:CA[3_365]	2.10	0.10
1:A:139:SER:CB	1:A:372:VAL:CG1[3_365]	2.10	0.10
1:A:141:ARG:CZ	1:A:439:GLN:N[3_365]	2.10	0.10
1:A:141:ARG:CA	1:A:435:ILE:O[3_365]	2.10	0.10
1:A:159:TYR:CD2	5:A:585:HOH:O[3_365]	2.10	0.10
1:A:163:GLY:N	1:A:270:THR:CG2[4_435]	2.10	0.10
1:A:197:ASP:OD2	1:B:261:ASN:OD1[4_435]	2.10	0.10
1:A:202:LEU:CG	5:A:553:HOH:O[3_365]	2.10	0.10
1:A:210:GLN:O	1:A:273:ASP:O[4_435]	2.10	0.10
1:A:217:GLU:OE1	1:B:275:ILE:CG1[4_435]	2.10	0.10
1:A:221:ASP:N	1:A:262:GLN:CA[4_435]	2.10	0.10
1:A:223:ILE:N	1:A:262:GLN:N[4_435]	2.10	0.10
1:A:300:ARG:N	1:A:300:ARG:CA[2_345]	2.10	0.10
1:A:334:LEU:CB	1:A:365:ALA:O[3_365]	2.10	0.10
1:A:335:LEU:CB	1:A:369:LYS:C[3_365]	2.10	0.10
1:A:336:HIS:C	1:A:372:VAL:CB[3_365]	2.10	0.10
1:A:356:ASN:ND2	4:A:502:ATP:C8[4_435]	2.10	0.10
1:A:449:ARG:NH2	1:B:275:ILE:CG2[4_435]	2.10	0.10
1:A:457:VAL:CG1	1:B:273:ASP:N[4_435]	2.10	0.10
1:B:99:ASP:C	1:B:450:LYS:CA[4_445]	2.10	0.10
1:B:100:TYR:CA	1:B:447:ALA:O[4_445]	2.10	0.10
1:B:108:GLY:C	1:B:297:PHE:O[3_365]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:SER:CB	1:B:471:GLN:N[3_365]	2.10	0.10
1:B:317:PHE:CB	1:B:474:HIS:CG[3_365]	2.10	0.10
1:B:334:LEU:O	1:B:473:HIS:CE1[3_365]	2.10	0.10
1:B:334:LEU:CD1	1:B:474:HIS:N[3_365]	2.10	0.10
1:B:340:PHE:CD2	1:B:364:THR:CB[4_445]	2.10	0.10
1:B:341:PRO:O	1:B:364:THR:O[4_445]	2.10	0.10
1:B:369:LYS:O	1:B:372:VAL:CA[3_465]	2.10	0.10
1:B:388:ARG:CA	1:B:413:LEU:CD2[4_445]	2.10	0.10
1:B:393:ASN:CB	1:B:406:PHE:CB[4_445]	2.10	0.10
1:B:395:ASP:C	1:B:441:LEU:CG[4_445]	2.10	0.10
1:B:408:GLU:O	5:B:521:HOH:O[3_465]	2.10	0.10
1:B:413:LEU:CA	1:B:423:GLY:CA[3_465]	2.10	0.10
1:B:416:ILE:CD1	1:B:436:GLU:OE1[4_445]	2.10	0.10
1:B:426:LEU:C	1:B:436:GLU:OE2[2_355]	2.10	0.10
1:B:428:GLY:CA	1:B:432:LYS:O[2_355]	2.10	0.10
1:B:430:LEU:CD1	1:B:436:GLU:N[4_445]	2.10	0.10
1:B:453:THR:CB	1:B:465:LYS:CA[2_345]	2.10	0.10
1:A:84:PHE:CE2	4:A:502:ATP:C6[3_365]	2.11	0.09
1:A:84:PHE:CG	4:A:502:ATP:N6[3_365]	2.11	0.09
1:A:93:SER:O	1:A:95:ALA:CA[2_245]	2.11	0.09
1:A:93:SER:O	1:A:97:GLY:N[3_365]	2.11	0.09
1:A:98:ILE:CG1	1:A:398:VAL:CB[3_365]	2.11	0.09
1:A:104:ILE:N	1:A:403:LEU:N[3_365]	2.11	0.09
1:A:106:ARG:C	1:A:406:PHE:CE2[3_365]	2.11	0.09
1:A:106:ARG:NH1	1:A:340:PHE:CE1[3_365]	2.11	0.09
1:A:107:PHE:CD1	1:A:406:PHE:CE2[3_365]	2.11	0.09
1:A:141:ARG:C	1:A:439:GLN:CD[3_365]	2.11	0.09
1:A:169:MET:N	1:A:267:PHE:CB[4_435]	2.11	0.09
1:A:212:TYR:CD2	1:B:259:THR:O[4_435]	2.11	0.09
1:A:217:GLU:CB	1:A:278:ILE:CA[4_435]	2.11	0.09
1:A:300:ARG:NH2	1:A:303:ILE:O[2_345]	2.11	0.09
1:A:306:LEU:O	1:A:366:LYS:CD[3_365]	2.11	0.09
1:A:321:ARG:NE	1:A:440:PRO:N[3_365]	2.11	0.09
1:A:321:ARG:O	1:A:443:ALA:O[3_365]	2.11	0.09
1:A:334:LEU:CG	1:A:368:ILE:CB[3_365]	2.11	0.09
1:A:337:SER:OG	1:A:371:LYS:O[3_365]	2.11	0.09
1:A:338:THR:N	1:A:375:HIS:N[3_365]	2.11	0.09
1:A:444:GLU:CG	5:A:613:HOH:O[4_435]	2.11	0.09
1:A:457:VAL:C	1:B:270:THR:OG1[4_435]	2.11	0.09
1:B:97:GLY:CA	1:B:445:HIS:ND1[4_445]	2.11	0.09
1:B:101:ASP:N	1:B:451:GLU:CG[4_445]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:HIS:O	1:B:472:HIS:N[3_365]	2.11	0.09
1:B:140:HIS:N	1:B:473:HIS:NE2[3_365]	2.11	0.09
1:B:141:ARG:N	1:B:473:HIS:CE1[3_365]	2.11	0.09
1:B:317:PHE:C	1:B:474:HIS:ND1[3_365]	2.11	0.09
1:B:321:ARG:NH1	5:B:519:HOH:O[3_365]	2.11	0.09
1:B:334:LEU:CA	1:B:473:HIS:CG[3_365]	2.11	0.09
1:B:340:PHE:O	1:B:364:THR:CB[4_445]	2.11	0.09
1:B:340:PHE:CE2	1:B:366:LYS:N[4_445]	2.11	0.09
1:B:342:ALA:N	1:B:363:ASP:C[4_445]	2.11	0.09
1:B:343:LEU:CA	1:B:367:GLN:C[4_445]	2.11	0.09
1:B:344:GLN:NE2	1:B:371:LYS:CE[4_445]	2.11	0.09
1:B:359:ILE:CG1	1:B:377:PHE:C[3_465]	2.11	0.09
1:B:371:LYS:CA	1:B:375:HIS:O[3_465]	2.11	0.09
1:B:373:ASN:ND2	1:B:431:LYS:CE[2_355]	2.11	0.09
1:B:379:GLY:O	5:B:537:HOH:O[2_355]	2.11	0.09
1:B:381:ARG:NE	1:B:405:PHE:C[4_445]	2.11	0.09
1:B:383:THR:CA	1:B:440:PRO:CA[2_355]	2.11	0.09
1:B:400:PHE:CD1	1:B:436:GLU:CA[4_445]	2.11	0.09
1:B:400:PHE:CE1	1:B:436:GLU:O[4_445]	2.11	0.09
1:B:400:PHE:CD2	1:B:436:GLU:O[4_445]	2.11	0.09
1:B:401:MET:CB	1:B:439:GLN:CB[4_445]	2.11	0.09
1:B:403:LEU:CD2	1:B:420:TYR:CD1[3_465]	2.11	0.09
1:B:416:ILE:CD1	1:B:436:GLU:CD[4_445]	2.11	0.09
1:B:430:LEU:O	1:B:432:LYS:N[4_445]	2.11	0.09
1:B:432:LYS:CG	1:B:434:LEU:N[3_465]	2.11	0.09
1:B:455:GLU:OE1	1:B:463:PRO:C[2_345]	2.11	0.09
1:A:87:PRO:N	1:A:170:HIS:CG[3_365]	2.12	0.08
1:A:87:PRO:CG	1:A:170:HIS:CB[3_365]	2.12	0.08
1:A:92:THR:CG2	1:A:347:GLN:OE1[2_245]	2.12	0.08
1:A:93:SER:O	1:A:347:GLN:NE2[2_245]	2.12	0.08
1:A:99:ASP:CA	1:A:397:ASP:O[3_365]	2.12	0.08
1:A:103:LEU:N	1:A:401:MET:O[3_365]	2.12	0.08
1:A:105:VAL:CG2	1:A:404:THR:N[3_365]	2.12	0.08
1:A:138:PHE:O	1:A:431:LYS:O[3_365]	2.12	0.08
1:A:167:GLU:CA	1:A:277:LYS:C[4_435]	2.12	0.08
1:A:169:MET:CG	1:A:267:PHE:N[4_435]	2.12	0.08
1:A:169:MET:CE	1:A:268:GLY:N[4_435]	2.12	0.08
1:A:195:MET:CG	1:A:271:ASP:OD1[4_435]	2.12	0.08
1:A:209:ASP:CA	1:B:258:VAL:O[4_435]	2.12	0.08
1:A:214:TYR:CB	1:A:273:ASP:CB[4_435]	2.12	0.08
1:A:236:SER:OG	1:B:261:ASN:CG[4_435]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:N	5:A:539:HOH:O[3_365]	2.12	0.08
1:A:262:GLN:OE1	1:A:449:ARG:N[3_365]	2.12	0.08
1:A:312:ASP:OD2	1:A:355:PRO:O[3_365]	2.12	0.08
1:A:312:ASP:OD1	1:A:355:PRO:O[3_365]	2.12	0.08
1:A:316:TYR:N	1:A:361:LEU:C[3_365]	2.12	0.08
1:A:317:PHE:O	1:A:442:ILE:CG2[3_365]	2.12	0.08
1:A:318:ARG:CA	1:A:442:ILE:CG1[3_365]	2.12	0.08
1:A:320:THR:CA	1:A:446:GLN:CB[3_365]	2.12	0.08
1:A:321:ARG:NH2	1:A:440:PRO:CA[3_365]	2.12	0.08
1:A:334:LEU:O	1:A:435:ILE:CG2[3_365]	2.12	0.08
1:A:335:LEU:O	1:A:369:LYS:CA[3_365]	2.12	0.08
1:A:339:PHE:CB	1:A:344:GLN:CA[3_365]	2.12	0.08
1:A:382:ASP:O	5:A:577:HOH:O[4_435]	2.12	0.08
1:A:449:ARG:NH2	1:B:275:ILE:CD1[4_435]	2.12	0.08
1:A:457:VAL:O	1:B:272:SER:N[4_435]	2.12	0.08
1:B:109:SER:C	1:B:470:PHE:CA[3_365]	2.12	0.08
1:B:109:SER:CA	1:B:470:PHE:C[3_365]	2.12	0.08
1:B:130:HIS:C	1:B:390:PHE:CD2[3_465]	2.12	0.08
1:B:370:THR:O	1:B:374:LYS:C[4_445]	2.12	0.08
1:B:370:THR:O	1:B:372:VAL:N[3_465]	2.12	0.08
1:B:382:ASP:N	1:B:405:PHE:CD1[4_445]	2.12	0.08
1:B:384:ILE:CG2	1:B:400:PHE:CE2[4_445]	2.12	0.08
1:B:384:ILE:N	1:B:440:PRO:N[2_355]	2.12	0.08
1:B:387:HIS:CA	1:B:413:LEU:CD1[4_445]	2.12	0.08
1:B:388:ARG:CA	5:B:535:HOH:O[4_445]	2.12	0.08
1:B:393:ASN:OD1	1:B:441:LEU:CD1[4_445]	2.12	0.08
1:B:400:PHE:CD1	1:B:426:LEU:CD2[3_465]	2.12	0.08
1:B:403:LEU:CD1	1:B:426:LEU:CA[3_465]	2.12	0.08
1:B:416:ILE:CG1	1:B:426:LEU:N[3_465]	2.12	0.08
1:B:426:LEU:CD2	1:B:436:GLU:CB[2_355]	2.12	0.08
1:B:453:THR:OG1	1:B:464:ARG:C[2_345]	2.12	0.08
1:B:455:GLU:N	1:B:464:ARG:CA[2_345]	2.12	0.08
1:A:92:THR:C	1:A:347:GLN:C[3_365]	2.13	0.07
1:A:99:ASP:CG	5:A:603:HOH:O[3_365]	2.13	0.07
1:A:100:TYR:CD2	1:A:398:VAL:CB[3_365]	2.13	0.07
1:A:103:LEU:C	1:A:402:TYR:N[3_365]	2.13	0.07
1:A:103:LEU:N	1:A:401:MET:CA[3_365]	2.13	0.07
1:A:109:SER:C	1:A:437:VAL:CA[3_365]	2.13	0.07
1:A:113:ASP:CA	1:A:429:GLU:C[3_365]	2.13	0.07
1:A:159:TYR:CA	5:A:585:HOH:O[3_365]	2.13	0.07
1:A:164:PRO:CG	1:A:270:THR:CB[4_435]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLN:CA	1:B:258:VAL:O[4_435]	2.13	0.07
1:A:212:TYR:N	1:B:259:THR:C[4_435]	2.13	0.07
1:A:213:SER:CA	1:A:275:ILE:CA[4_435]	2.13	0.07
1:A:218:ASN:OD1	1:A:269:PHE:CD1[4_435]	2.13	0.07
1:A:220:LYS:C	1:A:259:THR:C[4_435]	2.13	0.07
1:A:220:LYS:C	1:A:262:GLN:CB[4_435]	2.13	0.07
1:A:279:SER:O	5:A:555:HOH:O[3_365]	2.13	0.07
1:A:299:ASP:OD1	1:A:299:ASP:OD2[2_345]	2.13	0.07
1:A:335:LEU:CG	1:A:369:LYS:CB[3_365]	2.13	0.07
1:A:335:LEU:C	1:A:369:LYS:N[3_365]	2.13	0.07
1:A:337:SER:CA	1:A:372:VAL:C[3_365]	2.13	0.07
1:A:337:SER:OG	1:A:375:HIS:N[3_365]	2.13	0.07
1:A:338:THR:C	1:A:375:HIS:CB[3_365]	2.13	0.07
1:A:356:ASN:O	4:A:502:ATP:N3[4_435]	2.13	0.07
1:A:356:ASN:CB	4:A:502:ATP:C8[4_435]	2.13	0.07
1:B:264:LYS:NZ	5:A:560:HOH:O[3_365]	2.13	0.07
1:B:99:ASP:OD1	1:B:448:ARG:C[4_445]	2.13	0.07
1:B:102:LYS:CD	1:B:452:VAL:CB[4_445]	2.13	0.07
1:B:102:LYS:CD	1:B:452:VAL:N[4_445]	2.13	0.07
1:B:130:HIS:CA	1:B:390:PHE:CE2[3_465]	2.13	0.07
1:B:134:ARG:CD	1:B:390:PHE:CD1[3_465]	2.13	0.07
1:B:134:ARG:NE	1:B:390:PHE:CB[3_465]	2.13	0.07
1:B:341:PRO:CB	1:B:364:THR:C[4_445]	2.13	0.07
1:B:345:GLY:C	1:B:363:ASP:CG[4_445]	2.13	0.07
1:B:348:THR:CA	1:B:362:THR:OG1[4_445]	2.13	0.07
1:B:370:THR:O	1:B:375:HIS:N[2_355]	2.13	0.07
1:B:384:ILE:CA	1:B:400:PHE:CZ[4_445]	2.13	0.07
1:B:395:ASP:CB	5:B:514:HOH:O[4_445]	2.13	0.07
1:B:400:PHE:CG	1:B:440:PRO:CD[4_445]	2.13	0.07
1:B:401:MET:C	1:B:439:GLN:CB[4_445]	2.13	0.07
1:B:426:LEU:O	1:B:432:LYS:O[2_355]	2.13	0.07
1:B:428:GLY:O	1:B:430:LEU:CA[4_445]	2.13	0.07
1:B:455:GLU:CA	1:B:464:ARG:CD[2_345]	2.13	0.07
1:A:90:VAL:N	1:A:349:LYS:O[3_365]	2.14	0.06
1:A:94:SER:O	1:A:94:SER:CB[4_435]	2.14	0.06
1:A:94:SER:O	1:A:347:GLN:NE2[3_365]	2.14	0.06
1:A:103:LEU:C	1:A:402:TYR:CG[3_365]	2.14	0.06
1:A:103:LEU:CB	1:A:402:TYR:CB[3_365]	2.14	0.06
1:A:105:VAL:N	1:A:402:TYR:O[3_365]	2.14	0.06
1:A:111:LYS:C	1:A:432:LYS:N[3_365]	2.14	0.06
1:A:114:LYS:CE	1:A:388:ARG:NH1[3_365]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:O	1:A:373:ASN:OD1[3_365]	2.14	0.06
1:A:141:ARG:CG	1:A:435:ILE:O[3_365]	2.14	0.06
1:A:141:ARG:CB	1:A:439:GLN:OE1[3_365]	2.14	0.06
1:A:154:LYS:NZ	1:A:304:GLN:CB[2_345]	2.14	0.06
1:A:155:PRO:CB	5:A:618:HOH:O[2_345]	2.14	0.06
1:A:176:PRO:O	1:A:374:LYS:NZ[3_365]	2.14	0.06
1:A:195:MET:O	1:A:271:ASP:CB[4_435]	2.14	0.06
1:A:206:LEU:CG	5:A:529:HOH:O[4_435]	2.14	0.06
1:A:207:THR:CG2	1:B:257:HIS:O[4_435]	2.14	0.06
1:A:210:GLN:O	1:A:273:ASP:C[4_435]	2.14	0.06
1:A:211:ALA:CA	1:A:272:SER:O[4_435]	2.14	0.06
1:A:214:TYR:CE1	1:A:277:LYS:CB[4_435]	2.14	0.06
1:A:220:LYS:CD	1:B:275:ILE:CA[4_435]	2.14	0.06
1:A:221:ASP:OD1	1:A:319:MET:CE[4_435]	2.14	0.06
1:A:235:PHE:C	1:A:271:ASP:OD2[4_435]	2.14	0.06
1:A:257:HIS:CG	1:A:450:LYS:O[3_365]	2.14	0.06
1:A:262:GLN:OE1	1:A:449:ARG:CA[3_365]	2.14	0.06
1:A:281:PRO:O	1:A:362:THR:CG2[3_365]	2.14	0.06
1:A:299:ASP:N	1:A:299:ASP:C[2_345]	2.14	0.06
1:A:312:ASP:CB	1:A:357:SER:C[3_365]	2.14	0.06
1:A:318:ARG:O	1:A:442:ILE:CA[3_365]	2.14	0.06
1:A:326:ARG:NE	1:A:451:GLU:CG[3_365]	2.14	0.06
1:A:333:ALA:C	1:A:439:GLN:NE2[3_365]	2.14	0.06
1:A:333:ALA:CA	1:A:365:ALA:CB[3_365]	2.14	0.06
1:A:334:LEU:N	1:A:365:ALA:O[3_365]	2.14	0.06
1:A:440:PRO:CB	5:A:589:HOH:O[4_435]	2.14	0.06
1:A:457:VAL:O	1:B:270:THR:C[4_435]	2.14	0.06
1:A:461:MET:SD	1:B:270:THR:C[4_435]	2.14	0.06
1:B:99:ASP:OD1	1:B:451:GLU:N[4_445]	2.14	0.06
1:B:109:SER:O	1:B:471:GLN:N[3_365]	2.14	0.06
1:B:133:ARG:C	1:B:390:PHE:CZ[3_465]	2.14	0.06
1:B:171:VAL:CG1	1:B:377:PHE:CE1[3_465]	2.14	0.06
1:B:334:LEU:N	1:B:473:HIS:CA[3_365]	2.14	0.06
1:B:334:LEU:CD1	1:B:474:HIS:CD2[3_365]	2.14	0.06
1:B:342:ALA:CB	1:B:367:GLN:OE1[4_445]	2.14	0.06
1:B:369:LYS:CD	1:B:434:LEU:CD1[3_465]	2.14	0.06
1:B:371:LYS:CG	1:B:375:HIS:O[3_465]	2.14	0.06
1:B:372:VAL:CG2	5:B:479:HOH:O[3_465]	2.14	0.06
1:B:372:VAL:N	1:B:372:VAL:O[3_465]	2.14	0.06
1:B:374:LYS:CA	1:B:376:ALA:N[4_445]	2.14	0.06
1:B:378:SER:OG	1:B:402:TYR:CG[4_445]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:THR:C	1:B:440:PRO:CA[2_355]	2.14	0.06
1:B:397:ASP:O	1:B:438:LEU:CB[4_445]	2.14	0.06
1:B:398:VAL:N	1:B:438:LEU:CB[4_445]	2.14	0.06
1:B:416:ILE:CG2	1:B:426:LEU:CA[3_465]	2.14	0.06
1:B:426:LEU:CB	1:B:436:GLU:CA[2_355]	2.14	0.06
1:B:428:GLY:C	1:B:430:LEU:O[4_445]	2.14	0.06
1:B:428:GLY:CA	1:B:430:LEU:CA[4_445]	2.14	0.06
1:A:83:ASP:OD1	1:A:377:PHE:CE1[2_245]	2.15	0.05
1:A:84:PHE:O	1:A:349:LYS:C[3_365]	2.15	0.05
1:A:86:ASP:CA	1:A:350:MET:SD[3_365]	2.15	0.05
1:A:88:TRP:O	1:A:351:SER:C[3_365]	2.15	0.05
1:A:88:TRP:CA	1:A:351:SER:O[3_365]	2.15	0.05
1:A:88:TRP:C	1:A:352:ALA:C[3_365]	2.15	0.05
1:A:89:THR:N	1:A:351:SER:CB[3_365]	2.15	0.05
1:A:92:THR:CG2	1:A:347:GLN:N[3_365]	2.15	0.05
1:A:92:THR:CB	1:A:346:ALA:O[3_365]	2.15	0.05
1:A:100:TYR:O	1:A:399:SER:N[3_365]	2.15	0.05
1:A:101:ASP:O	1:A:400:PHE:CA[3_365]	2.15	0.05
1:A:103:LEU:CB	1:A:402:TYR:CE1[3_365]	2.15	0.05
1:A:114:LYS:CE	1:A:426:LEU:N[3_365]	2.15	0.05
1:A:141:ARG:CG	1:A:439:GLN:CG[3_365]	2.15	0.05
1:A:141:ARG:CZ	1:A:438:LEU:CB[3_365]	2.15	0.05
1:A:168:ALA:N	1:A:269:PHE:CZ[4_435]	2.15	0.05
1:A:197:ASP:OD2	1:B:261:ASN:ND2[4_435]	2.15	0.05
1:A:215:ALA:CB	1:A:271:ASP:CA[4_435]	2.15	0.05
1:A:216:VAL:O	1:A:260:PHE:CG[4_435]	2.15	0.05
1:A:217:GLU:CG	1:A:278:ILE:C[4_435]	2.15	0.05
1:A:219:ALA:N	1:A:260:PHE:CD1[4_435]	2.15	0.05
1:A:219:ALA:N	1:A:260:PHE:CG[4_435]	2.15	0.05
1:A:220:LYS:O	1:A:262:GLN:N[4_435]	2.15	0.05
1:A:221:ASP:CG	1:A:263:VAL:CB[4_435]	2.15	0.05
1:A:236:SER:CB	1:B:261:ASN:ND2[4_435]	2.15	0.05
1:A:257:HIS:CD2	1:A:450:LYS:CG[3_365]	2.15	0.05
1:A:310:ALA:C	1:A:371:LYS:CD[3_365]	2.15	0.05
1:A:316:TYR:CA	1:A:362:THR:CA[3_365]	2.15	0.05
1:A:336:HIS:N	1:A:369:LYS:CA[3_365]	2.15	0.05
1:A:336:HIS:ND1	1:A:368:ILE:CG2[3_365]	2.15	0.05
1:A:339:PHE:CD2	1:A:342:ALA:C[3_365]	2.15	0.05
1:A:344:GLN:CG	1:A:349:LYS:CB[4_435]	2.15	0.05
1:A:347:GLN:CA	1:A:347:GLN:OE1[3_365]	2.15	0.05
1:A:367:GLN:OE1	3:A:501:LTN:CZ2[4_435]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:TYR:CD1	1:B:447:ALA:CA[4_445]	2.15	0.05
1:B:107:PHE:O	1:B:299:ASP:N[3_365]	2.15	0.05
1:B:110:SER:CA	1:B:470:PHE:C[3_365]	2.15	0.05
1:B:171:VAL:CG1	1:B:366:LYS:CB[4_445]	2.15	0.05
1:B:342:ALA:CB	1:B:367:GLN:CD[4_445]	2.15	0.05
1:B:348:THR:O	1:B:362:THR:CB[4_445]	2.15	0.05
1:B:369:LYS:CB	1:B:378:SER:OG[2_355]	2.15	0.05
1:B:371:LYS:C	1:B:376:ALA:CA[3_465]	2.15	0.05
1:B:381:ARG:CA	1:B:404:THR:OG1[4_445]	2.15	0.05
1:B:384:ILE:CB	1:B:400:PHE:CD2[4_445]	2.15	0.05
1:B:387:HIS:ND1	1:B:404:THR:N[4_445]	2.15	0.05
1:B:394:CYS:CB	1:B:437:VAL:O[4_445]	2.15	0.05
1:B:397:ASP:OD2	1:B:434:LEU:CG[4_445]	2.15	0.05
1:B:400:PHE:CB	1:B:436:GLU:O[4_445]	2.15	0.05
1:B:420:TYR:CD2	1:B:437:VAL:CG1[4_445]	2.15	0.05
1:B:425:MET:CE	1:B:429:GLU:CD[3_465]	2.15	0.05
1:B:427:THR:CB	1:B:434:LEU:CB[4_445]	2.15	0.05
1:B:430:LEU:CB	1:B:433:ALA:O[4_445]	2.15	0.05
1:B:430:LEU:CG	1:B:435:ILE:N[4_445]	2.15	0.05
1:B:455:GLU:CD	5:B:563:HOH:O[2_345]	2.15	0.05
1:B:456:ILE:N	1:B:464:ARG:CB[2_345]	2.15	0.05
1:B:458:LYS:CA	1:B:462:THR:OG1[2_345]	2.15	0.05
1:A:87:PRO:C	1:A:360:PHE:CZ[3_365]	2.16	0.04
1:A:89:THR:CA	1:A:351:SER:O[3_365]	2.16	0.04
1:A:90:VAL:N	1:A:351:SER:N[3_365]	2.16	0.04
1:A:98:ILE:N	1:A:345:GLY:CA[3_365]	2.16	0.04
1:A:98:ILE:CB	1:A:398:VAL:CG2[3_365]	2.16	0.04
1:A:103:LEU:CD2	1:A:402:TYR:CD2[3_365]	2.16	0.04
1:A:106:ARG:O	1:A:406:PHE:CE2[3_365]	2.16	0.04
1:A:108:GLY:C	1:A:437:VAL:C[3_365]	2.16	0.04
1:A:109:SER:OG	1:A:434:LEU:CG[3_365]	2.16	0.04
1:A:110:SER:O	1:A:432:LYS:O[3_365]	2.16	0.04
1:A:111:LYS:N	1:A:433:ALA:N[3_365]	2.16	0.04
1:A:114:LYS:CD	5:A:536:HOH:O[3_365]	2.16	0.04
1:A:141:ARG:NE	1:A:438:LEU:CA[3_365]	2.16	0.04
1:A:167:GLU:O	1:A:269:PHE:CE2[4_435]	2.16	0.04
1:A:167:GLU:OE1	1:A:276:GLY:O[4_435]	2.16	0.04
1:A:167:GLU:CD	1:A:276:GLY:C[4_435]	2.16	0.04
1:A:167:GLU:OE1	1:A:279:SER:OG[4_435]	2.16	0.04
1:A:169:MET:CA	1:A:267:PHE:CA[4_435]	2.16	0.04
1:A:209:ASP:O	1:B:259:THR:N[4_435]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:CE	1:B:274:CYS:CA[4_435]	2.16	0.04
1:A:222:ILE:CG1	1:A:265:GLY:N[4_435]	2.16	0.04
1:A:223:ILE:CB	1:A:259:THR:OG1[4_435]	2.16	0.04
1:A:234:ILE:CB	1:B:271:ASP:CG[4_435]	2.16	0.04
1:A:258:VAL:CG2	1:A:449:ARG:CG[3_365]	2.16	0.04
1:A:299:ASP:CA	1:A:299:ASP:CB[2_345]	2.16	0.04
1:A:309:CYS:O	1:A:371:LYS:C[3_365]	2.16	0.04
1:A:317:PHE:O	5:A:527:HOH:O[3_365]	2.16	0.04
1:A:326:ARG:CZ	1:A:451:GLU:CB[3_365]	2.16	0.04
1:A:337:SER:C	1:A:375:HIS:N[3_365]	2.16	0.04
1:A:355:PRO:N	4:A:502:ATP:C5'[4_435]	2.16	0.04
1:A:355:PRO:CD	4:A:502:ATP:PA[4_435]	2.16	0.04
1:A:461:MET:SD	1:B:260:PHE:CZ[4_435]	2.16	0.04
1:A:471:GLN:N	5:A:568:HOH:O[2_345]	2.16	0.04
1:B:99:ASP:N	1:B:449:ARG:C[4_445]	2.16	0.04
1:B:321:ARG:CZ	1:B:472:HIS:ND1[3_365]	2.16	0.04
1:B:371:LYS:CB	1:B:376:ALA:N[3_465]	2.16	0.04
1:B:371:LYS:O	1:B:374:LYS:CB[2_355]	2.16	0.04
1:B:372:VAL:C	1:B:374:LYS:N[2_355]	2.16	0.04
1:B:380:GLY:N	1:B:402:TYR:O[4_445]	2.16	0.04
1:B:388:ARG:NH2	1:B:416:ILE:O[4_445]	2.16	0.04
1:B:390:PHE:O	1:B:407:LEU:O[4_445]	2.16	0.04
1:B:395:ASP:C	1:B:441:LEU:O[4_445]	2.16	0.04
1:B:399:SER:O	1:B:439:GLN:CD[4_445]	2.16	0.04
1:B:402:TYR:N	1:B:439:GLN:OE1[4_445]	2.16	0.04
1:B:407:LEU:C	1:B:421:THR:O[3_465]	2.16	0.04
1:B:409:ASP:O	1:B:423:GLY:N[3_465]	2.16	0.04
1:B:416:ILE:CG2	5:B:490:HOH:O[3_465]	2.16	0.04
1:B:420:TYR:CE2	1:B:437:VAL:CG1[4_445]	2.16	0.04
1:B:420:TYR:CE2	1:B:437:VAL:CG2[4_445]	2.16	0.04
1:B:427:THR:O	1:B:431:LYS:CA[4_445]	2.16	0.04
1:B:428:GLY:O	1:B:431:LYS:CA[2_355]	2.16	0.04
1:B:431:LYS:CD	1:B:435:ILE:CD1[2_355]	2.16	0.04
1:A:90:VAL:CG1	1:A:342:ALA:CA[3_365]	2.17	0.03
1:A:92:THR:OG1	1:A:345:GLY:C[3_365]	2.17	0.03
1:A:98:ILE:O	1:A:398:VAL:N[3_365]	2.17	0.03
1:A:99:ASP:O	1:A:401:MET:CG[3_365]	2.17	0.03
1:A:104:ILE:C	1:A:403:LEU:N[3_365]	2.17	0.03
1:A:106:ARG:C	1:A:406:PHE:CD1[3_365]	2.17	0.03
1:A:107:PHE:C	1:A:406:PHE:CG[3_365]	2.17	0.03
1:A:109:SER:N	1:A:438:LEU:N[3_365]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:O	1:A:434:LEU:CA[3_365]	2.17	0.03
1:A:111:LYS:N	1:A:433:ALA:O[3_365]	2.17	0.03
1:A:138:PHE:CD1	1:A:372:VAL:O[3_365]	2.17	0.03
1:A:138:PHE:CG	1:A:431:LYS:CD[3_365]	2.17	0.03
1:A:165:SER:N	5:A:620:HOH:O[4_435]	2.17	0.03
1:A:179:PHE:CD2	5:A:572:HOH:O[3_365]	2.17	0.03
1:A:218:ASN:CB	1:A:269:PHE:CB[4_435]	2.17	0.03
1:A:257:HIS:O	1:A:450:LYS:C[3_365]	2.17	0.03
1:A:313:GLN:CD	5:A:543:HOH:O[3_365]	2.17	0.03
1:A:321:ARG:CD	1:A:439:GLN:C[3_365]	2.17	0.03
1:A:336:HIS:CE1	1:A:368:ILE:CB[3_365]	2.17	0.03
1:A:336:HIS:O	1:A:372:VAL:O[3_365]	2.17	0.03
1:A:336:HIS:C	1:A:371:LYS:C[3_365]	2.17	0.03
1:A:336:HIS:CD2	1:A:372:VAL:CG2[3_365]	2.17	0.03
1:A:337:SER:CB	1:A:374:LYS:CA[3_365]	2.17	0.03
1:A:356:ASN:ND2	4:A:502:ATP:N9[4_435]	2.17	0.03
1:A:356:ASN:CG	4:A:502:ATP:C1'[4_435]	2.17	0.03
1:A:457:VAL:CG2	1:B:273:ASP:N[4_435]	2.17	0.03
1:B:109:SER:C	1:B:471:GLN:CA[3_365]	2.17	0.03
1:B:110:SER:N	1:B:471:GLN:CB[3_365]	2.17	0.03
1:B:140:HIS:CA	1:B:473:HIS:ND1[3_365]	2.17	0.03
1:B:345:GLY:C	1:B:360:PHE:C[4_445]	2.17	0.03
1:B:346:ALA:CA	1:B:360:PHE:O[4_445]	2.17	0.03
1:B:370:THR:O	1:B:374:LYS:CB[4_445]	2.17	0.03
1:B:371:LYS:CA	1:B:375:HIS:CA[3_465]	2.17	0.03
1:B:372:VAL:N	1:B:374:LYS:N[4_445]	2.17	0.03
1:B:379:GLY:N	1:B:438:LEU:CD2[4_445]	2.17	0.03
1:B:383:THR:CG2	1:B:443:ALA:CA[2_355]	2.17	0.03
1:B:392:GLY:C	1:B:407:LEU:CA[4_445]	2.17	0.03
1:B:400:PHE:C	1:B:439:GLN:OE1[4_445]	2.17	0.03
1:B:401:MET:C	1:B:439:GLN:CG[4_445]	2.17	0.03
1:B:426:LEU:CA	1:B:436:GLU:OE1[2_355]	2.17	0.03
1:B:428:GLY:O	1:B:432:LYS:CG[3_465]	2.17	0.03
1:B:430:LEU:CD1	1:B:436:GLU:CB[4_445]	2.17	0.03
1:A:88:TRP:CA	1:A:351:SER:C[3_365]	2.18	0.02
1:A:93:SER:OG	5:A:518:HOH:O[2_245]	2.18	0.02
1:A:93:SER:CB	1:A:346:ALA:CA[2_245]	2.18	0.02
1:A:112:ILE:O	1:A:430:LEU:N[3_365]	2.18	0.02
1:A:162:ARG:NH1	1:A:267:PHE:O[4_435]	2.18	0.02
1:A:197:ASP:CG	1:B:261:ASN:CG[4_435]	2.18	0.02
1:A:221:ASP:N	1:A:262:GLN:N[4_435]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:CG2	5:A:524:HOH:O[3_365]	2.18	0.02
1:A:314:ASP:C	1:A:442:ILE:CD1[3_365]	2.18	0.02
1:A:316:TYR:CA	1:A:360:PHE:O[3_365]	2.18	0.02
1:A:316:TYR:CG	1:A:360:PHE:CB[3_365]	2.18	0.02
1:A:316:TYR:C	1:A:362:THR:CA[3_365]	2.18	0.02
1:A:322:ASP:OD2	1:A:448:ARG:CG[3_365]	2.18	0.02
1:A:329:TYR:CE1	1:A:470:PHE:C[2_345]	2.18	0.02
1:A:337:SER:CB	1:A:371:LYS:O[3_365]	2.18	0.02
1:A:339:PHE:N	1:A:375:HIS:C[3_365]	2.18	0.02
1:A:454:ASP:OD1	1:B:277:LYS:CB[4_435]	2.18	0.02
1:A:460:PHE:CB	1:B:272:SER:CB[4_435]	2.18	0.02
1:B:99:ASP:CG	1:B:448:ARG:CA[4_445]	2.18	0.02
1:B:342:ALA:CA	1:B:367:GLN:CG[4_445]	2.18	0.02
1:B:343:LEU:C	1:B:371:LYS:CE[4_445]	2.18	0.02
1:B:344:GLN:C	1:B:371:LYS:NZ[4_445]	2.18	0.02
1:B:347:GLN:CA	1:B:361:LEU:C[4_445]	2.18	0.02
1:B:366:LYS:N	1:B:402:TYR:CD1[3_465]	2.18	0.02
1:B:369:LYS:CE	5:B:479:HOH:O[2_355]	2.18	0.02
1:B:382:ASP:N	1:B:404:THR:OG1[4_445]	2.18	0.02
1:B:410:ASP:C	5:B:538:HOH:O[3_465]	2.18	0.02
1:B:412:LYS:C	1:B:423:GLY:O[3_465]	2.18	0.02
1:B:427:THR:O	1:B:430:LEU:C[4_445]	2.18	0.02
1:B:430:LEU:CB	1:B:432:LYS:O[4_445]	2.18	0.02
1:B:459:GLU:CD	1:B:459:GLU:CD[2_345]	2.18	0.02
1:A:83:ASP:N	1:A:339:PHE:O[3_365]	2.19	0.01
1:A:83:ASP:OD1	1:A:377:PHE:CD1[2_245]	2.19	0.01
1:A:100:TYR:CG	1:A:398:VAL:CA[3_365]	2.19	0.01
1:A:102:LYS:N	1:A:400:PHE:CA[3_365]	2.19	0.01
1:A:102:LYS:C	1:A:402:TYR:CA[3_365]	2.19	0.01
1:A:103:LEU:O	1:A:402:TYR:O[3_365]	2.19	0.01
1:A:104:ILE:CB	1:A:434:LEU:CD1[3_365]	2.19	0.01
1:A:106:ARG:CD	1:A:405:PHE:CB[3_365]	2.19	0.01
1:A:111:LYS:CB	1:A:433:ALA:CB[3_365]	2.19	0.01
1:A:114:LYS:CG	1:A:429:GLU:CD[3_365]	2.19	0.01
1:A:138:PHE:CG	1:A:431:LYS:CE[3_365]	2.19	0.01
1:A:164:PRO:N	1:A:270:THR:CG2[4_435]	2.19	0.01
1:A:167:GLU:N	1:A:277:LYS:C[4_435]	2.19	0.01
1:A:209:ASP:CA	1:B:258:VAL:CB[4_435]	2.19	0.01
1:A:211:ALA:CB	1:A:272:SER:C[4_435]	2.19	0.01
1:A:218:ASN:C	1:A:263:VAL:CG2[4_435]	2.19	0.01
1:A:220:LYS:CB	1:A:259:THR:N[4_435]	2.19	0.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:O	1:A:262:GLN:CA[4_435]	2.19	0.01
1:A:223:ILE:N	1:A:261:ASN:C[4_435]	2.19	0.01
1:A:278:ILE:O	5:A:555:HOH:O[3_365]	2.19	0.01
1:A:281:PRO:CG	5:A:542:HOH:O[3_365]	2.19	0.01
1:A:289:PHE:CE1	1:A:471:GLN:O[2_345]	2.19	0.01
1:A:316:TYR:CA	1:A:361:LEU:N[3_365]	2.19	0.01
1:A:317:PHE:CE1	1:A:363:ASP:C[3_365]	2.19	0.01
1:A:319:MET:C	1:A:446:GLN:N[3_365]	2.19	0.01
1:A:333:ALA:C	1:A:365:ALA:C[3_365]	2.19	0.01
1:A:334:LEU:CD2	1:A:365:ALA:O[3_365]	2.19	0.01
1:A:336:HIS:O	1:A:372:VAL:CB[3_365]	2.19	0.01
1:A:458:LYS:C	1:B:270:THR:CG2[4_435]	2.19	0.01
1:B:97:GLY:N	1:B:445:HIS:CG[4_445]	2.19	0.01
1:B:102:LYS:CB	1:B:452:VAL:CA[4_445]	2.19	0.01
1:B:134:ARG:N	1:B:390:PHE:CZ[3_465]	2.19	0.01
1:B:134:ARG:NE	1:B:389:GLN:C[3_465]	2.19	0.01
1:B:307:ILE:CB	1:B:474:HIS:O[3_365]	2.19	0.01
1:B:344:GLN:C	1:B:360:PHE:N[4_445]	2.19	0.01
1:B:369:LYS:CD	1:B:434:LEU:CD2[3_465]	2.19	0.01
1:B:387:HIS:O	1:B:413:LEU:CD1[4_445]	2.19	0.01
1:B:388:ARG:CZ	1:B:416:ILE:C[4_445]	2.19	0.01
1:B:399:SER:CA	1:B:435:ILE:CB[4_445]	2.19	0.01
1:B:414:GLU:N	5:B:538:HOH:O[3_465]	2.19	0.01
1:B:415:GLN:CD	5:B:536:HOH:O[3_465]	2.19	0.01
1:B:428:GLY:N	1:B:430:LEU:C[4_445]	2.19	0.01
1:B:428:GLY:O	1:B:433:ALA:N[2_355]	2.19	0.01
1:B:429:GLU:O	1:B:432:LYS:CB[4_445]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	388/477 (81%)	366 (94%)	18 (5%)	4 (1%)	12 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	377/477 (79%)	359 (95%)	16 (4%)	2 (0%)	24	37
All	All	765/954 (80%)	725 (95%)	34 (4%)	6 (1%)	16	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	SER
1	B	351	SER
1	A	298	ARG
1	A	353	SER
1	B	350	MET
1	A	299	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/416 (82%)	320 (94%)	20 (6%)	18	31
1	B	331/416 (80%)	306 (92%)	25 (8%)	12	21
All	All	671/832 (81%)	626 (93%)	45 (7%)	15	26

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ILE
1	A	106	ARG
1	A	144	ASN
1	A	192	VAL
1	A	202	LEU
1	A	207	THR
1	A	232	THR
1	A	236	SER
1	A	239	ASP
1	A	291	ASN

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Mol	Chain	Res	Type
1	A	295	GLN
1	A	303	ILE
1	A	311	ILE
1	A	322	ASP
1	A	344	GLN
1	A	412	LYS
1	A	427	THR
1	A	430	LEU
1	A	452	VAL
1	A	457	VAL
1	B	114	LYS
1	B	148	ASP
1	B	171	VAL
1	B	186	VAL
1	B	192	VAL
1	B	202	LEU
1	B	232	THR
1	B	236	SER
1	B	239	ASP
1	B	291	ASN
1	B	295	GLN
1	B	296	ILE
1	B	301	THR
1	B	311	ILE
1	B	344	GLN
1	B	348	THR
1	B	354	ASP
1	B	393	ASN
1	B	407	LEU
1	B	412	LYS
1	B	418	LYS
1	B	427	THR
1	B	444	GLU
1	B	455	GLU
1	B	474	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	140	HIS
1	A	173	HIS

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Mol	Chain	Res	Type
1	A	257	HIS
1	A	262	GLN
1	A	291	ASN
1	A	295	GLN
1	A	304	GLN
1	A	336	HIS
1	A	344	GLN
1	A	393	ASN
1	A	445	HIS
1	B	129	HIS
1	B	140	HIS
1	B	145	GLN
1	B	170	HIS
1	B	188	ASN
1	B	255	GLN
1	B	257	HIS
1	B	261	ASN
1	B	262	GLN
1	B	291	ASN
1	B	295	GLN
1	B	336	HIS
1	B	344	GLN
1	B	356	ASN
1	B	373	ASN
1	B	375	HIS
1	B	393	ASN
1	B	445	HIS
1	B	474	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
3	LTN	A	501	-	16,16,16	3.43	11 (68%)	22,22,22	2.35	9 (40%)
3	LTN	B	478	-	16,16,16	3.52	11 (68%)	22,22,22	2.38	9 (40%)
4	ATP	A	502	-	32,33,33	1.20	2 (6%)	48,52,52	1.73	10 (20%)

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
3	LTN	A	501	-	-	2/8/8/8	0/2/2/2
3	LTN	B	478	-	-	3/8/8/8	0/2/2/2
4	ATP	A	502	-	-	0/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	478	LTN	O-C	8.37	1.38	1.23
3	A	501	LTN	O-C	8.18	1.38	1.23
3	B	478	LTN	C-N	-4.58	1.22	1.32
3	A	501	LTN	C-N	-4.54	1.22	1.32
3	B	478	LTN	CD2-CG	-4.50	1.36	1.44
3	A	501	LTN	CD2-CG	-4.34	1.36	1.44
3	B	478	LTN	CH2-CZ2	3.88	1.45	1.38
3	B	478	LTN	CZ2-CE2	3.72	1.45	1.39
3	A	501	LTN	CE2-NE1	-3.72	1.31	1.37
3	A	501	LTN	CZ2-CE2	3.66	1.45	1.39
3	A	501	LTN	CH2-CZ2	3.65	1.45	1.38
3	B	478	LTN	CE2-NE1	-3.40	1.32	1.37
3	A	501	LTN	CH2-CZ3	3.13	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	478	LTN	CE3-CD2	3.08	1.44	1.39
3	B	478	LTN	CH2-CZ3	3.08	1.45	1.38
4	A	502	ATP	C5-N7	-3.08	1.33	1.39
3	B	478	LTN	CD1-NE1	-3.07	1.32	1.37
3	B	478	LTN	CZ3-CE3	3.01	1.44	1.38
3	A	501	LTN	CE3-CD2	2.98	1.44	1.39
3	A	501	LTN	CD1-NE1	-2.90	1.32	1.37
3	A	501	LTN	CZ3-CE3	2.77	1.43	1.38
3	B	478	LTN	CD2-CE2	2.68	1.44	1.41
3	A	501	LTN	CD2-CE2	2.27	1.44	1.41
4	A	502	ATP	C8-N9	-2.22	1.33	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	478	LTN	CD2-CG-CD1	5.78	112.08	106.16
3	A	501	LTN	CD2-CG-CD1	5.63	111.91	106.16
3	B	478	LTN	CE2-CD2-CG	-5.47	101.64	107.17
3	A	501	LTN	CE2-CD2-CG	-5.34	101.78	107.17
4	A	502	ATP	C5-C4-N3	-5.25	119.49	126.72
4	A	502	ATP	N3-C2-N1	-4.53	121.72	128.58
4	A	502	ATP	N3-C4-N9	3.79	133.61	127.17
3	A	501	LTN	CG-CD1-NE1	-3.72	106.23	110.31
3	B	478	LTN	CG-CD1-NE1	-3.63	106.32	110.31
4	A	502	ATP	C2-N3-C4	3.57	120.56	111.83
3	B	478	LTN	O-C-N	-3.12	117.53	123.04
4	A	502	ATP	N9-C8-N7	-3.11	109.52	113.94
3	A	501	LTN	O-C-N	-3.07	117.63	123.04
3	A	501	LTN	CA-C-N	2.89	121.69	116.75
4	A	502	ATP	C5-N7-C8	2.83	107.90	103.45
3	B	478	LTN	CA-C-N	2.75	121.44	116.75
4	A	502	ATP	C4-C5-N7	-2.69	107.51	110.58
3	B	478	LTN	CZ2-CE2-CD2	-2.56	119.72	122.19
4	A	502	ATP	C3'-C2'-C1'	-2.50	96.74	101.46
3	A	501	LTN	CZ2-CE2-CD2	-2.47	119.80	122.19
4	A	502	ATP	O4'-C1'-N9	2.33	112.57	108.09
4	A	502	ATP	C4-N9-C8	2.32	108.17	105.74
3	A	501	LTN	CE3-CD2-CE2	2.30	121.23	118.84
3	B	478	LTN	CE3-CD2-CE2	2.27	121.20	118.84
3	B	478	LTN	CE3-CD2-CG	2.22	137.17	133.85
3	A	501	LTN	CE2-NE1-CD1	2.19	111.03	109.08
3	A	501	LTN	CE3-CD2-CG	2.11	137.00	133.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	478	LTN	CE2-NE1-CD1	2.06	110.91	109.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

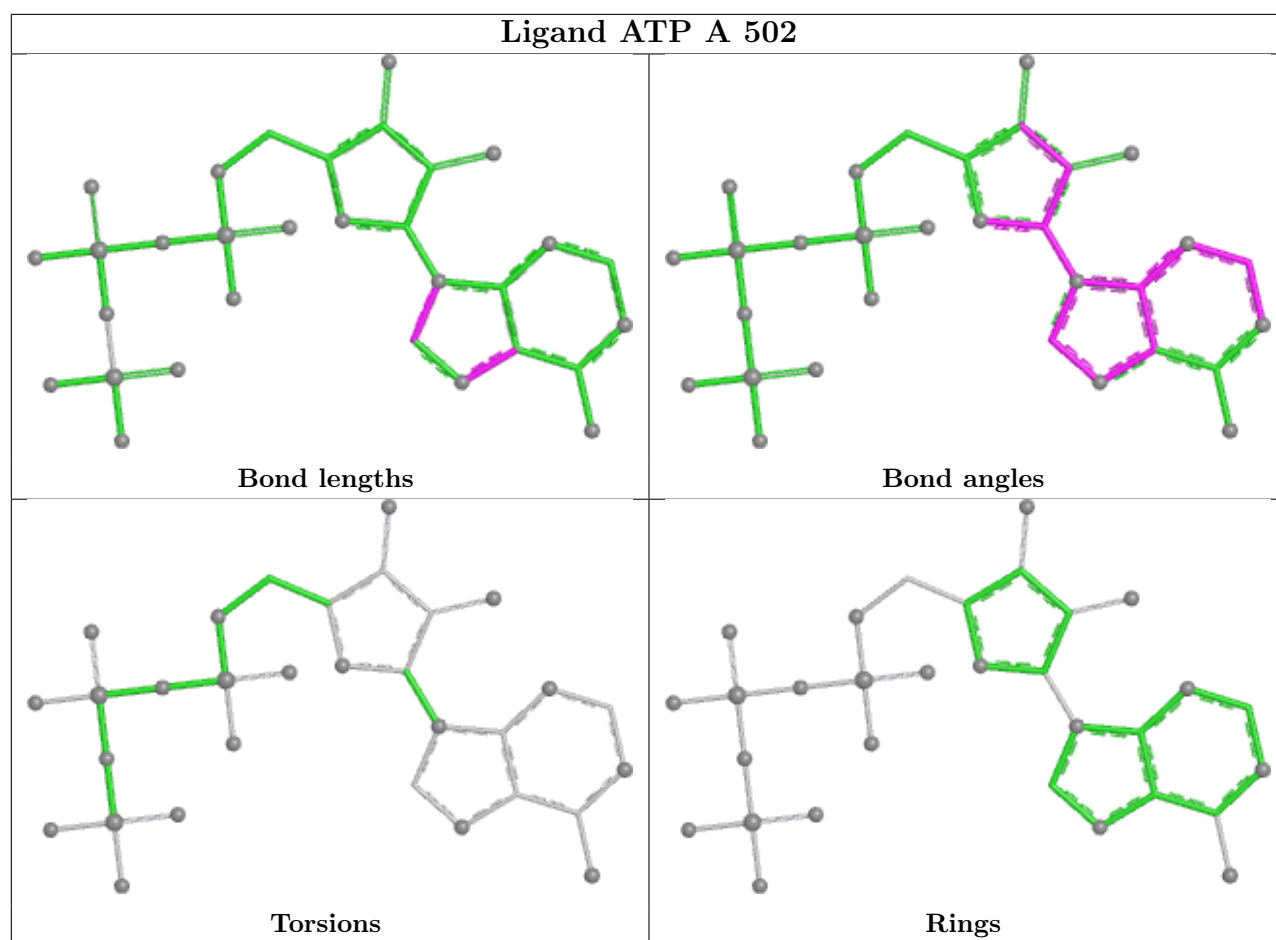
Mol	Chain	Res	Type	Atoms
3	A	501	LTN	O-C-CA-NH3
3	B	478	LTN	O-C-CA-NH3
3	A	501	LTN	O-C-CA-CB
3	B	478	LTN	O-C-CA-CB
3	B	478	LTN	N-C-CA-CB

There are no ring outliers.

3 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	LTN	1	7
3	B	478	LTN	1	0
4	A	502	ATP	10	77

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	390/477 (81%)	5.06	375 (96%) 0 0	33, 46, 93, 179	0
1	B	379/477 (79%)	5.55	374 (98%) 0 0	33, 48, 69, 92	0
All	All	769/954 (80%)	5.30	749 (97%) 0 0	33, 47, 80, 179	0

All (749) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	PHE	13.5
1	A	88	TRP	12.6
1	A	452	VAL	12.5
1	A	353	SER	12.2
1	B	426	LEU	11.4
1	B	378	SER	10.9
1	A	470	PHE	10.7
1	B	349	LYS	10.7
1	A	265	GLY	10.4
1	A	256	LYS	10.4
1	B	204	LYS	10.4
1	B	370	THR	10.4
1	B	299	ASP	10.3
1	A	90	VAL	10.0
1	B	352	ALA	9.9
1	B	276	GLY	9.8
1	A	104	ILE	9.7
1	B	108	GLY	9.7
1	B	333	ALA	9.7
1	B	385	GLU	9.6
1	B	350	MET	9.6
1	A	324	ALA	9.6
1	B	262	GLN	9.6
1	A	149	ALA	9.5

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Mol	Chain	Res	Type	RSRZ
1	A	341	PRO	9.5
1	B	200	LYS	9.5
1	B	106	ARG	9.5
1	B	351	SER	9.4
1	A	96	LYS	9.4
1	A	204	LYS	9.4
1	B	343	LEU	9.4
1	B	263	VAL	9.4
1	B	451	GLU	9.3
1	A	342	ALA	9.3
1	A	97	GLY	9.3
1	B	354	ASP	9.3
1	B	269	PHE	9.2
1	B	206	LEU	9.1
1	B	208	LEU	9.1
1	B	427	THR	9.1
1	B	224	ALA	9.1
1	A	467	SER	8.8
1	A	107	PHE	8.8
1	B	107	PHE	8.7
1	B	356	ASN	8.7
1	B	452	VAL	8.6
1	B	403	LEU	8.6
1	B	285	ALA	8.6
1	B	201	TYR	8.6
1	A	323	VAL	8.6
1	B	348	THR	8.5
1	B	399	SER	8.5
1	B	456	ILE	8.5
1	A	348	THR	8.4
1	B	318	ARG	8.4
1	B	355	PRO	8.4
1	A	354	ASP	8.4
1	A	201	TYR	8.4
1	B	237	ASP	8.3
1	A	203	TRP	8.3
1	B	211	ALA	8.3
1	B	125	GLY	8.3
1	A	423	GLY	8.2
1	B	376	ALA	8.2
1	B	100	TYR	8.2
1	A	466	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
1	B	435	ILE	8.2
1	B	203	TRP	8.1
1	B	283	ILE	8.1
1	B	322	ASP	8.1
1	B	357	SER	8.1
1	A	202	LEU	8.1
1	A	357	SER	8.1
1	A	232	THR	8.0
1	A	146	VAL	7.9
1	A	205	ASP	7.9
1	B	280	PHE	7.9
1	B	117	ILE	7.9
1	A	234	ILE	7.8
1	B	415	GLN	7.8
1	B	193	ILE	7.8
1	B	434	LEU	7.7
1	B	337	SER	7.7
1	A	83	ASP	7.7
1	A	171	VAL	7.7
1	A	224	ALA	7.7
1	A	195	MET	7.7
1	B	457	VAL	7.7
1	B	287	PRO	7.6
1	A	91	GLN	7.6
1	B	436	GLU	7.6
1	B	155	PRO	7.6
1	A	460	PHE	7.6
1	A	266	ILE	7.6
1	A	101	ASP	7.6
1	B	265	GLY	7.6
1	B	101	ASP	7.5
1	B	266	ILE	7.5
1	A	98	ILE	7.4
1	A	283	ILE	7.4
1	A	208	LEU	7.4
1	B	444	GLU	7.4
1	A	200	LYS	7.4
1	B	267	PHE	7.4
1	A	89	THR	7.3
1	B	138	PHE	7.3
1	B	172	GLY	7.3
1	B	216	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	241	MET	7.3
1	B	312	ASP	7.3
1	A	117	ILE	7.3
1	B	324	ALA	7.2
1	B	212	TYR	7.2
1	B	414	GLU	7.2
1	A	255	GLN	7.2
1	B	336	HIS	7.2
1	A	279	SER	7.2
1	A	282	ALA	7.2
1	B	443	ALA	7.2
1	B	242	GLY	7.2
1	A	136	ILE	7.2
1	B	98	ILE	7.2
1	A	87	PRO	7.1
1	B	190	PRO	7.1
1	A	85	VAL	7.1
1	A	157	TYR	7.1
1	B	420	TYR	7.1
1	A	378	SER	7.1
1	B	148	ASP	7.1
1	B	310	ALA	7.1
1	A	198	ASP	7.1
1	A	215	ALA	7.1
1	A	292	SER	7.1
1	B	353	SER	7.1
1	A	178	ILE	7.1
1	B	463	PRO	7.0
1	A	170	HIS	7.0
1	A	383	THR	7.0
1	B	102	LYS	7.0
1	A	153	LYS	7.0
1	B	406	PHE	7.0
1	B	144	ASN	7.0
1	B	154	LYS	7.0
1	B	325	PRO	7.0
1	A	407	LEU	6.9
1	A	426	LEU	6.9
1	B	179	PHE	6.9
1	B	308	PRO	6.9
1	B	207	THR	6.9
1	B	332	PRO	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	175	ILE	6.9
1	A	92	THR	6.9
1	B	120	ILE	6.9
1	B	278	ILE	6.9
1	B	202	LEU	6.9
1	A	126	GLN	6.9
1	B	314	ASP	6.9
1	B	238	LEU	6.8
1	B	105	VAL	6.8
1	B	115	GLU	6.8
1	B	339	PHE	6.8
1	B	429	GLU	6.8
1	A	176	PRO	6.8
1	B	128	PRO	6.8
1	A	259	THR	6.8
1	B	153	LYS	6.8
1	B	369	LYS	6.8
1	B	297	PHE	6.8
1	A	145	GLN	6.8
1	B	248	TYR	6.8
1	B	448	ARG	6.8
1	A	120	ILE	6.7
1	A	86	ASP	6.7
1	B	254	ILE	6.7
1	B	121	GLU	6.7
1	B	279	SER	6.7
1	B	327	ILE	6.7
1	A	193	ILE	6.7
1	A	271	ASP	6.6
1	B	335	LEU	6.6
1	B	393	ASN	6.6
1	B	252	VAL	6.6
1	B	311	ILE	6.6
1	A	251	VAL	6.6
1	A	302	ASP	6.6
1	B	419	ASP	6.6
1	B	145	GLN	6.6
1	B	274	CYS	6.6
1	A	154	LYS	6.6
1	B	226	GLY	6.5
1	B	320	THR	6.5
1	B	454	ASP	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	412	LYS	6.5
1	B	116	LEU	6.5
1	B	223	ILE	6.5
1	B	186	VAL	6.5
1	A	84	PHE	6.5
1	A	206	LEU	6.5
1	B	114	LYS	6.5
1	B	205	ASP	6.5
1	B	421	THR	6.4
1	A	301	THR	6.4
1	A	453	THR	6.4
1	B	368	ILE	6.4
1	B	360	PHE	6.4
1	A	395	ASP	6.4
1	A	387	HIS	6.4
1	A	247	PHE	6.4
1	B	213	SER	6.4
1	B	303	ILE	6.4
1	A	253	LYS	6.4
1	B	316	TYR	6.3
1	A	445	HIS	6.3
1	B	156	PHE	6.3
1	A	408	GLU	6.3
1	A	186	VAL	6.3
1	B	164	PRO	6.3
1	A	121	GLU	6.3
1	B	160	THR	6.3
1	B	220	LYS	6.3
1	B	210	GLN	6.3
1	A	102	LYS	6.3
1	A	165	SER	6.3
1	B	139	SER	6.3
1	B	282	ALA	6.3
1	B	271	ASP	6.3
1	A	394	CYS	6.3
1	A	464	ARG	6.3
1	A	156	PHE	6.2
1	B	418	LYS	6.2
1	B	152	ASN	6.2
1	B	221	ASP	6.2
1	B	396	VAL	6.2
1	B	165	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	127	ARG	6.2
1	A	456	ILE	6.2
1	A	270	THR	6.2
1	B	398	VAL	6.2
1	A	296	ILE	6.2
1	B	359	ILE	6.2
1	B	425	MET	6.2
1	A	150	TYR	6.2
1	A	177	PHE	6.1
1	B	264	LYS	6.1
1	A	396	VAL	6.1
1	A	471	GLN	6.1
1	B	408	GLU	6.1
1	A	420	TYR	6.1
1	A	172	GLY	6.1
1	A	379	GLY	6.1
1	B	97	GLY	6.1
1	B	305	CYS	6.1
1	A	404	THR	6.1
1	A	284	GLN	6.1
1	B	146	VAL	6.1
1	B	170	HIS	6.0
1	A	93	SER	6.0
1	A	304	GLN	6.0
1	A	334	LEU	6.0
1	B	136	ILE	6.0
1	A	380	GLY	6.0
1	A	409	ASP	6.0
1	A	182	TRP	6.0
1	A	455	GLU	6.0
1	A	447	ALA	6.0
1	B	249	LYS	5.9
1	B	445	HIS	5.9
1	A	416	ILE	5.9
1	B	433	ALA	5.9
1	A	393	ASN	5.9
1	B	437	VAL	5.9
1	A	115	GLU	5.9
1	A	465	LYS	5.9
1	B	137	PHE	5.9
1	A	243	MET	5.9
1	A	140	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	239	ASP	5.8
1	B	409	ASP	5.8
1	B	469	ASP	5.8
1	A	261	ASN	5.8
1	A	448	ARG	5.8
1	B	295	GLN	5.8
1	A	297	PHE	5.8
1	A	168	ALA	5.8
1	A	374	LYS	5.8
1	A	427	THR	5.8
1	B	253	LYS	5.7
1	B	122	ARG	5.7
1	A	163	GLY	5.7
1	B	135	GLY	5.7
1	A	192	VAL	5.7
1	A	194	GLN	5.7
1	B	192	VAL	5.7
1	A	174	LEU	5.7
1	A	235	PHE	5.7
1	B	233	PHE	5.7
1	A	411	ASP	5.7
1	A	275	ILE	5.7
1	B	104	ILE	5.7
1	A	332	PRO	5.7
1	A	179	PHE	5.7
1	A	436	GLU	5.7
1	A	356	ASN	5.7
1	A	345	GLY	5.7
1	B	461	MET	5.7
1	A	135	GLY	5.7
1	A	189	VAL	5.7
1	A	147	LEU	5.6
1	A	190	PRO	5.7
1	A	95	ALA	5.6
1	B	219	ALA	5.6
1	B	230	ASN	5.6
1	A	159	TYR	5.6
1	A	330	PRO	5.6
1	A	132	LEU	5.6
1	A	158	LEU	5.6
1	B	411	ASP	5.6
1	B	294	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	5.6
1	B	247	PHE	5.6
1	B	468	PHE	5.6
1	A	125	GLY	5.6
1	B	243	MET	5.6
1	A	262	GLN	5.6
1	A	118	ASN	5.6
1	B	474	HIS	5.6
1	B	129	HIS	5.5
1	A	142	ASP	5.5
1	A	382	ASP	5.5
1	B	317	PHE	5.5
1	A	130	HIS	5.5
1	A	166	SER	5.5
1	B	329	TYR	5.5
1	A	390	PHE	5.5
1	B	387	HIS	5.5
1	B	151	GLU	5.5
1	B	417	ARG	5.5
1	A	391	GLY	5.5
1	A	123	ALA	5.4
1	B	198	ASP	5.4
1	B	377	PHE	5.4
1	A	239	ASP	5.4
1	B	281	PRO	5.4
1	B	244	SER	5.4
1	B	358	SER	5.4
1	A	290	SER	5.4
1	B	166	SER	5.4
1	A	228	ASP	5.4
1	A	343	LEU	5.4
1	A	413	LEU	5.4
1	B	304	GLN	5.3
1	B	331	LYS	5.3
1	B	288	SER	5.3
1	A	144	ASN	5.3
1	B	118	ASN	5.3
1	B	184	GLN	5.3
1	B	209	ASP	5.3
1	A	462	THR	5.3
1	A	280	PHE	5.3
1	A	248	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	188	ASN	5.3
1	B	251	VAL	5.3
1	A	368	ILE	5.3
1	B	340	PHE	5.3
1	A	82	GLU	5.3
1	A	148	ASP	5.3
1	B	214	TYR	5.2
1	A	128	PRO	5.2
1	B	181	LYS	5.2
1	B	259	THR	5.2
1	A	233	PHE	5.2
1	B	131	PHE	5.2
1	A	295	GLN	5.2
1	A	281	PRO	5.2
1	B	168	ALA	5.2
1	A	213	SER	5.2
1	A	229	ILE	5.2
1	A	314	ASP	5.2
1	A	410	ASP	5.2
1	B	169	MET	5.2
1	B	467	SER	5.2
1	B	177	PHE	5.2
1	B	261	ASN	5.1
1	B	319	MET	5.1
1	A	286	ALA	5.1
1	B	163	GLY	5.1
1	A	191	LEU	5.1
1	A	303	ILE	5.1
1	B	323	VAL	5.1
1	B	222	ILE	5.1
1	B	466	LEU	5.1
1	A	230	ASN	5.1
1	A	242	GLY	5.1
1	A	377	PHE	5.1
1	A	346	ALA	5.1
1	B	367	GLN	5.0
1	A	99	ASP	5.0
1	A	320	THR	5.0
1	B	338	THR	5.0
1	A	355	PRO	5.0
1	B	111	LYS	5.0
1	B	161	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLN	5.0
1	B	195	MET	5.0
1	B	383	THR	5.0
1	A	258	VAL	5.0
1	A	94	SER	5.0
1	A	288	SER	5.0
1	B	127	ARG	5.0
1	B	386	GLU	5.0
1	B	215	ALA	5.0
1	A	196	THR	5.0
1	B	183	LEU	5.0
1	A	185	ASP	4.9
1	B	302	ASP	4.9
1	A	231	LYS	4.9
1	B	240	TYR	4.9
1	A	236	SER	4.9
1	B	147	LEU	4.9
1	B	438	LEU	4.9
1	A	139	SER	4.9
1	A	250	ASN	4.9
1	B	430	LEU	4.9
1	B	182	TRP	4.9
1	A	138	PHE	4.9
1	B	191	LEU	4.9
1	B	255	GLN	4.9
1	B	257	HIS	4.9
1	B	296	ILE	4.8
1	A	310	ALA	4.8
1	B	286	ALA	4.8
1	A	240	TYR	4.8
1	A	289	PHE	4.8
1	B	167	GLU	4.8
1	A	438	LEU	4.8
1	B	174	LEU	4.8
1	A	381	ARG	4.8
1	A	421	THR	4.8
1	B	460	PHE	4.8
1	B	132	LEU	4.8
1	B	173	HIS	4.8
1	A	122	ARG	4.8
1	A	252	VAL	4.8
1	A	433	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	131	PHE	4.8
1	B	291	ASN	4.8
1	A	325	PRO	4.7
1	B	217	GLU	4.7
1	B	458	LYS	4.7
1	B	284	GLN	4.7
1	A	405	PHE	4.7
1	B	290	SER	4.7
1	A	152	ASN	4.7
1	B	315	PRO	4.7
1	A	223	ILE	4.7
1	A	425	MET	4.7
1	A	254	ILE	4.6
1	B	394	CYS	4.6
1	A	187	PHE	4.6
1	A	311	ILE	4.6
1	B	149	ALA	4.6
1	B	157	TYR	4.6
1	A	173	HIS	4.6
1	B	379	GLY	4.6
1	A	264	LYS	4.6
1	B	175	ILE	4.6
1	B	229	ILE	4.6
1	B	234	ILE	4.6
1	B	275	ILE	4.6
1	B	309	CYS	4.5
1	A	237	ASP	4.5
1	B	246	GLY	4.5
1	A	212	TYR	4.5
1	B	159	TYR	4.5
1	A	151	GLU	4.5
1	A	392	GLY	4.5
1	B	293	PHE	4.5
1	A	373	ASN	4.5
1	A	352	ALA	4.5
1	A	207	THR	4.5
1	A	347	GLN	4.5
1	B	103	LEU	4.5
1	A	299	ASP	4.5
1	B	459	GLU	4.5
1	B	187	PHE	4.4
1	B	260	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	366	LYS	4.4
1	A	244	SER	4.4
1	B	109	SER	4.4
1	B	422	SER	4.4
1	A	134	ARG	4.4
1	A	362	THR	4.4
1	B	196	THR	4.4
1	A	214	TYR	4.4
1	A	305	CYS	4.4
1	B	446	GLN	4.4
1	A	441	LEU	4.4
1	B	306	LEU	4.4
1	A	444	GLU	4.4
1	A	160	THR	4.4
1	B	150	TYR	4.4
1	B	235	PHE	4.4
1	B	400	PHE	4.4
1	A	321	ARG	4.4
1	B	178	ILE	4.4
1	B	188	ASN	4.4
1	A	451	GLU	4.4
1	B	432	LYS	4.4
1	A	326	ARG	4.3
1	B	112	ILE	4.3
1	B	363	ASP	4.3
1	A	155	PRO	4.3
1	B	180	THR	4.3
1	B	300	ARG	4.3
1	A	227	PHE	4.3
1	A	291	ASN	4.3
1	A	386	GLU	4.3
1	B	158	LEU	4.3
1	B	447	ALA	4.3
1	A	161	GLY	4.3
1	A	268	GLY	4.3
1	B	313	GLN	4.3
1	A	285	ALA	4.3
1	B	245	SER	4.3
1	B	272	SER	4.3
1	A	133	ARG	4.3
1	A	119	ARG	4.3
1	B	442	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	465	LYS	4.2
1	A	287	PRO	4.2
1	B	197	ASP	4.2
1	A	339	PHE	4.2
1	B	162	ARG	4.2
1	A	180	THR	4.2
1	B	232	THR	4.2
1	B	405	PHE	4.2
1	A	418	LYS	4.2
1	A	422	SER	4.2
1	B	113	ASP	4.2
1	B	475	HIS	4.2
1	A	385	GLU	4.1
1	A	162	ARG	4.1
1	B	326	ARG	4.1
1	A	306	LEU	4.1
1	B	218	ASN	4.1
1	A	113	ASP	4.1
1	A	384	ILE	4.1
1	B	416	ILE	4.1
1	B	449	ARG	4.1
1	A	365	ALA	4.1
1	A	417	ARG	4.1
1	B	298	ARG	4.1
1	A	199	GLU	4.1
1	A	221	ASP	4.1
1	B	395	ASP	4.1
1	A	415	GLN	4.0
1	A	419	ASP	4.0
1	A	327	ILE	4.0
1	A	116	LEU	4.0
1	B	143	MET	4.0
1	A	269	PHE	4.0
1	A	108	GLY	4.0
1	B	231	LYS	4.0
1	B	140	HIS	4.0
1	B	268	GLY	4.0
1	A	211	ALA	4.0
1	B	292	SER	4.0
1	B	440	PRO	4.0
1	A	400	PHE	3.9
1	B	328	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	342	ALA	3.9
1	A	278	ILE	3.9
1	B	228	ASP	3.9
1	B	176	PRO	3.9
1	B	470	PHE	3.9
1	B	423	GLY	3.9
1	A	273	ASP	3.9
1	B	453	THR	3.9
1	A	294	PRO	3.9
1	A	143	MET	3.9
1	B	389	GLN	3.9
1	B	404	THR	3.8
1	A	137	PHE	3.8
1	A	428	GLY	3.8
1	B	431	LYS	3.8
1	A	183	LEU	3.8
1	B	441	LEU	3.8
1	B	225	CYS	3.8
1	B	189	VAL	3.8
1	A	293	PHE	3.8
1	A	375	HIS	3.8
1	A	226	GLY	3.8
1	B	301	THR	3.8
1	A	432	LYS	3.8
1	A	267	PHE	3.8
1	A	340	PHE	3.7
1	B	199	GLU	3.7
1	A	318	ARG	3.7
1	B	119	ARG	3.7
1	B	124	THR	3.7
1	B	345	GLY	3.7
1	A	329	TYR	3.7
1	A	349	LYS	3.7
1	A	245	SER	3.7
1	A	376	ALA	3.7
1	A	100	TYR	3.7
1	A	298	ARG	3.7
1	B	289	PHE	3.7
1	A	351	SER	3.6
1	A	106	ARG	3.6
1	B	256	LYS	3.6
1	A	184	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	330	PRO	3.6
1	A	322	ASP	3.6
1	A	105	VAL	3.6
1	A	124	THR	3.6
1	A	454	ASP	3.6
1	A	414	GLU	3.6
1	A	458	LYS	3.6
1	B	450	LYS	3.5
1	A	364	THR	3.5
1	A	110	SER	3.5
1	B	123	ALA	3.5
1	B	410	ASP	3.5
1	A	313	GLN	3.5
1	A	431	LYS	3.5
1	A	263	VAL	3.5
1	B	347	GLN	3.5
1	B	397	ASP	3.5
1	A	403	LEU	3.5
1	A	317	PHE	3.5
1	B	171	VAL	3.4
1	A	434	LEU	3.4
1	B	375	HIS	3.4
1	B	142	ASP	3.4
1	B	321	ARG	3.4
1	A	461	MET	3.4
1	A	103	LEU	3.4
1	B	371	LYS	3.4
1	B	374	LYS	3.4
1	A	333	ALA	3.4
1	B	402	TYR	3.4
1	B	401	MET	3.4
1	A	442	ILE	3.4
1	B	307	ILE	3.4
1	A	388	ARG	3.4
1	A	249	LYS	3.3
1	A	424	ALA	3.3
1	A	402	TYR	3.3
1	A	367	GLN	3.3
1	A	370	THR	3.3
1	A	435	ILE	3.3
1	A	350	MET	3.3
1	B	99	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	185	ASP	3.3
1	A	459	GLU	3.3
1	A	331	LYS	3.3
1	A	272	SER	3.3
1	B	236	SER	3.2
1	B	439	GLN	3.2
1	B	130	HIS	3.2
1	B	227	PHE	3.2
1	A	300	ARG	3.2
1	B	380	GLY	3.2
1	A	217	GLU	3.1
1	B	277	LYS	3.1
1	A	319	MET	3.1
1	B	361	LEU	3.1
1	A	406	PHE	3.1
1	A	316	TYR	3.1
1	B	455	GLU	3.1
1	B	407	LEU	3.1
1	A	344	GLN	3.1
1	B	472	HIS	3.1
1	B	384	ILE	3.1
1	A	336	HIS	3.0
1	B	250	ASN	3.0
1	A	246	GLY	3.0
1	B	344	GLN	3.0
1	A	443	ALA	3.0
1	B	241	MET	3.0
1	B	273	ASP	3.0
1	B	392	GLY	3.0
1	B	270	THR	3.0
1	A	360	PHE	3.0
1	A	363	ASP	3.0
1	A	469	ASP	3.0
1	B	382	ASP	3.0
1	A	309	CYS	3.0
1	B	194	GLN	3.0
1	A	257	HIS	3.0
1	A	449	ARG	3.0
1	A	397	ASP	2.9
1	A	129	HIS	2.9
1	B	372	VAL	2.9
1	A	463	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	372	VAL	2.9
1	A	308	PRO	2.8
1	A	389	GLN	2.8
1	A	114	LYS	2.8
1	A	277	LYS	2.8
1	B	412	LYS	2.8
1	B	464	ARG	2.8
1	B	334	LEU	2.8
1	A	401	MET	2.8
1	A	225	CYS	2.8
1	B	133	ARG	2.8
1	A	197	ASP	2.8
1	A	440	PRO	2.7
1	B	110	SER	2.7
1	B	381	ARG	2.7
1	A	315	PRO	2.7
1	B	391	GLY	2.7
1	A	181	LYS	2.7
1	B	373	ASN	2.7
1	B	141	ARG	2.7
1	A	359	ILE	2.6
1	B	471	GLN	2.6
1	A	109	SER	2.6
1	A	209	ASP	2.5
1	B	413	LEU	2.5
1	B	388	ARG	2.5
1	A	398	VAL	2.5
1	B	346	ALA	2.4
1	A	164	PRO	2.4
1	A	457	VAL	2.3
1	A	169	MET	2.3
1	B	462	THR	2.3
1	A	167	GLU	2.3
1	A	399	SER	2.3
1	A	218	ASN	2.2
1	B	428	GLY	2.2
1	A	430	LEU	2.2
1	A	111	LYS	2.2
1	A	366	LYS	2.2
1	B	362	THR	2.2
1	A	335	LEU	2.2
1	A	369	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	258	VAL	2.1
1	A	141	ARG	2.1
1	A	361	LEU	2.1
1	A	450	LYS	2.1
1	A	260	PHE	2.1
1	A	337	SER	2.1
1	A	338	THR	2.1
1	A	222	ILE	2.1
1	B	365	ALA	2.0
1	B	473	HIS	2.0
1	A	437	VAL	2.0

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](#)

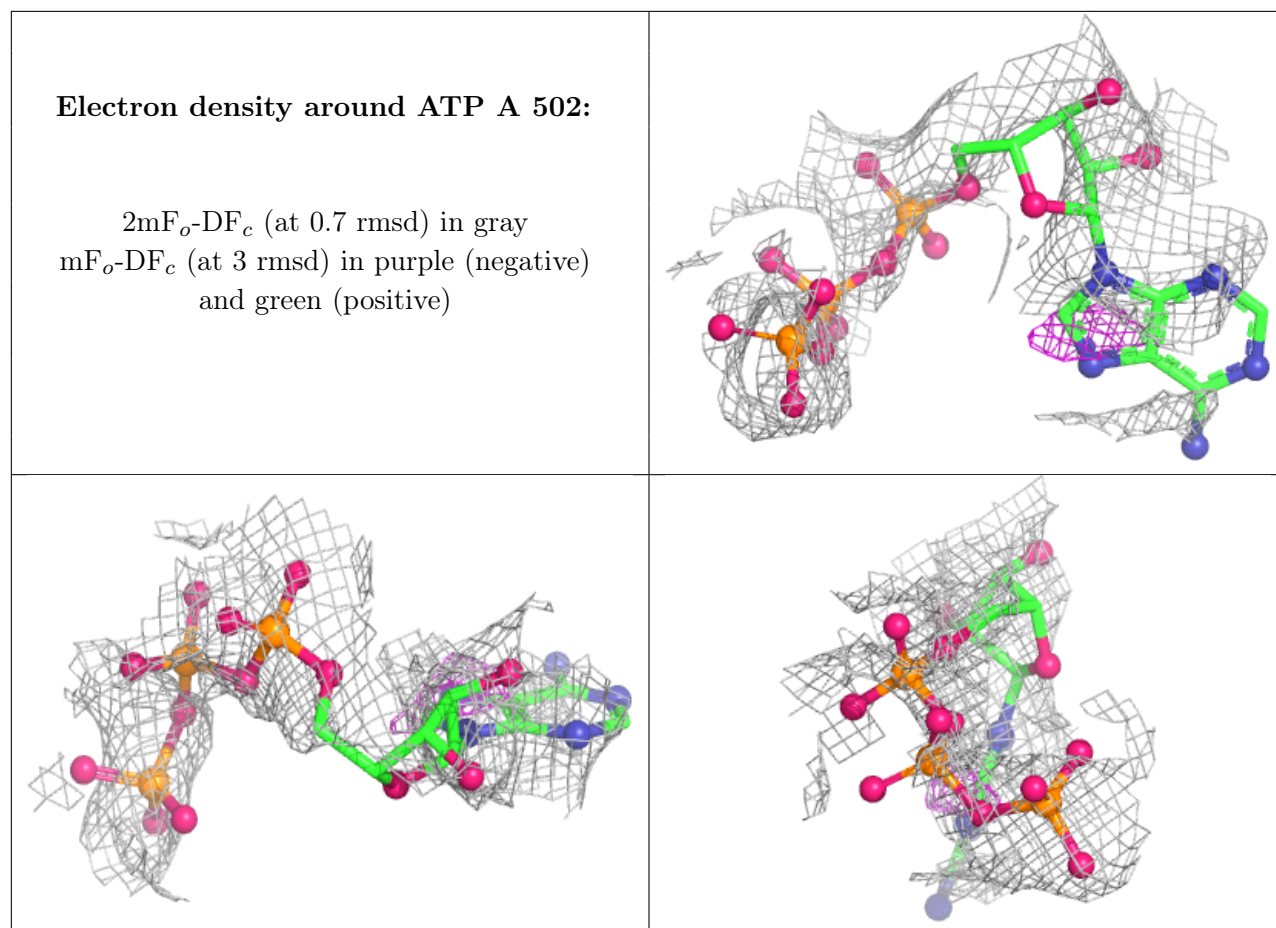
There are no oligosaccharides in this entry.

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	ATP	A	502	31/31	0.55	0.46	118,121,140,141	0
3	LTN	B	478	15/15	0.63	0.29	41,44,45,49	0
3	LTN	A	501	15/15	0.69	0.36	37,40,42,42	0
2	MG	A	500	1/1	0.84	0.46	74,74,74,74	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.