



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 03:21 AM UTC

PDB ID : 1IA0 / pdb_00001ia0
Title : KIF1A HEAD-MICROTUBULE COMPLEX STRUCTURE IN ATP-FORM
Authors : Kikkawa, M.; Sablin, E.P.; Okada, Y.; Yajima, H.; Fletterick, R.J.; Hirokawa, N.
Deposited on : 2001-03-22
Resolution : 15.00 Å(reported)
Based on initial model : 1TUB

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

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)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

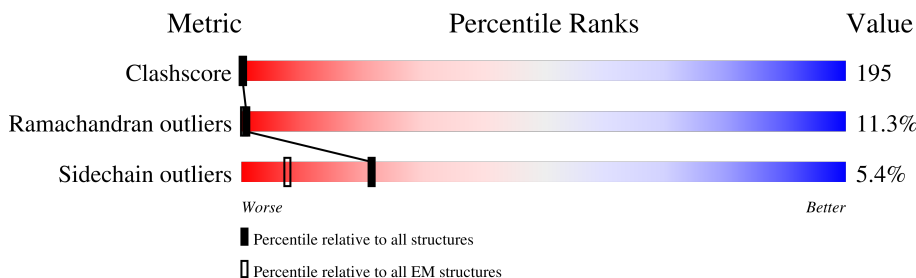
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	451	
2	B	445	
3	K	394	

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
4	GTP	A	500	-	-	X	-
5	GDP	B	501	-	-	X	-
6	TXL	B	502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9606 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 TUBULIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	440	Total	C	N	O	S	0	0
			3430	2168	583	657	22		

- Molecule 2 is a protein called TUBULIN BETA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	427	Total	C	N	O	S	0	0
			3359	2110	576	647	26		

- Molecule 3 is a protein called KINESIN-LIKE PROTEIN KIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	328	Total	C	N	O	S	10	0
			2667	1651	469	531	16		

There are 42 discrepancies between the modelled and reference sequences:

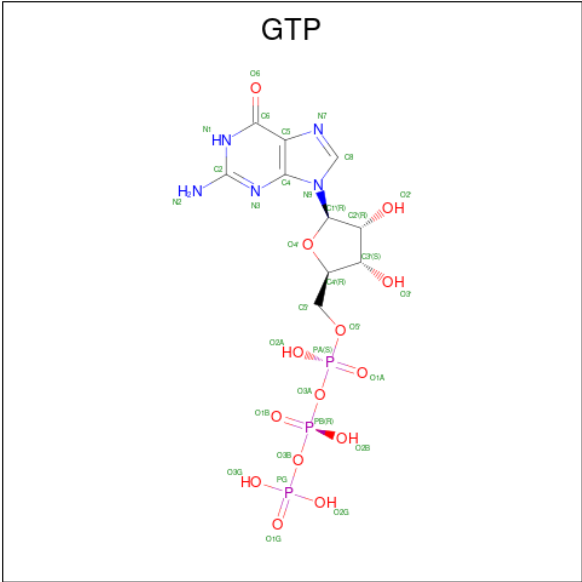
Chain	Residue	Modelled	Actual	Comment	Reference
K	-15	MET	-	see remark 999	UNP P33173
K	-14	ALA	-	see remark 999	UNP P33173
K	-13	SER	-	see remark 999	UNP P33173
K	-12	MET	-	see remark 999	UNP P33173
K	-11	THR	-	see remark 999	UNP P33173
K	-10	GLY	-	see remark 999	UNP P33173
K	-9	GLY	-	see remark 999	UNP P33173
K	-8	GLN	-	see remark 999	UNP P33173
K	-7	GLN	-	see remark 999	UNP P33173
K	-6	MET	-	see remark 999	UNP P33173
K	-5	GLY	-	see remark 999	UNP P33173
K	-4	ARG	-	see remark 999	UNP P33173
K	-3	ASP	-	see remark 999	UNP P33173
K	-2	PRO	-	see remark 999	UNP P33173
K	-1	ILE	-	see remark 999	UNP P33173

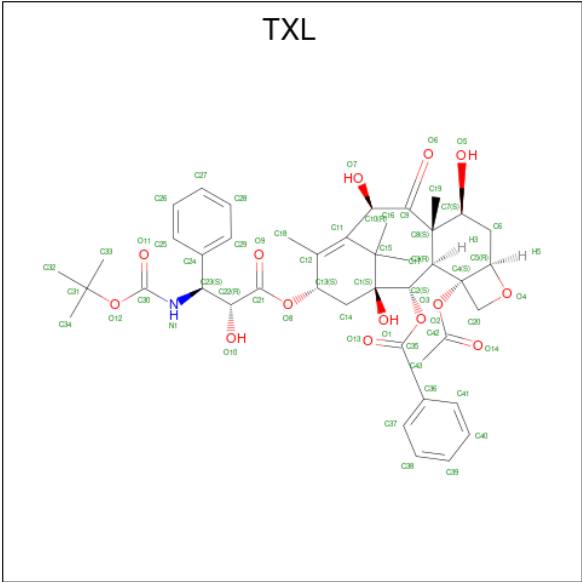
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Chain	Residue	Modelled	Actual	Comment	Reference
K	0	ASN	-	see remark 999	UNP P33173
K	1	MET	-	see remark 999	UNP P33173
K	2	PRO	-	see remark 999	UNP P33173
K	202	ALA	PRO	engineered mutation	UNP P33173
K	356	ASN	-	SEE REMARK 999	UNP P33173
K	357	THR	-	SEE REMARK 999	UNP P33173
K	358	VAL	-	SEE REMARK 999	UNP P33173
K	359	SER	-	SEE REMARK 999	UNP P33173
K	360	VAL	-	SEE REMARK 999	UNP P33173
K	361	ASN	-	SEE REMARK 999	UNP P33173
K	362	LEU	-	SEE REMARK 999	UNP P33173
K	363	GLU	-	SEE REMARK 999	UNP P33173
K	364	LEU	-	SEE REMARK 999	UNP P33173
K	365	THR	-	SEE REMARK 999	UNP P33173
K	366	ALA	-	SEE REMARK 999	UNP P33173
K	367	GLU	-	SEE REMARK 999	UNP P33173
K	368	GLU	-	SEE REMARK 999	UNP P33173
K	369	TRP	-	SEE REMARK 999	UNP P33173
K	370	LYS	-	SEE REMARK 999	UNP P33173
K	371	LYS	-	SEE REMARK 999	UNP P33173
K	372	LYS	-	SEE REMARK 999	UNP P33173
K	373	HIS	-	SEE REMARK 999	UNP P33173
K	374	HIS	-	SEE REMARK 999	UNP P33173
K	375	HIS	-	SEE REMARK 999	UNP P33173
K	376	HIS	-	SEE REMARK 999	UNP P33173
K	377	HIS	-	SEE REMARK 999	UNP P33173
K	378	HIS	-	SEE REMARK 999	UNP P33173

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



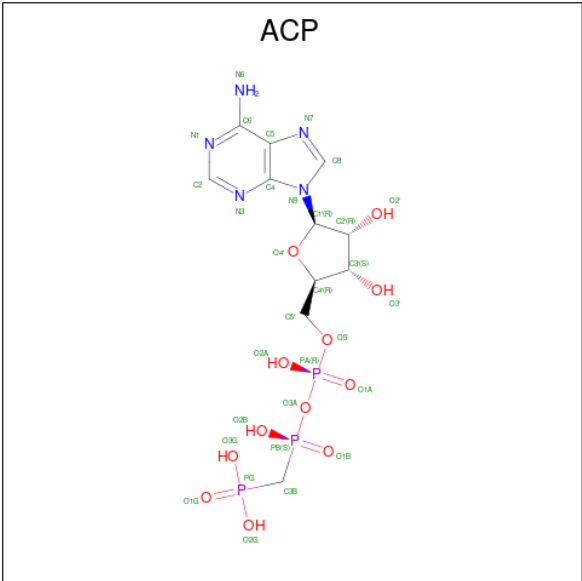


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	58	43	1	14	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
7	K	1	1	1	0

- Molecule 8 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).

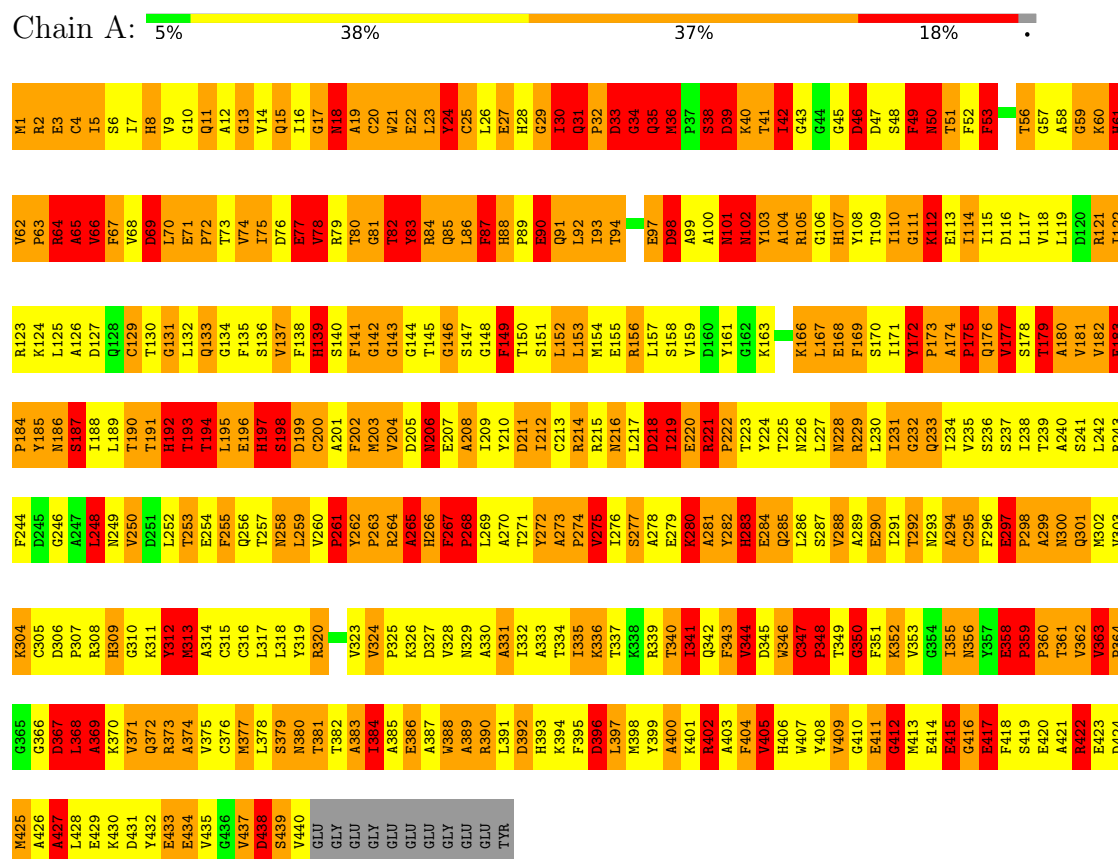


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	K	1	31	11	5	12	3	0

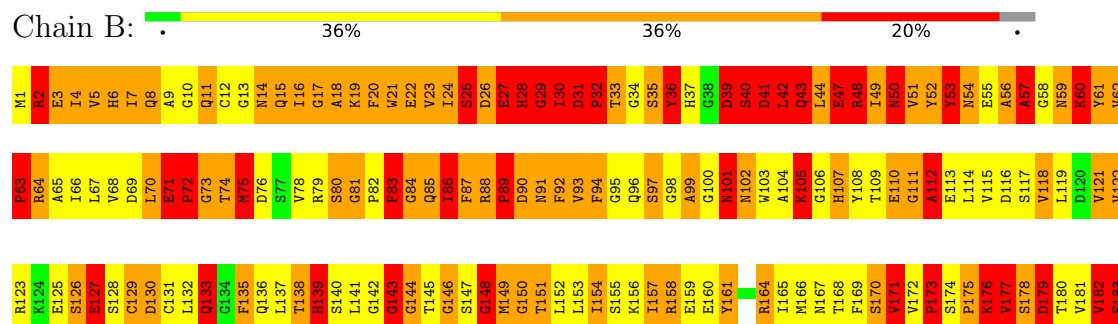
3 Residue-property plots

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

• Molecule 1: TUBULIN ALPHA CHAIN



• Molecule 2: TUBULIN BETA CHAIN



4 Data and refinement statistics

Xtrriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 15.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-15.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9606	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ACP, MG, GDP, TXL

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	3.36	243/3508 (6.9%)	3.46	307/4762 (6.4%)
2	B	3.61	243/3434 (7.1%)	3.81	360/4652 (7.7%)
3	K	0.57	0/2708	1.04	15/3655 (0.4%)
All	All	2.97	486/9650 (5.0%)	3.14	682/13069 (5.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	57
2	B	0	59
All	All	0	116

All (486) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	278	ARG	CA-CB	48.79	2.30	1.53
1	A	38	SER	C-N	-44.89	0.70	1.33
2	B	73	GLY	C-N	-44.03	0.69	1.33
2	B	105	LYS	C-N	-37.87	0.80	1.33
1	A	218	ASP	C-N	-35.87	0.84	1.33
2	B	200	GLU	C-N	-33.92	0.90	1.33
1	A	53	PHE	C-N	-33.50	0.90	1.33
2	B	321	GLY	C-N	-32.26	0.88	1.33
2	B	197	ASN	C-N	-30.32	0.90	1.33
1	A	358	GLU	C-N	-30.12	0.97	1.33
2	B	346	TRP	C-N	-30.05	0.99	1.33
2	B	340	SER	C-N	-29.38	0.92	1.33
1	A	416	GLY	C-N	-27.66	0.94	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	THR	C-N	-27.36	0.95	1.33
1	A	350	GLY	C-N	-27.31	0.95	1.33
2	B	247	GLN	C-N	-26.44	0.96	1.33
2	B	417	GLU	C-N	-26.40	0.98	1.33
1	A	415	GLU	C-N	-26.04	1.03	1.33
1	A	219	ILE	CB-CG1	-24.34	1.04	1.53
2	B	203	CYS	C-N	-23.24	1.02	1.33
1	A	69	ASP	C-N	-22.75	1.03	1.33
2	B	309	HIS	C-N	-22.45	1.00	1.33
2	B	275	LEU	C-N	-22.32	1.02	1.33
1	A	405	VAL	C-N	-21.70	1.03	1.33
2	B	182	VAL	C-N	-20.97	0.90	1.33
2	B	287	THR	C-N	20.85	1.56	1.33
1	A	221	ARG	C-N	-20.50	1.08	1.33
2	B	127	GLU	C-N	-20.27	1.05	1.33
2	B	400	ARG	C-N	-20.10	1.05	1.33
2	B	270	PRO	C-N	20.03	1.58	1.33
1	A	371	VAL	C-N	-19.81	1.02	1.33
2	B	331	GLN	C-N	-19.68	1.07	1.33
2	B	22	GLU	C-N	-19.19	1.07	1.33
1	A	347	CYS	C-N	-18.81	0.89	1.33
1	A	190	THR	C-N	-18.49	1.07	1.33
1	A	219	ILE	CB-CG2	18.34	2.13	1.52
2	B	334	ASN	C-N	-18.06	1.11	1.33
2	B	64	ARG	C-N	-17.98	1.11	1.33
1	A	409	VAL	C-N	17.64	1.59	1.33
2	B	380	ASN	C-N	-17.58	1.04	1.33
1	A	216	ASN	C-N	-17.57	1.09	1.33
2	B	387	LEU	C-N	17.39	1.63	1.33
2	B	344	VAL	C-N	-17.06	1.09	1.33
1	A	402	ARG	C-N	-16.96	1.09	1.33
1	A	187	SER	C-N	16.65	1.54	1.33
2	B	292	THR	C-N	-16.58	1.13	1.33
2	B	60	LYS	C-N	-16.48	1.10	1.33
2	B	371	LEU	C-N	-16.34	1.10	1.33
2	B	414	ASP	C-N	-15.82	1.11	1.33
2	B	337	ASN	C-N	-15.49	1.15	1.33
2	B	179	ASP	C-N	-15.27	1.10	1.33
1	A	280	LYS	C-N	-15.19	1.12	1.33
2	B	151	THR	C-N	-15.14	1.14	1.33
1	A	21	TRP	C-O	14.83	1.42	1.24
2	B	171	VAL	C-N	-14.78	1.16	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ASP	C-N	-14.74	1.11	1.33
1	A	34	GLY	N-CA	-14.51	1.24	1.45
2	B	146	GLY	C-N	14.44	1.53	1.33
2	B	259	MET	C-N	-14.18	1.19	1.32
1	A	233	GLN	C-N	-14.15	1.16	1.34
2	B	71	GLU	C-O	-14.02	1.06	1.24
1	A	259	LEU	C-N	-13.95	1.17	1.33
2	B	54	ASN	N-CA	-13.80	1.28	1.46
2	B	154	ILE	C-N	-13.77	1.15	1.33
1	A	90	GLU	C-N	-13.74	1.13	1.33
2	B	436	GLN	C-N	-13.39	1.14	1.33
1	A	346	TRP	C-N	-13.23	1.17	1.33
1	A	43	GLY	C-N	12.98	1.50	1.33
1	A	24	TYR	C-N	-12.92	1.15	1.33
1	A	231	ILE	C-O	12.85	1.39	1.24
1	A	181	VAL	C-N	12.64	1.47	1.34
1	A	438	ASP	C-O	12.48	1.38	1.23
2	B	193	GLN	C-O	12.44	1.40	1.24
2	B	89	PRO	C-N	-12.41	1.16	1.33
1	A	274	PRO	C-N	-12.36	1.16	1.33
2	B	218	LYS	C-N	12.34	1.50	1.33
2	B	299	LYS	C-N	-12.31	1.17	1.33
1	A	36	MET	C-N	-12.24	1.22	1.34
1	A	379	SER	C-N	-12.04	1.15	1.33
1	A	367	ASP	C-N	-11.92	1.17	1.33
2	B	72	PRO	C-N	-11.88	1.19	1.33
1	A	204	VAL	C-N	-11.85	1.16	1.33
2	B	71	GLU	C-N	-11.80	1.06	1.33
2	B	193	GLN	C-N	-11.78	1.19	1.33
1	A	31	GLN	C-N	-11.70	1.06	1.33
2	B	190	SER	C-N	11.66	1.49	1.33
2	B	291	LEU	N-CA	-11.64	1.31	1.46
2	B	53	TYR	C-N	-11.60	1.17	1.33
2	B	412	GLY	C-N	11.58	1.48	1.33
2	B	111	GLY	C-N	-11.46	1.19	1.33
1	A	32	PRO	N-CD	-11.44	1.31	1.47
1	A	111	GLY	C-N	-11.39	1.19	1.33
2	B	243	ARG	C-N	-11.38	1.16	1.33
1	A	176	GLN	C-N	11.37	1.49	1.33
1	A	1	MET	C-N	11.37	1.47	1.33
1	A	433	GLU	C-N	-11.13	1.18	1.33
1	A	87	PHE	C-N	-10.75	1.11	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	GLY	C-N	-10.73	1.18	1.33
2	B	167	ASN	C-N	10.53	1.47	1.33
1	A	184	PRO	CA-CB	-10.50	1.39	1.53
2	B	2	ARG	CA-C	-10.50	1.38	1.52
2	B	130	ASP	C-N	-10.47	1.18	1.33
2	B	221	THR	N-CA	10.45	1.57	1.46
1	A	140	SER	C-N	-10.44	1.19	1.33
1	A	384	ILE	C-O	-10.42	1.11	1.24
2	B	168	THR	C-N	10.40	1.47	1.33
2	B	139	HIS	C-N	10.39	1.47	1.33
1	A	2	ARG	N-CA	10.36	1.60	1.46
1	A	43	GLY	C-O	-10.34	1.11	1.23
2	B	383	ALA	C-N	-10.32	1.21	1.33
1	A	437	VAL	C-N	-10.32	1.20	1.33
2	B	164	ARG	C-N	10.31	1.45	1.33
2	B	234	THR	C-N	-10.31	1.19	1.33
1	A	77	GLU	C-N	10.27	1.46	1.34
1	A	383	ALA	C-N	-10.25	1.19	1.33
1	A	146	GLY	C-N	-10.23	1.19	1.33
2	B	348	PRO	C-N	-10.23	1.19	1.33
1	A	137	VAL	C-N	-10.19	1.19	1.33
1	A	339	ARG	CA-C	-10.19	1.39	1.52
1	A	91	GLN	C-N	10.06	1.48	1.33
1	A	46	ASP	C-N	10.02	1.47	1.33
1	A	273	ALA	C-N	-9.98	1.25	1.33
1	A	221	ARG	CB-CG	-9.97	1.22	1.52
2	B	92	PHE	C-N	-9.97	1.21	1.33
1	A	149	PHE	C-N	-9.94	1.19	1.33
2	B	178	SER	C-N	-9.93	1.19	1.33
1	A	33	ASP	CA-C	-9.91	1.39	1.52
1	A	17	GLY	C-N	9.89	1.47	1.34
2	B	393	GLU	C-O	-9.88	1.11	1.24
1	A	229	ARG	CA-CB	-9.86	1.37	1.53
2	B	194	LEU	C-N	-9.79	1.19	1.33
1	A	283	HIS	C-N	-9.65	1.20	1.33
2	B	52	TYR	C-N	-9.60	1.20	1.33
1	A	362	VAL	CA-CB	-9.60	1.48	1.55
2	B	192	HIS	C-O	9.58	1.36	1.24
1	A	380	ASN	C-N	-9.57	1.20	1.33
2	B	86	ILE	C-N	9.57	1.47	1.33
1	A	27	GLU	C-N	9.56	1.48	1.33
1	A	229	ARG	NE-CZ	-9.52	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	SER	CA-C	-9.48	1.41	1.52
2	B	2	ARG	C-N	-9.48	1.21	1.33
2	B	149	MET	C-N	-9.45	1.22	1.33
1	A	114	ILE	C-N	-9.40	1.21	1.33
1	A	22	GLU	C-O	9.38	1.35	1.24
2	B	349	ASN	N-CA	-9.32	1.34	1.46
1	A	183	GLU	C-O	-9.27	1.12	1.24
1	A	258	ASN	C-N	-9.20	1.21	1.33
2	B	346	TRP	N-CA	-9.19	1.34	1.45
1	A	94	THR	C-N	-9.17	1.29	1.33
2	B	298	ALA	C-N	9.15	1.46	1.33
1	A	19	ALA	C-N	-9.10	1.22	1.33
1	A	20	CYS	C-N	9.08	1.46	1.34
1	A	196	GLU	C-N	-9.08	1.21	1.33
2	B	40	SER	N-CA	-9.06	1.34	1.46
1	A	43	GLY	CA-C	9.06	1.61	1.52
2	B	273	ALA	C-N	-9.04	1.12	1.33
2	B	52	TYR	N-CA	-8.99	1.35	1.45
2	B	278	ARG	CD-NE	-8.99	1.33	1.46
2	B	133	GLN	C-N	-8.98	1.22	1.33
2	B	51	VAL	C-N	-8.94	1.21	1.33
2	B	107	HIS	C-O	8.90	1.34	1.24
2	B	222	PRO	C-N	-8.89	1.22	1.33
1	A	183	GLU	C-N	-8.80	1.22	1.33
1	A	107	HIS	C-O	8.78	1.34	1.24
2	B	290	GLU	C-O	-8.74	1.13	1.24
2	B	85	GLN	C-N	8.73	1.45	1.33
2	B	173	PRO	C-N	-8.72	1.15	1.33
1	A	141	PHE	N-CA	-8.72	1.34	1.46
1	A	220	GLU	CB-CG	8.67	1.78	1.52
1	A	222	PRO	N-CD	8.67	1.59	1.47
1	A	285	GLN	C-N	-8.67	1.21	1.33
2	B	76	ASP	C-O	8.66	1.34	1.24
2	B	296	PHE	C-N	-8.63	1.21	1.33
1	A	265	ALA	CA-C	-8.60	1.41	1.52
1	A	166	LYS	C-N	-8.58	1.21	1.33
1	A	112	LYS	C-O	-8.57	1.14	1.24
1	A	200	CYS	C-N	-8.57	1.21	1.33
2	B	27	GLU	C-N	-8.56	1.21	1.33
2	B	28	HIS	C-O	-8.55	1.13	1.24
2	B	242	LEU	C-N	-8.52	1.21	1.33
2	B	112	ALA	C-O	-8.51	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	THR	C-N	-8.50	1.21	1.33
2	B	143	GLY	C-N	-8.49	1.21	1.33
2	B	356	CYS	C-N	-8.47	1.21	1.33
2	B	25	SER	C-N	8.41	1.45	1.33
1	A	292	THR	C-N	-8.38	1.23	1.33
1	A	78	VAL	C-N	-8.36	1.20	1.33
1	A	232	GLY	CA-C	-8.35	1.42	1.52
1	A	355	ILE	C-N	-8.33	1.21	1.33
2	B	70	LEU	C-N	-8.31	1.16	1.33
1	A	85	GLN	CA-C	-8.31	1.43	1.53
2	B	244	PHE	N-CA	-8.29	1.33	1.45
1	A	41	THR	C-N	-8.28	1.22	1.33
1	A	377	MET	C-N	-8.26	1.20	1.33
1	A	277	SER	C-N	-8.24	1.22	1.33
2	B	143	GLY	CA-C	-8.20	1.37	1.51
1	A	406	HIS	C-N	-8.17	1.22	1.33
2	B	248	LEU	C-N	-8.17	1.21	1.33
1	A	66	VAL	N-CA	8.16	1.56	1.46
2	B	238	VAL	C-N	8.11	1.45	1.33
2	B	346	TRP	CA-C	-8.09	1.41	1.53
2	B	225	GLY	C-N	-7.99	1.23	1.34
1	A	266	HIS	N-CA	-7.98	1.35	1.45
1	A	102	ASN	C-N	-7.97	1.22	1.33
2	B	7	ILE	C-N	-7.96	1.23	1.33
1	A	166	LYS	CA-C	-7.93	1.43	1.52
2	B	4	ILE	CA-CB	-7.91	1.44	1.54
2	B	407	TRP	CA-CB	-7.88	1.40	1.53
1	A	194	THR	C-N	-7.86	1.23	1.33
1	A	295	CYS	C-N	-7.78	1.23	1.34
1	A	184	PRO	CA-C	-7.75	1.42	1.52
2	B	53	TYR	N-CA	-7.73	1.36	1.46
2	B	5	VAL	CA-C	-7.72	1.43	1.52
2	B	39	ASP	C-N	-7.68	1.23	1.33
2	B	118	VAL	C-N	-7.64	1.24	1.33
2	B	1	MET	CA-C	-7.64	1.36	1.52
2	B	1	MET	C-N	7.60	1.44	1.33
1	A	1	MET	CA-C	-7.60	1.36	1.52
1	A	19	ALA	C-O	-7.60	1.15	1.24
1	A	374	ALA	C-N	7.57	1.43	1.33
1	A	24	TYR	C-O	7.56	1.32	1.24
2	B	344	VAL	N-CA	-7.56	1.36	1.46
2	B	343	PHE	CA-C	-7.54	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ASP	N-CA	-7.53	1.36	1.46
2	B	199	ASP	C-N	-7.51	1.23	1.33
1	A	167	LEU	N-CA	-7.50	1.36	1.46
2	B	222	PRO	CA-C	-7.49	1.41	1.52
2	B	219	LEU	C-N	-7.48	1.23	1.33
1	A	23	LEU	C-N	-7.46	1.24	1.33
2	B	6	HIS	N-CA	-7.45	1.37	1.46
2	B	35	SER	C-N	-7.43	1.23	1.33
2	B	325	MET	C-N	-7.40	1.23	1.33
2	B	3	GLU	N-CA	-7.37	1.35	1.45
1	A	263	PRO	CA-CB	-7.36	1.45	1.53
1	A	391	LEU	C-N	-7.35	1.24	1.33
1	A	438	ASP	C-N	-7.32	1.23	1.34
1	A	47	ASP	N-CA	-7.32	1.38	1.46
2	B	113	GLU	C-N	7.31	1.44	1.33
1	A	222	PRO	CB-CG	7.29	1.86	1.49
1	A	228	ASN	C-N	-7.28	1.23	1.33
1	A	98	ASP	C-N	-7.26	1.24	1.33
2	B	276	THR	C-O	7.24	1.33	1.24
1	A	88	HIS	C-N	-7.24	1.24	1.33
2	B	256	ALA	C-N	-7.21	1.24	1.33
1	A	32	PRO	CA-CB	-7.19	1.43	1.53
1	A	405	VAL	CB-CG2	7.17	1.76	1.52
2	B	245	PRO	N-CD	-7.16	1.37	1.47
2	B	204	ILE	C-O	7.12	1.32	1.24
1	A	61	HIS	C-N	-7.10	1.25	1.33
2	B	138	THR	CA-C	-7.08	1.44	1.52
1	A	340	THR	C-N	-7.05	1.24	1.33
1	A	111	GLY	CA-C	-7.05	1.44	1.52
2	B	223	THR	N-CA	-7.04	1.37	1.46
1	A	267	PHE	N-CA	-7.03	1.36	1.45
2	B	345	GLU	CA-C	-7.02	1.43	1.52
2	B	111	GLY	CA-C	-7.02	1.44	1.52
2	B	53	TYR	CA-C	-7.01	1.43	1.52
2	B	406	HIS	C-N	-7.01	1.24	1.33
2	B	261	PRO	CA-C	-7.00	1.42	1.52
1	A	343	PHE	C-N	-6.97	1.24	1.33
1	A	263	PRO	N-CA	-6.96	1.42	1.47
2	B	44	LEU	C-N	6.96	1.43	1.33
1	A	366	GLY	C-N	6.95	1.44	1.33
2	B	300	ASN	C-O	-6.95	1.14	1.24
2	B	50	ASN	C-N	6.95	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	43	GLN	C-N	-6.91	1.24	1.33
1	A	93	ILE	C-N	-6.91	1.24	1.33
1	A	388	TRP	NE1-CE2	-6.90	1.29	1.37
1	A	266	HIS	CA-C	-6.89	1.44	1.52
2	B	20	PHE	C-N	-6.87	1.24	1.33
1	A	417	GLU	CA-C	-6.86	1.43	1.52
1	A	163	LYS	C-N	-6.85	1.21	1.33
2	B	224	TYR	C-O	-6.85	1.16	1.24
2	B	121	VAL	C-N	-6.84	1.25	1.33
2	B	62	VAL	CA-CB	-6.81	1.47	1.55
2	B	219	LEU	N-CA	6.80	1.54	1.46
1	A	197	HIS	C-N	6.78	1.43	1.33
1	A	64	ARG	C-N	-6.76	1.24	1.33
2	B	24	ILE	CA-CB	-6.72	1.47	1.55
1	A	50	ASN	C-N	-6.71	1.24	1.33
1	A	272	TYR	CA-C	-6.70	1.44	1.52
1	A	104	ALA	N-CA	-6.69	1.38	1.46
2	B	192	HIS	C-N	-6.63	1.23	1.33
2	B	332	MET	C-O	6.60	1.32	1.24
2	B	435	TYR	CA-C	-6.59	1.44	1.52
2	B	52	TYR	CA-C	-6.58	1.45	1.52
2	B	290	GLU	C-N	-6.57	1.24	1.33
1	A	232	GLY	C-N	-6.56	1.25	1.34
1	A	384	ILE	C-N	6.55	1.42	1.33
2	B	348	PRO	CA-C	-6.53	1.43	1.52
1	A	407	TRP	CA-CB	-6.49	1.42	1.53
1	A	281	ALA	C-N	-6.49	1.24	1.33
2	B	229	HIS	C-O	-6.49	1.15	1.24
2	B	255	LEU	C-N	-6.48	1.23	1.33
1	A	202	PHE	C-N	-6.47	1.25	1.33
1	A	268	PRO	C-N	-6.46	1.24	1.33
2	B	436	GLN	N-CA	-6.43	1.37	1.46
1	A	181	VAL	C-O	6.42	1.32	1.24
2	B	40	SER	C-N	-6.42	1.24	1.33
2	B	220	THR	C-N	6.42	1.39	1.33
2	B	219	LEU	CA-C	-6.41	1.44	1.52
1	A	434	GLU	C-O	6.40	1.32	1.24
1	A	169	PHE	C-N	-6.39	1.24	1.33
1	A	110	ILE	C-N	-6.37	1.25	1.33
2	B	21	TRP	NE1-CE2	-6.36	1.30	1.37
2	B	244	PHE	C-N	-6.36	1.19	1.33
1	A	198	SER	C-N	-6.34	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	LYS	CA-C	-6.32	1.47	1.53
2	B	358	ILE	C-N	-6.31	1.25	1.33
2	B	185	TYR	N-CA	6.30	1.53	1.46
2	B	110	GLU	C-N	-6.30	1.25	1.33
1	A	85	GLN	C-N	-6.29	1.24	1.33
1	A	283	HIS	CE1-NE2	-6.28	1.26	1.32
1	A	42	ILE	C-N	-6.27	1.26	1.33
1	A	229	ARG	CD-NE	-6.27	1.37	1.46
2	B	86	ILE	C-O	6.26	1.31	1.24
2	B	223	THR	CA-C	-6.26	1.44	1.52
2	B	51	VAL	CA-C	-6.24	1.45	1.52
2	B	278	ARG	NE-CZ	-6.23	1.26	1.33
2	B	51	VAL	N-CA	-6.23	1.38	1.46
1	A	324	VAL	CA-CB	-6.22	1.46	1.54
1	A	300	ASN	CA-C	-6.22	1.43	1.52
1	A	2	ARG	C-N	-6.21	1.25	1.33
2	B	224	TYR	N-CA	-6.20	1.38	1.46
1	A	74	VAL	C-N	-6.19	1.26	1.33
1	A	290	GLU	C-N	6.17	1.41	1.33
2	B	29	GLY	C-N	-6.17	1.25	1.33
2	B	347	ILE	C-N	-6.17	1.19	1.33
1	A	84	ARG	C-N	-6.15	1.25	1.33
1	A	21	TRP	NE1-CE2	-6.13	1.30	1.37
2	B	384	ILE	CA-CB	-6.12	1.46	1.54
2	B	230	LEU	N-CA	6.10	1.54	1.46
1	A	406	HIS	CE1-NE2	-6.08	1.26	1.32
1	A	348	PRO	CA-CB	-6.07	1.45	1.53
1	A	94	THR	CA-C	-6.06	1.45	1.53
1	A	5	ILE	CA-CB	-6.02	1.47	1.54
2	B	229	HIS	CB-CG	6.02	1.58	1.50
1	A	97	GLU	C-N	-6.01	1.25	1.33
1	A	103	TYR	CA-C	-5.98	1.44	1.52
1	A	175	PRO	CA-CB	-5.98	1.45	1.53
1	A	35	GLN	C-N	-5.96	1.26	1.33
2	B	351	VAL	CA-CB	-5.96	1.46	1.54
2	B	217	LEU	C-N	-5.96	1.25	1.33
1	A	346	TRP	CA-CB	-5.95	1.45	1.53
1	A	65	ALA	C-O	-5.95	1.16	1.24
1	A	221	ARG	CA-C	-5.94	1.45	1.52
1	A	389	ALA	C-N	-5.94	1.26	1.33
2	B	59	ASN	C-N	-5.92	1.25	1.33
1	A	156	ARG	C-N	-5.92	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	GLY	CA-C	-5.91	1.46	1.51
2	B	303	ALA	C-N	5.90	1.42	1.33
2	B	407	TRP	CA-C	-5.89	1.45	1.52
1	A	180	ALA	C-N	-5.87	1.26	1.34
2	B	173	PRO	CA-C	-5.84	1.44	1.52
1	A	411	GLU	C-O	5.81	1.31	1.24
1	A	405	VAL	CB-CG1	-5.79	1.33	1.52
1	A	39	ASP	N-CA	-5.77	1.38	1.46
2	B	422	GLU	C-N	-5.76	1.25	1.33
1	A	386	GLU	C-N	5.76	1.42	1.34
2	B	245	PRO	CA-CB	-5.72	1.45	1.53
2	B	122	VAL	C-N	-5.67	1.26	1.33
2	B	17	GLY	C-N	-5.67	1.26	1.33
2	B	23	VAL	C-O	-5.66	1.17	1.24
2	B	76	ASP	N-CA	-5.65	1.39	1.46
1	A	250	VAL	C-N	-5.65	1.25	1.33
2	B	215	ARG	C-N	-5.64	1.26	1.33
1	A	31	GLN	CA-C	5.63	1.59	1.52
2	B	385	GLN	C-O	-5.62	1.16	1.24
2	B	270	PRO	CA-C	-5.61	1.44	1.52
1	A	335	ILE	C-N	-5.60	1.25	1.33
1	A	346	TRP	NE1-CE2	-5.60	1.31	1.37
1	A	347	CYS	C-O	-5.60	1.18	1.24
2	B	42	LEU	C-N	-5.60	1.25	1.33
1	A	359	PRO	C-O	-5.56	1.18	1.24
1	A	211	ASP	C-N	-5.54	1.27	1.34
1	A	288	VAL	N-CA	-5.54	1.40	1.46
1	A	72	PRO	N-CD	-5.53	1.40	1.47
2	B	100	GLY	CA-C	-5.52	1.46	1.51
1	A	434	GLU	C-N	-5.52	1.27	1.34
1	A	97	GLU	CA-C	-5.50	1.45	1.52
1	A	331	ALA	C-N	-5.50	1.28	1.34
2	B	148	GLY	C-N	5.49	1.42	1.33
2	B	246	GLY	N-CA	5.49	1.53	1.45
2	B	139	HIS	CE1-NE2	-5.48	1.27	1.32
1	A	169	PHE	N-CA	-5.48	1.39	1.45
2	B	262	PHE	C-N	-5.47	1.27	1.34
1	A	152	LEU	C-N	-5.47	1.25	1.33
2	B	289	PRO	CA-CB	-5.47	1.46	1.53
2	B	84	GLY	C-N	-5.47	1.26	1.33
1	A	313	MET	N-CA	-5.46	1.39	1.46
2	B	217	LEU	CA-C	-5.46	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	TYR	C-N	-5.43	1.29	1.33
1	A	301	GLN	N-CA	-5.43	1.39	1.46
2	B	257	VAL	C-N	-5.43	1.26	1.33
1	A	13	GLY	C-N	-5.42	1.27	1.34
1	A	103	TYR	N-CA	-5.42	1.39	1.46
2	B	35	SER	CA-C	-5.41	1.47	1.52
1	A	261	PRO	CA-CB	-5.41	1.46	1.53
2	B	135	PHE	C-N	-5.41	1.26	1.33
2	B	19	LYS	C-N	-5.41	1.27	1.33
2	B	313	LEU	C-N	-5.41	1.26	1.33
1	A	407	TRP	NE1-CE2	-5.39	1.31	1.37
1	A	400	ALA	C-N	-5.39	1.26	1.33
2	B	72	PRO	C-O	5.39	1.30	1.24
2	B	332	MET	C-N	-5.38	1.26	1.33
1	A	283	HIS	C-O	5.37	1.30	1.24
1	A	360	PRO	N-CD	-5.37	1.40	1.47
1	A	422	ARG	C-N	-5.37	1.26	1.33
1	A	32	PRO	C-O	5.36	1.30	1.24
2	B	262	PHE	N-CA	-5.36	1.38	1.46
1	A	312	TYR	C-N	-5.36	1.26	1.33
2	B	189	LEU	C-N	-5.35	1.27	1.33
1	A	339	ARG	C-N	-5.35	1.24	1.33
2	B	346	TRP	NE1-CE2	-5.34	1.31	1.37
2	B	374	SER	C-N	-5.33	1.26	1.33
2	B	346	TRP	CA-CB	-5.33	1.44	1.53
1	A	282	TYR	N-CA	-5.33	1.39	1.46
2	B	345	GLU	C-N	-5.32	1.25	1.33
2	B	18	ALA	N-CA	-5.32	1.40	1.46
1	A	70	LEU	C-N	-5.31	1.27	1.33
1	A	177	VAL	C-N	-5.31	1.26	1.33
2	B	354	ALA	C-N	-5.30	1.26	1.33
1	A	253	THR	C-N	-5.30	1.25	1.33
1	A	286	LEU	C-N	-5.30	1.26	1.33
1	A	201	ALA	C-N	-5.29	1.26	1.33
1	A	46	ASP	N-CA	-5.28	1.39	1.46
2	B	261	PRO	CA-CB	-5.28	1.46	1.53
2	B	92	PHE	C-O	-5.28	1.17	1.24
1	A	4	CYS	C-N	-5.28	1.26	1.33
1	A	248	LEU	C-N	-5.27	1.26	1.33
2	B	138	THR	C-N	-5.26	1.26	1.33
2	B	178	SER	C-O	5.25	1.30	1.23
2	B	32	PRO	C-N	-5.25	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	ILE	C-O	-5.24	1.17	1.24
2	B	139	HIS	N-CA	-5.21	1.40	1.46
2	B	266	HIS	CE1-NE2	-5.21	1.27	1.32
2	B	212	ILE	CA-CB	-5.19	1.48	1.54
1	A	122	ILE	C-N	-5.19	1.27	1.33
2	B	39	ASP	CA-C	-5.19	1.45	1.52
2	B	216	THR	C-N	-5.18	1.25	1.33
1	A	86	LEU	N-CA	-5.17	1.39	1.46
2	B	32	PRO	N-CA	-5.17	1.40	1.47
2	B	26	ASP	C-N	5.16	1.41	1.33
2	B	59	ASN	CA-C	5.16	1.59	1.52
2	B	63	PRO	CA-C	-5.16	1.45	1.52
2	B	253	ARG	CD-NE	-5.15	1.39	1.46
2	B	74	THR	C-N	-5.15	1.26	1.33
2	B	21	TRP	N-CA	-5.14	1.39	1.46
1	A	8	HIS	CD2-NE2	-5.14	1.32	1.37
2	B	57	ALA	C-N	-5.14	1.25	1.33
2	B	16	ILE	C-O	-5.13	1.17	1.24
1	A	199	ASP	C-N	-5.12	1.26	1.33
1	A	192	HIS	CE1-NE2	-5.12	1.27	1.32
1	A	33	ASP	CA-CB	-5.12	1.44	1.53
2	B	101	ASN	N-CA	-5.12	1.39	1.46
2	B	307	PRO	C-N	-5.12	1.27	1.33
2	B	211	ASP	C-O	-5.11	1.18	1.24
1	A	64	ARG	C-O	-5.11	1.17	1.24
1	A	274	PRO	CA-C	-5.11	1.47	1.52
1	A	268	PRO	CA-C	-5.10	1.45	1.52
1	A	105	ARG	C-N	-5.10	1.25	1.33
1	A	3	GLU	C-N	-5.10	1.26	1.33
2	B	184	PRO	N-CA	-5.09	1.40	1.47
1	A	363	VAL	C-N	5.09	1.45	1.33
2	B	373	MET	C-N	5.08	1.40	1.33
1	A	281	ALA	CA-C	-5.08	1.46	1.52
1	A	361	THR	C-N	-5.08	1.30	1.33
2	B	183	GLU	C-N	-5.08	1.27	1.34
1	A	168	GLU	CA-C	-5.07	1.46	1.52
1	A	266	HIS	CE1-NE2	-5.07	1.27	1.32
2	B	343	PHE	CA-CB	-5.07	1.44	1.53
2	B	272	PHE	CA-C	-5.07	1.46	1.52
1	A	67	PHE	C-N	5.06	1.39	1.33
2	B	139	HIS	CG-CD2	-5.06	1.30	1.35
2	B	407	TRP	NE1-CE2	-5.05	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	GLU	CA-C	5.05	1.58	1.52
1	A	392	ASP	C-O	-5.05	1.18	1.24
2	B	14	ASN	CA-C	-5.05	1.46	1.52
2	B	258	ASN	N-CA	-5.04	1.40	1.46
2	B	403	ALA	C-N	5.04	1.39	1.33
2	B	192	HIS	CE1-NE2	-5.04	1.27	1.32
2	B	170	SER	C-N	-5.02	1.26	1.33
1	A	343	PHE	N-CA	-5.02	1.39	1.46
2	B	309	HIS	CD2-NE2	-5.02	1.32	1.37
1	A	312	TYR	CA-C	-5.01	1.46	1.52
1	A	199	ASP	CA-C	-5.00	1.46	1.52

All (682) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	O-C-N	-65.11	35.99	122.59
2	B	105	LYS	O-C-N	-56.44	47.53	122.59
2	B	73	GLY	O-C-N	-47.19	76.42	122.19
1	A	283	HIS	O-C-N	-41.56	67.31	122.59
2	B	275	LEU	O-C-N	-39.60	79.33	122.09
1	A	369	ALA	O-C-N	-39.53	70.02	122.59
1	A	415	GLU	CA-C-N	30.98	145.47	121.61
1	A	415	GLU	C-N-CA	30.98	145.47	121.61
1	A	24	TYR	O-C-N	-30.03	89.59	122.03
2	B	321	GLY	O-C-N	-30.00	83.71	122.70
2	B	194	LEU	O-C-N	-29.19	87.67	122.11
2	B	143	GLY	O-C-N	-28.20	79.60	122.18
1	A	363	VAL	C-N-CD	-27.19	13.50	125.00
2	B	344	VAL	O-C-N	-26.94	88.90	122.57
2	B	179	ASP	O-C-N	-26.92	86.78	122.59
1	A	221	ARG	CA-C-N	26.49	149.53	120.66
1	A	221	ARG	C-N-CA	26.49	149.53	120.66
2	B	273	ALA	C-N-CD	-26.02	18.32	125.00
1	A	1	MET	O-C-N	26.00	164.61	123.00
1	A	53	PHE	O-C-N	-25.88	88.17	122.59
2	B	321	GLY	CA-C-N	25.84	170.90	121.54
2	B	321	GLY	C-N-CA	25.84	170.90	121.54
1	A	218	ASP	O-C-N	-25.67	93.49	123.27
2	B	86	ILE	O-C-N	25.62	154.60	122.57
2	B	60	LYS	CA-C-N	24.91	169.13	121.54
2	B	60	LYS	C-N-CA	24.91	169.13	121.54
2	B	179	ASP	CA-C-N	24.81	161.19	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	ASP	C-N-CA	24.81	161.19	122.24
2	B	88	ARG	C-N-CD	-24.72	23.64	125.00
1	A	402	ARG	O-C-N	-24.30	78.22	122.44
2	B	247	GLN	O-C-N	-24.20	95.09	123.16
2	B	402	LYS	CA-C-N	23.95	167.29	121.54
2	B	402	LYS	C-N-CA	23.95	167.29	121.54
2	B	85	GLN	O-C-N	23.94	157.15	122.20
2	B	203	CYS	CA-C-N	23.58	164.42	121.97
2	B	203	CYS	C-N-CA	23.58	164.42	121.97
2	B	194	LEU	CA-C-N	23.48	163.97	121.70
2	B	194	LEU	C-N-CA	23.48	163.97	121.70
2	B	348	PRO	O-C-N	23.23	154.00	122.64
2	B	278	ARG	N-CA-CB	23.08	148.96	109.72
2	B	52	TYR	O-C-N	22.75	152.46	123.10
2	B	105	LYS	CA-C-N	21.59	147.13	120.14
2	B	105	LYS	C-N-CA	21.59	147.13	120.14
2	B	1	MET	O-C-N	20.81	156.29	123.00
1	A	34	GLY	O-C-N	-20.80	95.66	122.70
1	A	405	VAL	CA-C-N	20.74	157.61	121.52
1	A	405	VAL	C-N-CA	20.74	157.61	121.52
1	A	36	MET	CA-C-N	20.68	142.59	120.47
1	A	36	MET	C-N-CA	20.68	142.59	120.47
1	A	183	GLU	O-C-N	-20.50	97.75	121.32
2	B	127	GLU	O-C-N	-20.37	95.91	122.39
2	B	21	TRP	O-C-N	-20.25	96.00	122.33
2	B	60	LYS	O-C-N	-20.13	95.81	122.59
2	B	359	PRO	O-C-N	19.90	144.94	121.46
2	B	92	PHE	CA-CB-CG	-19.79	94.01	113.80
2	B	73	GLY	CA-C-N	19.55	153.91	120.68
2	B	73	GLY	C-N-CA	19.55	153.91	120.68
2	B	411	GLU	CA-C-N	19.28	159.19	121.41
2	B	411	GLU	C-N-CA	19.28	159.19	121.41
1	A	347	CYS	O-C-N	-19.21	97.47	121.10
2	B	53	TYR	O-C-N	18.99	147.85	122.59
1	A	87	PHE	O-C-N	-18.98	97.55	122.42
1	A	358	GLU	CA-C-N	18.65	139.59	120.38
1	A	358	GLU	C-N-CA	18.65	139.59	120.38
1	A	415	GLU	O-C-N	-18.56	103.93	121.56
2	B	344	VAL	CA-C-N	18.53	156.94	121.54
2	B	344	VAL	C-N-CA	18.53	156.94	121.54
2	B	30	ILE	CB-CA-C	18.43	141.52	111.29
1	A	67	PHE	CA-CB-CG	-18.23	95.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ASP	O-C-N	-18.07	93.33	122.42
1	A	283	HIS	CA-C-N	17.70	155.34	121.54
1	A	283	HIS	C-N-CA	17.70	155.34	121.54
1	A	1	MET	CB-CA-C	17.66	143.66	110.10
1	A	38	SER	O-C-N	-17.54	102.16	122.68
1	A	38	SER	CA-C-N	17.40	154.78	121.54
1	A	38	SER	C-N-CA	17.40	154.78	121.54
1	A	221	ARG	O-C-N	-17.11	101.64	121.32
1	A	50	ASN	O-C-N	-16.86	100.17	122.59
2	B	343	PHE	O-C-N	16.76	146.30	123.34
1	A	409	VAL	O-C-N	16.70	138.64	121.94
1	A	266	HIS	O-C-N	16.68	143.75	123.24
2	B	370	GLY	O-C-N	-16.62	101.71	122.32
1	A	297	GLU	CA-C-N	-16.55	99.15	119.84
1	A	297	GLU	C-N-CA	-16.55	99.15	119.84
2	B	247	GLN	CA-C-N	16.51	153.08	121.54
2	B	247	GLN	C-N-CA	16.51	153.08	121.54
1	A	347	CYS	CA-C-N	16.42	140.36	119.84
1	A	347	CYS	C-N-CA	16.42	140.36	119.84
1	A	405	VAL	CA-CB-CG1	16.35	138.20	110.40
2	B	49	ILE	O-C-N	-16.08	107.43	123.03
2	B	1	MET	CB-CA-C	16.06	140.62	110.10
1	A	218	ASP	CA-C-N	15.96	150.69	121.97
1	A	218	ASP	C-N-CA	15.96	150.69	121.97
2	B	347	ILE	CA-C-N	15.95	139.78	119.84
2	B	347	ILE	C-N-CA	15.95	139.78	119.84
2	B	171	VAL	O-C-N	-15.84	106.05	123.00
2	B	331	GLN	O-C-N	-15.73	99.16	122.28
2	B	411	GLU	O-C-N	-15.69	101.31	122.33
1	A	184	PRO	O-C-N	15.68	141.92	123.10
2	B	224	TYR	O-C-N	-15.64	104.32	122.15
2	B	400	ARG	O-C-N	-15.59	101.44	122.33
2	B	91	ASN	CA-CB-CG	15.41	128.01	112.60
2	B	402	LYS	O-C-N	-15.35	101.49	122.06
2	B	203	CYS	O-C-N	-15.14	103.51	123.19
1	A	69	ASP	O-C-N	-15.13	105.71	123.27
1	A	392	ASP	CA-C-O	-15.13	104.39	120.42
1	A	358	GLU	C-N-CD	-15.04	63.33	125.00
1	A	1	MET	CA-C-N	14.74	149.53	122.27
1	A	1	MET	C-N-CA	14.74	149.53	122.27
2	B	400	ARG	CA-C-N	14.61	149.45	121.54
2	B	400	ARG	C-N-CA	14.61	149.45	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	HIS	CA-CB-CG	14.57	128.37	113.80
2	B	30	ILE	O-C-N	-14.45	104.51	122.57
2	B	47	GLU	CA-C-N	14.43	149.09	121.54
2	B	47	GLU	C-N-CA	14.43	149.09	121.54
2	B	107	HIS	O-C-N	-14.41	106.47	122.03
1	A	107	HIS	O-C-N	-14.38	106.50	122.03
2	B	24	ILE	O-C-N	-14.31	109.25	121.98
2	B	1	MET	N-CA-C	-14.27	71.05	111.00
2	B	89	PRO	O-C-N	-14.22	103.44	122.64
2	B	406	HIS	CA-CB-CG	-13.96	99.84	113.80
1	A	41	THR	O-C-N	13.90	141.65	122.46
1	A	416	GLY	O-C-N	-13.89	111.14	123.37
1	A	355	ILE	CA-C-O	-13.86	105.79	120.48
1	A	219	ILE	CA-CB-CG2	-13.84	86.97	110.50
1	A	280	LYS	O-C-N	-13.82	104.20	122.59
2	B	253	ARG	CD-NE-CZ	13.80	143.72	124.40
1	A	183	GLU	CA-C-N	-13.77	105.99	119.76
1	A	183	GLU	C-N-CA	-13.77	105.99	119.76
1	A	42	ILE	CA-C-N	13.65	134.82	119.94
1	A	42	ILE	C-N-CA	13.65	134.82	119.94
1	A	297	GLU	O-C-N	13.53	136.88	121.32
1	A	280	LYS	CA-C-N	13.46	147.26	121.54
1	A	280	LYS	C-N-CA	13.46	147.26	121.54
1	A	179	THR	O-C-N	-13.43	104.73	122.59
1	A	412	GLY	O-C-N	-13.42	109.11	124.15
2	B	177	VAL	CA-C-O	13.35	137.47	120.78
1	A	396	ASP	O-C-N	-13.29	105.06	122.33
1	A	49	PHE	CA-C-N	13.18	146.72	121.54
1	A	49	PHE	C-N-CA	13.18	146.72	121.54
2	B	85	GLN	CA-C-N	13.07	145.49	121.97
2	B	85	GLN	C-N-CA	13.07	145.49	121.97
2	B	200	GLU	CA-C-N	12.98	142.38	121.86
2	B	200	GLU	C-N-CA	12.98	142.38	121.86
1	A	405	VAL	O-C-N	-12.96	106.70	122.77
2	B	182	VAL	CA-C-N	12.96	153.42	121.80
2	B	182	VAL	C-N-CA	12.96	153.42	121.80
1	A	21	TRP	CA-CB-CG	-12.90	89.09	113.60
2	B	113	GLU	CA-C-O	12.63	133.94	120.55
2	B	182	VAL	O-C-N	-12.54	106.89	122.57
1	A	1	MET	N-CA-C	-12.53	75.91	111.00
2	B	52	TYR	CA-C-N	12.51	145.43	121.54
2	B	52	TYR	C-N-CA	12.51	145.43	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	271	ILE	N-CA-C	12.41	122.33	110.42
2	B	275	LEU	CA-C-N	12.34	145.11	121.54
2	B	275	LEU	C-N-CA	12.34	145.11	121.54
1	A	416	GLY	CA-C-N	12.31	145.06	121.54
1	A	416	GLY	C-N-CA	12.31	145.06	121.54
2	B	414	ASP	CA-C-N	12.31	145.05	121.54
2	B	414	ASP	C-N-CA	12.31	145.05	121.54
2	B	289	PRO	O-C-N	12.28	138.69	122.24
1	A	113	GLU	CA-C-O	12.23	133.91	120.10
2	B	192	HIS	O-C-N	-12.18	105.66	122.46
1	A	30	ILE	CA-C-N	12.16	151.46	121.80
1	A	30	ILE	C-N-CA	12.16	151.46	121.80
2	B	154	ILE	CA-C-N	12.11	136.91	120.44
2	B	154	ILE	C-N-CA	12.11	136.91	120.44
2	B	127	GLU	CA-C-N	12.11	145.16	121.18
2	B	127	GLU	C-N-CA	12.11	145.16	121.18
2	B	414	ASP	O-C-N	-12.04	108.97	123.30
2	B	29	GLY	O-C-N	11.94	138.23	122.70
1	A	15	GLN	OE1-CD-NE2	-11.93	110.67	122.60
1	A	43	GLY	O-C-N	11.91	133.62	122.19
1	A	369	ALA	CA-C-N	11.89	141.95	123.04
1	A	369	ALA	C-N-CA	11.89	141.95	123.04
2	B	193	GLN	CA-C-N	11.84	138.65	120.89
2	B	193	GLN	C-N-CA	11.84	138.65	120.89
1	A	367	ASP	CA-C-N	11.84	144.15	121.54
1	A	367	ASP	C-N-CA	11.84	144.15	121.54
1	A	11	GLN	OE1-CD-NE2	-11.83	110.77	122.60
2	B	49	ILE	CA-C-N	11.82	144.11	121.54
2	B	49	ILE	C-N-CA	11.82	144.11	121.54
1	A	32	PRO	CA-N-CD	11.77	128.47	112.00
2	B	436	GLN	CA-C-N	11.73	142.82	121.70
2	B	436	GLN	C-N-CA	11.73	142.82	121.70
2	B	263	PRO	N-CA-C	11.73	129.12	113.40
2	B	11	GLN	OE1-CD-NE2	-11.73	110.87	122.60
1	A	87	PHE	CA-C-N	11.71	150.38	121.80
1	A	87	PHE	C-N-CA	11.71	150.38	121.80
2	B	29	GLY	CA-C-N	11.66	142.96	121.97
2	B	29	GLY	C-N-CA	11.66	142.96	121.97
1	A	2	ARG	CB-CA-C	-11.58	96.56	111.50
2	B	281	GLN	OE1-CD-NE2	-11.57	111.03	122.60
1	A	61	HIS	CA-CB-CG	11.53	125.33	113.80
2	B	219	LEU	O-C-N	-11.52	107.26	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	THR	O-C-N	-11.46	107.35	122.59
2	B	4	ILE	N-CA-C	11.37	123.35	108.35
2	B	200	GLU	O-C-N	-11.36	108.38	123.15
1	A	111	GLY	CA-C-O	-11.34	109.07	120.75
2	B	111	GLY	CA-C-O	-11.31	109.10	120.75
1	A	21	TRP	O-C-N	-11.28	108.39	122.27
1	A	24	TYR	CA-C-N	11.18	142.89	121.54
1	A	24	TYR	C-N-CA	11.18	142.89	121.54
2	B	412	GLY	CA-C-N	11.16	138.91	122.39
2	B	412	GLY	C-N-CA	11.16	138.91	122.39
1	A	186	ASN	CA-C-N	11.15	134.93	120.44
1	A	186	ASN	C-N-CA	11.15	134.93	120.44
2	B	167	ASN	CA-C-N	-11.14	107.28	122.99
2	B	167	ASN	C-N-CA	-11.14	107.28	122.99
2	B	178	SER	CA-C-O	-11.12	108.53	120.99
2	B	21	TRP	CA-C-N	-11.03	102.42	122.38
2	B	21	TRP	C-N-CA	-11.03	102.42	122.38
2	B	359	PRO	CA-C-N	-11.00	106.09	119.84
2	B	359	PRO	C-N-CA	-11.00	106.09	119.84
2	B	433	GLN	OE1-CD-NE2	-10.98	111.62	122.60
2	B	278	ARG	CB-CA-C	-10.91	92.73	110.84
2	B	370	GLY	CA-C-N	10.86	141.51	121.52
2	B	370	GLY	C-N-CA	10.86	141.51	121.52
2	B	293	GLN	OE1-CD-NE2	-10.75	111.85	122.60
2	B	193	GLN	O-C-N	-10.73	107.75	122.46
2	B	356	CYS	O-C-N	-10.62	107.47	122.76
2	B	15	GLN	OE1-CD-NE2	-10.52	112.08	122.60
2	B	290	GLU	O-C-N	10.52	134.14	122.15
2	B	89	PRO	CA-C-N	10.50	141.59	121.54
2	B	89	PRO	C-N-CA	10.50	141.59	121.54
2	B	385	GLN	OE1-CD-NE2	-10.48	112.12	122.60
1	A	15	GLN	O-C-N	10.48	134.85	122.17
1	A	17	GLY	O-C-N	10.46	133.68	122.28
1	A	113	GLU	O-C-N	-10.44	110.00	122.22
1	A	267	PHE	C-N-CD	-10.44	82.22	125.00
2	B	387	LEU	CA-C-N	-10.41	104.00	122.42
2	B	387	LEU	C-N-CA	-10.41	104.00	122.42
2	B	59	ASN	CA-C-N	10.39	141.38	121.54
2	B	59	ASN	C-N-CA	10.39	141.38	121.54
2	B	299	LYS	O-C-N	10.36	135.29	122.34
1	A	412	GLY	CA-C-N	10.33	137.16	120.94
1	A	412	GLY	C-N-CA	10.33	137.16	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	PRO	O-C-N	-10.30	112.94	122.93
2	B	394	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	A	172	TYR	CA-CB-CG	10.23	132.32	113.90
1	A	65	ALA	N-CA-C	10.17	132.46	110.80
2	B	85	GLN	OE1-CD-NE2	-10.15	112.45	122.60
1	A	92	LEU	CA-C-N	10.11	135.73	123.19
1	A	92	LEU	C-N-CA	10.11	135.73	123.19
2	B	161	TYR	CA-C-N	10.09	129.73	119.24
2	B	161	TYR	C-N-CA	10.09	129.73	119.24
1	A	18	ASN	O-C-N	10.07	134.66	122.27
2	B	47	GLU	O-C-N	-10.04	109.24	122.59
2	B	229	HIS	O-C-N	-10.02	109.27	122.59
2	B	309	HIS	O-C-N	-9.99	109.30	122.59
1	A	340	THR	O-C-N	9.98	134.93	123.05
2	B	331	GLN	CA-C-N	9.97	136.68	120.63
2	B	331	GLN	C-N-CA	9.97	136.68	120.63
2	B	282	GLN	OE1-CD-NE2	-9.94	112.66	122.60
2	B	94	PHE	CA-CB-CG	-9.90	103.90	113.80
1	A	32	PRO	N-CA-CB	-9.84	92.91	103.25
1	A	61	HIS	CB-CA-C	9.84	129.56	110.67
1	A	31	GLN	N-CA-C	9.72	131.30	109.81
1	A	298	PRO	CA-C-N	9.72	133.66	120.44
1	A	298	PRO	C-N-CA	9.72	133.66	120.44
1	A	190	THR	O-C-N	-9.69	109.35	122.33
2	B	8	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	A	34	GLY	CA-C-N	9.64	139.96	121.54
1	A	34	GLY	C-N-CA	9.64	139.96	121.54
1	A	78	VAL	O-C-N	-9.64	112.16	121.90
1	A	222	PRO	N-CA-CB	9.54	113.63	102.85
1	A	339	ARG	O-C-N	9.46	134.52	122.23
1	A	396	ASP	N-CA-C	-9.44	100.06	112.34
2	B	157	ILE	CA-C-O	-9.43	110.28	120.47
2	B	412	GLY	O-C-N	-9.42	110.45	122.70
2	B	185	TYR	CA-CB-CG	9.41	130.84	113.90
2	B	299	LYS	CA-C-N	-9.37	107.94	122.37
2	B	299	LYS	C-N-CA	-9.37	107.94	122.37
2	B	151	THR	O-C-N	-9.34	110.79	122.27
1	A	35	GLN	OE1-CD-NE2	-9.33	113.27	122.60
1	A	42	ILE	CA-C-O	-9.33	109.11	120.78
1	A	91	GLN	OE1-CD-NE2	-9.27	113.33	122.60
2	B	71	GLU	O-C-N	-9.24	110.69	121.32
2	B	72	PRO	CA-C-N	9.24	130.16	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	PRO	C-N-CA	9.24	130.16	120.00
2	B	24	ILE	CA-C-N	-9.15	104.06	121.54
2	B	24	ILE	C-N-CA	-9.15	104.06	121.54
2	B	276	THR	CA-C-N	9.13	138.97	121.54
2	B	276	THR	C-N-CA	9.13	138.97	121.54
1	A	90	GLU	O-C-N	-9.12	107.35	122.03
1	A	372	GLN	OE1-CD-NE2	-9.12	113.48	122.60
1	A	172	TYR	CB-CA-C	9.11	122.55	108.61
1	A	36	MET	O-C-N	-9.10	114.73	121.83
1	A	405	VAL	N-CA-CB	-9.08	100.14	111.31
2	B	273	ALA	CA-C-N	9.04	131.14	119.84
2	B	273	ALA	C-N-CA	9.04	131.14	119.84
1	A	298	PRO	O-C-N	-9.03	110.45	122.64
1	A	417	GLU	O-C-N	8.99	134.55	122.59
1	A	368	LEU	CA-C-N	8.97	138.67	121.54
1	A	368	LEU	C-N-CA	8.97	138.67	121.54
1	A	62	VAL	O-C-N	8.94	131.29	121.10
2	B	2	ARG	O-C-N	8.93	134.46	122.59
2	B	270	PRO	CA-C-N	8.87	129.21	121.58
2	B	270	PRO	C-N-CA	8.87	129.21	121.58
2	B	340	SER	CA-C-N	-8.87	104.60	121.54
2	B	340	SER	C-N-CA	-8.87	104.60	121.54
2	B	417	GLU	CA-C-N	8.86	135.82	122.17
2	B	417	GLU	C-N-CA	8.86	135.82	122.17
2	B	53	TYR	N-CA-CB	8.85	125.45	110.49
2	B	1	MET	CA-C-N	8.81	138.37	121.54
2	B	1	MET	C-N-CA	8.81	138.37	121.54
1	A	56	THR	CA-C-N	-8.74	104.27	121.41
1	A	56	THR	C-N-CA	-8.74	104.27	121.41
2	B	133	GLN	OE1-CD-NE2	-8.70	113.90	122.60
2	B	348	PRO	CA-C-N	8.70	138.15	121.54
2	B	348	PRO	C-N-CA	8.70	138.15	121.54
1	A	203	MET	O-C-N	8.69	133.68	123.17
1	A	391	LEU	CA-C-N	8.58	132.48	120.29
1	A	391	LEU	C-N-CA	8.58	132.48	120.29
1	A	371	VAL	O-C-N	8.58	132.78	122.83
2	B	433	GLN	O-C-N	8.56	132.24	122.22
1	A	38	SER	CA-C-O	-8.54	111.90	121.89
2	B	434	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	A	275	VAL	O-C-N	8.40	133.07	122.57
2	B	272	PHE	CA-C-O	-8.34	111.40	120.24
1	A	72	PRO	O-C-N	8.33	133.52	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	234	THR	CA-C-O	-8.33	110.39	119.97
1	A	195	LEU	CA-C-O	-8.30	109.17	119.38
1	A	31	GLN	O-C-N	8.29	130.86	121.32
1	A	182	VAL	CA-C-O	-8.26	109.61	119.85
2	B	183	GLU	CA-C-N	8.24	128.20	119.05
2	B	183	GLU	C-N-CA	8.24	128.20	119.05
1	A	18	ASN	CA-C-O	-8.24	110.50	119.97
1	A	347	CYS	C-N-CD	-8.24	91.23	125.00
2	B	143	GLY	CA-C-N	8.24	137.55	121.41
2	B	143	GLY	C-N-CA	8.24	137.55	121.41
2	B	32	PRO	O-C-N	8.17	133.67	122.64
1	A	56	THR	O-C-N	8.10	131.70	122.22
1	A	295	CYS	N-CA-C	8.04	120.83	111.02
1	A	31	GLN	CA-C-N	8.00	129.84	119.84
1	A	31	GLN	C-N-CA	8.00	129.84	119.84
2	B	59	ASN	O-C-N	-7.99	112.77	123.15
1	A	197	HIS	O-C-N	7.98	133.21	122.59
2	B	289	PRO	CA-C-N	-7.98	108.95	120.29
2	B	289	PRO	C-N-CA	-7.98	108.95	120.29
2	B	436	GLN	O-C-N	-7.97	111.98	122.59
2	B	247	GLN	OE1-CD-NE2	-7.95	114.65	122.60
2	B	50	ASN	CA-C-O	7.94	131.86	120.51
2	B	113	GLU	O-C-N	-7.93	113.71	122.12
2	B	281	GLN	O-C-N	-7.91	112.07	122.59
1	A	290	GLU	O-C-N	7.89	133.35	122.46
2	B	343	PHE	CA-CB-CG	-7.89	105.91	113.80
2	B	266	HIS	CA-CB-CG	-7.86	105.94	113.80
1	A	33	ASP	CA-C-N	-7.80	106.12	121.41
1	A	33	ASP	C-N-CA	-7.80	106.12	121.41
1	A	82	THR	CA-C-N	7.79	136.43	121.54
1	A	82	THR	C-N-CA	7.79	136.43	121.54
2	B	219	LEU	CA-C-N	-7.78	107.45	120.68
2	B	219	LEU	C-N-CA	-7.78	107.45	120.68
2	B	299	LYS	CA-C-O	-7.78	110.25	119.35
2	B	177	VAL	O-C-N	-7.74	112.90	122.57
1	A	90	GLU	CA-C-N	7.71	135.59	122.26
1	A	90	GLU	C-N-CA	7.71	135.59	122.26
2	B	154	ILE	O-C-N	-7.70	113.90	121.83
2	B	245	PRO	CA-N-CD	7.69	122.77	112.00
2	B	11	GLN	CG-CD-NE2	7.66	127.89	116.40
2	B	171	VAL	CA-C-N	7.66	136.30	122.13
2	B	171	VAL	C-N-CA	7.66	136.30	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	346	TRP	O-C-N	7.66	131.51	122.94
2	B	283	TYR	CA-C-N	7.65	136.16	121.54
2	B	283	TYR	C-N-CA	7.65	136.16	121.54
2	B	36	TYR	O-C-N	-7.64	112.42	122.59
1	A	11	GLN	CG-CD-NE2	7.64	127.86	116.40
1	A	50	ASN	CA-C-N	7.60	136.05	121.54
1	A	50	ASN	C-N-CA	7.60	136.05	121.54
2	B	85	GLN	CG-CD-NE2	7.55	127.72	116.40
2	B	281	GLN	CG-CD-NE2	7.54	127.70	116.40
1	A	402	ARG	CA-C-N	7.52	133.86	122.65
1	A	402	ARG	C-N-CA	7.52	133.86	122.65
1	A	21	TRP	CA-C-N	7.52	130.97	120.29
1	A	21	TRP	C-N-CA	7.52	130.97	120.29
2	B	260	VAL	O-C-N	7.51	128.45	121.61
2	B	407	TRP	CA-CB-CG	-7.50	99.35	113.60
1	A	184	PRO	N-CA-C	7.48	122.93	111.19
1	A	17	GLY	CA-C-N	-7.46	108.97	120.31
1	A	17	GLY	C-N-CA	-7.46	108.97	120.31
2	B	324	SER	O-C-N	7.46	132.20	122.95
2	B	259	MET	CA-C-N	-7.42	116.21	123.04
2	B	259	MET	C-N-CA	-7.42	116.21	123.04
1	A	71	GLU	N-CA-C	-7.36	98.62	108.11
2	B	5	VAL	N-CA-C	7.34	118.23	107.37
3	K	247	VAL	N-CA-C	7.33	118.44	108.17
1	A	15	GLN	CG-CD-NE2	7.33	127.39	116.40
2	B	385	GLN	CG-CD-NE2	7.32	127.38	116.40
1	A	62	VAL	CA-C-N	7.31	128.98	119.84
1	A	62	VAL	C-N-CA	7.31	128.98	119.84
2	B	224	TYR	N-CA-C	-7.29	103.41	111.36
3	K	234	THR	N-CA-C	-7.28	104.55	113.50
2	B	60	LYS	CA-C-O	7.25	130.88	120.51
2	B	284	ARG	NE-CZ-NH2	7.24	125.71	119.20
1	A	91	GLN	CG-CD-NE2	7.23	127.25	116.40
1	A	232	GLY	O-C-N	7.21	129.11	122.19
1	A	82	THR	O-C-N	7.18	132.14	122.59
2	B	86	ILE	CA-C-N	7.17	135.23	121.54
2	B	86	ILE	C-N-CA	7.17	135.23	121.54
1	A	343	PHE	O-C-N	7.16	131.62	122.81
1	A	32	PRO	N-CD-CG	-7.15	92.47	103.20
1	A	83	TYR	CA-CB-CG	-7.15	101.03	113.90
2	B	263	PRO	CB-CA-C	-7.14	101.83	112.55
2	B	373	MET	O-C-N	-7.13	115.07	123.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	ASP	O-C-N	-7.13	113.12	121.32
1	A	267	PHE	O-C-N	-7.12	112.09	121.34
2	B	346	TRP	N-CA-CB	7.12	121.85	110.46
2	B	433	GLN	CG-CD-NE2	7.09	127.03	116.40
1	A	140	SER	O-C-N	7.08	133.07	122.94
1	A	65	ALA	CB-CA-C	-7.07	96.35	110.42
2	B	282	GLN	CG-CD-NE2	7.06	126.99	116.40
2	B	243	ARG	O-C-N	7.06	132.66	122.28
2	B	4	ILE	O-C-N	7.05	131.27	123.09
1	A	97	GLU	O-C-N	7.05	131.15	122.34
1	A	71	GLU	O-C-N	-6.98	116.38	121.83
2	B	271	GLY	O-C-N	6.96	129.75	123.42
2	B	347	ILE	C-N-CD	-6.95	96.49	125.00
2	B	349	ASN	N-CA-C	-6.94	96.02	110.80
2	B	293	GLN	CG-CD-NE2	6.94	126.81	116.40
1	A	438	ASP	O-C-N	-6.93	114.81	122.92
1	A	88	HIS	CA-CB-CG	-6.92	106.88	113.80
1	A	92	LEU	O-C-N	-6.92	115.13	123.16
1	A	373	ARG	CD-NE-CZ	6.91	134.08	124.40
2	B	264	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	A	379	SER	O-C-N	6.88	131.26	123.27
2	B	269	MET	C-N-CD	-6.88	96.81	125.00
2	B	349	ASN	CB-CA-C	6.87	124.09	110.42
2	B	43	GLN	O-C-N	6.85	131.70	122.59
2	B	17	GLY	O-C-N	6.85	129.74	122.28
1	A	85	GLN	CA-C-N	-6.81	110.49	122.07
1	A	85	GLN	C-N-CA	-6.81	110.49	122.07
2	B	30	ILE	N-CA-CB	-6.80	100.02	111.23
1	A	112	LYS	CA-C-O	6.77	128.15	120.90
2	B	75	MET	CA-C-N	6.77	129.35	120.28
2	B	75	MET	C-N-CA	6.77	129.35	120.28
2	B	356	CYS	CA-C-O	-6.75	112.62	121.73
1	A	360	PRO	CA-C-N	-6.72	108.42	121.06
1	A	360	PRO	C-N-CA	-6.72	108.42	121.06
1	A	438	ASP	CA-C-O	-6.72	114.24	121.36
1	A	229	ARG	NE-CZ-NH2	6.72	125.25	119.20
2	B	269	MET	CA-C-O	-6.71	111.98	120.04
1	A	77	GLU	CA-C-N	-6.71	109.61	120.62
1	A	77	GLU	C-N-CA	-6.71	109.61	120.62
2	B	112	ALA	CA-C-O	6.71	128.08	120.90
2	B	433	GLN	CA-C-N	-6.69	108.76	121.54
2	B	433	GLN	C-N-CA	-6.69	108.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	TYR	CA-C-N	6.69	134.32	121.54
2	B	53	TYR	C-N-CA	6.69	134.32	121.54
2	B	311	ARG	NE-CZ-NH2	6.69	125.22	119.20
2	B	190	SER	CA-C-N	-6.68	109.95	121.97
2	B	190	SER	C-N-CA	-6.68	109.95	121.97
2	B	314	THR	N-CA-CB	6.67	121.77	110.49
3	K	334	ALA	N-CA-C	6.64	120.70	110.20
1	A	166	LYS	N-CA-C	-6.61	99.52	110.17
3	K	113	LYS	N-CA-C	6.60	124.85	110.80
2	B	158	ARG	NE-CZ-NH2	6.59	125.13	119.20
2	B	243	ARG	CA-C-N	-6.59	111.38	121.92
2	B	243	ARG	C-N-CA	-6.59	111.38	121.92
2	B	59	ASN	N-CA-C	-6.59	99.31	109.52
3	K	174	LEU	N-CA-C	6.58	121.01	112.92
1	A	121	ARG	NE-CZ-NH2	6.56	125.10	119.20
1	A	372	GLN	CG-CD-NE2	6.56	126.23	116.40
2	B	184	PRO	CA-C-N	6.55	129.38	120.54
2	B	184	PRO	C-N-CA	6.55	129.38	120.54
1	A	208	ALA	CA-C-N	6.52	128.90	120.56
1	A	208	ALA	C-N-CA	6.52	128.90	120.56
1	A	172	TYR	CB-CG-CD1	6.51	130.56	120.80
1	A	336	LYS	O-C-N	6.50	131.23	122.59
1	A	2	ARG	NE-CZ-NH2	6.49	125.04	119.20
2	B	337	ASN	O-C-N	-6.49	114.63	122.48
1	A	36	MET	CA-C-O	-6.46	113.49	119.76
1	A	32	PRO	CB-CA-C	-6.46	100.90	111.56
2	B	8	GLN	CG-CD-NE2	6.46	126.09	116.40
1	A	266	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	404	PHE	CA-C-N	-6.43	114.33	122.43
1	A	404	PHE	C-N-CA	-6.43	114.33	122.43
2	B	296	PHE	CA-C-N	-6.42	109.27	121.54
2	B	296	PHE	C-N-CA	-6.42	109.27	121.54
2	B	380	ASN	O-C-N	-6.40	115.78	123.27
2	B	272	PHE	CA-CB-CG	6.40	120.20	113.80
2	B	322	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	A	274	PRO	CA-C-N	6.40	133.49	121.97
1	A	274	PRO	C-N-CA	6.40	133.49	121.97
2	B	287	THR	CA-C-N	-6.40	110.29	122.13
2	B	287	THR	C-N-CA	-6.40	110.29	122.13
2	B	41	ASP	O-C-N	6.39	131.09	122.59
1	A	65	ALA	O-C-N	-6.39	114.10	122.59
1	A	101	ASN	CA-CB-CG	6.37	118.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	LEU	CB-CA-C	-6.37	97.75	110.42
2	B	26	ASP	CA-C-N	6.36	133.68	121.54
2	B	26	ASP	C-N-CA	6.36	133.68	121.54
2	B	245	PRO	N-CA-CB	-6.36	96.58	103.25
1	A	320	ARG	NE-CZ-NH2	6.35	124.92	119.20
2	B	28	HIS	O-C-N	6.34	131.03	122.59
2	B	76	ASP	CA-C-O	-6.34	113.83	120.55
2	B	72	PRO	O-C-N	-6.34	114.09	122.64
2	B	247	GLN	CG-CD-NE2	6.34	125.91	116.40
2	B	7	ILE	CA-C-O	-6.33	114.11	120.31
1	A	407	TRP	CA-CB-CG	-6.33	101.58	113.60
2	B	39	ASP	CA-CB-CG	-6.30	106.30	112.60
2	B	48	ARG	NE-CZ-NH2	6.29	124.86	119.20
2	B	133	GLN	CG-CD-NE2	6.28	125.82	116.40
1	A	411	GLU	CA-C-O	-6.25	112.03	119.15
1	A	299	ALA	O-C-N	-6.23	115.36	122.09
2	B	131	CYS	CA-C-N	6.22	129.66	120.95
2	B	131	CYS	C-N-CA	6.22	129.66	120.95
1	A	35	GLN	CG-CD-NE2	6.21	125.72	116.40
1	A	439	SER	CA-C-N	6.21	132.88	121.70
1	A	439	SER	C-N-CA	6.21	132.88	121.70
2	B	176	LYS	O-C-N	-6.21	114.34	122.59
1	A	29	GLY	O-C-N	-6.20	117.80	123.56
1	A	427	ALA	O-C-N	6.20	130.83	122.59
2	B	264	ARG	CB-CA-C	6.20	120.71	109.62
1	A	219	ILE	CG1-CB-CG2	-6.19	92.12	110.70
2	B	173	PRO	O-C-N	-6.19	114.28	122.64
2	B	220	THR	CA-C-N	6.19	131.15	122.74
2	B	220	THR	C-N-CA	6.19	131.15	122.74
1	A	356	ASN	CA-C-O	-6.17	114.22	121.44
2	B	356	CYS	CA-C-N	6.17	131.89	122.08
2	B	356	CYS	C-N-CA	6.17	131.89	122.08
1	A	72	PRO	CB-CA-C	-6.16	103.12	112.11
2	B	188	THR	CA-C-O	6.16	127.06	119.79
2	B	255	LEU	O-C-N	-6.16	115.59	122.12
1	A	187	SER	CA-C-N	-6.14	112.82	120.56
1	A	187	SER	C-N-CA	-6.14	112.82	120.56
2	B	15	GLN	CG-CD-NE2	6.14	125.62	116.40
2	B	269	MET	O-C-N	6.14	127.43	121.66
2	B	290	GLU	CA-C-N	-6.14	110.24	120.68
2	B	290	GLU	C-N-CA	-6.14	110.24	120.68
2	B	84	GLY	O-C-N	6.13	130.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	GLU	O-C-N	6.11	129.12	122.15
1	A	32	PRO	N-CA-C	6.07	124.97	112.47
2	B	182	VAL	CA-C-O	-6.07	113.20	120.78
1	A	71	GLU	CA-C-N	6.06	125.62	119.19
1	A	71	GLU	C-N-CA	6.06	125.62	119.19
1	A	41	THR	CA-C-N	-6.05	111.08	121.97
1	A	41	THR	C-N-CA	-6.05	111.08	121.97
2	B	200	GLU	CA-C-O	-6.05	114.36	121.44
2	B	394	GLN	CG-CD-NE2	6.03	125.45	116.40
1	A	381	THR	CA-C-O	6.02	128.84	121.56
1	A	373	ARG	CB-CA-C	6.01	120.05	109.89
2	B	427	ASP	O-C-N	6.00	130.57	122.59
3	K	77[A]	ILE	N-CA-C	6.00	117.54	111.00
3	K	77[B]	ILE	N-CA-C	6.00	117.54	111.00
1	A	335	ILE	O-C-N	5.98	127.67	121.87
1	A	363	VAL	O-C-N	-5.98	114.29	121.10
2	B	264	ARG	NH1-CZ-NH2	-5.97	111.53	119.30
2	B	139	HIS	N-CA-CB	-5.96	101.55	111.57
1	A	438	ASP	CA-C-N	5.95	129.35	120.31
1	A	438	ASP	C-N-CA	5.95	129.35	120.31
1	A	344	VAL	N-CA-CB	-5.94	101.43	111.23
1	A	262	TYR	O-C-N	-5.93	114.50	121.32
2	B	281	GLN	CA-C-N	5.92	133.08	122.06
2	B	281	GLN	C-N-CA	5.92	133.08	122.06
1	A	211	ASP	CA-CB-CG	-5.92	106.68	112.60
2	B	26	ASP	CA-C-O	5.91	126.64	119.49
1	A	63	PRO	N-CA-C	5.89	124.60	112.47
2	B	185	TYR	N-CA-CB	-5.89	101.17	109.94
1	A	63	PRO	O-C-N	5.89	130.59	122.64
3	K	332	SER	N-CA-C	-5.88	102.63	109.93
1	A	124	LYS	O-C-N	5.88	128.35	122.12
1	A	139	HIS	N-CA-CB	-5.87	100.61	111.53
1	A	13	GLY	O-C-N	-5.87	115.07	122.70
1	A	229	ARG	NE-CZ-NH1	-5.86	115.64	121.50
2	B	244	PHE	N-CA-C	-5.86	101.51	110.07
1	A	374	ALA	O-C-N	-5.84	116.05	123.24
2	B	270	PRO	O-C-N	-5.83	114.78	122.64
2	B	400	ARG	NE-CZ-NH2	5.81	124.42	119.20
3	K	249	LEU	N-CA-C	5.80	118.38	110.55
1	A	265	ALA	CA-C-N	-5.80	113.58	122.62
1	A	265	ALA	C-N-CA	-5.80	113.58	122.62
2	B	345	GLU	CA-C-N	-5.80	110.42	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	345	GLU	C-N-CA	-5.80	110.42	122.07
1	A	233	GLN	O-C-N	-5.79	115.15	122.27
1	A	366	GLY	N-CA-C	-5.79	107.16	114.16
2	B	434	GLN	CG-CD-NE2	5.78	125.07	116.40
2	B	261	PRO	O-C-N	5.75	130.40	122.64
2	B	23	VAL	CA-C-N	-5.73	117.30	123.08
2	B	23	VAL	C-N-CA	-5.73	117.30	123.08
2	B	42	LEU	O-C-N	5.73	130.21	122.59
1	A	422	ARG	NE-CZ-NH2	5.71	124.34	119.20
2	B	215	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	31	GLN	C-N-CD	-5.70	101.62	125.00
1	A	434	GLU	CA-C-O	-5.70	111.64	119.05
1	A	350	GLY	O-C-N	5.69	130.10	122.70
1	A	413	MET	CA-C-O	-5.69	115.36	121.56
1	A	187	SER	O-C-N	5.68	127.92	122.07
1	A	222	PRO	CA-CB-CG	-5.68	93.71	104.50
1	A	105	ARG	CD-NE-CZ	5.68	132.35	124.40
1	A	396	ASP	CA-CB-CG	5.66	118.26	112.60
2	B	424	ASN	CA-C-N	5.66	131.04	121.14
2	B	424	ASN	C-N-CA	5.66	131.04	121.14
1	A	273	ALA	CA-C-N	5.65	128.76	120.46
1	A	273	ALA	C-N-CA	5.65	128.76	120.46
1	A	221	ARG	CA-CB-CG	5.63	125.37	114.10
1	A	352	LYS	CA-C-O	-5.63	114.12	120.32
1	A	107	HIS	CA-C-O	5.63	126.70	120.90
1	A	215	ARG	NE-CZ-NH2	5.62	124.25	119.20
2	B	256	ALA	CA-C-N	5.61	129.52	121.55
2	B	256	ALA	C-N-CA	5.61	129.52	121.55
2	B	164	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	A	294	ALA	CA-C-N	-5.60	113.00	120.79
1	A	294	ALA	C-N-CA	-5.60	113.00	120.79
2	B	107	HIS	CA-C-O	5.60	126.67	120.90
1	A	255	PHE	CA-CB-CG	5.60	119.40	113.80
2	B	224	TYR	CA-C-N	-5.58	113.14	120.22
2	B	224	TYR	C-N-CA	-5.58	113.14	120.22
2	B	244	PHE	CB-CA-C	5.57	122.09	110.50
2	B	389	LYS	CB-CA-C	5.56	121.48	110.42
2	B	76	ASP	CA-C-N	5.55	127.72	120.28
2	B	76	ASP	C-N-CA	5.55	127.72	120.28
1	A	437	VAL	CA-C-O	-5.55	113.85	120.78
2	B	23	VAL	O-C-N	5.55	129.50	122.57
2	B	4	ILE	N-CA-CB	-5.54	102.27	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	THR	CA-C-N	5.54	131.84	122.26
1	A	179	THR	C-N-CA	5.54	131.84	122.26
1	A	415	GLU	CA-C-O	-5.53	113.47	119.00
1	A	206	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	309	HIS	O-C-N	5.51	129.47	123.13
2	B	390	ARG	CB-CA-C	5.50	117.87	109.34
2	B	384	ILE	CA-C-N	-5.50	111.04	121.54
2	B	384	ILE	C-N-CA	-5.50	111.04	121.54
1	A	411	GLU	N-CA-C	-5.48	106.64	113.38
1	A	374	ALA	CA-C-O	5.47	127.51	121.11
1	A	262	TYR	CA-CB-CG	5.46	123.72	113.90
2	B	150	GLY	CA-C-O	-5.42	114.34	120.30
2	B	224	TYR	CA-C-O	5.42	126.16	120.42
1	A	229	ARG	CD-NE-CZ	-5.39	116.85	124.40
2	B	278	ARG	CA-CB-CG	5.39	124.88	114.10
2	B	64	ARG	NE-CZ-NH2	5.38	124.05	119.20
2	B	302	MET	CG-SD-CE	5.38	112.74	100.90
1	A	299	ALA	CA-C-O	-5.37	115.17	120.70
3	K	165	ASN	N-CA-C	-5.37	97.76	107.75
1	A	33	ASP	CA-C-O	5.37	128.18	120.51
2	B	93	VAL	O-C-N	5.37	128.89	123.20
1	A	103	TYR	O-C-N	5.36	129.51	122.33
2	B	253	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	60	LYS	CB-CA-C	-5.34	102.26	110.81
2	B	83	PHE	CA-CB-CG	5.33	119.13	113.80
2	B	254	LYS	N-CA-C	-5.33	105.64	111.82
1	A	59	GLY	O-C-N	5.32	127.67	122.19
2	B	126	SER	O-C-N	5.31	127.75	122.12
2	B	246	GLY	N-CA-C	5.30	125.74	113.18
2	B	22	GLU	CA-C-O	5.29	125.67	119.28
1	A	304	LYS	O-C-N	5.28	129.98	121.53
2	B	308	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	114	ILE	O-C-N	-5.27	115.99	122.57
1	A	191	THR	CA-C-N	5.24	129.53	121.19
1	A	191	THR	C-N-CA	5.24	129.53	121.19
1	A	86	LEU	N-CA-C	5.23	117.00	108.63
2	B	247	GLN	CA-C-O	-5.22	114.92	120.92
1	A	221	ARG	C-N-CD	-5.22	103.59	125.00
2	B	291	LEU	CA-C-N	5.22	127.54	120.44
2	B	291	LEU	C-N-CA	5.22	127.54	120.44
3	K	118	ILE	N-CA-C	5.22	115.43	110.42
2	B	407	TRP	CB-CA-C	5.21	119.70	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLN	O-C-N	-5.20	112.06	121.63
2	B	319	PHE	N-CA-C	5.20	116.86	108.34
2	B	186	ASN	CA-C-O	-5.16	112.50	119.11
3	K	8	VAL	N-CA-C	5.16	115.55	108.12
1	A	101	ASN	CB-CA-C	-5.16	102.31	110.81
1	A	283	HIS	CA-C-O	-5.14	113.16	120.51
1	A	172	TYR	CA-C-N	5.14	125.11	120.03
1	A	172	TYR	C-N-CA	5.14	125.11	120.03
2	B	220	THR	O-C-N	5.14	129.21	122.33
1	A	262	TYR	N-CA-CB	5.13	119.50	110.37
1	A	200	CYS	O-C-N	5.12	128.90	122.86
2	B	19	LYS	CD-CE-NZ	5.11	128.26	111.90
3	K	184	LEU	N-CA-C	5.10	117.56	109.24
2	B	40	SER	O-C-N	5.09	129.35	122.59
2	B	264	ARG	N-CA-C	-5.08	103.43	110.35
3	K	270	ASN	N-CA-CB	-5.08	102.06	111.52
2	B	160	GLU	O-C-N	5.08	129.30	122.49
2	B	71	GLU	CA-C-N	5.07	126.18	119.84
2	B	71	GLU	C-N-CA	5.07	126.18	119.84
1	A	93	ILE	O-C-N	5.06	128.49	123.18
1	A	320	ARG	O-C-N	5.03	129.49	123.36
1	A	53	PHE	CA-C-N	5.02	129.85	122.77
1	A	53	PHE	C-N-CA	5.02	129.85	122.77
1	A	339	ARG	N-CA-C	-5.02	105.51	111.69
1	A	173	PRO	CB-CA-C	-5.01	104.39	110.95

There are no chirality outliers.

All (116) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LYS	Mainchain
1	A	143	GLY	Mainchain
1	A	149	PHE	Mainchain
1	A	153	LEU	Mainchain
1	A	179	THR	Mainchain,Peptide
1	A	18	ASN	Mainchain
1	A	187	SER	Mainchain
1	A	193	THR	Mainchain
1	A	218	ASP	Peptide
1	A	221	ARG	Mainchain,Peptide
1	A	24	TYR	Mainchain,Peptide
1	A	267	PHE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	280	LYS	Mainchain,Peptide
1	A	283	HIS	Mainchain,Peptide
1	A	297	GLU	Mainchain
1	A	30	ILE	Mainchain,Peptide
1	A	34	GLY	Peptide
1	A	347	CYS	Mainchain
1	A	350	GLY	Mainchain
1	A	358	GLU	Peptide
1	A	36	MET	Mainchain
1	A	363	VAL	Mainchain
1	A	367	ASP	Mainchain
1	A	368	LEU	Mainchain,Peptide
1	A	369	ALA	Mainchain,Peptide
1	A	38	SER	Mainchain,Peptide
1	A	384	ILE	Mainchain
1	A	392	ASP	Mainchain
1	A	397	LEU	Mainchain
1	A	402	ARG	Mainchain,Peptide
1	A	405	VAL	Peptide
1	A	412	GLY	Peptide
1	A	415	GLU	Mainchain,Peptide
1	A	438	ASP	Mainchain
1	A	49	PHE	Mainchain,Peptide
1	A	50	ASN	Mainchain,Peptide
1	A	53	PHE	Mainchain
1	A	64	ARG	Peptide
1	A	69	ASP	Mainchain
1	A	75	ILE	Mainchain
1	A	77	GLU	Mainchain
1	A	78	VAL	Mainchain
1	A	87	PHE	Peptide
1	A	90	GLU	Mainchain
2	B	105	LYS	Mainchain
2	B	112	ALA	Mainchain
2	B	127	GLU	Mainchain,Peptide
2	B	133	GLN	Mainchain
2	B	143	GLY	Mainchain,Peptide
2	B	148	GLY	Mainchain
2	B	171	VAL	Mainchain,Peptide
2	B	173	PRO	Mainchain
2	B	179	ASP	Mainchain,Peptide
2	B	182	VAL	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
2	B	185	TYR	Sidechain
2	B	187	ALA	Mainchain
2	B	193	GLN	Mainchain
2	B	194	LEU	Mainchain
2	B	200	GLU	Mainchain
2	B	203	CYS	Peptide
2	B	239	THR	Mainchain
2	B	242	LEU	Mainchain
2	B	247	GLN	Mainchain,Peptide
2	B	273	ALA	Peptide
2	B	275	LEU	Mainchain,Peptide
2	B	281	GLN	Mainchain
2	B	284	ARG	Mainchain
2	B	309	HIS	Mainchain
2	B	316	ALA	Mainchain
2	B	321	GLY	Mainchain
2	B	331	GLN	Mainchain
2	B	337	ASN	Mainchain
2	B	340	SER	Mainchain
2	B	344	VAL	Mainchain,Peptide
2	B	347	ILE	Mainchain,Peptide
2	B	356	CYS	Mainchain,Peptide
2	B	393	GLU	Mainchain
2	B	402	LYS	Mainchain,Peptide
2	B	411	GLU	Mainchain,Peptide
2	B	414	ASP	Mainchain,Peptide
2	B	436	GLN	Mainchain,Peptide
2	B	47	GLU	Mainchain,Peptide
2	B	56	ALA	Mainchain
2	B	60	LYS	Mainchain,Peptide
2	B	71	GLU	Peptide
2	B	89	PRO	Mainchain,Peptide

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	3430	0	3272	1721	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3359	0	3181	1900	0
3	K	2667	0	2614	160	0
4	A	32	0	11	22	0
5	B	28	0	12	20	0
6	B	58	0	51	61	0
7	K	1	0	0	0	0
8	K	31	0	14	2	0
All	All	9606	0	9155	3654	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 195.

All (3654) 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)
2:B:405:LEU:HD22	2:B:418:PHE:CZ	1.17	1.68
2:B:151:THR:CB	2:B:192:HIS:CD2	1.75	1.68
2:B:229:HIS:CE1	6:B:502:TXL:H343	1.28	1.67
1:A:115:ILE:HD12	1:A:152:LEU:CG	1.26	1.64
2:B:184:PRO:HG2	2:B:399:PHE:CE2	1.12	1.63
2:B:147:SER:HB3	2:B:189:LEU:CD1	1.19	1.63
2:B:287:THR:HB	2:B:290:GLU:CB	1.26	1.63
1:A:217:LEU:HD13	1:A:368:LEU:CD1	1.25	1.63
1:A:405:VAL:CG2	1:A:405:VAL:CB	1.76	1.63
2:B:295:MET:HE3	2:B:375:ALA:CB	1.18	1.63
2:B:346:TRP:CE3	2:B:347:ILE:HG13	1.25	1.63
1:A:53:PHE:N	1:A:88:HIS:CE1	1.68	1.62
2:B:405:LEU:CD1	2:B:408:TYR:CB	1.75	1.61
2:B:103:TRP:CE3	2:B:413:MET:HE1	1.30	1.60
1:A:424:ASP:CG	3:K:307:ARG:HH12	1.03	1.60
2:B:158:ARG:CB	2:B:197:ASN:CB	1.76	1.60
1:A:326:LYS:NZ	2:B:214:PHE:CZ	1.67	1.59
1:A:115:ILE:CD1	1:A:152:LEU:HG	1.15	1.59
1:A:220:GLU:CB	1:A:220:GLU:CG	1.78	1.58
1:A:212:ILE:HD11	1:A:230:LEU:CD2	1.25	1.57
2:B:181:VAL:CG1	2:B:399:PHE:HZ	1.17	1.57
2:B:158:ARG:HB2	2:B:197:ASN:CB	1.14	1.57
1:A:296:PHE:CE1	1:A:335:ILE:HD13	1.38	1.57
2:B:346:TRP:CZ3	2:B:347:ILE:HD11	1.34	1.57
1:A:204:VAL:CG1	1:A:209:ILE:HD11	1.17	1.57
2:B:6:HIS:CE1	2:B:30:ILE:HD12	1.39	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:HIS:CD2	6:B:502:TXL:C38	1.86	1.57
2:B:158:ARG:CD	2:B:197:ASN:HB2	1.30	1.56
2:B:151:THR:HG22	2:B:192:HIS:CE1	1.39	1.56
2:B:158:ARG:CG	2:B:197:ASN:HB2	1.13	1.56
1:A:31:GLN:HE22	1:A:243:ARG:CG	1.15	1.55
2:B:70:LEU:HD12	2:B:94:PHE:CD2	1.40	1.54
1:A:103:TYR:CE2	1:A:189:LEU:HD23	1.41	1.54
1:A:349:THR:CB	2:B:177:VAL:CG1	1.78	1.53
1:A:70:LEU:HD12	1:A:145:THR:CG2	1.07	1.53
1:A:100:ALA:CB	1:A:105:ARG:HD3	1.38	1.53
1:A:103:TYR:CD2	1:A:189:LEU:HD23	1.44	1.53
2:B:295:MET:CE	2:B:375:ALA:HB1	1.08	1.53
2:B:399:PHE:CE1	2:B:408:TYR:HE2	1.22	1.53
2:B:151:THR:CA	2:B:192:HIS:CD2	1.89	1.51
2:B:181:VAL:HG13	2:B:399:PHE:CZ	1.40	1.51
1:A:31:GLN:CD	1:A:243:ARG:HD2	1.08	1.50
2:B:158:ARG:CA	2:B:197:ASN:HD22	0.89	1.50
2:B:169:PHE:CE1	2:B:235:MET:HG2	1.45	1.50
1:A:62:VAL:CG1	1:A:63:PRO:HD2	1.39	1.50
2:B:184:PRO:CG	2:B:399:PHE:CG	1.92	1.50
2:B:346:TRP:CE3	2:B:347:ILE:CG1	1.90	1.50
1:A:210:TYR:CE2	1:A:227:LEU:HD22	1.45	1.49
1:A:64:ARG:HH22	1:A:132:LEU:CD2	1.22	1.49
1:A:264:ARG:NH2	3:K:307:ARG:HD2	1.24	1.49
2:B:405:LEU:CD2	2:B:418:PHE:CZ	1.91	1.49
2:B:405:LEU:HD13	2:B:408:TYR:CD2	1.48	1.49
1:A:107:HIS:HB2	1:A:148:GLY:CA	1.42	1.48
2:B:192:HIS:CA	2:B:196:GLU:HG3	1.42	1.48
2:B:259:MET:HB3	2:B:268:PHE:CE1	1.47	1.48
2:B:107:HIS:C	2:B:152:LEU:HD11	1.35	1.48
1:A:272:TYR:CE1	1:A:274:PRO:O	1.64	1.47
1:A:349:THR:HB	2:B:177:VAL:CG1	1.00	1.47
2:B:399:PHE:HE1	2:B:408:TYR:CE2	1.30	1.47
1:A:70:LEU:CD1	1:A:145:THR:HG22	0.98	1.46
1:A:349:THR:CB	2:B:177:VAL:HG11	1.34	1.46
2:B:405:LEU:CD2	2:B:418:PHE:CE2	2.00	1.46
2:B:405:LEU:HD11	2:B:408:TYR:CB	1.34	1.45
1:A:212:ILE:CD1	1:A:230:LEU:HD21	1.45	1.45
2:B:399:PHE:CE1	2:B:408:TYR:CE2	2.03	1.45
1:A:158:SER:CB	1:A:197:HIS:CB	1.84	1.44
2:B:405:LEU:CD1	2:B:408:TYR:HB2	0.96	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CD2	1:A:147:SER:HB2	1.50	1.44
2:B:151:THR:HB	2:B:192:HIS:CD2	1.39	1.44
1:A:397:LEU:CD2	1:A:401:LYS:HD2	1.47	1.44
1:A:107:HIS:CB	1:A:148:GLY:HA3	1.47	1.44
2:B:239:THR:O	2:B:243:ARG:CD	1.65	1.44
2:B:19:LYS:CB	2:B:228:ASN:HB3	1.45	1.43
2:B:286:LEU:CD1	2:B:372:LYS:HB2	1.47	1.43
2:B:135:PHE:HB3	2:B:166:MET:CE	1.47	1.43
2:B:158:ARG:HD2	2:B:197:ASN:CA	1.44	1.43
2:B:70:LEU:CD1	2:B:94:PHE:CD2	1.99	1.43
2:B:172:VAL:CG1	2:B:173:PRO:HD2	1.46	1.42
2:B:19:LYS:HG3	2:B:228:ASN:CB	1.46	1.42
1:A:264:ARG:HH21	3:K:307:ARG:CB	1.31	1.42
2:B:87:PHE:CE1	2:B:89:PRO:HG2	1.52	1.42
2:B:151:THR:HA	2:B:192:HIS:CD2	1.49	1.42
1:A:53:PHE:CA	1:A:88:HIS:CE1	2.01	1.41
1:A:222:PRO:CB	1:A:222:PRO:CG	1.86	1.41
2:B:151:THR:HG22	2:B:192:HIS:ND1	1.24	1.41
1:A:64:ARG:NH2	1:A:132:LEU:HD22	1.31	1.41
1:A:424:ASP:CB	3:K:307:ARG:HH12	1.34	1.40
2:B:147:SER:CB	2:B:189:LEU:HD11	0.95	1.40
1:A:250:VAL:HG13	1:A:254:GLU:CB	1.48	1.40
1:A:172:TYR:OH	1:A:387:ALA:CB	1.64	1.40
2:B:184:PRO:CB	2:B:399:PHE:CD2	2.05	1.40
1:A:68:VAL:HG11	1:A:149:PHE:CZ	1.57	1.39
1:A:277:SER:OG	1:A:280:LYS:CG	1.68	1.39
2:B:19:LYS:CG	2:B:228:ASN:HB3	1.50	1.39
2:B:57:ALA:HA	2:B:64:ARG:CB	1.52	1.39
1:A:204:VAL:CG2	1:A:231:ILE:HG23	1.50	1.39
2:B:7:ILE:HB	2:B:137:LEU:CD2	1.51	1.39
2:B:229:HIS:CD2	6:B:502:TXL:C37	2.02	1.39
2:B:87:PHE:CD1	2:B:88:ARG:O	1.76	1.38
1:A:250:VAL:HG13	1:A:254:GLU:CG	1.54	1.38
2:B:175:PRO:O	2:B:176:LYS:CE	1.70	1.38
1:A:176:GLN:O	1:A:177:VAL:CG2	1.69	1.37
1:A:288:VAL:CG2	1:A:373:ARG:HD3	1.52	1.37
2:B:103:TRP:CD1	2:B:189:LEU:HD23	1.57	1.37
2:B:184:PRO:CD	2:B:399:PHE:CD2	2.07	1.37
2:B:158:ARG:HA	2:B:197:ASN:ND2	1.04	1.36
2:B:184:PRO:HG2	2:B:399:PHE:CG	1.55	1.36
1:A:264:ARG:NH2	3:K:307:ARG:HB3	1.40	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:CG	3:K:307:ARG:NH1	1.81	1.36
2:B:158:ARG:CB	2:B:197:ASN:HB2	1.44	1.36
2:B:147:SER:CB	2:B:189:LEU:CD1	1.79	1.36
1:A:179:THR:HG22	1:A:181:VAL:N	1.42	1.35
2:B:20:PHE:CE2	2:B:235:MET:HB3	1.50	1.35
2:B:97:SER:HB2	2:B:110:GLU:OE1	1.19	1.35
2:B:24:ILE:O	2:B:26:ASP:N	1.60	1.35
2:B:32:PRO:CB	2:B:59:ASN:HD22	1.25	1.35
2:B:435:TYR:O	2:B:436:GLN:CG	1.72	1.35
1:A:31:GLN:CD	1:A:243:ARG:CD	1.99	1.35
1:A:182:VAL:HG13	1:A:186:ASN:ND2	1.40	1.35
1:A:217:LEU:CD1	1:A:368:LEU:HD11	1.55	1.34
1:A:272:TYR:CZ	1:A:274:PRO:HG2	1.62	1.34
2:B:175:PRO:O	2:B:176:LYS:CD	1.74	1.34
2:B:192:HIS:HA	2:B:196:GLU:CG	1.55	1.34
1:A:212:ILE:CD1	1:A:230:LEU:CD2	2.02	1.34
2:B:96:GLN:O	2:B:98:GLY:N	1.59	1.34
2:B:201:THR:CG2	2:B:265:LEU:HD21	1.57	1.34
2:B:151:THR:HA	2:B:192:HIS:NE2	1.04	1.33
2:B:305:CYS:SG	2:B:384:ILE:HD13	1.67	1.33
1:A:2:ARG:NH2	2:B:71:GLU:HB3	1.42	1.33
1:A:53:PHE:N	1:A:88:HIS:NE2	1.75	1.33
1:A:158:SER:CB	1:A:197:HIS:HB3	1.49	1.33
2:B:4:ILE:HD12	2:B:30:ILE:C	1.53	1.33
2:B:19:LYS:CG	2:B:228:ASN:CB	2.02	1.33
2:B:294:GLN:CG	2:B:300:ASN:OD1	1.77	1.33
2:B:405:LEU:HD22	2:B:418:PHE:CE2	1.56	1.33
1:A:31:GLN:N	1:A:32:PRO:CD	1.76	1.32
1:A:31:GLN:NE2	1:A:243:ARG:CD	1.92	1.32
1:A:306:ASP:OD1	1:A:308:ARG:CG	1.76	1.32
2:B:346:TRP:CZ3	2:B:347:ILE:CD1	2.10	1.32
2:B:22:GLU:HG2	2:B:83:PHE:CD2	1.63	1.32
1:A:277:SER:CB	1:A:280:LYS:HG2	1.59	1.32
2:B:75:MET:CE	2:B:79:ARG:HD2	1.60	1.32
1:A:101:ASN:O	1:A:102:ASN:CG	1.72	1.32
1:A:179:THR:CG2	1:A:181:VAL:H	1.42	1.32
1:A:369:ALA:CB	1:A:371:VAL:HG23	1.56	1.32
2:B:142:GLY:C	2:B:185:TYR:CE1	2.07	1.32
2:B:158:ARG:CG	2:B:197:ASN:CB	1.95	1.32
1:A:184:PRO:HG3	1:A:395:PHE:CB	1.57	1.31
2:B:107:HIS:O	2:B:152:LEU:HD11	1.28	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:CG1	2:B:399:PHE:CZ	2.03	1.31
2:B:244:PHE:CD2	2:B:245:PRO:HD2	1.65	1.31
2:B:335:VAL:O	2:B:339:ASN:ND2	1.60	1.31
2:B:158:ARG:HD2	2:B:197:ASN:CB	1.59	1.31
2:B:175:PRO:O	2:B:176:LYS:HE2	1.22	1.31
1:A:30:ILE:O	1:A:32:PRO:CG	1.78	1.31
1:A:38:SER:C	1:A:39:ASP:CA	2.04	1.31
1:A:108:TYR:O	1:A:112:LYS:CD	1.76	1.31
2:B:311:ARG:HG2	2:B:341:SER:O	1.21	1.30
1:A:250:VAL:CG2	1:A:352:LYS:HE2	1.60	1.30
1:A:250:VAL:CG1	1:A:254:GLU:HB3	1.61	1.30
2:B:192:HIS:O	2:B:196:GLU:CB	1.80	1.30
1:A:103:TYR:CD2	1:A:189:LEU:CD2	2.13	1.29
1:A:291:ILE:HG22	1:A:375:VAL:CG2	1.62	1.29
2:B:201:THR:HG21	2:B:265:LEU:CD2	1.60	1.29
2:B:12:CYS:O	2:B:16:ILE:HG12	1.25	1.29
1:A:266:HIS:CD2	1:A:432:TYR:HE1	1.50	1.29
1:A:423:GLU:OE2	3:K:172:PRO:HA	1.23	1.29
2:B:189:LEU:O	2:B:193:GLN:HG3	1.31	1.29
2:B:435:TYR:O	2:B:436:GLN:HG3	1.20	1.29
1:A:38:SER:O	1:A:39:ASP:N	1.58	1.29
2:B:107:HIS:CA	2:B:152:LEU:HD11	1.63	1.29
2:B:229:HIS:CG	6:B:502:TXL:H38	1.67	1.29
2:B:268:PHE:CE1	2:B:380:ASN:ND2	1.99	1.29
2:B:107:HIS:CD2	2:B:152:LEU:HG	1.66	1.28
2:B:114:LEU:HD12	2:B:117:SER:OG	1.24	1.28
2:B:180:THR:O	2:B:398:MET:CE	1.78	1.28
1:A:2:ARG:CG	1:A:133:GLN:OE1	1.82	1.28
2:B:151:THR:CG2	2:B:192:HIS:CG	2.16	1.28
2:B:259:MET:HE1	2:B:379:GLY:CA	1.64	1.28
1:A:184:PRO:CG	1:A:395:PHE:CD2	2.17	1.28
2:B:192:HIS:O	2:B:196:GLU:HB2	1.17	1.28
2:B:319:PHE:CE1	2:B:353:THR:HG23	1.67	1.28
1:A:31:GLN:N	1:A:32:PRO:HD3	1.05	1.27
1:A:433:GLU:O	1:A:437:VAL:HG23	1.32	1.27
1:A:306:ASP:OD1	1:A:308:ARG:HG3	1.17	1.27
2:B:151:THR:HG22	2:B:192:HIS:CG	1.67	1.27
2:B:151:THR:CA	2:B:192:HIS:NE2	1.82	1.27
2:B:312:TYR:HA	2:B:381:SER:CB	1.63	1.27
2:B:183:GLU:HB2	2:B:184:PRO:CD	1.59	1.27
2:B:237:GLY:HA2	2:B:241:CYS:SG	1.74	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:NE2	1:A:243:ARG:CG	1.93	1.27
1:A:53:PHE:HA	1:A:88:HIS:CE1	1.64	1.27
2:B:145:THR:O	2:B:149:MET:HB3	1.19	1.27
2:B:405:LEU:CD1	2:B:408:TYR:CD2	2.06	1.26
2:B:182:VAL:HG13	2:B:186:ASN:ND2	1.48	1.26
1:A:383:ALA:O	1:A:385:ALA:N	1.69	1.26
2:B:87:PHE:CE1	2:B:88:ARG:O	1.87	1.26
2:B:94:PHE:HD1	2:B:94:PHE:O	1.16	1.26
1:A:108:TYR:C	1:A:112:LYS:HE3	1.59	1.26
1:A:204:VAL:CG1	1:A:209:ILE:CD1	2.13	1.26
1:A:219:ILE:CB	1:A:219:ILE:CG2	2.13	1.26
1:A:220:GLU:C	1:A:222:PRO:HD3	1.61	1.26
1:A:204:VAL:HG21	1:A:231:ILE:CG2	1.47	1.26
2:B:193:GLN:O	2:B:265:LEU:CD2	1.82	1.26
1:A:424:ASP:OD1	3:K:307:ARG:NH2	1.70	1.25
2:B:3:GLU:OE1	2:B:130:ASP:CB	1.84	1.25
2:B:183:GLU:CB	2:B:184:PRO:HD3	1.63	1.25
2:B:312:TYR:O	2:B:344:VAL:CG2	1.84	1.25
1:A:172:TYR:OH	1:A:387:ALA:HB3	1.11	1.25
2:B:12:CYS:O	2:B:16:ILE:CG1	1.82	1.25
1:A:288:VAL:HG22	1:A:373:ARG:CD	1.65	1.25
2:B:57:ALA:CA	2:B:64:ARG:HB2	1.64	1.25
2:B:92:PHE:CD2	2:B:114:LEU:HD11	1.70	1.25
2:B:103:TRP:HD1	2:B:189:LEU:CD2	1.49	1.25
2:B:287:THR:O	2:B:291:LEU:CG	1.81	1.25
1:A:107:HIS:HB2	1:A:148:GLY:C	1.59	1.25
1:A:264:ARG:HH22	3:K:307:ARG:CD	1.48	1.25
2:B:405:LEU:CD1	2:B:408:TYR:CG	2.20	1.25
2:B:435:TYR:C	2:B:436:GLN:HG3	1.17	1.25
1:A:424:ASP:HA	3:K:307:ARG:CZ	1.65	1.24
2:B:103:TRP:CD1	2:B:189:LEU:CD2	2.18	1.24
1:A:97:GLU:CB	1:A:110:ILE:HG21	1.65	1.24
1:A:206:ASN:ND2	1:A:227:LEU:CD2	2.00	1.24
1:A:257:THR:HG22	2:B:407:TRP:CE3	1.71	1.24
1:A:108:TYR:CA	1:A:112:LYS:HE3	1.67	1.24
2:B:44:LEU:HD23	2:B:85:GLN:CG	1.35	1.24
2:B:103:TRP:CE3	2:B:413:MET:CE	2.21	1.24
1:A:30:ILE:C	1:A:32:PRO:CD	2.11	1.24
1:A:77:GLU:HA	1:A:80:THR:OG1	1.09	1.24
1:A:108:TYR:O	1:A:112:LYS:CE	1.85	1.24
2:B:4:ILE:HD13	2:B:30:ILE:CG2	1.68	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:O	2:B:37:HIS:N	1.71	1.24
2:B:319:PHE:HE1	2:B:353:THR:CG2	1.50	1.24
1:A:30:ILE:CG2	1:A:64:ARG:HG2	1.68	1.23
1:A:31:GLN:OE1	1:A:243:ARG:CD	1.85	1.23
1:A:259:LEU:O	1:A:261:PRO:HD3	1.38	1.23
1:A:276:ILE:O	1:A:368:LEU:HB3	1.31	1.23
1:A:326:LYS:NZ	2:B:214:PHE:CE1	2.06	1.23
2:B:382:THR:CG2	2:B:436:GLN:OE1	1.78	1.23
1:A:9:VAL:HG11	1:A:150:THR:CG2	1.67	1.23
1:A:185:TYR:HD2	1:A:408:TYR:OH	0.92	1.23
1:A:291:ILE:CG2	1:A:375:VAL:HG23	1.65	1.23
2:B:287:THR:CG2	2:B:289:PRO:HD2	1.67	1.23
1:A:360:PRO:CG	1:A:371:VAL:O	1.86	1.23
2:B:107:HIS:HA	2:B:152:LEU:CD1	1.67	1.23
2:B:111:GLY:O	2:B:115:VAL:HG23	1.32	1.23
2:B:244:PHE:CE2	2:B:358:ILE:HD12	1.73	1.23
2:B:20:PHE:CE2	2:B:235:MET:CB	2.01	1.23
1:A:77:GLU:CA	1:A:80:THR:OG1	1.86	1.23
2:B:143:GLY:N	2:B:185:TYR:CE1	2.05	1.23
1:A:30:ILE:O	1:A:32:PRO:HG2	1.27	1.22
1:A:206:ASN:ND2	1:A:227:LEU:HD21	1.51	1.22
2:B:87:PHE:HE1	2:B:89:PRO:CG	1.51	1.22
2:B:102:ASN:HD22	2:B:105:LYS:CE	1.49	1.22
2:B:435:TYR:C	2:B:436:GLN:CG	2.06	1.22
2:B:75:MET:CE	2:B:79:ARG:CD	2.17	1.22
2:B:75:MET:HE2	2:B:79:ARG:CD	1.70	1.22
1:A:20:CYS:O	1:A:24:TYR:CD2	1.91	1.22
1:A:312:TYR:O	1:A:344:VAL:CG2	1.87	1.22
2:B:229:HIS:CD2	6:B:502:TXL:H38	1.54	1.22
2:B:287:THR:CB	2:B:290:GLU:HB2	1.67	1.22
1:A:26:LEU:HD11	1:A:361:THR:CG2	1.69	1.22
1:A:48:SER:O	1:A:56:THR:CG2	1.87	1.22
1:A:78:VAL:CG1	1:A:87:PHE:HE1	1.53	1.22
1:A:424:ASP:CB	3:K:307:ARG:NH1	2.00	1.22
1:A:3:GLU:HA	1:A:31:GLN:CB	1.70	1.22
1:A:272:TYR:HE1	1:A:274:PRO:O	0.94	1.22
2:B:6:HIS:HE1	2:B:30:ILE:CD1	1.53	1.22
2:B:69:ASP:OD2	2:B:74:THR:HB	1.32	1.22
1:A:93:ILE:CD1	1:A:118:VAL:HG22	1.70	1.21
1:A:210:TYR:CE2	1:A:227:LEU:CD2	2.21	1.21
2:B:36:TYR:CE2	2:B:244:PHE:CE1	1.94	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:CYS:HB2	1:A:30:ILE:CG2	1.68	1.21
1:A:423:GLU:OE1	3:K:170:GLU:HG3	1.30	1.21
2:B:97:SER:CB	2:B:110:GLU:OE1	1.89	1.21
2:B:175:PRO:O	2:B:176:LYS:CG	1.88	1.21
2:B:175:PRO:C	2:B:176:LYS:HG2	1.54	1.21
1:A:242:LEU:HD12	1:A:255:PHE:CZ	1.73	1.21
2:B:184:PRO:CD	2:B:399:PHE:HD2	1.49	1.21
2:B:183:GLU:CD	2:B:394:GLN:HB3	1.66	1.21
2:B:237:GLY:O	2:B:241:CYS:HB2	1.33	1.21
1:A:416:GLY:HA3	3:K:169:ARG:NH2	1.54	1.21
2:B:319:PHE:CE1	2:B:328:VAL:CG1	2.24	1.21
1:A:217:LEU:HD13	1:A:368:LEU:HD13	1.21	1.20
2:B:143:GLY:N	2:B:185:TYR:HE1	1.35	1.20
2:B:312:TYR:HA	2:B:381:SER:CA	1.71	1.20
1:A:217:LEU:CD1	1:A:368:LEU:CD1	2.14	1.20
1:A:272:TYR:CE1	1:A:274:PRO:HG2	1.75	1.20
2:B:229:HIS:CE1	6:B:502:TXL:C34	2.23	1.20
1:A:28:HIS:CE1	1:A:29:GLY:O	1.93	1.20
1:A:184:PRO:HG3	1:A:395:PHE:CD2	1.74	1.20
2:B:192:HIS:CA	2:B:196:GLU:CG	2.12	1.20
1:A:396:ASP:O	1:A:401:LYS:HB2	1.40	1.20
2:B:87:PHE:CE1	2:B:89:PRO:CG	2.23	1.20
2:B:175:PRO:HD3	2:B:390:ARG:NH2	1.57	1.20
2:B:20:PHE:HE2	2:B:235:MET:CB	1.24	1.19
1:A:176:GLN:O	1:A:177:VAL:HG23	1.03	1.19
1:A:220:GLU:O	1:A:222:PRO:CD	1.89	1.19
1:A:344:VAL:HB	1:A:347:CYS:SG	1.80	1.19
2:B:107:HIS:O	2:B:152:LEU:CD1	1.89	1.19
2:B:169:PHE:CE1	2:B:235:MET:CG	2.25	1.19
1:A:16:ILE:HD13	1:A:138:PHE:CD1	1.75	1.19
2:B:135:PHE:CB	2:B:166:MET:CE	2.20	1.19
1:A:174:ALA:CB	1:A:175:PRO:CD	2.20	1.19
2:B:321:GLY:HA3	2:B:373:MET:HG3	1.22	1.19
1:A:343:PHE:CE2	1:A:351:PHE:CZ	2.30	1.19
2:B:151:THR:CG2	2:B:192:HIS:CE1	2.26	1.19
1:A:115:ILE:CD1	1:A:152:LEU:CG	1.92	1.18
1:A:332:ILE:CD1	1:A:353:VAL:HG21	1.70	1.18
1:A:2:ARG:HG2	1:A:133:GLN:OE1	1.06	1.18
2:B:259:MET:CE	2:B:379:GLY:HA2	1.72	1.18
2:B:346:TRP:HE3	2:B:347:ILE:CG1	1.34	1.18
1:A:4:CYS:SG	1:A:252:LEU:HD11	1.83	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:O	2:B:47:GLU:HG3	1.01	1.18
2:B:250:ALA:HA	2:B:254:LYS:HD2	1.25	1.18
1:A:184:PRO:CB	1:A:395:PHE:HD2	1.55	1.18
1:A:312:TYR:HA	1:A:381:THR:HG22	1.26	1.18
2:B:32:PRO:CB	2:B:59:ASN:ND2	1.79	1.18
1:A:31:GLN:OE1	1:A:243:ARG:HD2	1.03	1.17
1:A:103:TYR:CD1	1:A:188:ILE:CG2	2.26	1.17
1:A:115:ILE:HD13	1:A:156:ARG:CZ	1.74	1.17
1:A:3:GLU:O	1:A:132:LEU:O	1.59	1.17
1:A:48:SER:O	1:A:56:THR:HG21	1.02	1.17
2:B:33:THR:N	2:B:59:ASN:HD22	1.42	1.17
2:B:370:GLY:O	6:B:502:TXL:H183	1.43	1.17
1:A:264:ARG:NH2	3:K:307:ARG:CD	2.04	1.17
1:A:437:VAL:O	1:A:438:ASP:OD1	1.62	1.17
1:A:108:TYR:O	1:A:112:LYS:HE3	1.40	1.17
1:A:312:TYR:CE2	1:A:377:MET:HE1	1.79	1.17
2:B:41:ASP:O	2:B:42:LEU:HG	1.45	1.17
1:A:62:VAL:CG1	1:A:63:PRO:CD	2.22	1.16
2:B:234:THR:OG1	2:B:302:MET:HE1	1.44	1.16
1:A:2:ARG:HH21	2:B:71:GLU:CB	1.57	1.16
1:A:105:ARG:HH21	1:A:110:ILE:HD11	1.03	1.16
1:A:220:GLU:O	1:A:222:PRO:HD2	1.45	1.16
2:B:7:ILE:HA	2:B:66:ILE:CG2	1.75	1.16
2:B:294:GLN:HG2	2:B:300:ASN:OD1	1.01	1.16
1:A:31:GLN:NE2	1:A:243:ARG:HD2	1.51	1.16
2:B:174:SER:CB	2:B:207:GLU:HB3	1.73	1.16
2:B:44:LEU:O	2:B:47:GLU:CG	1.91	1.16
1:A:100:ALA:CB	1:A:105:ARG:CD	2.23	1.16
1:A:115:ILE:HD12	1:A:152:LEU:CD2	1.75	1.16
1:A:137:VAL:HG21	1:A:154:MET:SD	1.85	1.16
2:B:103:TRP:CZ3	2:B:413:MET:HE1	1.81	1.16
2:B:191:VAL:CG2	2:B:421:ALA:HA	1.75	1.15
2:B:97:SER:HB2	2:B:110:GLU:CD	1.71	1.15
2:B:111:GLY:C	2:B:115:VAL:HG23	1.69	1.15
2:B:180:THR:O	2:B:398:MET:HE3	1.44	1.15
2:B:183:GLU:HB2	2:B:398:MET:SD	1.85	1.15
2:B:287:THR:HB	2:B:290:GLU:HB3	1.21	1.15
2:B:287:THR:HG22	2:B:289:PRO:HD2	1.20	1.15
2:B:80:SER:C	2:B:82:PRO:HD2	1.70	1.15
2:B:103:TRP:CZ3	2:B:413:MET:CE	2.28	1.15
2:B:151:THR:CG2	2:B:192:HIS:CD2	2.27	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:CB	2:B:197:ASN:CG	2.19	1.15
2:B:209:LEU:HD13	2:B:227:LEU:HG	1.21	1.15
2:B:260:VAL:HG22	2:B:266:HIS:HB2	1.21	1.15
2:B:405:LEU:HD12	2:B:408:TYR:CB	1.56	1.15
2:B:22:GLU:HB3	2:B:83:PHE:CE2	1.81	1.15
2:B:22:GLU:HB3	2:B:83:PHE:CZ	1.82	1.15
2:B:50:ASN:N	2:B:61:TYR:CD2	2.15	1.15
2:B:158:ARG:CB	2:B:197:ASN:HD22	1.60	1.15
2:B:234:THR:OG1	2:B:302:MET:SD	2.05	1.15
2:B:234:THR:OG1	2:B:302:MET:CE	1.95	1.15
2:B:241:CYS:SG	2:B:320:ARG:NH1	2.20	1.15
1:A:217:LEU:HD11	1:A:368:LEU:HD21	1.15	1.14
2:B:141:LEU:HD22	2:B:186:ASN:HB3	1.21	1.14
1:A:176:GLN:C	1:A:177:VAL:HG23	1.71	1.14
2:B:135:PHE:HB3	2:B:166:MET:HE1	1.27	1.14
2:B:172:VAL:CG1	2:B:173:PRO:CD	2.25	1.14
2:B:242:LEU:HD13	2:B:250:ALA:HB3	1.28	1.14
3:K:159:ASN:ND2	3:K:161:LYS:HG3	1.62	1.14
1:A:231:ILE:HD13	1:A:302:MET:HE2	1.25	1.14
2:B:104:ALA:HA	2:B:108:TYR:CD2	1.83	1.14
2:B:105:LYS:HE2	2:B:411:GLU:OE2	1.48	1.14
2:B:151:THR:HB	2:B:192:HIS:CG	1.81	1.14
2:B:313:LEU:CD2	2:B:344:VAL:HG11	1.75	1.14
1:A:174:ALA:HB1	1:A:175:PRO:CD	1.75	1.14
1:A:155:GLU:HG3	1:A:192:HIS:CD2	1.82	1.14
1:A:184:PRO:HG3	1:A:395:PHE:CG	1.81	1.14
1:A:224:TYR:OH	4:A:500:GTP:O2'	1.65	1.14
2:B:277:SER:HB2	2:B:280:SER:HB2	1.30	1.14
1:A:296:PHE:CE1	1:A:335:ILE:CD1	2.31	1.13
2:B:151:THR:CB	2:B:192:HIS:CG	2.31	1.13
2:B:158:ARG:HB2	2:B:197:ASN:CG	1.72	1.13
2:B:296:PHE:CZ	2:B:335:VAL:HG11	1.83	1.13
1:A:397:LEU:HD23	1:A:401:LYS:HD2	1.19	1.13
2:B:22:GLU:CG	2:B:83:PHE:CD2	2.30	1.13
2:B:180:THR:O	2:B:398:MET:HE1	1.48	1.13
2:B:313:LEU:HD23	2:B:344:VAL:CG2	1.79	1.13
2:B:7:ILE:CG1	2:B:66:ILE:HG21	1.77	1.13
2:B:56:ALA:HB3	2:B:62:VAL:CB	1.78	1.13
2:B:244:PHE:HE2	2:B:358:ILE:CD1	1.60	1.13
2:B:405:LEU:CD1	2:B:408:TYR:HD2	1.53	1.13
1:A:59:GLY:O	1:A:62:VAL:O	1.63	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:CG	1:A:368:LEU:HD11	1.78	1.13
2:B:154:ILE:HG21	2:B:198:THR:CG2	1.79	1.13
2:B:154:ILE:CG2	2:B:198:THR:HG23	1.78	1.13
2:B:184:PRO:CG	2:B:399:PHE:CE2	1.90	1.13
2:B:193:GLN:O	2:B:265:LEU:HD22	0.96	1.13
1:A:206:ASN:HD22	1:A:227:LEU:HD21	0.97	1.13
1:A:62:VAL:HG13	1:A:63:PRO:CD	1.77	1.12
2:B:24:ILE:O	2:B:25:SER:C	1.80	1.12
1:A:57:GLY:HA3	1:A:61:HIS:CE1	1.83	1.12
1:A:266:HIS:CD2	1:A:432:TYR:CE1	2.38	1.12
1:A:312:TYR:CE2	1:A:377:MET:CE	2.32	1.12
2:B:36:TYR:CE2	2:B:244:PHE:HE1	1.46	1.12
2:B:107:HIS:CE1	2:B:152:LEU:HD21	1.84	1.12
2:B:135:PHE:HB3	2:B:166:MET:HE3	1.24	1.12
2:B:320:ARG:HG2	2:B:374:SER:OG	1.47	1.12
2:B:385:GLN:CG	2:B:389:LYS:HE3	1.79	1.12
1:A:31:GLN:NE2	1:A:243:ARG:HG3	1.56	1.12
1:A:62:VAL:HG12	1:A:63:PRO:HD2	1.24	1.12
1:A:182:VAL:CG1	1:A:186:ASN:ND2	2.12	1.12
2:B:102:ASN:HD22	2:B:105:LYS:NZ	1.45	1.12
1:A:38:SER:CA	1:A:39:ASP:N	2.11	1.12
1:A:97:GLU:CB	1:A:110:ILE:CG2	2.27	1.12
1:A:103:TYR:HD2	1:A:147:SER:CB	1.59	1.12
2:B:135:PHE:CG	2:B:166:MET:HE1	1.85	1.12
2:B:192:HIS:O	2:B:196:GLU:CG	1.98	1.12
2:B:286:LEU:HD11	2:B:372:LYS:HB2	1.13	1.12
2:B:287:THR:HG22	2:B:289:PRO:CD	1.79	1.12
2:B:390:ARG:O	2:B:394:GLN:HG2	1.46	1.12
2:B:154:ILE:HG21	2:B:198:THR:HG23	1.21	1.11
2:B:319:PHE:CD1	2:B:328:VAL:HG11	1.85	1.11
1:A:10:GLY:O	1:A:13:GLY:N	1.83	1.11
1:A:30:ILE:HG21	1:A:64:ARG:HG2	1.15	1.11
1:A:328:VAL:HG13	1:A:332:ILE:HD11	1.31	1.11
2:B:24:ILE:C	2:B:26:ASP:N	2.01	1.11
2:B:107:HIS:CA	2:B:152:LEU:CD1	2.25	1.11
2:B:107:HIS:NE2	2:B:152:LEU:HD23	1.64	1.11
2:B:192:HIS:C	2:B:196:GLU:HG3	1.73	1.11
1:A:179:THR:HG21	1:A:181:VAL:HB	1.13	1.11
1:A:184:PRO:CG	1:A:395:PHE:HD2	1.56	1.11
2:B:181:VAL:HG12	2:B:399:PHE:HZ	1.05	1.11
1:A:48:SER:OG	1:A:56:THR:HB	1.51	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:CB	1:A:148:GLY:CA	2.17	1.11
2:B:48:ARG:HH11	2:B:60:LYS:CA	1.62	1.11
2:B:135:PHE:CD2	2:B:166:MET:HE1	1.86	1.11
2:B:201:THR:CG2	2:B:265:LEU:HD11	1.79	1.11
2:B:295:MET:CE	2:B:375:ALA:CB	1.93	1.11
1:A:30:ILE:HB	1:A:64:ARG:HB2	1.24	1.11
1:A:397:LEU:HD22	1:A:401:LYS:HD2	1.27	1.11
2:B:107:HIS:CD2	2:B:152:LEU:CD2	2.34	1.11
2:B:176:LYS:HE3	2:B:207:GLU:OE2	1.49	1.11
2:B:385:GLN:HG3	2:B:389:LYS:HE3	1.21	1.11
2:B:192:HIS:C	2:B:196:GLU:CG	2.24	1.10
2:B:287:THR:CB	2:B:290:GLU:CB	2.23	1.10
1:A:97:GLU:HB3	1:A:110:ILE:CG2	1.81	1.10
1:A:177:VAL:HG12	1:A:178:SER:H	1.04	1.10
1:A:191:THR:HG21	1:A:421:ALA:CB	1.81	1.10
1:A:204:VAL:HG11	1:A:209:ILE:HD11	1.10	1.10
1:A:313:MET:HE1	1:A:346:TRP:CZ2	1.85	1.10
2:B:158:ARG:CB	2:B:197:ASN:ND2	2.10	1.10
1:A:2:ARG:O	1:A:31:GLN:HG3	1.51	1.10
1:A:266:HIS:NE2	1:A:432:TYR:HE1	1.48	1.10
2:B:107:HIS:CD2	2:B:152:LEU:CG	2.32	1.10
2:B:435:TYR:O	2:B:436:GLN:CD	1.95	1.10
1:A:59:GLY:C	1:A:62:VAL:O	1.95	1.10
1:A:210:TYR:CZ	1:A:227:LEU:HD22	1.87	1.10
1:A:420:GLU:CD	3:K:170:GLU:O	1.93	1.10
1:A:169:PHE:CZ	1:A:235:VAL:HG22	1.85	1.10
2:B:41:ASP:C	2:B:42:LEU:HG	1.76	1.10
1:A:3:GLU:CA	1:A:31:GLN:HB2	1.82	1.09
1:A:105:ARG:NH2	1:A:110:ILE:HD11	1.67	1.09
2:B:4:ILE:CD1	2:B:30:ILE:HA	1.83	1.09
2:B:66:ILE:HG13	2:B:121:VAL:CG1	1.82	1.09
2:B:312:TYR:HA	2:B:381:SER:HB3	1.30	1.09
1:A:277:SER:OG	1:A:280:LYS:HG2	0.93	1.09
2:B:158:ARG:CD	2:B:197:ASN:CB	2.09	1.09
2:B:242:LEU:N	2:B:356:CYS:SG	2.25	1.09
1:A:22:GLU:HG2	1:A:85:GLN:HE22	0.94	1.09
1:A:70:LEU:CG	1:A:145:THR:HG22	1.81	1.09
1:A:158:SER:HB3	1:A:197:HIS:CB	1.35	1.09
1:A:174:ALA:HB1	1:A:175:PRO:HD3	1.27	1.09
1:A:174:ALA:HB1	1:A:390:ARG:HH22	1.03	1.09
2:B:44:LEU:CD2	2:B:85:GLN:HG3	1.78	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:CA	2:B:278:ARG:CB	2.30	1.09
2:B:312:TYR:O	2:B:344:VAL:HG23	1.47	1.09
1:A:100:ALA:HB1	1:A:105:ARG:HD3	1.13	1.09
1:A:183:GLU:HB3	1:A:394:LYS:HB3	1.24	1.09
2:B:3:GLU:HA	2:B:31:ASP:CB	1.83	1.09
2:B:414:ASP:OD2	3:K:253:GLU:OE2	1.67	1.09
2:B:56:ALA:HB3	2:B:62:VAL:HB	1.35	1.09
2:B:94:PHE:O	2:B:94:PHE:CD1	2.05	1.09
2:B:135:PHE:CB	2:B:166:MET:HE1	1.80	1.09
3:K:18[B]:ARG:HH21	3:K:336:ILE:HD12	1.15	1.09
1:A:45:GLY:O	1:A:46:ASP:CG	1.96	1.08
1:A:108:TYR:CE2	1:A:417:GLU:OE2	2.06	1.08
1:A:349:THR:CB	2:B:177:VAL:HG12	1.58	1.08
2:B:3:GLU:C	2:B:4:ILE:HG13	1.77	1.08
2:B:7:ILE:CA	2:B:66:ILE:HG23	1.75	1.08
2:B:44:LEU:HD23	2:B:85:GLN:HG3	1.12	1.08
2:B:175:PRO:CD	2:B:390:ARG:HH21	1.66	1.08
1:A:100:ALA:HB2	1:A:105:ARG:HD3	1.18	1.08
1:A:184:PRO:HG3	1:A:395:PHE:HB2	1.33	1.08
1:A:217:LEU:HG	1:A:218:ASP:H	0.96	1.08
2:B:7:ILE:HG12	2:B:66:ILE:HD13	1.09	1.08
2:B:103:TRP:HZ3	2:B:108:TYR:OH	1.33	1.08
2:B:150:GLY:O	2:B:154:ILE:HG13	1.52	1.08
3:K:252:SER:O	3:K:253:GLU:HG2	1.53	1.08
1:A:103:TYR:CD1	1:A:188:ILE:HG21	1.86	1.08
1:A:332:ILE:HD13	1:A:353:VAL:HG21	1.35	1.08
2:B:233:ALA:HB1	2:B:272:PHE:CD2	1.87	1.08
1:A:204:VAL:HG12	1:A:209:ILE:HD11	1.09	1.08
1:A:262:TYR:HB3	1:A:263:PRO:CD	1.84	1.08
1:A:296:PHE:HE1	1:A:335:ILE:CD1	1.67	1.08
2:B:33:THR:H	2:B:59:ASN:ND2	1.47	1.08
2:B:56:ALA:HB3	2:B:62:VAL:CG2	1.81	1.08
2:B:80:SER:O	2:B:82:PRO:HD2	1.52	1.08
2:B:147:SER:OG	2:B:189:LEU:HD11	1.50	1.08
2:B:243:ARG:HH21	2:B:252:LEU:HD21	1.17	1.08
2:B:382:THR:HG21	2:B:436:GLN:OE1	1.51	1.08
1:A:237:SER:O	1:A:241:SER:OG	1.69	1.08
1:A:423:GLU:OE1	3:K:170:GLU:CG	2.01	1.08
2:B:44:LEU:C	2:B:47:GLU:HG3	1.79	1.08
2:B:405:LEU:HD21	2:B:418:PHE:CE2	1.82	1.08
1:A:26:LEU:HD11	1:A:361:THR:HG21	1.23	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:HG13	1:A:254:GLU:HB3	1.08	1.07
2:B:36:TYR:CD2	2:B:244:PHE:HE1	1.43	1.07
2:B:49:ILE:C	2:B:61:TYR:CD2	2.32	1.07
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.10	1.07
1:A:24:TYR:O	1:A:26:LEU:N	1.87	1.07
1:A:100:ALA:HB2	1:A:105:ARG:CD	1.80	1.07
1:A:250:VAL:HG21	1:A:352:LYS:HE2	1.13	1.07
2:B:69:ASP:CG	2:B:74:THR:HB	1.77	1.07
2:B:313:LEU:CD2	2:B:344:VAL:CG1	2.31	1.07
2:B:313:LEU:HD22	2:B:344:VAL:HG11	1.13	1.07
2:B:346:TRP:O	2:B:347:ILE:HB	1.50	1.07
1:A:184:PRO:CG	1:A:395:PHE:HA	1.84	1.07
1:A:292:THR:HG22	1:A:319:TYR:OH	1.53	1.07
2:B:33:THR:O	2:B:59:ASN:ND2	1.87	1.07
2:B:305:CYS:SG	2:B:384:ILE:CD1	2.41	1.07
1:A:171:ILE:N	1:A:203:MET:HE1	1.69	1.07
1:A:360:PRO:HG3	1:A:371:VAL:O	0.91	1.07
2:B:3:GLU:OE1	2:B:130:ASP:HB2	0.91	1.07
2:B:158:ARG:HD2	2:B:197:ASN:N	1.70	1.07
2:B:259:MET:CB	2:B:268:PHE:CE1	2.38	1.07
1:A:103:TYR:CD2	1:A:147:SER:CB	2.36	1.07
1:A:192:HIS:ND1	1:A:193:THR:N	2.03	1.06
2:B:48:ARG:HB2	2:B:61:TYR:HA	1.34	1.06
2:B:103:TRP:NE1	2:B:189:LEU:HD23	1.70	1.06
2:B:319:PHE:CE1	2:B:328:VAL:HG11	1.87	1.06
2:B:3:GLU:HB3	2:B:132:LEU:HD23	1.33	1.06
2:B:19:LYS:CD	2:B:228:ASN:HB2	1.84	1.06
2:B:35:SER:N	2:B:60:LYS:HE3	1.71	1.06
2:B:49:ILE:C	2:B:61:TYR:HD2	1.63	1.06
2:B:154:ILE:HD12	2:B:192:HIS:CE1	1.90	1.06
2:B:244:PHE:CG	2:B:245:PRO:HD2	1.89	1.06
2:B:397:ALA:HA	2:B:401:ARG:HD3	1.33	1.06
2:B:405:LEU:HD12	2:B:408:TYR:CG	1.88	1.06
2:B:102:ASN:HB2	2:B:105:LYS:HD2	1.33	1.06
1:A:78:VAL:HG11	1:A:87:PHE:HE1	1.19	1.06
1:A:103:TYR:CD1	1:A:188:ILE:HG22	1.89	1.06
2:B:102:ASN:HD22	2:B:105:LYS:HE3	1.17	1.06
2:B:141:LEU:CD1	2:B:172:VAL:HA	1.86	1.06
2:B:174:SER:OG	2:B:207:GLU:CB	2.02	1.06
2:B:178:SER:CB	5:B:501:GDP:O3'	2.03	1.06
1:A:103:TYR:OH	1:A:151:SER:CB	2.04	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:SER:OG	1:A:280:LYS:N	1.87	1.06
2:B:53:TYR:CD1	2:B:87:PHE:CZ	2.44	1.06
2:B:107:HIS:NE2	2:B:152:LEU:CD2	2.18	1.06
1:A:93:ILE:HD13	1:A:118:VAL:HG22	1.11	1.05
1:A:97:GLU:HB2	1:A:110:ILE:HG21	1.38	1.05
3:K:233:GLU:HG3	3:K:234:THR:H	0.90	1.05
1:A:70:LEU:HD12	1:A:145:THR:CB	1.86	1.05
2:B:7:ILE:CB	2:B:137:LEU:CD2	2.34	1.05
2:B:22:GLU:CB	2:B:83:PHE:CE2	2.39	1.05
2:B:75:MET:HE2	2:B:79:ARG:HD3	1.35	1.05
2:B:265:LEU:HD23	2:B:267:PHE:CZ	1.92	1.05
2:B:311:ARG:CG	2:B:341:SER:O	2.04	1.05
2:B:313:LEU:N	2:B:380:ASN:O	1.86	1.05
2:B:370:GLY:C	6:B:502:TXL:H183	1.81	1.05
2:B:107:HIS:HA	2:B:152:LEU:HD12	1.35	1.05
1:A:174:ALA:CB	1:A:175:PRO:HD2	1.86	1.05
1:A:324:VAL:HB	1:A:327:ASP:CG	1.82	1.05
2:B:48:ARG:HH11	2:B:60:LYS:HA	1.17	1.05
2:B:141:LEU:HD12	2:B:172:VAL:CA	1.86	1.05
2:B:259:MET:CE	2:B:379:GLY:CA	2.29	1.05
1:A:205:ASP:OD1	1:A:303:VAL:CG2	1.98	1.05
1:A:217:LEU:HD11	1:A:368:LEU:CD2	1.86	1.05
2:B:32:PRO:HB2	2:B:59:ASN:ND2	1.00	1.05
2:B:75:MET:HE1	2:B:79:ARG:HD2	1.06	1.05
2:B:75:MET:HA	2:B:75:MET:HE3	1.38	1.05
2:B:103:TRP:HD1	2:B:189:LEU:HD21	1.17	1.05
2:B:326:LYS:O	2:B:330:GLU:HG3	1.56	1.05
1:A:31:GLN:HE22	1:A:243:ARG:HG3	0.94	1.04
1:A:256:GLN:HB3	2:B:407:TRP:CH2	1.91	1.04
1:A:312:TYR:CD2	1:A:381:THR:CG2	2.40	1.04
1:A:45:GLY:O	1:A:46:ASP:CB	1.98	1.04
1:A:183:GLU:HB3	1:A:394:LYS:CB	1.87	1.04
2:B:24:ILE:C	2:B:26:ASP:H	1.55	1.04
2:B:102:ASN:OD1	2:B:408:TYR:CE1	2.09	1.04
2:B:44:LEU:HD21	2:B:86:ILE:N	1.67	1.04
2:B:70:LEU:CD1	2:B:94:PHE:HD2	1.47	1.04
2:B:244:PHE:CD2	2:B:245:PRO:CD	2.39	1.04
1:A:30:ILE:HB	1:A:64:ARG:CB	1.87	1.04
1:A:121:ARG:O	1:A:125:LEU:HG	1.56	1.04
1:A:306:ASP:OD1	1:A:308:ARG:CB	2.05	1.04
2:B:4:ILE:CD1	2:B:30:ILE:HG22	1.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:HD2	2:B:228:ASN:HB2	1.39	1.04
2:B:56:ALA:O	2:B:59:ASN:O	1.73	1.04
2:B:172:VAL:HG13	2:B:173:PRO:HD2	1.05	1.04
2:B:308:ARG:HD3	2:B:342:TYR:CE2	1.92	1.04
1:A:126:ALA:O	1:A:132:LEU:HD11	1.57	1.04
2:B:69:ASP:OD2	2:B:74:THR:CB	2.06	1.04
2:B:70:LEU:HD23	2:B:145:THR:HG22	1.04	1.04
2:B:147:SER:HB3	2:B:189:LEU:CG	1.77	1.04
2:B:147:SER:CA	2:B:189:LEU:CD1	2.36	1.04
1:A:32:PRO:O	1:A:34:GLY:N	1.89	1.03
1:A:62:VAL:HG13	1:A:63:PRO:HD2	1.07	1.03
1:A:155:GLU:CG	1:A:192:HIS:CD2	2.41	1.03
2:B:66:ILE:HG13	2:B:121:VAL:HG11	1.04	1.03
2:B:92:PHE:HD2	2:B:114:LEU:HD11	1.04	1.03
2:B:384:ILE:C	2:B:386:GLU:H	1.52	1.03
2:B:172:VAL:HG12	2:B:173:PRO:CD	1.88	1.03
2:B:275:LEU:HG	2:B:294:GLN:NE2	1.73	1.03
1:A:179:THR:HG21	1:A:181:VAL:CB	1.87	1.03
2:B:194:LEU:HA	2:B:265:LEU:CB	1.88	1.03
1:A:193:THR:O	1:A:194:THR:O	1.77	1.03
1:A:217:LEU:CD2	1:A:368:LEU:HD11	1.88	1.03
1:A:266:HIS:NE2	1:A:432:TYR:CE1	2.26	1.03
1:A:424:ASP:OD1	3:K:307:ARG:CZ	2.05	1.03
3:K:233:GLU:HG3	3:K:234:THR:N	1.73	1.03
2:B:78:VAL:O	2:B:82:PRO:HG2	1.59	1.02
2:B:275:LEU:HG	2:B:294:GLN:HE22	1.21	1.02
2:B:287:THR:O	2:B:291:LEU:HG	0.85	1.02
1:A:16:ILE:HD13	1:A:138:PHE:HD1	0.88	1.02
2:B:4:ILE:HD12	2:B:30:ILE:O	1.57	1.02
2:B:6:HIS:CE1	2:B:30:ILE:CD1	2.32	1.02
2:B:145:THR:O	2:B:149:MET:CB	2.05	1.02
1:A:191:THR:O	1:A:194:THR:HB	1.56	1.02
2:B:7:ILE:HG12	2:B:66:ILE:HG21	1.34	1.02
2:B:80:SER:O	2:B:82:PRO:CD	2.07	1.02
2:B:384:ILE:C	2:B:386:GLU:N	2.11	1.02
2:B:414:ASP:HB2	3:K:253:GLU:CD	1.83	1.02
1:A:206:ASN:O	1:A:210:TYR:HD2	1.41	1.02
1:A:328:VAL:HG13	1:A:332:ILE:CD1	1.90	1.02
2:B:23:VAL:HG22	6:B:502:TXL:H333	1.41	1.02
2:B:268:PHE:CD1	2:B:380:ASN:ND2	2.28	1.02
1:A:4:CYS:HB2	1:A:30:ILE:HG23	1.03	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ALA:HA	2:B:413:MET:HE3	1.38	1.02
2:B:107:HIS:CE1	2:B:152:LEU:CD2	2.42	1.02
1:A:70:LEU:CG	1:A:145:THR:CG2	2.36	1.01
1:A:252:LEU:HA	1:A:255:PHE:HD2	1.18	1.01
2:B:19:LYS:HB2	2:B:228:ASN:HB3	1.42	1.01
2:B:151:THR:CG2	2:B:192:HIS:ND1	2.14	1.01
2:B:175:PRO:O	2:B:176:LYS:HG2	1.49	1.01
2:B:190:SER:O	2:B:193:GLN:N	1.92	1.01
2:B:201:THR:HG23	2:B:265:LEU:CD1	1.91	1.01
1:A:115:ILE:HD11	1:A:152:LEU:HG	1.40	1.01
1:A:405:VAL:HG22	1:A:409:VAL:HG23	1.39	1.01
2:B:22:GLU:CD	2:B:83:PHE:CG	2.39	1.01
2:B:107:HIS:C	2:B:152:LEU:CD1	2.27	1.01
2:B:286:LEU:CD1	2:B:372:LYS:CB	2.39	1.01
1:A:2:ARG:HG2	1:A:133:GLN:CD	1.85	1.00
1:A:108:TYR:O	1:A:112:LYS:HD2	1.61	1.00
1:A:296:PHE:CZ	1:A:335:ILE:HG21	1.95	1.00
2:B:200:GLU:OE2	2:B:256:ALA:HA	1.56	1.00
2:B:260:VAL:CG1	2:B:262:PHE:O	2.08	1.00
2:B:384:ILE:O	2:B:386:GLU:N	1.93	1.00
2:B:385:GLN:CG	2:B:389:LYS:CE	2.37	1.00
1:A:103:TYR:HD2	1:A:189:LEU:CD2	1.59	1.00
1:A:343:PHE:HE2	1:A:351:PHE:HZ	1.08	1.00
2:B:242:LEU:HD22	2:B:250:ALA:H	1.23	1.00
2:B:396:THR:OG1	2:B:422:GLU:OE2	1.79	1.00
2:B:422:GLU:O	2:B:426:ASN:HB2	1.60	1.00
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.42	1.00
2:B:343:PHE:HB3	2:B:350:ASN:HD22	1.26	1.00
2:B:101:ASN:O	2:B:102:ASN:CG	2.05	1.00
2:B:103:TRP:NE1	2:B:148:GLY:HA2	1.75	1.00
1:A:103:TYR:CE1	1:A:188:ILE:HG22	1.96	1.00
1:A:143:GLY:O	1:A:146:GLY:N	1.95	1.00
1:A:431:ASP:HA	3:K:303:PHE:CD1	1.96	1.00
2:B:296:PHE:CE1	2:B:335:VAL:HG11	1.96	1.00
2:B:313:LEU:HA	2:B:344:VAL:HG21	1.43	1.00
2:B:194:LEU:HA	2:B:265:LEU:HB3	1.44	1.00
2:B:320:ARG:HG2	2:B:374:SER:HG	1.25	1.00
2:B:405:LEU:HD12	2:B:408:TYR:HB2	1.03	1.00
1:A:88:HIS:CG	1:A:89:PRO:HD2	1.95	1.00
1:A:174:ALA:CB	1:A:390:ARG:HH22	1.75	1.00
1:A:185:TYR:CD2	1:A:408:TYR:OH	1.85	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:CG2	1:A:219:ILE:CG1	2.40	1.00
1:A:433:GLU:O	1:A:437:VAL:CG2	2.10	1.00
2:B:243:ARG:NH2	2:B:252:LEU:HD11	1.77	1.00
2:B:343:PHE:HD1	2:B:350:ASN:CG	1.67	1.00
1:A:312:TYR:O	1:A:344:VAL:HG23	1.58	0.99
1:A:397:LEU:CD2	1:A:401:LYS:CD	2.40	0.99
1:A:424:ASP:HA	3:K:307:ARG:NH2	1.77	0.99
2:B:111:GLY:O	2:B:115:VAL:N	1.95	0.99
2:B:181:VAL:HG22	2:B:404:PHE:CE2	1.97	0.99
2:B:275:LEU:HD11	2:B:300:ASN:ND2	1.78	0.99
2:B:284:ARG:HD2	2:B:290:GLU:OE1	1.62	0.99
1:A:45:GLY:O	1:A:46:ASP:HB2	1.60	0.99
1:A:145:THR:O	1:A:149:PHE:HB3	1.62	0.99
2:B:192:HIS:CB	2:B:196:GLU:HG3	1.90	0.99
1:A:256:GLN:O	1:A:260:VAL:HG23	1.61	0.99
2:B:191:VAL:HG21	2:B:421:ALA:HA	1.42	0.99
2:B:312:TYR:HA	2:B:381:SER:HA	1.43	0.99
1:A:184:PRO:CD	1:A:395:PHE:HA	1.91	0.99
1:A:276:ILE:HD12	1:A:371:VAL:HG22	1.41	0.99
1:A:397:LEU:HD22	1:A:401:LYS:CD	1.93	0.99
1:A:31:GLN:HE22	1:A:243:ARG:CD	1.67	0.99
2:B:44:LEU:HD11	2:B:86:ILE:O	1.63	0.99
1:A:204:VAL:HG23	1:A:231:ILE:HG23	1.41	0.99
1:A:104:ALA:HA	1:A:108:TYR:CD2	1.97	0.99
1:A:174:ALA:HB3	1:A:175:PRO:HD2	1.44	0.99
1:A:269:LEU:O	1:A:378:LEU:HA	1.61	0.99
1:A:78:VAL:CG1	1:A:87:PHE:CE1	2.46	0.99
1:A:205:ASP:CB	1:A:303:VAL:HA	1.92	0.99
1:A:313:MET:HE1	1:A:346:TRP:CH2	1.97	0.99
1:A:343:PHE:CZ	1:A:351:PHE:CZ	2.50	0.99
1:A:416:GLY:CA	3:K:169:ARG:NH2	2.25	0.99
2:B:70:LEU:HD11	2:B:94:PHE:CD2	1.92	0.99
1:A:242:LEU:HB3	1:A:250:VAL:O	1.63	0.99
1:A:270:ALA:O	1:A:302:MET:HG2	1.63	0.99
1:A:312:TYR:O	1:A:344:VAL:HG22	1.62	0.99
1:A:22:GLU:HG2	1:A:85:GLN:NE2	1.78	0.98
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.58	0.98
2:B:199:ASP:OD2	2:B:256:ALA:HB2	1.62	0.98
2:B:405:LEU:HD22	2:B:418:PHE:CE1	1.98	0.98
2:B:70:LEU:HD23	2:B:145:THR:CG2	1.93	0.98
2:B:155:SER:O	2:B:159:GLU:HG3	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:PHE:HD1	2:B:350:ASN:ND2	1.62	0.98
1:A:42:ILE:O	1:A:42:ILE:HG22	1.60	0.98
1:A:72:PRO:O	1:A:76:ASP:N	1.96	0.98
1:A:97:GLU:HB3	1:A:110:ILE:HG21	1.36	0.98
2:B:154:ILE:CG2	2:B:198:THR:CG2	2.40	0.98
1:A:103:TYR:CE2	1:A:189:LEU:HA	1.98	0.98
2:B:102:ASN:HB2	2:B:105:LYS:CD	1.92	0.98
2:B:173:PRO:CG	2:B:391:ILE:HD11	1.92	0.98
2:B:275:LEU:CD1	2:B:294:GLN:HE21	1.75	0.98
2:B:279:GLY:C	2:B:281:GLN:H	1.62	0.98
2:B:79:ARG:O	2:B:80:SER:CB	2.10	0.98
1:A:51:THR:HG22	1:A:52:PHE:N	1.74	0.98
1:A:68:VAL:CG1	1:A:149:PHE:CZ	2.47	0.98
1:A:76:ASP:O	1:A:80:THR:N	1.97	0.98
2:B:174:SER:OG	2:B:207:GLU:HB2	1.63	0.98
1:A:30:ILE:O	1:A:32:PRO:CD	2.08	0.98
2:B:36:TYR:CD2	2:B:244:PHE:CE1	2.22	0.98
2:B:173:PRO:HG3	2:B:391:ILE:HD11	1.45	0.98
2:B:286:LEU:HD11	2:B:371:LEU:O	1.62	0.98
2:B:182:VAL:HG13	2:B:186:ASN:HD22	1.29	0.97
1:A:101:ASN:O	1:A:102:ASN:ND2	1.97	0.97
1:A:206:ASN:ND2	1:A:227:LEU:HD23	1.79	0.97
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.46	0.97
2:B:6:HIS:HB2	2:B:65:ALA:HA	1.46	0.97
2:B:102:ASN:ND2	2:B:105:LYS:NZ	2.12	0.97
2:B:103:TRP:CD1	2:B:148:GLY:CA	2.48	0.97
2:B:201:THR:HG23	2:B:265:LEU:HD11	0.97	0.97
1:A:194:THR:HG22	1:A:195:LEU:HG	1.44	0.97
1:A:419:SER:HB2	3:K:172:PRO:HB3	1.46	0.97
1:A:429:GLU:O	1:A:433:GLU:HG3	1.63	0.97
2:B:181:VAL:HG13	2:B:399:PHE:CE1	1.97	0.97
2:B:414:ASP:CB	3:K:253:GLU:CD	2.37	0.97
1:A:51:THR:HG22	1:A:52:PHE:H	1.26	0.97
1:A:115:ILE:HG21	1:A:152:LEU:HD21	1.45	0.97
1:A:241:SER:HB2	1:A:356:ASN:ND2	1.78	0.97
1:A:250:VAL:HG13	1:A:254:GLU:HG2	1.44	0.97
2:B:142:GLY:CA	2:B:182:VAL:HG22	1.94	0.97
2:B:262:PHE:HB3	2:B:263:PRO:HD2	1.43	0.97
1:A:36:MET:SD	1:A:61:HIS:N	2.33	0.97
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.06	0.97
1:A:217:LEU:CD1	1:A:368:LEU:HD21	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:CG1	1:A:150:THR:CG2	2.42	0.97
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.29	0.97
1:A:177:VAL:CG1	1:A:178:SER:H	1.78	0.97
1:A:241:SER:HB2	1:A:356:ASN:HD22	1.27	0.97
1:A:310:GLY:O	1:A:342:GLN:OE1	1.82	0.97
1:A:115:ILE:HD13	1:A:156:ARG:NE	1.80	0.97
1:A:217:LEU:HD13	1:A:368:LEU:HD11	1.02	0.97
1:A:313:MET:CE	1:A:346:TRP:CH2	2.47	0.97
2:B:68:VAL:HG11	2:B:149:MET:HE2	1.47	0.97
1:A:107:HIS:HB2	1:A:148:GLY:HA3	1.01	0.97
2:B:111:GLY:O	2:B:115:VAL:CG2	2.12	0.97
2:B:7:ILE:HB	2:B:137:LEU:HD23	1.01	0.96
2:B:33:THR:N	2:B:59:ASN:ND2	2.04	0.96
2:B:158:ARG:CA	2:B:197:ASN:ND2	1.74	0.96
3:K:233:GLU:CG	3:K:234:THR:H	1.76	0.96
1:A:424:ASP:CA	3:K:307:ARG:CZ	2.43	0.96
2:B:19:LYS:CG	2:B:228:ASN:HB2	1.86	0.96
2:B:206:ASN:O	2:B:210:TYR:CE2	2.18	0.96
2:B:206:ASN:O	2:B:210:TYR:CD2	2.18	0.96
1:A:107:HIS:CB	1:A:148:GLY:C	2.36	0.96
2:B:70:LEU:HD11	2:B:94:PHE:CE2	2.00	0.96
2:B:229:HIS:CD2	6:B:502:TXL:H37	1.98	0.96
1:A:108:TYR:HA	1:A:112:LYS:HE3	1.47	0.96
2:B:7:ILE:CB	2:B:137:LEU:HD23	1.95	0.96
1:A:78:VAL:HG11	1:A:87:PHE:CE1	2.00	0.96
1:A:177:VAL:HG12	1:A:178:SER:N	1.79	0.96
2:B:3:GLU:HG2	2:B:4:ILE:H	1.27	0.96
2:B:39:ASP:O	2:B:40:SER:OG	1.82	0.96
2:B:405:LEU:HD11	2:B:408:TYR:HB3	1.44	0.96
1:A:2:ARG:NH2	2:B:71:GLU:CB	2.22	0.96
1:A:204:VAL:HG12	1:A:209:ILE:CD1	1.87	0.96
1:A:422:ARG:O	1:A:426:ALA:HB2	1.63	0.96
2:B:229:HIS:HE1	6:B:502:TXL:H343	1.30	0.96
2:B:229:HIS:HD2	6:B:502:TXL:C38	1.47	0.96
2:B:287:THR:CG2	2:B:289:PRO:CD	2.38	0.96
1:A:31:GLN:N	1:A:32:PRO:HD2	1.81	0.96
2:B:260:VAL:HG13	2:B:266:HIS:ND1	1.78	0.96
2:B:346:TRP:CE3	2:B:347:ILE:CD1	2.43	0.96
1:A:119:LEU:HD11	1:A:156:ARG:HD3	1.48	0.96
1:A:191:THR:O	1:A:194:THR:CB	2.14	0.96
1:A:420:GLU:CD	3:K:170:GLU:H	1.73	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:VAL:C	2:B:82:PRO:HG2	1.91	0.96
2:B:208:ALA:CB	2:B:303:ALA:O	2.13	0.96
1:A:68:VAL:HG11	1:A:149:PHE:HZ	1.30	0.95
1:A:333:ALA:O	1:A:337:THR:HG23	1.66	0.95
2:B:275:LEU:HD12	2:B:294:GLN:HE21	1.29	0.95
1:A:372:GLN:O	1:A:373:ARG:HG3	1.65	0.95
2:B:53:TYR:HE1	2:B:89:PRO:HG3	1.29	0.95
2:B:346:TRP:O	2:B:347:ILE:CB	2.09	0.95
1:A:68:VAL:HG11	1:A:149:PHE:CE1	2.01	0.95
1:A:250:VAL:CG2	1:A:352:LYS:CE	2.43	0.95
1:A:309:HIS:CG	1:A:386:GLU:OE2	2.19	0.95
2:B:181:VAL:O	2:B:399:PHE:CE2	2.19	0.95
1:A:212:ILE:HD13	1:A:230:LEU:HD21	1.49	0.95
1:A:424:ASP:CA	3:K:307:ARG:NH2	2.30	0.95
1:A:426:ALA:O	1:A:429:GLU:N	2.00	0.95
2:B:243:ARG:HH21	2:B:252:LEU:CD2	1.78	0.95
2:B:346:TRP:CZ3	2:B:347:ILE:CG1	2.45	0.95
1:A:2:ARG:HH21	2:B:71:GLU:HB3	0.79	0.95
1:A:171:ILE:N	1:A:203:MET:CE	2.24	0.95
1:A:141:PHE:O	1:A:182:VAL:HG13	1.66	0.95
2:B:158:ARG:CG	2:B:197:ASN:CG	2.38	0.95
1:A:184:PRO:CB	1:A:395:PHE:CD2	2.45	0.95
2:B:4:ILE:CD1	2:B:30:ILE:O	2.14	0.95
2:B:79:ARG:O	2:B:80:SER:HB3	1.66	0.95
2:B:151:THR:HG22	2:B:192:HIS:CD2	1.96	0.95
2:B:426:ASN:O	2:B:429:VAL:N	2.00	0.95
1:A:16:ILE:CD1	1:A:138:PHE:HD1	1.78	0.95
1:A:229:ARG:O	1:A:233:GLN:HG3	1.66	0.95
2:B:3:GLU:HA	2:B:31:ASP:HB3	1.47	0.95
2:B:151:THR:HB	2:B:192:HIS:HD2	1.31	0.95
2:B:147:SER:HA	2:B:189:LEU:HD13	1.47	0.95
2:B:274:PRO:O	2:B:276:THR:HG23	1.67	0.95
2:B:287:THR:HG21	2:B:289:PRO:HG2	1.49	0.95
1:A:53:PHE:N	1:A:88:HIS:HE2	1.54	0.95
1:A:158:SER:HB2	1:A:197:HIS:CB	1.67	0.95
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.49	0.95
1:A:314:ALA:HB3	1:A:380:ASN:HD22	1.31	0.95
2:B:259:MET:HB3	2:B:268:PHE:CZ	2.02	0.95
1:A:141:PHE:O	1:A:186:ASN:ND2	1.58	0.94
2:B:4:ILE:CD1	2:B:30:ILE:C	2.40	0.94
2:B:398:MET:O	2:B:401:ARG:HB3	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:SER:OG	2:B:207:GLU:HB3	1.65	0.94
1:A:3:GLU:O	1:A:132:LEU:C	2.08	0.94
1:A:59:GLY:CA	1:A:62:VAL:O	2.15	0.94
2:B:184:PRO:CD	2:B:399:PHE:CE2	2.37	0.94
1:A:20:CYS:O	1:A:24:TYR:HD2	1.46	0.94
1:A:252:LEU:HA	1:A:255:PHE:CD2	2.02	0.94
1:A:294:ALA:O	1:A:300:ASN:ND2	1.99	0.94
1:A:257:THR:CG2	2:B:407:TRP:CE3	2.50	0.94
1:A:405:VAL:CG2	1:A:405:VAL:CG1	2.44	0.94
2:B:19:LYS:HG3	2:B:228:ASN:HB2	1.43	0.94
2:B:103:TRP:CZ3	2:B:413:MET:HE2	2.03	0.94
2:B:241:CYS:SG	2:B:320:ARG:HD3	2.08	0.94
2:B:287:THR:HG22	2:B:290:GLU:H	1.29	0.94
2:B:382:THR:HG23	2:B:436:GLN:OE1	1.64	0.94
1:A:3:GLU:HA	1:A:31:GLN:HB2	0.94	0.94
1:A:30:ILE:C	1:A:32:PRO:HD3	1.81	0.94
2:B:56:ALA:HB1	2:B:60:LYS:O	1.68	0.94
2:B:433:GLN:HG2	2:B:437:ASP:OD2	1.65	0.94
1:A:103:TYR:CE2	1:A:189:LEU:CD2	2.38	0.94
1:A:212:ILE:HD11	1:A:230:LEU:HD22	0.96	0.94
1:A:217:LEU:HD22	1:A:368:LEU:HD11	1.47	0.94
2:B:182:VAL:CG1	2:B:186:ASN:ND2	2.30	0.94
1:A:65:ALA:CB	1:A:91:GLN:OE1	2.16	0.94
2:B:126:SER:HA	2:B:132:LEU:HD12	1.50	0.94
2:B:295:MET:CE	2:B:375:ALA:CA	2.45	0.94
2:B:319:PHE:HE1	2:B:353:THR:HG23	0.77	0.94
1:A:220:GLU:C	1:A:222:PRO:CD	2.37	0.93
2:B:15:GLN:OE1	5:B:501:GDP:O6	1.84	0.93
2:B:158:ARG:CD	2:B:197:ASN:CA	2.39	0.93
1:A:343:PHE:CE2	1:A:351:PHE:HZ	1.81	0.93
1:A:397:LEU:HA	1:A:401:LYS:CB	1.96	0.93
2:B:97:SER:O	2:B:110:GLU:OE2	1.84	0.93
1:A:36:MET:SD	1:A:61:HIS:CA	2.56	0.93
1:A:119:LEU:O	1:A:122:ILE:HG22	1.65	0.93
1:A:369:ALA:HB2	1:A:371:VAL:HG23	1.46	0.93
2:B:19:LYS:HG3	2:B:228:ASN:CG	1.93	0.93
1:A:64:ARG:NH2	1:A:132:LEU:CD2	2.05	0.93
2:B:48:ARG:NH1	2:B:60:LYS:HA	1.83	0.93
1:A:154:MET:HE3	1:A:166:LYS:HD3	1.50	0.93
1:A:181:VAL:O	1:A:184:PRO:O	1.87	0.93
1:A:272:TYR:CD1	1:A:274:PRO:O	2.22	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:CA	1:A:381:THR:HG22	1.99	0.93
2:B:33:THR:C	2:B:59:ASN:HD21	1.76	0.93
2:B:151:THR:HG22	2:B:192:HIS:NE2	1.83	0.93
2:B:184:PRO:CD	2:B:398:MET:SD	2.57	0.93
2:B:274:PRO:HB3	2:B:371:LEU:HD21	1.50	0.93
2:B:343:PHE:CD1	2:B:350:ASN:ND2	2.37	0.93
3:K:159:ASN:HD22	3:K:161:LYS:HG3	1.26	0.93
1:A:217:LEU:CD1	1:A:368:LEU:CD2	2.46	0.93
1:A:250:VAL:HG22	1:A:352:LYS:HE2	1.49	0.93
2:B:48:ARG:NH1	2:B:60:LYS:CA	2.31	0.93
2:B:343:PHE:HB3	2:B:350:ASN:ND2	1.83	0.93
1:A:32:PRO:C	1:A:34:GLY:H	1.69	0.93
1:A:258:ASN:OD1	1:A:352:LYS:HD2	1.69	0.93
2:B:142:GLY:HA2	2:B:185:TYR:CD1	2.03	0.93
1:A:15:GLN:HA	1:A:18:ASN:ND2	1.83	0.93
1:A:204:VAL:CG2	1:A:231:ILE:CG2	2.24	0.93
1:A:230:LEU:HG	1:A:302:MET:HE1	1.51	0.93
2:B:142:GLY:HA2	2:B:182:VAL:HG22	1.49	0.93
2:B:154:ILE:HD12	2:B:192:HIS:NE2	1.83	0.93
1:A:250:VAL:CG1	1:A:254:GLU:CG	2.46	0.93
1:A:405:VAL:CG2	1:A:409:VAL:HG23	1.98	0.93
2:B:101:ASN:O	2:B:102:ASN:CB	2.17	0.93
3:K:252:SER:HA	3:K:275:LEU:HD11	1.50	0.93
1:A:108:TYR:O	1:A:112:LYS:CG	2.17	0.92
1:A:180:ALA:HB1	1:A:398:MET:HE3	1.51	0.92
1:A:217:LEU:HG	1:A:218:ASP:N	1.76	0.92
1:A:256:GLN:O	1:A:260:VAL:CG2	2.16	0.92
1:A:369:ALA:HB3	1:A:371:VAL:HG23	1.50	0.92
1:A:83:TYR:CD2	1:A:83:TYR:O	2.22	0.92
1:A:155:GLU:HG2	1:A:196:GLU:HG3	1.51	0.92
1:A:423:GLU:OE2	3:K:172:PRO:CA	2.17	0.92
2:B:7:ILE:CA	2:B:66:ILE:CG2	2.38	0.92
2:B:106:GLY:O	2:B:111:GLY:HA3	1.70	0.92
2:B:183:GLU:CD	2:B:394:GLN:CB	2.41	0.92
2:B:275:LEU:CG	2:B:294:GLN:NE2	2.32	0.92
1:A:31:GLN:HE22	1:A:243:ARG:CB	1.81	0.92
1:A:59:GLY:HA2	1:A:62:VAL:O	1.70	0.92
1:A:106:GLY:O	1:A:111:GLY:HA3	1.70	0.92
1:A:53:PHE:CA	1:A:88:HIS:NE2	2.20	0.92
1:A:107:HIS:CD2	1:A:148:GLY:O	2.23	0.92
1:A:258:ASN:CG	1:A:352:LYS:HD2	1.93	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:HIS:ND1	2:B:152:LEU:HD21	1.85	0.92
2:B:386:GLU:O	2:B:388:PHE:N	2.01	0.92
1:A:238:ILE:HG23	1:A:255:PHE:CE1	2.05	0.92
1:A:250:VAL:HG22	1:A:254:GLU:HG2	1.50	0.92
1:A:288:VAL:HG22	1:A:373:ARG:HD3	0.93	0.92
3:K:216:ARG:HH11	3:K:216:ARG:HG3	1.33	0.92
1:A:277:SER:H	1:A:280:LYS:CG	1.82	0.92
1:A:349:THR:CG2	2:B:177:VAL:CG1	2.46	0.92
1:A:420:GLU:OE1	3:K:170:GLU:O	1.87	0.92
1:A:428:LEU:O	1:A:432:TYR:HB2	1.70	0.92
2:B:71:GLU:O	2:B:73:GLY:N	2.01	0.92
1:A:59:GLY:O	1:A:62:VAL:C	2.12	0.92
1:A:158:SER:HB3	1:A:197:HIS:HB2	1.51	0.92
1:A:184:PRO:CG	1:A:395:PHE:CA	2.47	0.92
1:A:184:PRO:CG	1:A:395:PHE:CB	2.45	0.92
2:B:33:THR:H	2:B:59:ASN:HD22	0.93	0.92
2:B:433:GLN:HG2	2:B:437:ASP:CG	1.95	0.92
1:A:107:HIS:HD2	1:A:148:GLY:O	1.51	0.91
2:B:49:ILE:CA	2:B:61:TYR:HD2	1.82	0.91
2:B:70:LEU:CD2	2:B:145:THR:HG22	1.98	0.91
2:B:104:ALA:HA	2:B:108:TYR:HD2	1.20	0.91
2:B:239:THR:C	2:B:243:ARG:HD2	1.95	0.91
1:A:383:ALA:O	1:A:384:ILE:C	2.07	0.91
2:B:181:VAL:O	2:B:399:PHE:HE2	1.50	0.91
2:B:8:GLN:HE21	2:B:21:TRP:NE1	1.68	0.91
2:B:158:ARG:HD2	2:B:197:ASN:HA	1.52	0.91
2:B:241:CYS:O	2:B:242:LEU:HB2	1.69	0.91
1:A:332:ILE:HD13	1:A:353:VAL:CG2	1.99	0.91
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.05	0.91
2:B:126:SER:HA	2:B:132:LEU:CD1	2.01	0.91
2:B:19:LYS:CB	2:B:228:ASN:CB	2.40	0.91
2:B:70:LEU:CD1	2:B:94:PHE:CE2	2.52	0.91
2:B:103:TRP:HE3	2:B:413:MET:HE1	1.09	0.91
1:A:26:LEU:CD1	1:A:361:THR:OG1	2.19	0.91
1:A:103:TYR:HE2	1:A:189:LEU:HA	1.32	0.91
1:A:103:TYR:CG	1:A:188:ILE:CG2	2.54	0.91
1:A:277:SER:H	1:A:280:LYS:HG3	1.34	0.91
1:A:349:THR:CG2	2:B:177:VAL:HG12	2.00	0.91
2:B:44:LEU:CD2	2:B:86:ILE:H	1.61	0.91
2:B:319:PHE:CZ	2:B:328:VAL:CG1	2.54	0.91
2:B:24:ILE:O	2:B:27:GLU:N	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:GLY:O	2:B:58:GLY:C	2.14	0.91
2:B:158:ARG:HG3	2:B:197:ASN:CG	1.94	0.91
2:B:184:PRO:CB	2:B:399:PHE:CG	2.41	0.91
2:B:102:ASN:ND2	2:B:105:LYS:CE	2.33	0.91
2:B:260:VAL:HG12	2:B:262:PHE:O	1.69	0.91
1:A:9:VAL:HG11	1:A:150:THR:HG21	1.53	0.91
1:A:100:ALA:HB1	1:A:105:ARG:CD	1.91	0.91
1:A:115:ILE:HD13	1:A:152:LEU:CG	2.01	0.91
1:A:250:VAL:HG22	1:A:352:LYS:CE	2.00	0.91
2:B:385:GLN:HE22	2:B:433:GLN:CD	1.79	0.91
2:B:229:HIS:CB	6:B:502:TXL:H38	2.01	0.90
2:B:229:HIS:NE2	6:B:502:TXL:H343	1.82	0.90
2:B:312:TYR:CA	2:B:381:SER:HB3	2.01	0.90
1:A:420:GLU:OE2	3:K:170:GLU:O	1.89	0.90
2:B:11:GLN:HB3	5:B:501:GDP:PA	2.11	0.90
2:B:14:ASN:HB3	2:B:74:THR:CG2	2.01	0.90
2:B:56:ALA:HB3	2:B:62:VAL:HG23	1.54	0.90
2:B:143:GLY:O	5:B:501:GDP:O3B	1.89	0.90
2:B:268:PHE:HE1	2:B:380:ASN:ND2	1.65	0.90
1:A:72:PRO:O	1:A:75:ILE:CG2	2.19	0.90
1:A:328:VAL:CG1	1:A:353:VAL:HG11	2.00	0.90
2:B:66:ILE:CG1	2:B:121:VAL:HG11	1.99	0.90
1:A:254:GLU:OE1	2:B:101:ASN:OD1	1.87	0.90
1:A:305:CYS:O	1:A:307:PRO:HD3	1.71	0.90
2:B:200:GLU:HB3	2:B:268:PHE:HE2	1.37	0.90
2:B:405:LEU:CD2	2:B:418:PHE:HZ	1.84	0.90
2:B:44:LEU:CG	2:B:85:GLN:HG3	2.02	0.90
2:B:75:MET:HE1	2:B:79:ARG:CD	1.93	0.90
2:B:158:ARG:HA	2:B:197:ASN:HD21	1.35	0.90
2:B:183:GLU:HB2	2:B:184:PRO:HD3	0.90	0.90
2:B:229:HIS:CG	6:B:502:TXL:C38	2.41	0.90
1:A:257:THR:HG22	2:B:407:TRP:HE3	1.36	0.90
2:B:185:TYR:O	2:B:189:LEU:HG	1.72	0.90
2:B:243:ARG:NH2	2:B:252:LEU:HD21	1.86	0.90
1:A:184:PRO:HB3	1:A:395:PHE:HD2	1.33	0.90
2:B:39:ASP:O	2:B:40:SER:CB	2.16	0.90
2:B:259:MET:CB	2:B:268:PHE:CZ	2.55	0.90
2:B:275:LEU:CD1	2:B:294:GLN:NE2	2.35	0.90
1:A:67:PHE:HB2	1:A:92:LEU:HD23	1.53	0.90
1:A:312:TYR:CD2	1:A:381:THR:HG21	2.06	0.90
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:LEU:CD1	2:B:418:PHE:HZ	1.85	0.90
1:A:5:ILE:HG21	1:A:135:PHE:HE1	1.35	0.90
1:A:107:HIS:CG	1:A:148:GLY:CA	2.54	0.90
1:A:328:VAL:HG12	1:A:332:ILE:HD12	1.53	0.90
2:B:4:ILE:HD13	2:B:30:ILE:HG22	0.93	0.90
2:B:86:ILE:HD12	2:B:91:ASN:HD21	1.33	0.90
1:A:204:VAL:HG11	1:A:209:ILE:CD1	1.92	0.90
1:A:206:ASN:O	1:A:210:TYR:CD2	2.25	0.90
2:B:151:THR:CG2	2:B:192:HIS:NE2	2.35	0.90
1:A:383:ALA:C	1:A:385:ALA:N	2.23	0.89
1:A:405:VAL:HG22	1:A:409:VAL:CG2	2.01	0.89
2:B:102:ASN:ND2	2:B:105:LYS:HE3	1.85	0.89
2:B:192:HIS:HA	2:B:196:GLU:HG2	1.53	0.89
2:B:94:PHE:CD1	2:B:97:SER:HB3	2.06	0.89
2:B:189:LEU:O	2:B:193:GLN:CG	2.19	0.89
2:B:312:TYR:CA	2:B:381:SER:CB	2.49	0.89
2:B:369:ARG:O	6:B:502:TXL:O9	1.88	0.89
1:A:93:ILE:HD13	1:A:118:VAL:CG2	2.01	0.89
1:A:155:GLU:O	1:A:159:VAL:HG23	1.72	0.89
1:A:276:ILE:O	1:A:368:LEU:CB	2.21	0.89
1:A:420:GLU:OE1	3:K:170:GLU:N	2.05	0.89
2:B:172:VAL:HG11	2:B:387:LEU:HD11	1.54	0.89
2:B:184:PRO:HD2	2:B:399:PHE:CE2	2.06	0.89
2:B:234:THR:CB	2:B:302:MET:HE1	2.03	0.89
2:B:278:ARG:O	2:B:281:GLN:HB3	1.71	0.89
1:A:431:ASP:HA	3:K:303:PHE:CE1	2.07	0.89
2:B:239:THR:O	2:B:243:ARG:HD2	0.72	0.89
1:A:100:ALA:HB1	1:A:105:ARG:HB3	1.55	0.89
1:A:194:THR:HG22	1:A:195:LEU:H	1.38	0.89
2:B:25:SER:O	2:B:27:GLU:HG3	1.73	0.89
2:B:311:ARG:O	2:B:382:THR:N	2.05	0.89
1:A:64:ARG:HH22	1:A:132:LEU:HD22	0.76	0.89
1:A:72:PRO:HA	1:A:75:ILE:CG2	2.02	0.89
1:A:103:TYR:H	1:A:408:TYR:HE1	0.96	0.89
1:A:183:GLU:OE2	1:A:394:LYS:NZ	1.77	0.89
1:A:250:VAL:HG13	1:A:352:LYS:NZ	1.86	0.89
2:B:80:SER:O	2:B:82:PRO:N	2.05	0.89
1:A:291:ILE:CD1	1:A:373:ARG:HB3	2.03	0.89
1:A:326:LYS:NZ	2:B:214:PHE:CE2	2.40	0.89
1:A:4:CYS:CB	1:A:30:ILE:HG23	1.99	0.89
1:A:276:ILE:HG21	1:A:282:TYR:CD1	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:HE21	2:B:21:TRP:HE1	1.21	0.89
2:B:173:PRO:HG3	2:B:391:ILE:CD1	2.03	0.89
2:B:405:LEU:HD13	2:B:408:TYR:HD2	0.74	0.89
1:A:328:VAL:CG1	1:A:332:ILE:CD1	2.50	0.89
1:A:191:THR:CG2	1:A:421:ALA:HB1	2.03	0.89
2:B:7:ILE:HD12	2:B:137:LEU:HD21	1.55	0.89
2:B:183:GLU:OE1	2:B:394:GLN:CB	2.21	0.89
1:A:2:ARG:NH2	2:B:71:GLU:OE1	2.06	0.88
1:A:88:HIS:ND1	1:A:89:PRO:HD2	1.88	0.88
1:A:239:THR:HG23	1:A:243:ARG:HG3	1.54	0.88
2:B:20:PHE:CE2	2:B:235:MET:HB2	2.06	0.88
2:B:200:GLU:OE2	2:B:256:ALA:CA	2.15	0.88
2:B:346:TRP:HE3	2:B:347:ILE:HG12	1.33	0.88
3:K:252:SER:HA	3:K:275:LEU:CD1	2.02	0.88
1:A:382:THR:O	1:A:385:ALA:HB3	1.71	0.88
2:B:346:TRP:CE3	2:B:347:ILE:HG12	2.06	0.88
1:A:231:ILE:HD13	1:A:302:MET:CE	2.03	0.88
2:B:87:PHE:HD1	2:B:88:ARG:O	1.47	0.88
2:B:435:TYR:N	2:B:435:TYR:HD1	1.66	0.88
1:A:41:THR:O	1:A:42:ILE:HB	1.73	0.88
1:A:328:VAL:CG1	1:A:332:ILE:HD12	2.03	0.88
2:B:11:GLN:CB	5:B:501:GDP:O2A	2.20	0.88
2:B:42:LEU:O	2:B:43:GLN:HG3	1.74	0.88
3:K:234:THR:HB	3:K:236:ILE:HD11	1.55	0.88
1:A:154:MET:HE3	1:A:166:LYS:CD	2.04	0.88
1:A:166:LYS:O	1:A:199:ASP:HB2	1.72	0.88
2:B:169:PHE:CE1	2:B:235:MET:SD	2.67	0.88
2:B:313:LEU:HD23	2:B:344:VAL:HG21	1.52	0.88
1:A:277:SER:HB3	1:A:280:LYS:HE2	1.56	0.88
2:B:20:PHE:HE2	2:B:235:MET:HB3	0.80	0.88
2:B:53:TYR:CE1	2:B:87:PHE:CZ	2.62	0.88
2:B:151:THR:CA	2:B:192:HIS:HD2	1.82	0.88
2:B:313:LEU:HD22	2:B:344:VAL:CG1	1.98	0.88
1:A:133:GLN:O	1:A:252:LEU:HD12	1.73	0.88
1:A:382:THR:O	1:A:385:ALA:CB	2.22	0.88
2:B:295:MET:HE1	2:B:375:ALA:CB	2.02	0.88
2:B:385:GLN:NE2	2:B:433:GLN:OE1	2.07	0.88
2:B:98:GLY:O	2:B:99:ALA:O	1.91	0.88
2:B:284:ARG:CD	2:B:290:GLU:OE1	2.22	0.88
1:A:76:ASP:O	1:A:80:THR:OG1	1.91	0.87
1:A:183:GLU:CB	1:A:394:LYS:HB3	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:HD12	2:B:30:ILE:CA	2.03	0.87
2:B:142:GLY:HA3	2:B:182:VAL:CG2	2.04	0.87
2:B:154:ILE:HD13	2:B:198:THR:HG21	1.56	0.87
2:B:301:MET:HE1	2:B:377:PHE:CD1	2.09	0.87
2:B:104:ALA:CA	2:B:108:TYR:HD2	1.85	0.87
2:B:114:LEU:CD1	2:B:117:SER:OG	2.19	0.87
1:A:72:PRO:C	1:A:75:ILE:HG22	1.99	0.87
1:A:220:GLU:O	1:A:222:PRO:HD3	1.60	0.87
2:B:302:MET:O	2:B:302:MET:HG2	1.72	0.87
6:B:502:TXL:H173	6:B:502:TXL:H13	1.57	0.87
1:A:277:SER:HA	1:A:368:LEU:HD22	1.56	0.87
1:A:311:LYS:HB3	1:A:342:GLN:O	1.74	0.87
1:A:53:PHE:N	1:A:88:HIS:HE1	1.41	0.87
1:A:191:THR:CG2	1:A:421:ALA:CB	2.53	0.87
1:A:425:MET:O	1:A:428:LEU:HB3	1.73	0.87
2:B:275:LEU:CG	2:B:294:GLN:HE22	1.85	0.87
2:B:388:PHE:C	2:B:390:ARG:H	1.80	0.87
1:A:23:LEU:CD2	1:A:236:SER:HB3	2.04	0.87
2:B:48:ARG:HD2	2:B:60:LYS:HA	1.55	0.87
2:B:184:PRO:HD3	2:B:398:MET:SD	2.14	0.87
1:A:424:ASP:CA	3:K:307:ARG:NH1	2.37	0.87
2:B:274:PRO:CB	2:B:371:LEU:HD21	2.04	0.87
1:A:115:ILE:O	1:A:119:LEU:HG	1.75	0.87
1:A:196:GLU:O	1:A:197:HIS:ND1	2.08	0.87
2:B:6:HIS:CD2	2:B:21:TRP:HH2	1.92	0.87
1:A:208:ALA:O	1:A:212:ILE:HG23	1.75	0.86
2:B:22:GLU:OE2	2:B:83:PHE:HB2	1.74	0.86
2:B:226:ASP:CG	6:B:502:TXL:H39	2.00	0.86
2:B:320:ARG:CG	2:B:374:SER:OG	2.23	0.86
1:A:81:GLY:O	1:A:82:THR:C	2.18	0.86
1:A:209:ILE:CD1	1:A:227:LEU:HD11	1.93	0.86
2:B:53:TYR:CE1	2:B:87:PHE:CE1	2.62	0.86
2:B:151:THR:CA	2:B:192:HIS:HE2	1.68	0.86
2:B:172:VAL:HG12	2:B:173:PRO:N	1.89	0.86
2:B:244:PHE:HE2	2:B:358:ILE:HD12	1.06	0.86
2:B:312:TYR:CA	2:B:381:SER:HA	2.06	0.86
1:A:313:MET:HB2	1:A:380:ASN:O	1.75	0.86
2:B:384:ILE:CG2	2:B:388:PHE:HE2	1.88	0.86
1:A:9:VAL:HG11	1:A:150:THR:HG22	1.57	0.86
1:A:103:TYR:HE2	1:A:189:LEU:HD23	1.29	0.86
1:A:231:ILE:CD1	1:A:302:MET:HE2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:GLY:O	2:B:281:GLN:N	2.08	0.86
1:A:158:SER:HB2	1:A:197:HIS:HB3	0.87	0.86
2:B:118:VAL:HG11	2:B:153:LEU:HD22	1.54	0.86
2:B:276:THR:OG1	6:B:502:TXL:H62	1.74	0.86
1:A:303:VAL:CG1	1:A:305:CYS:SG	2.64	0.86
2:B:49:ILE:CA	2:B:61:TYR:CD2	2.57	0.86
2:B:339:ASN:O	2:B:342:TYR:N	2.09	0.86
2:B:369:ARG:O	6:B:502:TXL:O10	1.93	0.86
1:A:65:ALA:HB1	1:A:91:GLN:OE1	1.73	0.86
1:A:224:TYR:HE1	4:A:500:GTP:N3	1.73	0.86
2:B:87:PHE:CD1	2:B:89:PRO:HG2	2.03	0.86
2:B:405:LEU:HD12	2:B:408:TYR:CD2	2.00	0.86
3:K:317:GLU:OE1	3:K:322:ASN:HB3	1.74	0.86
1:A:184:PRO:HG3	1:A:395:PHE:CA	2.06	0.86
1:A:250:VAL:CG1	1:A:254:GLU:CB	2.34	0.86
1:A:424:ASP:OD1	3:K:307:ARG:NH1	2.06	0.86
1:A:30:ILE:C	1:A:32:PRO:HD2	1.98	0.86
1:A:108:TYR:HA	1:A:112:LYS:CE	2.05	0.86
1:A:109:THR:HG21	1:A:411:GLU:OE1	1.75	0.86
2:B:144:GLY:N	2:B:185:TYR:CE1	2.44	0.86
2:B:435:TYR:N	2:B:435:TYR:CD1	2.31	0.86
1:A:424:ASP:N	3:K:307:ARG:HH22	1.74	0.86
2:B:7:ILE:HA	2:B:66:ILE:HG23	0.89	0.86
2:B:80:SER:C	2:B:82:PRO:CD	2.48	0.86
2:B:107:HIS:CG	2:B:152:LEU:HD21	2.11	0.86
2:B:194:LEU:CD2	2:B:267:PHE:CE2	2.58	0.86
2:B:226:ASP:CG	6:B:502:TXL:C39	2.49	0.86
2:B:327:GLU:O	2:B:331:GLN:HG2	1.75	0.86
1:A:193:THR:O	1:A:194:THR:C	2.05	0.85
1:A:272:TYR:CE1	1:A:274:PRO:CG	2.59	0.85
2:B:184:PRO:CG	2:B:399:PHE:CD2	0.91	0.85
2:B:241:CYS:HG	2:B:320:ARG:NH1	1.70	0.85
2:B:430:SER:O	2:B:434:GLN:HG3	1.76	0.85
2:B:127:GLU:O	2:B:129:CYS:N	2.09	0.85
2:B:147:SER:CA	2:B:189:LEU:HD13	2.04	0.85
2:B:313:LEU:HD23	2:B:344:VAL:HG22	1.58	0.85
2:B:53:TYR:CD1	2:B:87:PHE:CE1	2.63	0.85
2:B:178:SER:HB3	5:B:501:GDP:O3'	1.74	0.85
1:A:306:ASP:OD2	1:A:308:ARG:HD2	1.76	0.85
2:B:13:GLY:CA	2:B:138:THR:OG1	2.24	0.85
2:B:254:LYS:O	2:B:258:ASN:OD1	1.94	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD23	1:A:236:SER:HB3	1.57	0.85
1:A:250:VAL:HG12	1:A:254:GLU:HB3	1.55	0.85
1:A:276:ILE:HD12	1:A:371:VAL:CG2	2.06	0.85
2:B:14:ASN:CG	2:B:69:ASP:OD1	2.20	0.85
2:B:44:LEU:HD21	2:B:86:ILE:H	1.00	0.85
2:B:102:ASN:HA	2:B:408:TYR:HE1	1.42	0.85
1:A:83:TYR:O	1:A:84:ARG:HG3	1.76	0.85
1:A:88:HIS:CE1	1:A:89:PRO:HD2	2.12	0.85
1:A:103:TYR:HA	1:A:147:SER:OG	1.77	0.85
1:A:174:ALA:HB1	1:A:390:ARG:NH2	1.81	0.85
2:B:7:ILE:HG13	2:B:66:ILE:HG21	1.58	0.85
1:A:154:MET:HB2	1:A:192:HIS:CE1	2.11	0.85
2:B:287:THR:HB	2:B:290:GLU:HB2	0.86	0.85
2:B:405:LEU:HD21	2:B:418:PHE:HE2	1.41	0.85
1:A:184:PRO:HB2	1:A:399:TYR:CD2	2.12	0.85
1:A:282:TYR:CD2	1:A:285:GLN:HA	2.11	0.85
2:B:41:ASP:O	2:B:42:LEU:CG	2.25	0.85
2:B:57:ALA:CA	2:B:64:ARG:CB	2.38	0.85
2:B:229:HIS:NE2	6:B:502:TXL:C37	2.40	0.85
1:A:383:ALA:C	1:A:385:ALA:H	1.84	0.84
1:A:80:THR:O	1:A:81:GLY:C	2.19	0.84
1:A:193:THR:O	1:A:197:HIS:O	1.94	0.84
1:A:276:ILE:HD13	1:A:282:TYR:CD1	2.11	0.84
1:A:64:ARG:HH22	1:A:132:LEU:HD23	1.41	0.84
1:A:175:PRO:HD3	1:A:390:ARG:NH2	1.91	0.84
2:B:244:PHE:CG	2:B:245:PRO:CD	2.56	0.84
2:B:405:LEU:O	2:B:405:LEU:HG	1.75	0.84
1:A:420:GLU:OE2	3:K:170:GLU:C	2.20	0.84
2:B:96:GLN:C	2:B:98:GLY:N	2.31	0.84
2:B:174:SER:HB2	2:B:207:GLU:HB3	1.59	0.84
2:B:181:VAL:HA	2:B:398:MET:CE	2.06	0.84
1:A:107:HIS:CG	1:A:148:GLY:HA3	2.13	0.84
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.10	0.84
2:B:158:ARG:CB	2:B:197:ASN:HB3	1.70	0.84
2:B:226:ASP:OD2	6:B:502:TXL:H40	1.77	0.84
2:B:233:ALA:HB1	2:B:272:PHE:CG	2.12	0.84
1:A:271:THR:OG1	1:A:377:MET:HB3	1.76	0.84
1:A:273:ALA:HB1	1:A:294:ALA:HB3	1.60	0.84
1:A:416:GLY:C	3:K:169:ARG:HH22	1.84	0.84
2:B:49:ILE:N	2:B:61:TYR:HD2	1.75	0.84
2:B:385:GLN:HG2	2:B:389:LYS:HD2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:HB2	2:B:197:ASN:HB3	0.85	0.84
2:B:199:ASP:OD2	2:B:256:ALA:CB	2.26	0.84
2:B:428:LEU:O	2:B:432:TYR:HB2	1.77	0.84
2:B:182:VAL:HG13	2:B:186:ASN:HD21	1.41	0.84
2:B:184:PRO:HG3	2:B:399:PHE:CB	2.07	0.84
1:A:16:ILE:CD1	1:A:138:PHE:CD1	2.59	0.84
1:A:349:THR:OG1	2:B:177:VAL:HG12	1.77	0.84
2:B:275:LEU:HD12	2:B:294:GLN:NE2	1.92	0.84
1:A:1:MET:O	1:A:130:THR:O	1.94	0.83
2:B:158:ARG:HG3	2:B:197:ASN:CB	2.08	0.83
2:B:201:THR:OG1	2:B:267:PHE:HA	1.78	0.83
2:B:289:PRO:O	2:B:293:GLN:HB2	1.78	0.83
1:A:104:ALA:HA	1:A:108:TYR:HD2	1.39	0.83
1:A:176:GLN:O	1:A:177:VAL:HG22	1.77	0.83
2:B:23:VAL:CG2	6:B:502:TXL:H333	2.09	0.83
2:B:166:MET:HB2	2:B:198:THR:HA	1.61	0.83
2:B:172:VAL:HG12	2:B:173:PRO:HD2	1.43	0.83
2:B:295:MET:HE1	2:B:375:ALA:HB1	1.50	0.83
1:A:217:LEU:HD22	1:A:368:LEU:CD1	2.08	0.83
2:B:169:PHE:HE1	2:B:235:MET:HG2	0.82	0.83
2:B:226:ASP:OD1	6:B:502:TXL:C39	2.25	0.83
2:B:244:PHE:CB	2:B:245:PRO:HD2	2.05	0.83
1:A:70:LEU:CD1	1:A:145:THR:CG2	1.89	0.83
1:A:133:GLN:NE2	2:B:96:GLN:O	2.11	0.83
1:A:292:THR:HG22	1:A:319:TYR:CZ	2.12	0.83
2:B:183:GLU:CB	2:B:398:MET:SD	2.65	0.83
2:B:401:ARG:HG3	2:B:402:LYS:H	1.41	0.83
1:A:115:ILE:CD1	1:A:152:LEU:CD2	2.45	0.83
2:B:433:GLN:HG2	2:B:437:ASP:OD1	1.78	0.83
1:A:33:ASP:OD2	1:A:244:PHE:HD2	1.62	0.83
1:A:277:SER:OG	1:A:280:LYS:CB	2.25	0.83
2:B:343:PHE:CD1	2:B:350:ASN:CG	2.55	0.83
1:A:288:VAL:HG22	1:A:373:ARG:CG	2.08	0.83
2:B:14:ASN:HB3	2:B:74:THR:HG21	1.59	0.83
2:B:68:VAL:CG1	2:B:149:MET:HE2	2.09	0.83
1:A:77:GLU:HA	1:A:80:THR:CB	2.08	0.83
2:B:11:GLN:HB3	5:B:501:GDP:O2A	1.79	0.83
2:B:142:GLY:C	2:B:185:TYR:CZ	2.56	0.83
2:B:222:PRO:O	2:B:223:THR:HG23	1.79	0.83
2:B:279:GLY:C	2:B:281:GLN:N	2.35	0.83
1:A:51:THR:CG2	1:A:52:PHE:H	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:HB1	1:A:294:ALA:CB	2.07	0.83
2:B:339:ASN:O	2:B:342:TYR:HB2	1.79	0.83
2:B:414:ASP:CG	3:K:253:GLU:OE2	2.22	0.83
1:A:97:GLU:HB3	1:A:110:ILE:HG23	1.61	0.82
1:A:424:ASP:N	3:K:307:ARG:NH2	2.26	0.82
2:B:35:SER:N	2:B:60:LYS:CE	2.42	0.82
2:B:174:SER:CB	2:B:207:GLU:CB	2.52	0.82
2:B:174:SER:HB2	2:B:175:PRO:HD2	1.59	0.82
2:B:288:VAL:N	2:B:289:PRO:HD2	1.92	0.82
1:A:202:PHE:CE1	1:A:378:LEU:HD13	2.14	0.82
2:B:19:LYS:HB3	2:B:228:ASN:HB3	1.60	0.82
2:B:68:VAL:CG1	2:B:149:MET:CE	2.58	0.82
2:B:105:LYS:HG2	2:B:411:GLU:CG	2.09	0.82
2:B:48:ARG:NH1	2:B:60:LYS:CG	2.42	0.82
2:B:105:LYS:HE2	2:B:411:GLU:CD	2.03	0.82
2:B:143:GLY:N	2:B:147:SER:OG	2.12	0.82
2:B:313:LEU:HD23	2:B:344:VAL:CG1	2.08	0.82
1:A:2:ARG:CB	1:A:133:GLN:OE1	2.27	0.82
1:A:18:ASN:O	1:A:22:GLU:HG3	1.78	0.82
2:B:14:ASN:CB	2:B:74:THR:OG1	2.27	0.82
1:A:219:ILE:CG2	1:A:219:ILE:CA	2.57	0.82
1:A:264:ARG:O	1:A:266:HIS:CE1	2.32	0.82
2:B:53:TYR:CD1	2:B:87:PHE:HZ	1.96	0.82
2:B:229:HIS:CG	6:B:502:TXL:C37	2.62	0.82
2:B:414:ASP:CB	3:K:253:GLU:OE2	2.28	0.82
1:A:13:GLY:O	1:A:16:ILE:HG22	1.80	0.82
1:A:264:ARG:NH2	3:K:307:ARG:CG	2.41	0.82
1:A:184:PRO:CD	1:A:395:PHE:CA	2.58	0.82
1:A:313:MET:HA	1:A:344:VAL:HG21	1.60	0.82
2:B:22:GLU:OE2	2:B:83:PHE:CB	2.27	0.82
2:B:175:PRO:HD3	2:B:390:ARG:HH21	0.74	0.82
2:B:194:LEU:HA	2:B:265:LEU:HB2	1.60	0.82
2:B:194:LEU:HD23	2:B:265:LEU:HB3	1.62	0.82
1:A:424:ASP:HB3	3:K:307:ARG:NH1	1.90	0.82
2:B:169:PHE:CZ	2:B:235:MET:SD	2.73	0.82
2:B:311:ARG:O	2:B:381:SER:HB2	1.80	0.82
1:A:76:ASP:C	1:A:80:THR:HG1	1.87	0.82
1:A:194:THR:HG22	1:A:195:LEU:N	1.95	0.82
1:A:291:ILE:HG22	1:A:375:VAL:HG23	0.84	0.82
1:A:332:ILE:CD1	1:A:353:VAL:CG2	2.54	0.82
2:B:87:PHE:HE1	2:B:89:PRO:HG2	0.84	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PHE:HE1	2:B:235:MET:CG	1.76	0.82
2:B:241:CYS:O	2:B:242:LEU:CB	2.27	0.82
1:A:70:LEU:HB2	1:A:145:THR:HG21	1.62	0.81
1:A:107:HIS:HB3	1:A:148:GLY:HA3	1.60	0.81
1:A:264:ARG:NH2	3:K:307:ARG:CB	2.13	0.81
2:B:165:ILE:HD13	2:B:199:ASP:OD2	1.79	0.81
3:K:234:THR:HB	3:K:236:ILE:CD1	2.10	0.81
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.62	0.81
1:A:76:ASP:O	1:A:80:THR:CA	2.27	0.81
1:A:108:TYR:O	1:A:112:LYS:HG3	1.80	0.81
1:A:250:VAL:CG1	1:A:352:LYS:NZ	2.43	0.81
1:A:256:GLN:HB3	2:B:407:TRP:HH2	1.45	0.81
1:A:306:ASP:CG	1:A:308:ARG:HB2	2.06	0.81
1:A:320:ARG:HG2	1:A:374:ALA:HB3	1.60	0.81
2:B:6:HIS:CD2	2:B:21:TRP:CH2	2.68	0.81
2:B:30:ILE:CG2	2:B:243:ARG:NH1	2.44	0.81
2:B:35:SER:HA	2:B:60:LYS:HE2	1.62	0.81
2:B:119:LEU:O	2:B:123:ARG:HG3	1.80	0.81
2:B:184:PRO:HB3	2:B:395:PHE:CE1	2.16	0.81
1:A:20:CYS:O	1:A:24:TYR:CE2	2.33	0.81
1:A:106:GLY:O	1:A:111:GLY:CA	2.29	0.81
2:B:106:GLY:O	2:B:111:GLY:CA	2.29	0.81
2:B:287:THR:CG2	2:B:290:GLU:H	1.92	0.81
1:A:30:ILE:CG2	1:A:64:ARG:CG	2.55	0.81
1:A:64:ARG:CZ	1:A:132:LEU:HD22	2.10	0.81
1:A:205:ASP:OD1	1:A:303:VAL:HG22	1.18	0.81
1:A:312:TYR:HA	1:A:381:THR:CG2	2.09	0.81
1:A:416:GLY:C	3:K:169:ARG:NH2	2.39	0.81
2:B:13:GLY:HA2	2:B:138:THR:CB	2.10	0.81
1:A:154:MET:CE	1:A:166:LYS:HD3	2.11	0.81
1:A:397:LEU:HA	1:A:401:LYS:HB2	1.57	0.81
2:B:102:ASN:HB3	2:B:408:TYR:HD1	1.46	0.81
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.11	0.81
1:A:101:ASN:HA	4:A:500:GTP:O2G	1.81	0.81
2:B:141:LEU:HD22	2:B:186:ASN:CB	2.09	0.81
2:B:405:LEU:CG	2:B:408:TYR:HB2	2.07	0.81
2:B:287:THR:CB	2:B:290:GLU:HB3	1.99	0.81
1:A:9:VAL:CG1	1:A:150:THR:HG22	2.08	0.80
2:B:4:ILE:CD1	2:B:30:ILE:CA	2.58	0.80
2:B:105:LYS:HG2	2:B:411:GLU:CD	2.06	0.80
1:A:38:SER:C	1:A:39:ASP:N	0.70	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PHE:HZ	1:A:351:PHE:CE2	1.99	0.80
1:A:423:GLU:C	3:K:307:ARG:NH2	2.39	0.80
2:B:4:ILE:HD12	2:B:30:ILE:HA	1.48	0.80
2:B:22:GLU:HG2	2:B:83:PHE:HD2	1.47	0.80
2:B:48:ARG:NH1	2:B:60:LYS:HG2	1.95	0.80
2:B:142:GLY:CA	2:B:185:TYR:CE1	2.64	0.80
1:A:301:GLN:NE2	1:A:305:CYS:O	2.12	0.80
2:B:6:HIS:NE2	2:B:21:TRP:HH2	1.77	0.80
2:B:190:SER:O	2:B:192:HIS:N	2.14	0.80
2:B:250:ALA:CA	2:B:254:LYS:HD2	2.09	0.80
1:A:88:HIS:CG	1:A:89:PRO:CD	2.63	0.80
1:A:144:GLY:HA2	1:A:185:TYR:OH	1.81	0.80
1:A:276:ILE:HG21	1:A:282:TYR:HD1	1.44	0.80
1:A:361:THR:HG22	1:A:362:VAL:N	1.96	0.80
2:B:286:LEU:HD12	2:B:372:LYS:HB2	1.61	0.80
1:A:116:ASP:O	1:A:119:LEU:N	2.15	0.80
1:A:221:ARG:N	1:A:222:PRO:HD3	1.97	0.80
2:B:385:GLN:HG2	2:B:389:LYS:CE	2.09	0.80
2:B:64:ARG:NH2	2:B:125:GLU:O	2.13	0.80
2:B:12:CYS:O	2:B:16:ILE:CB	2.29	0.80
2:B:42:LEU:C	2:B:43:GLN:HG3	2.07	0.80
2:B:56:ALA:CB	2:B:62:VAL:HB	2.11	0.80
2:B:102:ASN:CG	2:B:408:TYR:CD1	2.59	0.80
2:B:268:PHE:CD1	2:B:380:ASN:CG	2.59	0.80
2:B:287:THR:HG22	2:B:288:VAL:N	1.95	0.80
2:B:10:GLY:O	2:B:14:ASN:ND2	2.14	0.80
2:B:13:GLY:HA2	2:B:138:THR:HB	1.62	0.80
2:B:96:GLN:O	2:B:97:SER:C	2.21	0.80
2:B:385:GLN:HG2	2:B:389:LYS:CD	2.11	0.80
1:A:83:TYR:C	1:A:84:ARG:HG3	2.05	0.80
1:A:103:TYR:CG	1:A:188:ILE:HG22	2.16	0.80
2:B:95:GLY:O	2:B:96:GLN:HB2	1.81	0.80
2:B:286:LEU:HD13	2:B:373:MET:N	1.96	0.80
1:A:176:GLN:C	1:A:177:VAL:CG2	2.42	0.80
1:A:212:ILE:CD1	1:A:230:LEU:HD22	1.89	0.80
2:B:102:ASN:CG	2:B:408:TYR:CE1	2.60	0.80
2:B:175:PRO:HB2	2:B:176:LYS:HE2	1.64	0.80
2:B:208:ALA:HB1	2:B:303:ALA:O	1.82	0.80
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.58	0.80
2:B:385:GLN:HG3	2:B:389:LYS:CE	2.04	0.80
1:A:179:THR:CG2	1:A:181:VAL:HB	2.04	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLN:HB3	2:B:407:TRP:CZ3	2.16	0.79
2:B:142:GLY:CA	2:B:185:TYR:CD1	2.65	0.79
2:B:194:LEU:CD2	2:B:267:PHE:HE2	1.93	0.79
1:A:15:GLN:O	1:A:18:ASN:N	2.14	0.79
1:A:396:ASP:OD2	1:A:422:ARG:NH1	2.15	0.79
2:B:35:SER:CA	2:B:60:LYS:CE	2.60	0.79
2:B:105:LYS:CE	2:B:411:GLU:OE2	2.27	0.79
1:A:6:SER:HA	1:A:136:SER:OG	1.81	0.79
1:A:108:TYR:CA	1:A:112:LYS:CE	2.54	0.79
1:A:271:THR:OG1	1:A:377:MET:CB	2.30	0.79
1:A:424:ASP:HA	3:K:307:ARG:NH1	1.96	0.79
2:B:178:SER:CB	5:B:501:GDP:HO3'	1.94	0.79
2:B:259:MET:HE2	2:B:379:GLY:N	1.97	0.79
2:B:265:LEU:HD23	2:B:267:PHE:CE1	2.17	0.79
1:A:179:THR:CG2	1:A:181:VAL:CB	2.58	0.79
1:A:431:ASP:HB3	3:K:303:PHE:HE1	1.47	0.79
2:B:30:ILE:HG21	2:B:136:GLN:HE22	1.47	0.79
2:B:176:LYS:CE	2:B:207:GLU:OE2	2.29	0.79
1:A:5:ILE:HG21	1:A:135:PHE:CE1	2.18	0.79
1:A:133:GLN:NE2	2:B:98:GLY:HA2	1.96	0.79
1:A:343:PHE:CZ	1:A:351:PHE:CE2	2.69	0.79
1:A:369:ALA:CB	1:A:371:VAL:CG2	2.51	0.79
1:A:119:LEU:O	1:A:122:ILE:CG2	2.30	0.79
1:A:272:TYR:CZ	1:A:274:PRO:CG	2.56	0.79
1:A:420:GLU:HG3	3:K:169:ARG:HE	1.44	0.79
2:B:48:ARG:NH1	2:B:60:LYS:H	1.81	0.79
2:B:49:ILE:N	2:B:61:TYR:CD2	2.51	0.79
2:B:259:MET:HE1	2:B:379:GLY:HA2	0.83	0.79
1:A:206:ASN:HD21	1:A:227:LEU:HD23	1.42	0.79
2:B:243:ARG:HH21	2:B:252:LEU:HD11	1.47	0.79
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.65	0.79
2:B:405:LEU:HD13	2:B:418:PHE:HZ	1.47	0.79
1:A:196:GLU:O	1:A:197:HIS:CB	2.30	0.79
2:B:7:ILE:CG1	2:B:66:ILE:CG2	2.58	0.79
2:B:7:ILE:HG12	2:B:66:ILE:CD1	2.04	0.79
2:B:287:THR:CG2	2:B:289:PRO:HG2	2.12	0.79
1:A:258:ASN:OD1	1:A:352:LYS:CD	2.29	0.79
1:A:309:HIS:CD2	1:A:386:GLU:OE2	2.36	0.79
2:B:184:PRO:HG3	2:B:399:PHE:CD2	1.33	0.79
1:A:306:ASP:OD1	1:A:308:ARG:HB2	1.79	0.79
2:B:218:LYS:O	2:B:219:LEU:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ARG:HD2	2:B:290:GLU:CD	2.08	0.79
2:B:323:MET:HG2	2:B:324:SER:N	1.98	0.79
2:B:340:SER:HG	2:B:341:SER:N	1.79	0.79
1:A:17:GLY:O	1:A:21:TRP:N	2.11	0.78
1:A:172:TYR:CE2	1:A:388:TRP:CZ3	2.70	0.78
2:B:69:ASP:OD2	2:B:74:THR:CG2	2.31	0.78
2:B:192:HIS:HA	2:B:196:GLU:CD	2.08	0.78
2:B:213:CYS:HB3	2:B:219:LEU:HD11	1.64	0.78
1:A:109:THR:CG2	1:A:411:GLU:HB3	2.12	0.78
1:A:155:GLU:OE2	1:A:192:HIS:HD2	1.65	0.78
2:B:48:ARG:NH1	2:B:60:LYS:N	2.32	0.78
1:A:115:ILE:CG2	1:A:152:LEU:HD21	2.12	0.78
2:B:66:ILE:HB	2:B:125:GLU:OE2	1.84	0.78
2:B:244:PHE:CD2	2:B:358:ILE:HD12	2.18	0.78
2:B:300:ASN:ND2	2:B:300:ASN:O	2.16	0.78
2:B:401:ARG:HG3	2:B:402:LYS:N	1.99	0.78
1:A:179:THR:HG22	1:A:181:VAL:H	0.63	0.78
1:A:420:GLU:CD	3:K:170:GLU:N	2.40	0.78
2:B:44:LEU:CD2	2:B:85:GLN:CG	2.15	0.78
2:B:53:TYR:CE1	2:B:89:PRO:HG3	2.17	0.78
1:A:191:THR:HG21	1:A:421:ALA:HB2	1.63	0.78
1:A:312:TYR:HE2	1:A:377:MET:CE	1.80	0.78
1:A:409:VAL:HG22	1:A:414:GLU:HG2	1.64	0.78
2:B:305:CYS:SG	2:B:387:LEU:HB2	2.24	0.78
1:A:3:GLU:HA	1:A:31:GLN:CG	2.11	0.78
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.56	0.78
2:B:111:GLY:C	2:B:115:VAL:CG2	2.56	0.78
1:A:4:CYS:CB	1:A:30:ILE:CG2	2.57	0.78
1:A:303:VAL:HG11	1:A:305:CYS:SG	2.22	0.78
2:B:4:ILE:HD13	2:B:30:ILE:CB	2.13	0.78
2:B:7:ILE:CD1	2:B:137:LEU:HD21	2.14	0.78
2:B:34:GLY:O	2:B:35:SER:OG	2.01	0.78
2:B:194:LEU:HD23	2:B:267:PHE:CZ	2.19	0.78
1:A:65:ALA:O	1:A:66:VAL:HG23	1.83	0.78
1:A:72:PRO:O	1:A:75:ILE:HG22	1.83	0.78
2:B:4:ILE:HG21	2:B:30:ILE:CG2	2.12	0.78
2:B:44:LEU:HD11	2:B:86:ILE:C	2.09	0.78
2:B:102:ASN:HA	2:B:408:TYR:CE1	2.18	0.78
2:B:107:HIS:CG	2:B:152:LEU:HG	2.19	0.78
2:B:144:GLY:N	2:B:185:TYR:CZ	2.52	0.78
1:A:93:ILE:HD11	1:A:121:ARG:HD2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:NE2	2:B:21:TRP:NE1	2.31	0.78
1:A:142:GLY:C	1:A:185:TYR:CE1	2.62	0.78
1:A:153:LEU:O	1:A:157:LEU:HG	1.84	0.78
1:A:344:VAL:CB	1:A:347:CYS:SG	2.69	0.78
2:B:7:ILE:CG1	2:B:66:ILE:HD13	2.05	0.78
2:B:48:ARG:CD	2:B:60:LYS:HA	2.13	0.78
2:B:128:SER:O	2:B:129:CYS:HB2	1.84	0.78
2:B:184:PRO:CG	2:B:399:PHE:HD2	0.66	0.78
2:B:273:ALA:HB1	2:B:294:GLN:OE1	1.83	0.78
2:B:286:LEU:CD1	2:B:371:LEU:O	2.32	0.78
1:A:158:SER:OG	1:A:196:GLU:O	2.02	0.77
1:A:277:SER:OG	1:A:280:LYS:CA	2.32	0.77
2:B:103:TRP:CZ3	2:B:108:TYR:OH	2.18	0.77
2:B:184:PRO:HD2	2:B:399:PHE:HE2	1.46	0.77
2:B:275:LEU:HD11	2:B:300:ASN:HD21	1.49	0.77
2:B:319:PHE:CZ	2:B:328:VAL:HG13	2.19	0.77
1:A:152:LEU:HD11	1:A:156:ARG:CZ	2.13	0.77
1:A:155:GLU:OE2	1:A:192:HIS:CD2	2.37	0.77
1:A:296:PHE:HE1	1:A:335:ILE:HD13	0.98	0.77
2:B:107:HIS:CG	2:B:152:LEU:CD2	2.67	0.77
2:B:320:ARG:NH2	6:B:502:TXL:H27	1.98	0.77
2:B:346:TRP:CD2	2:B:347:ILE:HG13	2.14	0.77
2:B:399:PHE:CZ	2:B:408:TYR:OH	2.37	0.77
1:A:155:GLU:HG3	1:A:192:HIS:NE2	1.99	0.77
1:A:206:ASN:HD21	4:A:500:GTP:N2	1.82	0.77
2:B:102:ASN:OD1	2:B:408:TYR:HE1	1.62	0.77
2:B:192:HIS:C	2:B:196:GLU:HG2	2.09	0.77
2:B:383:ALA:O	2:B:386:GLU:HG3	1.84	0.77
1:A:70:LEU:CG	1:A:145:THR:HG21	2.14	0.77
1:A:103:TYR:O	1:A:107:HIS:HB3	1.85	0.77
1:A:262:TYR:HB3	1:A:263:PRO:HD3	1.65	0.77
2:B:229:HIS:CE1	6:B:502:TXL:O11	2.38	0.77
1:A:70:LEU:HB2	1:A:145:THR:CG2	2.14	0.77
2:B:107:HIS:HD2	2:B:152:LEU:HG	1.48	0.77
2:B:92:PHE:CE2	2:B:114:LEU:HD11	2.20	0.77
2:B:105:LYS:CG	2:B:411:GLU:HG3	2.14	0.77
2:B:243:ARG:HH21	2:B:252:LEU:CD1	1.98	0.77
2:B:262:PHE:HB3	2:B:263:PRO:CD	2.14	0.77
6:B:502:TXL:H162	6:B:502:TXL:C9	2.15	0.77
1:A:105:ARG:NH2	1:A:110:ILE:CD1	2.46	0.77
1:A:252:LEU:HD23	1:A:255:PHE:CE2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG23	1:A:373:ARG:HD3	1.62	0.77
1:A:416:GLY:CA	3:K:169:ARG:HH22	1.94	0.77
2:B:154:ILE:HG22	2:B:196:GLU:O	1.85	0.77
2:B:249:ASN:O	2:B:254:LYS:NZ	2.16	0.77
2:B:319:PHE:CD1	2:B:328:VAL:CG1	2.58	0.77
2:B:229:HIS:ND1	6:B:502:TXL:O11	2.18	0.77
2:B:252:LEU:O	2:B:255:LEU:HB2	1.85	0.77
2:B:425:MET:O	2:B:428:LEU:HB3	1.84	0.77
1:A:72:PRO:O	1:A:75:ILE:HG23	1.82	0.77
1:A:105:ARG:HH21	1:A:110:ILE:CD1	1.92	0.77
1:A:192:HIS:O	1:A:196:GLU:HG2	1.85	0.77
2:B:107:HIS:O	2:B:152:LEU:HD13	1.82	0.77
1:A:108:TYR:HE2	1:A:417:GLU:OE2	1.63	0.77
1:A:206:ASN:HD21	1:A:227:LEU:CD2	1.87	0.77
2:B:104:ALA:CA	2:B:108:TYR:CD2	2.63	0.77
2:B:147:SER:CB	2:B:189:LEU:HD13	2.08	0.77
2:B:277:SER:CB	2:B:280:SER:HB2	2.12	0.77
1:A:1:MET:C	2:B:96:GLN:CD	2.42	0.76
1:A:217:LEU:HD13	1:A:368:LEU:CG	2.12	0.76
1:A:291:ILE:C	1:A:375:VAL:HG21	2.10	0.76
2:B:15:GLN:CD	5:B:501:GDP:O6	2.29	0.76
2:B:86:ILE:HD12	2:B:91:ASN:ND2	1.99	0.76
2:B:222:PRO:O	2:B:223:THR:CG2	2.32	0.76
1:A:3:GLU:OE2	1:A:129:CYS:HB3	1.82	0.76
1:A:97:GLU:CG	1:A:110:ILE:CG2	2.63	0.76
2:B:181:VAL:HA	2:B:398:MET:HE2	1.65	0.76
3:K:216:ARG:HH11	3:K:216:ARG:CG	1.98	0.76
1:A:148:GLY:HA2	1:A:151:SER:OG	1.85	0.76
2:B:107:HIS:CG	2:B:152:LEU:CG	2.69	0.76
2:B:213:CYS:HB3	2:B:219:LEU:CD1	2.16	0.76
2:B:346:TRP:HZ3	2:B:347:ILE:HD11	0.95	0.76
1:A:115:ILE:CD1	1:A:152:LEU:CD1	2.63	0.76
1:A:115:ILE:HD13	1:A:152:LEU:CD1	2.16	0.76
2:B:27:GLU:O	2:B:36:TYR:HB3	1.86	0.76
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.20	0.76
1:A:273:ALA:CB	1:A:294:ALA:HB3	2.16	0.76
2:B:103:TRP:CZ3	2:B:108:TYR:CZ	2.73	0.76
2:B:254:LYS:O	2:B:258:ASN:CG	2.28	0.76
1:A:294:ALA:C	1:A:300:ASN:ND2	2.43	0.76
1:A:420:GLU:OE1	3:K:170:GLU:CA	2.34	0.76
2:B:104:ALA:HA	2:B:108:TYR:CE2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:ARG:HD3	2:B:422:GLU:OE1	1.85	0.76
1:A:254:GLU:CD	2:B:101:ASN:OD1	2.28	0.76
2:B:200:GLU:HB3	2:B:268:PHE:CE2	2.21	0.76
2:B:237:GLY:CA	2:B:241:CYS:SG	2.68	0.76
1:A:80:THR:O	1:A:83:TYR:N	2.19	0.76
2:B:12:CYS:SG	5:B:501:GDP:C4	2.79	0.76
2:B:308:ARG:HD3	2:B:342:TYR:CZ	2.21	0.76
2:B:399:PHE:HZ	2:B:408:TYR:OH	1.68	0.76
2:B:399:PHE:O	2:B:403:ALA:HA	1.86	0.76
1:A:173:PRO:HG3	1:A:182:VAL:HG12	1.66	0.76
2:B:181:VAL:HG12	2:B:399:PHE:CZ	1.95	0.76
1:A:62:VAL:HG12	1:A:63:PRO:CD	2.06	0.75
1:A:97:GLU:HG3	1:A:110:ILE:CG2	2.16	0.75
1:A:97:GLU:O	1:A:98:ASP:HB3	1.85	0.75
1:A:183:GLU:HB2	1:A:398:MET:SD	2.26	0.75
1:A:228:ASN:ND2	4:A:500:GTP:HN1	1.84	0.75
2:B:142:GLY:HA3	2:B:182:VAL:HG22	1.65	0.75
2:B:273:ALA:N	2:B:274:PRO:HD2	1.45	0.75
2:B:311:ARG:C	2:B:381:SER:HB2	2.11	0.75
1:A:266:HIS:HD2	1:A:432:TYR:CE1	2.04	0.75
2:B:48:ARG:HH11	2:B:60:LYS:CG	1.97	0.75
2:B:135:PHE:CB	2:B:166:MET:SD	2.74	0.75
2:B:237:GLY:O	2:B:241:CYS:CB	2.26	0.75
2:B:384:ILE:CG2	2:B:388:PHE:CE2	2.69	0.75
1:A:420:GLU:OE1	3:K:170:GLU:HB3	1.87	0.75
2:B:75:MET:HE2	2:B:79:ARG:CB	2.16	0.75
2:B:169:PHE:CZ	2:B:235:MET:HG2	2.17	0.75
2:B:338:LYS:O	2:B:339:ASN:CG	2.29	0.75
1:A:383:ALA:O	1:A:386:GLU:N	2.18	0.75
2:B:105:LYS:HG2	2:B:411:GLU:HG3	1.67	0.75
2:B:184:PRO:HA	2:B:395:PHE:HD1	1.52	0.75
1:A:66:VAL:CG2	1:A:125:LEU:CD1	2.64	0.75
1:A:313:MET:CB	1:A:380:ASN:O	2.34	0.75
2:B:141:LEU:CD1	2:B:173:PRO:HD3	2.16	0.75
2:B:170:SER:OG	2:B:203:CYS:HA	1.86	0.75
2:B:222:PRO:C	2:B:223:THR:HG23	2.11	0.75
2:B:405:LEU:HD11	2:B:408:TYR:HB2	0.78	0.75
1:A:76:ASP:C	1:A:80:THR:OG1	2.29	0.75
1:A:431:ASP:CA	3:K:303:PHE:CE1	2.70	0.75
2:B:87:PHE:CD1	2:B:89:PRO:HD2	2.20	0.75
2:B:192:HIS:CA	2:B:196:GLU:HG2	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:C	1:A:122:ILE:HG22	2.11	0.75
1:A:151:SER:HB2	1:A:192:HIS:CB	2.15	0.75
1:A:431:ASP:CB	3:K:303:PHE:HE1	2.00	0.75
2:B:70:LEU:HD12	2:B:94:PHE:HD2	0.68	0.75
2:B:143:GLY:O	5:B:501:GDP:PB	2.40	0.75
2:B:398:MET:HG2	2:B:399:PHE:N	2.01	0.75
2:B:53:TYR:HE1	2:B:89:PRO:CG	1.98	0.75
1:A:103:TYR:HD2	1:A:189:LEU:CG	2.00	0.74
1:A:184:PRO:HD3	1:A:395:PHE:N	2.01	0.74
1:A:311:LYS:CB	1:A:342:GLN:O	2.34	0.74
2:B:6:HIS:NE2	2:B:21:TRP:CH2	2.55	0.74
2:B:103:TRP:CZ3	2:B:108:TYR:CE2	2.75	0.74
2:B:154:ILE:HD13	2:B:198:THR:CG2	2.17	0.74
2:B:312:TYR:O	2:B:344:VAL:HG22	1.84	0.74
2:B:22:GLU:CG	2:B:83:PHE:CE2	2.70	0.74
2:B:326:LYS:O	2:B:330:GLU:CG	2.35	0.74
2:B:343:PHE:CB	2:B:350:ASN:ND2	2.50	0.74
2:B:405:LEU:HD21	2:B:418:PHE:CZ	2.03	0.74
1:A:42:ILE:O	1:A:42:ILE:CG2	2.30	0.74
1:A:326:LYS:O	1:A:330:ALA:HB3	1.87	0.74
1:A:361:THR:O	1:A:362:VAL:HG23	1.86	0.74
1:A:416:GLY:HA3	3:K:169:ARG:HH21	1.47	0.74
1:A:88:HIS:CD2	1:A:89:PRO:CD	2.70	0.74
1:A:287:SER:OG	1:A:290:GLU:HB2	1.87	0.74
1:A:349:THR:OG1	2:B:177:VAL:CG1	2.35	0.74
2:B:229:HIS:NE2	6:B:502:TXL:H37	2.01	0.74
1:A:26:LEU:HD11	1:A:361:THR:CB	2.17	0.74
1:A:312:TYR:HE2	1:A:377:MET:HE1	1.34	0.74
1:A:319:TYR:O	1:A:355:ILE:HA	1.87	0.74
2:B:89:PRO:O	2:B:90:ASP:OD1	2.05	0.74
2:B:190:SER:O	2:B:191:VAL:C	2.30	0.74
2:B:287:THR:CG2	2:B:289:PRO:CG	2.65	0.74
2:B:319:PHE:CE1	2:B:328:VAL:HG12	2.18	0.74
2:B:188:THR:HG22	2:B:417:GLU:O	1.87	0.74
2:B:226:ASP:OD1	6:B:502:TXL:H39	1.87	0.74
1:A:103:TYR:OH	1:A:151:SER:HB3	1.87	0.74
1:A:179:THR:CG2	1:A:181:VAL:HG23	2.18	0.74
1:A:219:ILE:CG2	1:A:219:ILE:HG12	2.16	0.74
1:A:224:TYR:CE1	4:A:500:GTP:N3	2.55	0.74
2:B:7:ILE:HB	2:B:137:LEU:HD21	1.62	0.74
2:B:56:ALA:CB	2:B:62:VAL:HG23	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:PHE:CE1	2:B:353:THR:CG2	2.42	0.74
1:A:57:GLY:HA3	1:A:61:HIS:NE2	2.01	0.74
1:A:196:GLU:O	1:A:197:HIS:HB3	1.87	0.74
1:A:206:ASN:HD21	4:A:500:GTP:HN22	1.35	0.74
2:B:6:HIS:CG	2:B:21:TRP:HZ2	2.05	0.74
2:B:35:SER:CA	2:B:60:LYS:HE3	2.16	0.74
2:B:265:LEU:CD2	2:B:267:PHE:CE1	2.71	0.74
2:B:296:PHE:CE2	2:B:335:VAL:HG11	2.22	0.74
1:A:137:VAL:HB	1:A:168:GLU:HG2	1.70	0.74
1:A:440:VAL:N	2:B:402:LYS:HZ1	1.70	0.74
2:B:213:CYS:SG	2:B:227:LEU:CD1	2.75	0.74
1:A:33:ASP:OD2	1:A:244:PHE:CD2	2.39	0.74
1:A:209:ILE:HG23	1:A:230:LEU:CD2	2.17	0.74
2:B:9:ALA:HA	2:B:68:VAL:O	1.86	0.74
2:B:386:GLU:C	2:B:388:PHE:N	2.43	0.74
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.18	0.73
1:A:277:SER:CA	1:A:280:LYS:HG2	2.18	0.73
1:A:369:ALA:HB1	1:A:371:VAL:HG23	1.67	0.73
1:A:107:HIS:CD2	1:A:148:GLY:CA	2.71	0.73
2:B:123:ARG:O	2:B:127:GLU:HG3	1.87	0.73
2:B:184:PRO:HG2	2:B:399:PHE:CD2	0.29	0.73
2:B:244:PHE:CE2	2:B:358:ILE:CD1	2.48	0.73
2:B:272:PHE:CD1	2:B:274:PRO:HG2	2.24	0.73
2:B:336:GLN:NE2	2:B:351:VAL:HB	2.03	0.73
2:B:397:ALA:O	2:B:401:ARG:HG2	1.87	0.73
1:A:70:LEU:CB	1:A:145:THR:CG2	2.65	0.73
1:A:172:TYR:CZ	1:A:387:ALA:HB1	2.22	0.73
1:A:206:ASN:ND2	4:A:500:GTP:HN22	1.85	0.73
1:A:431:ASP:O	1:A:435:VAL:HG23	1.88	0.73
2:B:244:PHE:HD2	2:B:245:PRO:HD2	1.45	0.73
1:A:2:ARG:NH2	2:B:99:ALA:CB	2.52	0.73
2:B:8:GLN:NE2	2:B:21:TRP:CD1	2.56	0.73
2:B:75:MET:CE	2:B:79:ARG:HD3	1.99	0.73
1:A:65:ALA:HB2	1:A:91:GLN:OE1	1.87	0.73
1:A:153:LEU:O	1:A:157:LEU:CD1	2.37	0.73
1:A:158:SER:H	1:A:166:LYS:NZ	1.86	0.73
1:A:179:THR:HG23	1:A:181:VAL:HG23	1.70	0.73
2:B:265:LEU:O	2:B:267:PHE:CE2	2.41	0.73
2:B:313:LEU:CD2	2:B:344:VAL:HG13	2.17	0.73
1:A:3:GLU:HB3	1:A:64:ARG:CZ	2.18	0.73
1:A:264:ARG:HH21	3:K:307:ARG:HB3	0.57	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:SER:CB	1:A:280:LYS:CG	2.51	0.73
1:A:282:TYR:HD2	1:A:285:GLN:HA	1.52	0.73
1:A:282:TYR:HD2	1:A:285:GLN:CA	2.01	0.73
2:B:53:TYR:CE1	2:B:87:PHE:HZ	2.07	0.73
2:B:181:VAL:CG2	2:B:404:PHE:CE2	2.70	0.73
2:B:265:LEU:CD2	2:B:267:PHE:CZ	2.71	0.73
1:A:100:ALA:HB2	1:A:105:ARG:NE	2.04	0.73
1:A:210:TYR:CD2	1:A:227:LEU:HD22	2.20	0.73
1:A:344:VAL:HB	1:A:347:CYS:HG	1.51	0.73
1:A:349:THR:HG21	2:B:177:VAL:HG12	1.71	0.73
2:B:35:SER:H	2:B:60:LYS:HE3	1.53	0.73
2:B:142:GLY:HA3	2:B:182:VAL:HG21	1.71	0.73
2:B:229:HIS:HB2	6:B:502:TXL:H38	1.68	0.73
2:B:239:THR:HA	2:B:243:ARG:CZ	2.19	0.73
1:A:314:ALA:O	1:A:379:SER:HA	1.89	0.73
2:B:21:TRP:HA	2:B:24:ILE:HD12	1.71	0.73
2:B:92:PHE:CE1	2:B:121:VAL:HG21	2.23	0.73
2:B:288:VAL:H	2:B:289:PRO:HD2	1.54	0.73
2:B:383:ALA:O	2:B:386:GLU:CG	2.37	0.73
3:K:159:ASN:HD22	3:K:161:LYS:CG	2.02	0.73
1:A:97:GLU:O	1:A:110:ILE:HD13	1.88	0.73
1:A:250:VAL:CG1	1:A:254:GLU:HG2	2.15	0.73
2:B:286:LEU:HD11	2:B:372:LYS:CB	2.07	0.73
2:B:14:ASN:HB2	2:B:74:THR:OG1	1.89	0.73
2:B:105:LYS:HE2	2:B:411:GLU:CG	2.18	0.73
2:B:259:MET:HB2	2:B:268:PHE:CZ	2.23	0.73
1:A:250:VAL:CG2	1:A:254:GLU:HG2	2.19	0.72
2:B:101:ASN:O	2:B:102:ASN:HB2	1.88	0.72
2:B:194:LEU:HD21	2:B:267:PHE:CE2	2.23	0.72
2:B:280:SER:O	2:B:282:GLN:N	2.21	0.72
1:A:36:MET:SD	1:A:60:LYS:HB2	2.29	0.72
2:B:231:VAL:HG12	2:B:235:MET:HE2	1.71	0.72
1:A:145:THR:C	1:A:149:PHE:HB3	2.13	0.72
1:A:234:ILE:HD12	1:A:270:ALA:HB1	1.71	0.72
2:B:184:PRO:HG3	2:B:399:PHE:CG	1.84	0.72
1:A:277:SER:HB2	1:A:279:GLU:H	1.53	0.72
1:A:312:TYR:CD2	1:A:381:THR:HG22	2.23	0.72
1:A:397:LEU:HD22	1:A:401:LYS:CE	2.20	0.72
2:B:19:LYS:CD	2:B:228:ASN:CB	2.53	0.72
2:B:158:ARG:CD	2:B:197:ASN:N	2.51	0.72
1:A:102:ASN:C	1:A:185:TYR:HE2	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:PHE:CZ	2:B:235:MET:HB3	2.22	0.72
2:B:242:LEU:HD22	2:B:250:ALA:N	2.01	0.72
2:B:286:LEU:HB3	2:B:373:MET:HB3	1.71	0.72
1:A:144:GLY:N	4:A:500:GTP:O2G	2.19	0.72
2:B:3:GLU:CB	2:B:132:LEU:HD23	2.14	0.72
2:B:133:GLN:NE2	2:B:253:ARG:NH1	2.38	0.72
2:B:178:SER:HB2	5:B:501:GDP:O3'	1.89	0.72
2:B:259:MET:CE	2:B:379:GLY:N	2.51	0.72
1:A:6:SER:HB3	1:A:30:ILE:CD1	2.19	0.72
2:B:53:TYR:CE1	2:B:87:PHE:HE1	2.07	0.72
6:B:502:TXL:H181	6:B:502:TXL:C21	2.19	0.72
1:A:5:ILE:CD1	1:A:135:PHE:CE1	2.73	0.72
1:A:70:LEU:CB	1:A:145:THR:HG21	2.20	0.72
1:A:115:ILE:CD1	1:A:156:ARG:CZ	2.62	0.72
1:A:184:PRO:HD3	1:A:395:PHE:CA	2.19	0.72
2:B:6:HIS:CG	2:B:21:TRP:CZ2	2.77	0.72
2:B:226:ASP:OD2	6:B:502:TXL:C40	2.37	0.72
1:A:101:ASN:O	1:A:102:ASN:OD1	2.07	0.72
1:A:179:THR:HG22	1:A:180:ALA:N	1.95	0.72
2:B:7:ILE:CG2	2:B:137:LEU:HD22	2.19	0.72
2:B:128:SER:O	2:B:129:CYS:CB	2.37	0.72
1:A:152:LEU:HD11	1:A:156:ARG:NH2	2.05	0.72
1:A:210:TYR:CZ	1:A:227:LEU:CD2	2.60	0.72
1:A:341:ILE:CG2	1:A:343:PHE:CE2	2.72	0.72
2:B:175:PRO:C	2:B:176:LYS:HE2	2.12	0.72
1:A:9:VAL:HB	1:A:138:PHE:O	1.88	0.71
2:B:288:VAL:O	2:B:292:THR:N	2.19	0.71
1:A:152:LEU:HD11	1:A:156:ARG:NE	2.04	0.71
1:A:179:THR:CG2	1:A:181:VAL:N	2.21	0.71
1:A:228:ASN:ND2	4:A:500:GTP:O6	2.23	0.71
3:K:18[B]:ARG:NH2	3:K:336:ILE:HD12	1.98	0.71
1:A:104:ALA:HA	1:A:108:TYR:CE2	2.25	0.71
1:A:291:ILE:HD11	1:A:373:ARG:HB3	1.72	0.71
2:B:143:GLY:CA	2:B:185:TYR:HE1	2.03	0.71
2:B:183:GLU:OE1	2:B:394:GLN:HB3	1.83	0.71
2:B:323:MET:HG2	2:B:324:SER:H	1.55	0.71
1:A:184:PRO:CB	1:A:399:TYR:CD2	2.73	0.71
1:A:184:PRO:HG2	1:A:395:PHE:CD2	2.20	0.71
1:A:289:ALA:HB1	1:A:331:ALA:CB	2.20	0.71
1:A:319:TYR:CE2	1:A:375:VAL:HG22	2.26	0.71
1:A:336:LYS:HG2	1:A:336:LYS:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:PRO:CD	2:B:374:SER:HB3	2.20	0.71
2:B:397:ALA:CA	2:B:401:ARG:HD3	2.19	0.71
1:A:53:PHE:HA	1:A:88:HIS:NE2	1.92	0.71
2:B:3:GLU:HG2	2:B:4:ILE:N	2.04	0.71
2:B:204:ILE:O	2:B:204:ILE:HG22	1.90	0.71
1:A:220:GLU:CG	1:A:220:GLU:CA	2.67	0.71
2:B:111:GLY:CA	2:B:115:VAL:HG23	2.20	0.71
2:B:183:GLU:HB2	2:B:184:PRO:HD2	1.70	0.71
1:A:36:MET:SD	1:A:61:HIS:HA	2.30	0.71
1:A:217:LEU:CG	1:A:218:ASP:H	1.86	0.71
1:A:292:THR:HG22	1:A:319:TYR:CE2	2.25	0.71
2:B:405:LEU:HD13	2:B:418:PHE:CZ	2.25	0.71
2:B:414:ASP:HB2	3:K:253:GLU:OE1	1.89	0.71
2:B:95:GLY:O	2:B:96:GLN:CB	2.39	0.71
2:B:191:VAL:CG2	2:B:421:ALA:CA	2.61	0.71
2:B:242:LEU:HD13	2:B:250:ALA:CB	2.15	0.71
2:B:431:GLU:HA	2:B:434:GLN:CD	2.15	0.71
1:A:241:SER:CB	1:A:356:ASN:ND2	2.53	0.71
2:B:213:CYS:SG	2:B:227:LEU:HD12	2.31	0.71
1:A:256:GLN:CB	2:B:407:TRP:CZ3	2.74	0.71
1:A:312:TYR:CE2	1:A:377:MET:HE2	2.26	0.71
2:B:7:ILE:CG2	2:B:137:LEU:CD2	2.69	0.71
2:B:132:LEU:HB2	2:B:164:ARG:NH1	2.06	0.71
2:B:184:PRO:HB2	2:B:399:PHE:CD2	2.23	0.71
2:B:259:MET:SD	2:B:378:ILE:HG22	2.31	0.71
2:B:284:ARG:HB3	2:B:287:THR:OG1	1.90	0.71
2:B:388:PHE:C	2:B:390:ARG:N	2.49	0.71
1:A:341:ILE:HG21	1:A:343:PHE:CE2	2.26	0.70
1:A:349:THR:CA	2:B:177:VAL:HG11	2.18	0.70
1:A:424:ASP:CG	3:K:307:ARG:CZ	2.53	0.70
2:B:102:ASN:HB3	2:B:408:TYR:CD1	2.25	0.70
2:B:184:PRO:HG3	2:B:399:PHE:HB2	1.70	0.70
2:B:243:ARG:NH2	2:B:252:LEU:CD1	2.52	0.70
1:A:100:ALA:O	1:A:144:GLY:HA3	1.90	0.70
1:A:184:PRO:HG2	1:A:395:PHE:HA	1.72	0.70
1:A:253:THR:O	1:A:253:THR:HG22	1.90	0.70
2:B:416:MET:O	2:B:417:GLU:HB2	1.90	0.70
3:K:168:VAL:HG21	3:K:310:VAL:HG13	1.72	0.70
1:A:4:CYS:SG	1:A:252:LEU:CD1	2.72	0.70
1:A:30:ILE:HD12	1:A:64:ARG:HB3	1.72	0.70
1:A:239:THR:O	1:A:243:ARG:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PHE:CE1	1:A:422:ARG:HG3	2.26	0.70
2:B:142:GLY:CA	2:B:182:VAL:CG2	2.65	0.70
2:B:287:THR:CG2	2:B:288:VAL:N	2.55	0.70
1:A:167:LEU:CD1	1:A:252:LEU:HD22	2.21	0.70
2:B:147:SER:OG	2:B:189:LEU:CD1	2.21	0.70
2:B:175:PRO:O	2:B:176:LYS:HD3	1.88	0.70
1:A:264:ARG:HH21	3:K:307:ARG:CG	1.97	0.70
2:B:2:ARG:CG	2:B:2:ARG:O	2.36	0.70
2:B:3:GLU:C	2:B:4:ILE:CG1	2.58	0.70
2:B:7:ILE:HG12	2:B:66:ILE:CG2	2.16	0.70
2:B:102:ASN:CB	2:B:408:TYR:CD1	2.73	0.70
2:B:183:GLU:CG	2:B:394:GLN:HB3	2.21	0.70
1:A:28:HIS:CG	1:A:29:GLY:H	2.10	0.70
1:A:242:LEU:HD22	1:A:250:VAL:H	1.56	0.70
2:B:19:LYS:HD2	2:B:228:ASN:CB	2.18	0.70
2:B:35:SER:H	2:B:60:LYS:CE	2.02	0.70
3:K:252:SER:O	3:K:253:GLU:CG	2.37	0.70
1:A:16:ILE:HG21	1:A:138:PHE:CD1	2.26	0.70
1:A:30:ILE:CB	1:A:64:ARG:CB	2.66	0.70
1:A:30:ILE:CB	1:A:64:ARG:HB2	2.15	0.70
1:A:437:VAL:C	1:A:438:ASP:OD1	2.33	0.70
2:B:53:TYR:HE1	2:B:87:PHE:CE1	2.08	0.70
1:A:3:GLU:HB2	1:A:132:LEU:HA	1.74	0.70
1:A:143:GLY:O	1:A:144:GLY:C	2.35	0.70
1:A:273:ALA:N	1:A:274:PRO:HD2	2.07	0.70
1:A:70:LEU:CD1	1:A:145:THR:CB	2.60	0.70
1:A:103:TYR:OH	1:A:151:SER:OG	2.08	0.70
1:A:288:VAL:O	1:A:291:ILE:HG13	1.92	0.70
1:A:312:TYR:CB	1:A:381:THR:HG22	2.21	0.70
1:A:369:ALA:HB2	1:A:371:VAL:CG2	2.21	0.70
2:B:44:LEU:HB2	2:B:84:GLY:HA2	1.74	0.70
2:B:133:GLN:HE21	2:B:253:ARG:HH11	1.39	0.70
1:A:311:LYS:C	1:A:312:TYR:O	2.31	0.70
2:B:35:SER:HB3	2:B:60:LYS:CG	2.22	0.70
2:B:57:ALA:C	2:B:64:ARG:H	2.00	0.70
2:B:313:LEU:CA	2:B:344:VAL:HG21	2.22	0.70
1:A:66:VAL:HG22	1:A:125:LEU:CD1	2.23	0.69
1:A:420:GLU:CD	3:K:170:GLU:C	2.58	0.69
2:B:169:PHE:CZ	2:B:235:MET:CG	2.75	0.69
2:B:242:LEU:CA	2:B:356:CYS:SG	2.79	0.69
2:B:265:LEU:O	2:B:267:PHE:CD2	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:CD1	1:A:157:LEU:HD22	2.23	0.69
2:B:48:ARG:HH11	2:B:60:LYS:CB	2.04	0.69
2:B:103:TRP:CD1	2:B:189:LEU:HD21	2.08	0.69
2:B:165:ILE:CD1	2:B:199:ASP:OD2	2.40	0.69
1:A:30:ILE:HG22	1:A:64:ARG:HG2	1.70	0.69
1:A:158:SER:N	1:A:166:LYS:NZ	2.40	0.69
1:A:219:ILE:CG2	1:A:219:ILE:C	2.65	0.69
1:A:291:ILE:HD11	1:A:373:ARG:CB	2.22	0.69
2:B:183:GLU:CB	2:B:184:PRO:CD	2.29	0.69
2:B:183:GLU:CD	2:B:394:GLN:CG	2.65	0.69
2:B:201:THR:CG2	2:B:265:LEU:CD1	2.59	0.69
2:B:191:VAL:HG21	2:B:421:ALA:CA	2.21	0.69
2:B:253:ARG:HH11	2:B:253:ARG:HB2	1.58	0.69
1:A:17:GLY:O	1:A:21:TRP:HD1	1.76	0.69
2:B:242:LEU:HD23	2:B:356:CYS:SG	2.33	0.69
2:B:259:MET:CE	2:B:378:ILE:HG22	2.22	0.69
2:B:342:TYR:C	2:B:343:PHE:CD2	2.71	0.69
1:A:5:ILE:HD12	1:A:135:PHE:CE1	2.28	0.69
1:A:13:GLY:HA2	1:A:16:ILE:HG22	1.75	0.69
1:A:48:SER:OG	1:A:56:THR:CB	2.37	0.69
1:A:72:PRO:C	1:A:75:ILE:CG2	2.64	0.69
1:A:108:TYR:OH	1:A:417:GLU:HG3	1.91	0.69
1:A:115:ILE:CD1	1:A:156:ARG:HD2	2.23	0.69
1:A:271:THR:O	1:A:376:CYS:HA	1.92	0.69
2:B:3:GLU:OE2	2:B:64:ARG:NH1	2.25	0.69
2:B:289:PRO:HA	2:B:292:THR:OG1	1.93	0.69
2:B:397:ALA:C	2:B:401:ARG:HB2	2.17	0.69
1:A:395:PHE:CD1	1:A:422:ARG:HG3	2.28	0.69
1:A:401:LYS:HG2	1:A:402:ARG:HG3	1.75	0.69
1:A:405:VAL:CG2	1:A:409:VAL:CG2	2.65	0.69
2:B:229:HIS:CE1	6:B:502:TXL:H37	2.27	0.69
1:A:51:THR:CG2	1:A:52:PHE:N	2.45	0.69
1:A:72:PRO:CA	1:A:75:ILE:CG2	2.70	0.69
1:A:77:GLU:C	1:A:80:THR:H	2.01	0.69
1:A:115:ILE:HD13	1:A:152:LEU:HD11	1.73	0.69
1:A:230:LEU:CG	1:A:302:MET:HE1	2.23	0.69
2:B:2:ARG:O	2:B:2:ARG:HG2	1.91	0.69
2:B:184:PRO:HD2	2:B:398:MET:SD	2.32	0.69
2:B:244:PHE:CB	2:B:245:PRO:CD	2.71	0.69
2:B:259:MET:O	2:B:261:PRO:HD3	1.93	0.69
2:B:384:ILE:O	2:B:385:GLN:C	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:ARG:O	2:B:394:GLN:CG	2.33	0.69
1:A:258:ASN:O	1:A:314:ALA:HB1	1.92	0.69
2:B:135:PHE:CG	2:B:166:MET:CE	2.63	0.69
2:B:183:GLU:OE2	2:B:394:GLN:CD	2.36	0.69
2:B:246:GLY:HA2	2:B:357:ASP:CG	2.18	0.69
2:B:53:TYR:HD1	2:B:87:PHE:CZ	2.05	0.69
2:B:320:ARG:HE	2:B:360:PRO:HG3	1.58	0.69
1:A:13:GLY:C	1:A:16:ILE:HG22	2.18	0.68
1:A:155:GLU:CD	1:A:192:HIS:CD2	2.68	0.68
1:A:158:SER:CB	1:A:196:GLU:O	2.41	0.68
1:A:422:ARG:O	1:A:426:ALA:CB	2.41	0.68
2:B:14:ASN:ND2	2:B:69:ASP:OD1	2.25	0.68
2:B:97:SER:OG	2:B:110:GLU:OE1	2.10	0.68
1:A:45:GLY:C	1:A:46:ASP:CG	2.58	0.68
1:A:103:TYR:CE2	1:A:189:LEU:CA	2.75	0.68
1:A:107:HIS:CD2	1:A:148:GLY:HA2	2.29	0.68
2:B:194:LEU:HD23	2:B:267:PHE:CE2	2.28	0.68
1:A:17:GLY:O	1:A:21:TRP:CD1	2.46	0.68
2:B:80:SER:O	2:B:81:GLY:C	2.35	0.68
2:B:102:ASN:ND2	2:B:105:LYS:HZ1	1.88	0.68
2:B:141:LEU:CD2	2:B:186:ASN:HB3	2.12	0.68
2:B:184:PRO:HG3	2:B:399:PHE:HD2	0.76	0.68
1:A:241:SER:CB	1:A:356:ASN:HD22	2.04	0.68
1:A:361:THR:C	1:A:362:VAL:HG23	2.18	0.68
2:B:75:MET:HE2	2:B:79:ARG:HB3	1.76	0.68
2:B:183:GLU:CG	2:B:398:MET:SD	2.82	0.68
2:B:339:ASN:O	2:B:342:TYR:CB	2.40	0.68
2:B:405:LEU:O	2:B:409:THR:N	2.26	0.68
1:A:5:ILE:HD11	1:A:132:LEU:HD13	1.76	0.68
1:A:172:TYR:CZ	1:A:387:ALA:CB	2.74	0.68
1:A:184:PRO:CG	1:A:399:TYR:HD2	2.05	0.68
1:A:200:CYS:SG	1:A:259:LEU:HB2	2.32	0.68
1:A:397:LEU:HD22	1:A:401:LYS:NZ	2.08	0.68
2:B:35:SER:CA	2:B:60:LYS:HE2	2.21	0.68
2:B:194:LEU:CD2	2:B:267:PHE:CZ	2.75	0.68
2:B:369:ARG:O	6:B:502:TXL:C21	2.41	0.68
1:A:58:ALA:HB3	1:A:60:LYS:HG3	1.75	0.68
1:A:202:PHE:HE1	1:A:378:LEU:HD13	1.55	0.68
1:A:257:THR:CG2	2:B:407:TRP:HE3	2.01	0.68
1:A:294:ALA:C	1:A:300:ASN:HD22	2.00	0.68
2:B:31:ASP:H	2:B:32:PRO:HD3	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CG	1:A:89:PRO:N	2.62	0.68
1:A:200:CYS:SG	1:A:260:VAL:HG23	2.33	0.68
1:A:312:TYR:CG	1:A:381:THR:HG22	2.28	0.68
1:A:5:ILE:HD12	1:A:135:PHE:CZ	2.28	0.68
2:B:328:VAL:O	2:B:332:MET:HG2	1.93	0.68
1:A:16:ILE:CG2	1:A:138:PHE:CD1	2.77	0.68
1:A:155:GLU:HG2	1:A:196:GLU:CG	2.21	0.68
1:A:155:GLU:CD	1:A:192:HIS:HD2	1.88	0.68
1:A:184:PRO:HB3	1:A:395:PHE:CD2	2.19	0.68
1:A:420:GLU:OE1	3:K:170:GLU:C	2.36	0.68
2:B:42:LEU:O	2:B:43:GLN:CG	2.42	0.68
2:B:135:PHE:HB2	2:B:166:MET:SD	2.34	0.68
2:B:230:LEU:HG	2:B:302:MET:HE3	1.76	0.68
1:A:66:VAL:CG2	1:A:125:LEU:HD13	2.24	0.68
1:A:97:GLU:HB3	1:A:110:ILE:HD13	1.74	0.67
2:B:75:MET:CE	2:B:75:MET:HA	2.21	0.67
2:B:229:HIS:CG	6:B:502:TXL:H37	2.28	0.67
2:B:296:PHE:O	2:B:297:ASP:C	2.34	0.67
1:A:313:MET:HE3	1:A:346:TRP:CH2	2.27	0.67
1:A:315:CYS:SG	1:A:343:PHE:CE1	2.87	0.67
2:B:11:GLN:HB2	5:B:501:GDP:O2A	1.95	0.67
1:A:100:ALA:HB1	1:A:105:ARG:CB	2.22	0.67
1:A:103:TYR:N	1:A:408:TYR:HE1	1.81	0.67
2:B:371:LEU:O	2:B:372:LYS:HB2	1.93	0.67
1:A:275:VAL:O	1:A:275:VAL:HG12	1.94	0.67
1:A:296:PHE:CE1	1:A:335:ILE:HG21	2.28	0.67
1:A:426:ALA:C	1:A:428:LEU:N	2.51	0.67
2:B:242:LEU:HD21	2:B:354:ALA:HB1	1.77	0.67
2:B:352:LYS:HG2	2:B:353:THR:N	2.09	0.67
2:B:386:GLU:C	2:B:388:PHE:H	2.01	0.67
3:K:303:PHE:C	3:K:303:PHE:CD2	2.72	0.67
1:A:83:TYR:O	1:A:84:ARG:CG	2.41	0.67
1:A:220:GLU:H	1:A:220:GLU:HG3	1.58	0.67
1:A:317:LEU:HA	1:A:376:CYS:O	1.94	0.67
2:B:22:GLU:HG2	2:B:83:PHE:CE2	2.26	0.67
2:B:144:GLY:N	2:B:185:TYR:OH	2.27	0.67
1:A:57:GLY:HA3	1:A:61:HIS:ND1	2.08	0.67
1:A:77:GLU:O	1:A:80:THR:HB	1.95	0.67
1:A:196:GLU:O	1:A:197:HIS:CG	2.48	0.67
2:B:96:GLN:O	2:B:98:GLY:CA	2.42	0.67
2:B:405:LEU:CG	2:B:418:PHE:CZ	2.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HG21	1:A:64:ARG:CG	2.09	0.67
1:A:204:VAL:HG13	1:A:302:MET:HE3	1.75	0.67
2:B:22:GLU:CD	2:B:83:PHE:CD2	2.70	0.67
2:B:69:ASP:CG	2:B:74:THR:CB	2.60	0.67
2:B:201:THR:HG21	2:B:265:LEU:CG	2.24	0.67
2:B:244:PHE:O	2:B:245:PRO:O	2.12	0.67
2:B:286:LEU:HD13	2:B:372:LYS:HB2	1.67	0.67
1:A:239:THR:O	1:A:243:ARG:CG	2.43	0.67
2:B:44:LEU:O	2:B:44:LEU:HG	1.93	0.67
2:B:259:MET:HE2	2:B:379:GLY:CA	2.22	0.67
2:B:426:ASN:C	2:B:428:LEU:N	2.51	0.67
1:A:107:HIS:CD2	1:A:148:GLY:C	2.72	0.67
1:A:234:ILE:O	1:A:237:SER:OG	2.11	0.67
1:A:361:THR:O	1:A:362:VAL:CG2	2.41	0.67
1:A:399:TYR:O	1:A:403:ALA:HA	1.94	0.67
2:B:40:SER:O	2:B:41:ASP:CG	2.38	0.67
2:B:44:LEU:CB	2:B:85:GLN:HG3	2.24	0.67
1:A:311:LYS:O	1:A:312:TYR:O	2.12	0.66
2:B:6:HIS:O	2:B:66:ILE:N	2.23	0.66
2:B:30:ILE:HG23	2:B:243:ARG:NH1	2.08	0.66
1:A:38:SER:C	1:A:39:ASP:CB	2.68	0.66
1:A:205:ASP:HB2	1:A:302:MET:O	1.96	0.66
2:B:272:PHE:CE1	2:B:274:PRO:HG2	2.30	0.66
2:B:359:PRO:CB	2:B:372:LYS:O	2.43	0.66
2:B:401:ARG:CG	2:B:402:LYS:H	2.03	0.66
1:A:22:GLU:O	1:A:25:CYS:CB	2.44	0.66
1:A:191:THR:HG21	1:A:421:ALA:CA	2.24	0.66
2:B:181:VAL:CG2	2:B:404:PHE:HE2	2.08	0.66
1:A:48:SER:O	1:A:50:ASN:ND2	2.22	0.66
1:A:103:TYR:N	1:A:408:TYR:CE1	2.61	0.66
1:A:153:LEU:O	1:A:157:LEU:CG	2.42	0.66
1:A:254:GLU:OE2	2:B:101:ASN:OD1	2.13	0.66
1:A:272:TYR:CE2	1:A:274:PRO:HG2	2.26	0.66
1:A:328:VAL:HG13	1:A:353:VAL:HG11	1.77	0.66
2:B:184:PRO:HA	2:B:395:PHE:CD1	2.30	0.66
2:B:284:ARG:O	2:B:286:LEU:N	2.28	0.66
1:A:14:VAL:HB	1:A:74:VAL:HG21	1.78	0.66
1:A:41:THR:O	1:A:42:ILE:CB	2.44	0.66
1:A:126:ALA:O	1:A:132:LEU:CD1	2.41	0.66
1:A:312:TYR:HD2	1:A:381:THR:CG2	2.04	0.66
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:GLU:CA	2:B:83:PHE:CE2	2.79	0.66
2:B:30:ILE:CG2	2:B:136:GLN:HE22	2.09	0.66
2:B:158:ARG:HH11	2:B:197:ASN:H	1.41	0.66
2:B:184:PRO:HB3	2:B:395:PHE:CD1	2.30	0.66
2:B:197:ASN:OD1	2:B:197:ASN:O	2.13	0.66
1:A:88:HIS:CD2	1:A:89:PRO:N	2.63	0.66
1:A:172:TYR:HD1	1:A:173:PRO:O	1.79	0.66
2:B:229:HIS:NE2	6:B:502:TXL:C34	2.50	0.66
2:B:433:GLN:O	2:B:434:GLN:C	2.34	0.66
1:A:75:ILE:HD12	1:A:93:ILE:O	1.95	0.66
1:A:193:THR:HG1	1:A:194:THR:N	1.92	0.66
1:A:262:TYR:CE1	1:A:435:VAL:HG13	2.31	0.66
1:A:262:TYR:CB	1:A:263:PRO:CD	2.57	0.66
2:B:182:VAL:CG1	2:B:186:ASN:HD22	2.01	0.66
2:B:407:TRP:N	2:B:407:TRP:CD1	2.58	0.66
1:A:313:MET:HA	1:A:344:VAL:CG2	2.25	0.66
1:A:405:VAL:CG2	1:A:405:VAL:HG11	2.25	0.66
2:B:158:ARG:HA	2:B:197:ASN:HD22	0.52	0.66
2:B:274:PRO:C	2:B:276:THR:HG23	2.21	0.66
1:A:146:GLY:HA2	1:A:150:THR:HG23	1.76	0.66
1:A:202:PHE:CD1	1:A:378:LEU:HD22	2.30	0.66
1:A:242:LEU:CD1	1:A:255:PHE:CZ	2.67	0.66
2:B:151:THR:HA	2:B:192:HIS:HE2	0.85	0.66
1:A:184:PRO:CG	1:A:395:PHE:CG	2.60	0.66
1:A:223:THR:H	1:A:226:ASN:HD22	1.44	0.66
2:B:141:LEU:HD12	2:B:172:VAL:HA	0.91	0.66
2:B:391:ILE:O	2:B:394:GLN:HB2	1.95	0.66
1:A:65:ALA:O	1:A:66:VAL:CG2	2.43	0.65
1:A:291:ILE:CD1	1:A:373:ARG:CB	2.74	0.65
1:A:348:PRO:O	1:A:349:THR:OG1	2.13	0.65
2:B:8:GLN:HB2	2:B:67:LEU:HD12	1.78	0.65
2:B:44:LEU:CG	2:B:85:GLN:CG	2.67	0.65
2:B:142:GLY:O	2:B:185:TYR:CZ	2.49	0.65
2:B:398:MET:HE2	2:B:399:PHE:CE2	2.31	0.65
1:A:107:HIS:CD2	1:A:151:SER:OG	2.49	0.65
1:A:109:THR:HG21	1:A:411:GLU:HB3	1.78	0.65
1:A:179:THR:CG2	1:A:181:VAL:CG2	2.74	0.65
1:A:231:ILE:CD1	1:A:302:MET:CE	2.69	0.65
2:B:44:LEU:HB3	2:B:85:GLN:HG3	1.76	0.65
2:B:87:PHE:CE1	2:B:89:PRO:HG3	2.28	0.65
2:B:92:PHE:CD2	2:B:114:LEU:CD1	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ALA:HA	2:B:413:MET:CE	2.22	0.65
1:A:2:ARG:HH21	2:B:71:GLU:CG	2.08	0.65
1:A:239:THR:CG2	1:A:243:ARG:HG3	2.23	0.65
2:B:153:LEU:O	2:B:157:ILE:HG13	1.95	0.65
1:A:238:ILE:HG23	1:A:255:PHE:CZ	2.32	0.65
1:A:239:THR:O	1:A:243:ARG:CB	2.44	0.65
1:A:288:VAL:O	1:A:291:ILE:CG1	2.44	0.65
1:A:306:ASP:CG	1:A:308:ARG:CG	2.69	0.65
2:B:107:HIS:CD2	2:B:152:LEU:HD23	2.19	0.65
2:B:181:VAL:CA	2:B:398:MET:HE1	2.27	0.65
2:B:190:SER:C	2:B:192:HIS:N	2.53	0.65
1:A:197:HIS:O	1:A:198:SER:CB	2.45	0.65
2:B:34:GLY:O	2:B:36:TYR:CD2	2.49	0.65
2:B:103:TRP:CD1	2:B:148:GLY:HA3	2.31	0.65
1:A:2:ARG:HH21	2:B:99:ALA:HB2	1.61	0.65
2:B:23:VAL:HG21	2:B:232:SER:CB	2.26	0.65
2:B:53:TYR:CE1	2:B:89:PRO:CG	2.78	0.65
2:B:94:PHE:CD2	2:B:114:LEU:HD22	2.32	0.65
2:B:104:ALA:CA	2:B:413:MET:HE3	2.19	0.65
2:B:111:GLY:O	2:B:115:VAL:CB	2.45	0.65
2:B:336:GLN:HE21	2:B:351:VAL:HB	1.60	0.65
2:B:399:PHE:CZ	2:B:408:TYR:CE2	2.80	0.65
1:A:115:ILE:HD11	1:A:156:ARG:HD2	1.79	0.65
1:A:142:GLY:HA2	1:A:185:TYR:CD1	2.32	0.65
1:A:277:SER:CA	1:A:368:LEU:HD22	2.24	0.65
2:B:49:ILE:O	2:B:50:ASN:CG	2.40	0.65
2:B:141:LEU:HD12	2:B:173:PRO:HD3	1.77	0.65
1:A:5:ILE:HG13	1:A:64:ARG:HH21	1.60	0.65
1:A:277:SER:N	1:A:280:LYS:HG2	2.11	0.65
2:B:151:THR:C	2:B:192:HIS:CD2	2.73	0.65
2:B:296:PHE:CE1	2:B:335:VAL:HG21	2.32	0.65
2:B:405:LEU:O	2:B:409:THR:OG1	2.07	0.65
3:K:231:ASP:O	3:K:233:GLU:HG2	1.96	0.65
1:A:77:GLU:N	1:A:80:THR:OG1	2.30	0.65
1:A:80:THR:O	1:A:82:THR:N	2.30	0.65
2:B:12:CYS:SG	5:B:501:GDP:O4'	2.55	0.65
2:B:165:ILE:HD13	2:B:256:ALA:CB	2.26	0.65
2:B:226:ASP:CG	6:B:502:TXL:C40	2.70	0.65
2:B:435:TYR:CA	2:B:436:GLN:HG3	2.18	0.65
1:A:154:MET:HE1	1:A:166:LYS:HB3	1.78	0.65
1:A:296:PHE:O	1:A:297:GLU:C	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD23	1:A:401:LYS:CD	2.11	0.65
2:B:92:PHE:CE1	2:B:121:VAL:CG2	2.80	0.65
1:A:2:ARG:NH2	2:B:99:ALA:HB3	2.11	0.64
1:A:5:ILE:HB	1:A:135:PHE:CD1	2.32	0.64
1:A:83:TYR:O	1:A:84:ARG:CB	2.44	0.64
1:A:104:ALA:CA	1:A:108:TYR:HD2	2.08	0.64
1:A:209:ILE:HD13	1:A:227:LEU:CD1	2.24	0.64
2:B:259:MET:HB3	2:B:268:PHE:HE1	1.45	0.64
2:B:399:PHE:CE1	2:B:408:TYR:CZ	2.80	0.64
1:A:41:THR:O	1:A:41:THR:HG22	1.97	0.64
1:A:217:LEU:CD1	1:A:277:SER:HA	2.27	0.64
1:A:297:GLU:C	1:A:299:ALA:N	2.55	0.64
2:B:13:GLY:HA2	2:B:138:THR:OG1	1.95	0.64
2:B:41:ASP:C	2:B:42:LEU:CG	2.54	0.64
2:B:200:GLU:CB	2:B:268:PHE:HE2	2.09	0.64
1:A:13:GLY:CA	1:A:16:ILE:HG22	2.26	0.64
1:A:22:GLU:O	1:A:25:CYS:HB3	1.97	0.64
1:A:238:ILE:O	1:A:255:PHE:HZ	1.80	0.64
1:A:250:VAL:HG21	1:A:352:LYS:CE	2.08	0.64
1:A:287:SER:OG	1:A:290:GLU:CB	2.45	0.64
2:B:33:THR:HG22	2:B:34:GLY:N	2.11	0.64
2:B:53:TYR:HD1	2:B:87:PHE:CE1	2.11	0.64
2:B:92:PHE:HE1	2:B:121:VAL:CG2	2.10	0.64
2:B:118:VAL:O	2:B:118:VAL:HG12	1.98	0.64
2:B:268:PHE:CD1	2:B:380:ASN:OD1	2.49	0.64
2:B:422:GLU:O	2:B:426:ASN:CB	2.41	0.64
1:A:57:GLY:CA	1:A:61:HIS:CE1	2.71	0.64
2:B:103:TRP:HE1	2:B:189:LEU:HD23	1.59	0.64
2:B:166:MET:O	2:B:199:ASP:HB3	1.97	0.64
1:A:97:GLU:CB	1:A:110:ILE:HG23	2.21	0.64
1:A:209:ILE:HG12	1:A:302:MET:HE3	1.78	0.64
1:A:267:PHE:O	1:A:380:ASN:OD1	2.15	0.64
1:A:296:PHE:CZ	1:A:335:ILE:HD13	2.22	0.64
2:B:5:VAL:HG11	2:B:135:PHE:CE2	2.33	0.64
2:B:183:GLU:OE1	2:B:394:GLN:HG3	1.98	0.64
1:A:291:ILE:HD12	1:A:373:ARG:HB3	1.77	0.64
1:A:317:LEU:O	1:A:353:VAL:HA	1.98	0.64
1:A:426:ALA:O	1:A:428:LEU:N	2.31	0.64
2:B:319:PHE:CE2	2:B:328:VAL:HG13	2.32	0.64
2:B:32:PRO:CA	2:B:59:ASN:HD22	2.05	0.64
2:B:133:GLN:NE2	2:B:253:ARG:HH11	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CG	1:A:188:ILE:HG21	2.22	0.64
1:A:282:TYR:O	1:A:284:GLU:N	2.31	0.64
1:A:361:THR:CG2	1:A:362:VAL:N	2.59	0.64
1:A:65:ALA:CB	1:A:91:GLN:CD	2.71	0.64
1:A:312:TYR:CZ	1:A:377:MET:HE1	2.29	0.64
2:B:12:CYS:SG	5:B:501:GDP:N9	2.71	0.64
2:B:57:ALA:O	2:B:62:VAL:O	2.16	0.64
2:B:92:PHE:HE1	2:B:121:VAL:HG21	1.62	0.64
2:B:154:ILE:HG23	2:B:198:THR:CG2	2.26	0.64
2:B:272:PHE:CZ	6:B:502:TXL:H28	2.33	0.64
1:A:1:MET:N	2:B:96:GLN:OE1	2.31	0.63
1:A:102:ASN:CA	1:A:185:TYR:HE2	2.11	0.63
1:A:179:THR:HB	1:A:182:VAL:HG23	1.79	0.63
1:A:192:HIS:O	1:A:196:GLU:CG	2.46	0.63
1:A:196:GLU:C	1:A:197:HIS:ND1	2.56	0.63
2:B:6:HIS:CE1	2:B:21:TRP:CH2	2.86	0.63
2:B:154:ILE:HD12	2:B:192:HIS:HE2	1.60	0.63
1:A:65:ALA:HB1	1:A:91:GLN:CD	2.23	0.63
1:A:72:PRO:HA	1:A:75:ILE:HG21	1.80	0.63
1:A:237:SER:HA	1:A:320:ARG:NH1	2.13	0.63
1:A:264:ARG:NH1	1:A:424:ASP:O	2.32	0.63
1:A:303:VAL:HG12	1:A:305:CYS:SG	2.38	0.63
2:B:166:MET:CG	2:B:197:ASN:O	2.46	0.63
2:B:192:HIS:ND1	2:B:192:HIS:C	2.57	0.63
2:B:201:THR:HG21	2:B:265:LEU:HD21	0.74	0.63
1:A:2:ARG:NH2	2:B:99:ALA:HB2	2.13	0.63
1:A:172:TYR:HE2	1:A:388:TRP:CZ3	2.12	0.63
2:B:32:PRO:C	2:B:59:ASN:HD22	2.06	0.63
2:B:47:GLU:HG2	2:B:63:PRO:HD3	1.80	0.63
2:B:48:ARG:C	2:B:61:TYR:CD2	2.76	0.63
2:B:101:ASN:O	2:B:105:LYS:HD2	1.97	0.63
2:B:231:VAL:HA	2:B:302:MET:CE	2.28	0.63
3:K:159:ASN:ND2	3:K:161:LYS:CG	2.52	0.63
1:A:67:PHE:HB2	1:A:92:LEU:CD2	2.28	0.63
2:B:22:GLU:C	2:B:24:ILE:H	2.06	0.63
2:B:174:SER:HB2	2:B:175:PRO:CD	2.29	0.63
1:A:28:HIS:CG	1:A:29:GLY:N	2.64	0.63
1:A:82:THR:C	1:A:84:ARG:H	2.07	0.63
1:A:103:TYR:CZ	1:A:188:ILE:HG22	2.34	0.63
1:A:204:VAL:HG13	1:A:302:MET:CE	2.28	0.63
1:A:282:TYR:CE2	1:A:284:GLU:O	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:O	1:A:327:ASP:HB2	1.97	0.63
2:B:66:ILE:CG1	2:B:121:VAL:CG1	2.69	0.63
2:B:250:ALA:HB2	2:B:352:LYS:NZ	2.13	0.63
2:B:288:VAL:N	2:B:289:PRO:CD	2.59	0.63
2:B:313:LEU:CD2	2:B:344:VAL:HG21	2.28	0.63
2:B:414:ASP:OD2	3:K:253:GLU:CD	2.40	0.63
2:B:426:ASN:O	2:B:428:LEU:N	2.32	0.63
1:A:132:LEU:O	1:A:134:GLY:N	2.30	0.63
1:A:191:THR:CG2	1:A:421:ALA:HA	2.28	0.63
1:A:270:ALA:O	1:A:302:MET:CG	2.43	0.63
2:B:405:LEU:CD1	2:B:418:PHE:CZ	2.71	0.63
6:B:502:TXL:H192	6:B:502:TXL:C20	2.29	0.63
1:A:304:LYS:HG2	1:A:304:LYS:O	1.98	0.63
1:A:335:ILE:C	1:A:337:THR:H	2.06	0.63
2:B:22:GLU:CD	2:B:83:PHE:CB	2.72	0.63
2:B:30:ILE:HG22	2:B:243:ARG:NH1	2.14	0.63
2:B:274:PRO:HB2	2:B:371:LEU:HD11	1.81	0.63
2:B:398:MET:O	2:B:401:ARG:CB	2.45	0.63
1:A:97:GLU:HA	1:A:97:GLU:OE1	1.97	0.63
1:A:142:GLY:CA	1:A:185:TYR:CE1	2.82	0.63
1:A:151:SER:HB2	1:A:192:HIS:HB2	1.79	0.63
1:A:184:PRO:CG	1:A:395:PHE:HB2	2.19	0.63
1:A:1:MET:O	2:B:96:GLN:NE2	2.27	0.63
1:A:14:VAL:HA	1:A:67:PHE:CE1	2.34	0.63
1:A:210:TYR:HE2	1:A:227:LEU:CD2	2.02	0.63
1:A:282:TYR:CE2	1:A:285:GLN:HA	2.33	0.63
2:B:4:ILE:CD1	2:B:30:ILE:CB	2.77	0.63
2:B:35:SER:HB3	2:B:60:LYS:HG3	1.81	0.63
2:B:70:LEU:O	2:B:71:GLU:CG	2.47	0.63
2:B:101:ASN:ND2	2:B:185:TYR:OH	2.31	0.63
1:A:404:PHE:CD2	1:A:404:PHE:O	2.52	0.62
2:B:11:GLN:HB3	5:B:501:GDP:O1A	1.97	0.62
2:B:133:GLN:O	2:B:133:GLN:HG2	1.99	0.62
1:A:133:GLN:NE2	2:B:98:GLY:CA	2.61	0.62
1:A:154:MET:HB2	1:A:192:HIS:NE2	2.14	0.62
1:A:202:PHE:CE1	1:A:378:LEU:HD22	2.34	0.62
1:A:103:TYR:CE2	1:A:147:SER:C	2.76	0.62
1:A:115:ILE:CD1	1:A:156:ARG:NE	2.59	0.62
2:B:23:VAL:O	2:B:26:ASP:CB	2.47	0.62
2:B:181:VAL:CA	2:B:398:MET:CE	2.77	0.62
1:A:2:ARG:O	1:A:243:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLY:HA3	1:A:61:HIS:CD2	2.34	0.62
1:A:192:HIS:ND1	1:A:192:HIS:C	2.57	0.62
1:A:224:TYR:CE1	4:A:500:GTP:C2	2.86	0.62
1:A:277:SER:N	1:A:280:LYS:CG	2.58	0.62
2:B:55:GLU:C	2:B:57:ALA:N	2.56	0.62
2:B:102:ASN:HD22	2:B:105:LYS:HZ1	1.39	0.62
1:A:103:TYR:CD2	1:A:189:LEU:CG	2.78	0.62
1:A:257:THR:HG22	2:B:407:TRP:CD2	2.32	0.62
2:B:241:CYS:SG	2:B:320:ARG:CD	2.84	0.62
1:A:107:HIS:CG	1:A:148:GLY:C	2.77	0.62
1:A:224:TYR:CD1	4:A:500:GTP:C2	2.88	0.62
1:A:288:VAL:O	1:A:291:ILE:HB	2.00	0.62
1:A:331:ALA:O	1:A:334:THR:OG1	2.13	0.62
2:B:40:SER:C	2:B:41:ASP:CG	2.67	0.62
2:B:89:PRO:O	2:B:90:ASP:CG	2.43	0.62
2:B:103:TRP:CG	2:B:188:THR:HG1	2.17	0.62
2:B:169:PHE:HA	2:B:202:TYR:HB2	1.81	0.62
2:B:424:ASN:O	2:B:424:ASN:ND2	2.32	0.62
2:B:427:ASP:O	2:B:431:GLU:N	2.18	0.62
3:K:171:HIS:CD2	3:K:174:LEU:H	2.17	0.62
1:A:106:GLY:O	1:A:111:GLY:N	2.32	0.62
1:A:108:TYR:CZ	1:A:417:GLU:OE2	2.53	0.62
1:A:122:ILE:CD1	1:A:157:LEU:CD2	2.77	0.62
1:A:313:MET:CE	1:A:346:TRP:CZ2	2.70	0.62
2:B:18:ALA:O	2:B:22:GLU:HG3	2.00	0.62
2:B:94:PHE:CD1	2:B:94:PHE:C	2.68	0.62
2:B:106:GLY:O	2:B:111:GLY:N	2.32	0.62
2:B:165:ILE:HD13	2:B:256:ALA:HB1	1.80	0.62
2:B:246:GLY:HA2	2:B:357:ASP:OD2	2.00	0.62
2:B:342:TYR:O	2:B:343:PHE:CD2	2.52	0.62
1:A:102:ASN:C	1:A:185:TYR:CE2	2.78	0.62
1:A:206:ASN:CG	4:A:500:GTP:HN22	2.06	0.62
2:B:289:PRO:O	2:B:293:GLN:CB	2.48	0.62
1:A:259:LEU:HB3	1:A:380:ASN:HD21	1.64	0.62
2:B:209:LEU:HD13	2:B:227:LEU:CG	2.15	0.62
2:B:295:MET:CE	2:B:375:ALA:C	2.72	0.62
1:A:289:ALA:HB1	1:A:331:ALA:HB2	1.82	0.62
2:B:71:GLU:O	2:B:72:PRO:C	2.38	0.62
2:B:183:GLU:OE1	2:B:394:GLN:CG	2.48	0.62
1:A:14:VAL:HB	1:A:74:VAL:CG2	2.30	0.61
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:HG22	1:A:343:PHE:CE2	2.35	0.61
2:B:13:GLY:HA3	2:B:138:THR:OG1	1.97	0.61
2:B:102:ASN:CB	2:B:408:TYR:HD1	2.07	0.61
2:B:216:THR:HG21	2:B:275:LEU:CD1	2.29	0.61
2:B:288:VAL:O	2:B:291:LEU:N	2.33	0.61
2:B:360:PRO:CG	2:B:374:SER:HB3	2.30	0.61
2:B:433:GLN:CG	2:B:437:ASP:OD1	2.48	0.61
1:A:3:GLU:CB	1:A:64:ARG:CZ	2.77	0.61
1:A:361:THR:HG22	1:A:362:VAL:H	1.63	0.61
2:B:3:GLU:HA	2:B:31:ASP:CG	2.19	0.61
2:B:238:VAL:HG13	2:B:255:LEU:CD1	2.30	0.61
2:B:241:CYS:SG	2:B:320:ARG:CZ	2.89	0.61
2:B:313:LEU:HD13	2:B:435:TYR:HD2	1.65	0.61
1:A:139:HIS:HB3	1:A:169:PHE:O	2.00	0.61
1:A:420:GLU:OE1	3:K:170:GLU:CB	2.47	0.61
2:B:4:ILE:HD11	2:B:30:ILE:O	1.98	0.61
2:B:22:GLU:HA	2:B:83:PHE:CE2	2.35	0.61
2:B:102:ASN:HB2	2:B:105:LYS:CG	2.29	0.61
2:B:173:PRO:HG2	2:B:391:ILE:HD11	1.78	0.61
1:A:276:ILE:HD13	1:A:282:TYR:CG	2.35	0.61
1:A:397:LEU:HA	1:A:401:LYS:HB3	1.78	0.61
2:B:78:VAL:CA	2:B:82:PRO:HG2	2.29	0.61
2:B:165:ILE:CD1	2:B:256:ALA:CB	2.79	0.61
2:B:250:ALA:CB	2:B:352:LYS:NZ	2.63	0.61
1:A:175:PRO:HD3	1:A:390:ARG:HH22	1.62	0.61
1:A:194:THR:CG2	1:A:195:LEU:HG	2.27	0.61
1:A:242:LEU:HD13	1:A:250:VAL:O	2.00	0.61
1:A:269:LEU:HD21	1:A:384:ILE:HD11	1.83	0.61
1:A:273:ALA:CB	1:A:294:ALA:CB	2.78	0.61
2:B:104:ALA:O	2:B:108:TYR:HB2	2.01	0.61
2:B:246:GLY:CA	2:B:357:ASP:OD2	2.48	0.61
1:A:313:MET:CE	1:A:346:TRP:HH2	2.12	0.61
2:B:3:GLU:CD	2:B:64:ARG:HH12	2.09	0.61
1:A:34:GLY:O	1:A:60:LYS:NZ	2.34	0.61
2:B:30:ILE:CG2	2:B:243:ARG:HH12	2.13	0.61
2:B:33:THR:C	2:B:59:ASN:ND2	2.44	0.61
2:B:346:TRP:HZ3	2:B:347:ILE:CD1	1.79	0.61
1:A:9:VAL:CG1	1:A:146:GLY:HA2	2.31	0.61
1:A:209:ILE:CD1	1:A:227:LEU:CD1	2.67	0.61
1:A:277:SER:OG	1:A:280:LYS:CD	2.47	0.61
2:B:12:CYS:O	2:B:16:ILE:HB	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:N	2:B:32:PRO:CD	2.64	0.61
2:B:250:ALA:CB	2:B:352:LYS:HZ3	2.13	0.61
2:B:287:THR:HG22	2:B:289:PRO:N	2.14	0.61
1:A:30:ILE:C	1:A:32:PRO:CG	2.55	0.61
1:A:83:TYR:O	1:A:83:TYR:CG	2.54	0.61
1:A:115:ILE:HD12	1:A:152:LEU:HG	0.67	0.61
1:A:172:TYR:CE1	1:A:387:ALA:HB1	2.34	0.61
2:B:15:GLN:O	2:B:18:ALA:HB3	2.00	0.61
2:B:68:VAL:CG1	2:B:149:MET:HE1	2.30	0.61
2:B:295:MET:SD	2:B:375:ALA:HB1	2.36	0.61
2:B:433:GLN:CG	2:B:437:ASP:OD2	2.43	0.61
1:A:158:SER:CB	1:A:197:HIS:HB2	2.14	0.61
1:A:262:TYR:HE1	1:A:435:VAL:HG13	1.65	0.61
1:A:358:GLU:O	1:A:359:PRO:O	2.19	0.61
2:B:30:ILE:HG23	2:B:243:ARG:HH11	1.65	0.61
2:B:398:MET:HG2	2:B:399:PHE:H	1.64	0.61
1:A:97:GLU:O	1:A:110:ILE:CD1	2.48	0.60
1:A:109:THR:HG23	1:A:411:GLU:HB3	1.81	0.60
2:B:19:LYS:HG3	2:B:228:ASN:ND2	2.16	0.60
2:B:34:GLY:HA2	2:B:37:HIS:CD2	2.36	0.60
2:B:78:VAL:HA	2:B:82:PRO:CG	2.32	0.60
2:B:79:ARG:O	2:B:80:SER:OG	2.19	0.60
2:B:223:THR:OG1	2:B:226:ASP:HB2	2.00	0.60
2:B:398:MET:CG	2:B:399:PHE:H	2.12	0.60
6:B:502:TXL:C9	6:B:502:TXL:C16	2.79	0.60
3:K:252:SER:HA	3:K:275:LEU:HD12	1.83	0.60
1:A:14:VAL:HG11	1:A:74:VAL:HG13	1.84	0.60
1:A:122:ILE:HD13	1:A:157:LEU:CD2	2.31	0.60
1:A:219:ILE:C	1:A:219:ILE:HG22	2.26	0.60
1:A:184:PRO:HG2	1:A:399:TYR:HD2	1.67	0.60
2:B:141:LEU:HD13	2:B:173:PRO:HD3	1.81	0.60
2:B:176:LYS:C	2:B:177:VAL:HG13	2.25	0.60
2:B:184:PRO:HB2	2:B:399:PHE:CG	2.33	0.60
2:B:323:MET:CG	2:B:324:SER:H	2.13	0.60
1:A:151:SER:HB2	1:A:155:GLU:OE2	2.01	0.60
1:A:315:CYS:SG	1:A:343:PHE:HE1	2.21	0.60
2:B:4:ILE:HG21	2:B:30:ILE:HB	1.82	0.60
2:B:53:TYR:HE1	2:B:87:PHE:HE1	1.46	0.60
2:B:339:ASN:O	2:B:342:TYR:CA	2.50	0.60
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.83	0.60
1:A:420:GLU:HG3	3:K:169:ARG:NE	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TRP:O	2:B:107:HIS:HB3	2.02	0.60
2:B:107:HIS:CE1	2:B:152:LEU:HD23	2.22	0.60
2:B:136:GLN:HE22	2:B:243:ARG:HH12	1.49	0.60
2:B:151:THR:CB	2:B:192:HIS:NE2	2.28	0.60
1:A:5:ILE:CG2	1:A:135:PHE:CE1	2.83	0.60
1:A:264:ARG:O	1:A:265:ALA:O	2.19	0.60
1:A:327:ASP:O	1:A:331:ALA:HB3	2.01	0.60
1:A:396:ASP:O	1:A:401:LYS:CB	2.34	0.60
2:B:55:GLU:C	2:B:57:ALA:H	2.07	0.60
2:B:414:ASP:C	2:B:416:MET:H	2.05	0.60
1:A:237:SER:HB2	1:A:376:CYS:SG	2.41	0.60
1:A:362:VAL:HG13	1:A:367:ASP:HB3	1.83	0.60
2:B:139:HIS:NE2	2:B:193:GLN:NE2	2.49	0.60
1:A:237:SER:CB	1:A:376:CYS:SG	2.90	0.60
1:A:427:ALA:O	1:A:431:ASP:N	2.19	0.60
2:B:78:VAL:O	2:B:82:PRO:CG	2.43	0.60
2:B:115:VAL:HG12	2:B:156:LYS:NZ	2.16	0.60
2:B:141:LEU:HG	2:B:171:VAL:O	2.01	0.60
2:B:385:GLN:CD	2:B:433:GLN:HB2	2.26	0.60
1:A:33:ASP:C	1:A:33:ASP:OD1	2.40	0.60
1:A:191:THR:CG2	1:A:421:ALA:CA	2.79	0.60
1:A:217:LEU:CD1	1:A:368:LEU:CG	2.75	0.60
1:A:434:GLU:HB2	3:K:303:PHE:CG	2.37	0.60
1:A:437:VAL:O	1:A:437:VAL:HG12	2.01	0.60
2:B:22:GLU:OE1	2:B:83:PHE:CD1	2.55	0.60
2:B:198:THR:O	2:B:265:LEU:HD13	2.02	0.60
2:B:325:MET:HE1	2:B:355:VAL:HB	1.83	0.60
1:A:2:ARG:HB3	1:A:243:ARG:HH12	1.67	0.60
1:A:100:ALA:HB1	1:A:105:ARG:CG	2.31	0.60
1:A:350:GLY:HA2	2:B:180:THR:HG22	1.84	0.60
2:B:20:PHE:HZ	2:B:239:THR:HG21	1.67	0.60
2:B:320:ARG:HG3	2:B:320:ARG:O	2.00	0.60
3:K:159:ASN:HD21	3:K:161:LYS:HG3	1.64	0.60
1:A:6:SER:OG	1:A:65:ALA:N	2.34	0.59
1:A:8:HIS:HE1	1:A:17:GLY:HA3	1.65	0.59
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.02	0.59
1:A:26:LEU:HD11	1:A:361:THR:OG1	1.94	0.59
1:A:57:GLY:HA3	1:A:61:HIS:CG	2.37	0.59
1:A:153:LEU:O	1:A:157:LEU:HD12	2.01	0.59
1:A:180:ALA:CB	1:A:398:MET:HE3	2.26	0.59
1:A:190:THR:OG1	1:A:425:MET:HE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:HE2	1:A:377:MET:HE2	1.63	0.59
2:B:219:LEU:CD2	2:B:226:ASP:OD2	2.50	0.59
2:B:294:GLN:CD	2:B:300:ASN:OD1	2.45	0.59
1:A:219:ILE:HG22	1:A:219:ILE:O	2.02	0.59
1:A:362:VAL:HG12	1:A:363:VAL:N	2.17	0.59
2:B:182:VAL:CG1	2:B:186:ASN:HD21	2.05	0.59
2:B:274:PRO:O	2:B:276:THR:CG2	2.46	0.59
2:B:288:VAL:C	2:B:291:LEU:H	2.10	0.59
1:A:4:CYS:HB2	1:A:30:ILE:HG21	1.76	0.59
1:A:144:GLY:CA	1:A:185:TYR:OH	2.50	0.59
1:A:154:MET:HE3	1:A:166:LYS:HD2	1.82	0.59
2:B:158:ARG:CG	2:B:197:ASN:ND2	2.61	0.59
2:B:174:SER:HB2	2:B:207:GLU:CB	2.26	0.59
2:B:229:HIS:O	2:B:230:LEU:C	2.43	0.59
1:A:173:PRO:HG3	1:A:182:VAL:CG1	2.32	0.59
1:A:324:VAL:CG1	1:A:325:PRO:HD2	2.33	0.59
2:B:14:ASN:HB3	2:B:74:THR:OG1	2.01	0.59
3:K:159:ASN:C	3:K:161:LYS:H	2.09	0.59
1:A:74:VAL:O	1:A:77:GLU:HB2	2.03	0.59
1:A:209:ILE:O	1:A:212:ILE:HG12	2.02	0.59
2:B:62:VAL:HG12	2:B:63:PRO:N	2.18	0.59
2:B:268:PHE:HA	2:B:380:ASN:OD1	2.03	0.59
2:B:383:ALA:O	2:B:386:GLU:CB	2.51	0.59
2:B:431:GLU:HA	2:B:434:GLN:NE2	2.17	0.59
1:A:101:ASN:C	1:A:102:ASN:CG	2.59	0.59
1:A:236:SER:O	1:A:240:ALA:HB3	2.02	0.59
1:A:324:VAL:HB	1:A:327:ASP:OD2	2.03	0.59
2:B:175:PRO:CB	2:B:176:LYS:HE2	2.32	0.59
2:B:178:SER:O	2:B:179:ASP:HB2	2.00	0.59
2:B:216:THR:HG21	2:B:275:LEU:HD12	1.83	0.59
1:A:100:ALA:CB	1:A:105:ARG:CG	2.81	0.59
1:A:117:LEU:O	1:A:121:ARG:HG3	2.02	0.59
1:A:385:ALA:HB2	1:A:432:TYR:HD2	1.68	0.59
1:A:397:LEU:HA	1:A:401:LYS:CD	2.33	0.59
1:A:423:GLU:OE1	3:K:170:GLU:HG2	1.99	0.59
2:B:23:VAL:O	2:B:26:ASP:HB2	2.02	0.59
2:B:102:ASN:ND2	2:B:105:LYS:HZ2	2.01	0.59
2:B:346:TRP:HZ2	2:B:435:TYR:CD2	2.21	0.59
3:K:83[A]:GLN:NE2	3:K:87:GLU:OE2	2.36	0.59
1:A:36:MET:SD	1:A:60:LYS:CB	2.90	0.59
1:A:310:GLY:HA3	1:A:382:THR:OG1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLU:HB2	2:B:36:TYR:HB3	1.84	0.59
2:B:251:ASP:O	2:B:253:ARG:N	2.35	0.59
2:B:274:PRO:CB	2:B:371:LEU:HD11	2.32	0.59
2:B:397:ALA:O	2:B:401:ARG:CG	2.50	0.59
1:A:171:ILE:H	1:A:203:MET:HE1	1.64	0.59
1:A:282:TYR:O	1:A:284:GLU:CA	2.50	0.59
1:A:78:VAL:HG13	1:A:87:PHE:HE1	1.61	0.59
1:A:143:GLY:O	1:A:145:THR:N	2.36	0.59
1:A:191:THR:O	1:A:194:THR:OG1	2.19	0.59
1:A:202:PHE:HA	1:A:268:PRO:HG2	1.85	0.59
1:A:223:THR:OG1	1:A:225:THR:OG1	2.10	0.59
2:B:143:GLY:C	2:B:185:TYR:CE1	2.80	0.59
2:B:180:THR:C	2:B:398:MET:HE1	2.27	0.59
2:B:340:SER:O	2:B:343:PHE:N	2.35	0.59
2:B:383:ALA:O	2:B:386:GLU:HB2	2.03	0.59
1:A:291:ILE:O	1:A:294:ALA:HB3	2.03	0.58
1:A:264:ARG:HH22	3:K:307:ARG:HD2	0.55	0.58
1:A:273:ALA:N	1:A:274:PRO:CD	2.66	0.58
2:B:6:HIS:CD2	2:B:64:ARG:O	2.56	0.58
2:B:194:LEU:HD21	2:B:267:PHE:HE2	1.65	0.58
2:B:234:THR:CB	2:B:302:MET:CE	2.75	0.58
3:K:171:HIS:HD2	3:K:173:LEU:H	1.51	0.58
3:K:303:PHE:CD2	3:K:303:PHE:O	2.56	0.58
1:A:28:HIS:ND1	1:A:29:GLY:O	2.32	0.58
1:A:103:TYR:CE1	1:A:188:ILE:CG2	2.67	0.58
1:A:185:TYR:CE1	1:A:189:LEU:HD11	2.39	0.58
2:B:4:ILE:HD13	2:B:30:ILE:HA	1.66	0.58
2:B:29:GLY:HA2	2:B:30:ILE:HG12	1.85	0.58
2:B:78:VAL:HA	2:B:82:PRO:HG2	1.86	0.58
2:B:181:VAL:HG22	2:B:404:PHE:CD2	2.39	0.58
2:B:272:PHE:CE2	6:B:502:TXL:H28	2.38	0.58
2:B:346:TRP:O	2:B:347:ILE:CG1	2.51	0.58
3:K:100:GLY:H	8:K:503:ACP:H3B1	1.68	0.58
1:A:76:ASP:O	1:A:80:THR:CB	2.51	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.03	0.58
2:B:29:GLY:O	2:B:58:GLY:CA	2.52	0.58
2:B:133:GLN:HE21	2:B:253:ARG:HB2	1.68	0.58
2:B:143:GLY:C	2:B:185:TYR:HE1	2.11	0.58
2:B:184:PRO:CG	2:B:399:PHE:CB	2.69	0.58
2:B:400:ARG:CD	2:B:422:GLU:OE1	2.51	0.58
1:A:18:ASN:O	1:A:22:GLU:CG	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:171:HIS:HD2	3:K:174:LEU:H	1.51	0.58
1:A:361:THR:CG2	1:A:362:VAL:H	2.15	0.58
2:B:70:LEU:O	2:B:71:GLU:HG3	2.03	0.58
3:K:234:THR:CB	3:K:236:ILE:HD11	2.31	0.58
1:A:141:PHE:HB3	1:A:173:PRO:HD3	1.84	0.58
1:A:197:HIS:O	1:A:198:SER:HB3	2.03	0.58
1:A:328:VAL:O	1:A:332:ILE:HG13	2.04	0.58
1:A:100:ALA:CB	1:A:105:ARG:HB3	2.31	0.58
1:A:208:ALA:HB2	1:A:303:VAL:HA	1.85	0.58
1:A:312:TYR:CE1	1:A:341:ILE:HG23	2.38	0.58
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.86	0.58
2:B:385:GLN:O	2:B:389:LYS:HG3	2.04	0.58
1:A:9:VAL:HG11	1:A:150:THR:HG23	1.78	0.58
1:A:72:PRO:CA	1:A:75:ILE:HG22	2.33	0.58
1:A:97:GLU:CG	1:A:110:ILE:HG23	2.33	0.58
1:A:108:TYR:C	1:A:112:LYS:HG3	2.29	0.58
1:A:169:PHE:HZ	1:A:235:VAL:HG22	1.61	0.58
1:A:242:LEU:CB	1:A:250:VAL:O	2.47	0.58
2:B:280:SER:C	2:B:282:GLN:H	2.07	0.58
2:B:338:LYS:O	2:B:339:ASN:OD1	2.22	0.58
1:A:2:ARG:O	1:A:31:GLN:CG	2.39	0.58
1:A:30:ILE:O	1:A:32:PRO:HG3	1.95	0.58
1:A:45:GLY:O	1:A:46:ASP:OD2	2.22	0.58
1:A:85:GLN:O	1:A:87:PHE:N	2.37	0.58
1:A:275:VAL:O	1:A:368:LEU:HD13	2.04	0.58
1:A:324:VAL:HB	1:A:327:ASP:OD1	2.03	0.58
1:A:346:TRP:CE3	1:A:346:TRP:O	2.56	0.58
2:B:4:ILE:HG21	2:B:30:ILE:CB	2.34	0.58
2:B:105:LYS:CE	2:B:411:GLU:HG3	2.34	0.58
2:B:142:GLY:HA2	2:B:185:TYR:CG	2.37	0.58
2:B:181:VAL:O	2:B:399:PHE:CZ	2.57	0.58
2:B:302:MET:O	2:B:302:MET:CG	2.47	0.58
1:A:34:GLY:C	1:A:35:GLN:HG3	2.29	0.57
1:A:85:GLN:O	1:A:86:LEU:C	2.39	0.57
1:A:115:ILE:CD1	1:A:156:ARG:CD	2.82	0.57
1:A:175:PRO:HG2	1:A:207:GLU:HG2	1.86	0.57
1:A:303:VAL:HG12	1:A:304:LYS:N	2.17	0.57
2:B:213:CYS:HA	2:B:217:LEU:CD1	2.06	0.57
1:A:26:LEU:CD1	1:A:361:THR:HG21	2.15	0.57
2:B:308:ARG:O	2:B:342:TYR:HE2	1.86	0.57
1:A:182:VAL:HG12	1:A:186:ASN:ND2	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:ARG:O	2:B:381:SER:CB	2.52	0.57
1:A:14:VAL:CG1	1:A:74:VAL:HG22	2.35	0.57
1:A:14:VAL:CG2	1:A:69:ASP:OD1	2.52	0.57
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.30	0.57
1:A:171:ILE:N	1:A:203:MET:HE3	2.03	0.57
2:B:7:ILE:CB	2:B:137:LEU:HD21	2.28	0.57
2:B:57:ALA:HA	2:B:64:ARG:HB2	0.68	0.57
2:B:104:ALA:HB2	2:B:413:MET:SD	2.44	0.57
2:B:180:THR:C	2:B:398:MET:CE	2.73	0.57
1:A:8:HIS:CE1	1:A:17:GLY:HA3	2.39	0.57
1:A:23:LEU:CD2	1:A:236:SER:CB	2.81	0.57
1:A:23:LEU:HD21	1:A:236:SER:CB	2.34	0.57
1:A:242:LEU:HD12	1:A:255:PHE:CE2	2.34	0.57
1:A:271:THR:CG2	1:A:377:MET:HB3	2.35	0.57
1:A:340:THR:O	1:A:341:ILE:HG12	2.04	0.57
2:B:288:VAL:C	2:B:290:GLU:N	2.57	0.57
3:K:18[A]:ARG:HE	3:K:22[A]:ARG:NH2	2.03	0.57
1:A:141:PHE:O	1:A:182:VAL:CG1	2.48	0.57
2:B:181:VAL:C	2:B:399:PHE:HE2	2.12	0.57
2:B:319:PHE:CZ	2:B:328:VAL:HG12	2.36	0.57
1:A:13:GLY:HA2	1:A:16:ILE:HG21	1.87	0.57
1:A:103:TYR:OH	1:A:151:SER:HB2	1.98	0.57
1:A:434:GLU:CB	3:K:303:PHE:CG	2.87	0.57
2:B:64:ARG:HH21	2:B:125:GLU:C	2.13	0.57
2:B:242:LEU:HA	2:B:356:CYS:SG	2.45	0.57
2:B:371:LEU:O	2:B:372:LYS:CB	2.50	0.57
1:A:77:GLU:O	1:A:83:TYR:HB2	2.05	0.57
1:A:191:THR:HG23	1:A:421:ALA:HB1	1.86	0.57
2:B:7:ILE:O	2:B:137:LEU:HA	2.04	0.57
2:B:26:ASP:OD1	2:B:26:ASP:O	2.23	0.57
2:B:123:ARG:O	2:B:126:SER:OG	2.20	0.57
2:B:141:LEU:C	2:B:186:ASN:ND2	2.63	0.57
1:A:184:PRO:CB	1:A:399:TYR:HD2	2.15	0.57
1:A:217:LEU:CB	1:A:368:LEU:HD11	2.35	0.57
1:A:254:GLU:OE2	1:A:352:LYS:HE3	2.04	0.57
2:B:192:HIS:HA	2:B:196:GLU:HG3	1.24	0.57
2:B:230:LEU:O	2:B:233:ALA:HB3	2.04	0.57
2:B:274:PRO:HB2	2:B:371:LEU:CD1	2.34	0.57
1:A:32:PRO:C	1:A:34:GLY:N	2.32	0.56
1:A:267:PHE:CG	1:A:388:TRP:HZ2	2.23	0.56
1:A:335:ILE:CG2	1:A:341:ILE:HG13	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:THR:OG1	2:B:267:PHE:CD1	2.58	0.56
2:B:268:PHE:HD1	2:B:380:ASN:CG	2.13	0.56
2:B:371:LEU:N	6:B:502:TXL:H183	2.20	0.56
3:K:18[B]:ARG:HH21	3:K:336:ILE:CD1	2.04	0.56
1:A:48:SER:HG	1:A:56:THR:HB	1.63	0.56
1:A:64:ARG:HH22	1:A:132:LEU:CG	2.09	0.56
1:A:122:ILE:O	1:A:126:ALA:N	2.35	0.56
2:B:56:ALA:HB1	2:B:62:VAL:H	1.70	0.56
2:B:92:PHE:HD2	2:B:114:LEU:CD1	1.97	0.56
2:B:158:ARG:NH1	2:B:197:ASN:H	2.03	0.56
3:K:119:ILE:HB	3:K:120:PRO:HD3	1.87	0.56
1:A:10:GLY:O	1:A:13:GLY:CA	2.53	0.56
1:A:33:ASP:OD1	1:A:33:ASP:O	2.23	0.56
1:A:40:LYS:C	1:A:42:ILE:H	2.08	0.56
1:A:89:PRO:O	1:A:90:GLU:HB2	2.04	0.56
1:A:97:GLU:CB	1:A:110:ILE:HD13	2.35	0.56
1:A:106:GLY:HA2	1:A:111:GLY:H	1.69	0.56
1:A:170:SER:OG	1:A:203:MET:CG	1.65	0.56
1:A:228:ASN:ND2	4:A:500:GTP:N1	2.49	0.56
1:A:239:THR:O	1:A:243:ARG:HG2	2.05	0.56
1:A:242:LEU:HD11	1:A:318:LEU:HD11	1.87	0.56
1:A:292:THR:O	1:A:295:CYS:HB2	2.05	0.56
1:A:327:ASP:O	1:A:331:ALA:CB	2.53	0.56
2:B:21:TRP:HA	2:B:24:ILE:CD1	2.34	0.56
2:B:102:ASN:CB	2:B:408:TYR:CE1	2.88	0.56
2:B:154:ILE:HG23	2:B:198:THR:HG22	1.87	0.56
2:B:239:THR:HB	2:B:243:ARG:NH1	2.20	0.56
2:B:244:PHE:CG	2:B:245:PRO:HD3	2.40	0.56
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.87	0.56
3:K:77[B]:ILE:H	3:K:77[B]:ILE:HD12	1.70	0.56
3:K:207:ALA:HA	3:K:211:ASN:OD1	2.06	0.56
1:A:28:HIS:ND1	1:A:29:GLY:N	2.54	0.56
1:A:326:LYS:NZ	2:B:214:PHE:HZ	1.81	0.56
2:B:241:CYS:C	2:B:242:LEU:HG	2.31	0.56
2:B:434:GLN:C	2:B:435:TYR:HD1	2.14	0.56
1:A:14:VAL:HG21	1:A:69:ASP:OD1	2.06	0.56
1:A:325:PRO:CG	2:B:223:THR:HA	2.36	0.56
1:A:341:ILE:HG22	1:A:343:PHE:CD2	2.40	0.56
1:A:405:VAL:HG11	1:A:405:VAL:HG21	1.87	0.56
1:A:431:ASP:HA	3:K:303:PHE:HD1	1.64	0.56
2:B:49:ILE:HA	2:B:61:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:CD1	2:B:88:ARG:C	2.76	0.56
2:B:262:PHE:HB2	2:B:266:HIS:HE1	1.71	0.56
1:A:219:ILE:HG21	1:A:219:ILE:HD13	1.87	0.56
1:A:258:ASN:OD1	1:A:352:LYS:CE	2.53	0.56
2:B:12:CYS:C	2:B:16:ILE:HG12	2.21	0.56
2:B:141:LEU:C	2:B:186:ASN:HD21	2.13	0.56
2:B:259:MET:CE	2:B:379:GLY:C	2.78	0.56
2:B:274:PRO:CB	2:B:371:LEU:CD2	2.81	0.56
2:B:359:PRO:HB2	2:B:372:LYS:O	2.05	0.56
1:A:9:VAL:CG2	1:A:138:PHE:O	2.54	0.56
1:A:267:PHE:CE1	1:A:388:TRP:CZ2	2.93	0.56
1:A:288:VAL:O	1:A:291:ILE:CB	2.54	0.56
2:B:6:HIS:ND1	2:B:21:TRP:CZ2	2.74	0.56
2:B:64:ARG:HH21	2:B:125:GLU:HB3	1.69	0.56
2:B:388:PHE:O	2:B:390:ARG:N	2.38	0.56
3:K:252:SER:CA	3:K:275:LEU:HD11	2.31	0.56
1:A:2:ARG:HB3	1:A:243:ARG:NH1	2.21	0.56
1:A:14:VAL:HG21	1:A:74:VAL:HG13	1.88	0.56
1:A:23:LEU:HD21	1:A:236:SER:HB3	1.86	0.56
1:A:103:TYR:HA	1:A:147:SER:HG	1.70	0.56
1:A:192:HIS:CG	1:A:193:THR:N	2.73	0.56
1:A:332:ILE:HD11	1:A:353:VAL:HG21	1.78	0.56
2:B:183:GLU:OE2	2:B:394:GLN:CG	2.53	0.56
2:B:212:ILE:CD1	2:B:302:MET:HB2	2.35	0.56
2:B:311:ARG:CD	2:B:341:SER:O	2.54	0.56
1:A:17:GLY:C	1:A:21:TRP:HD1	2.13	0.56
1:A:62:VAL:HG13	1:A:63:PRO:HD3	1.80	0.56
1:A:228:ASN:HD21	4:A:500:GTP:HN1	1.48	0.56
2:B:40:SER:C	2:B:41:ASP:OD1	2.49	0.56
2:B:170:SER:O	2:B:204:ILE:HB	2.06	0.56
2:B:191:VAL:HG23	2:B:421:ALA:CB	2.36	0.56
1:A:35:GLN:O	1:A:36:MET:CG	2.54	0.55
1:A:107:HIS:HD2	1:A:151:SER:OG	1.88	0.55
1:A:174:ALA:HB3	1:A:175:PRO:CD	2.10	0.55
1:A:187:SER:O	1:A:191:THR:HG23	2.07	0.55
1:A:324:VAL:HG13	1:A:325:PRO:HD2	1.87	0.55
2:B:44:LEU:O	2:B:47:GLU:CB	2.54	0.55
2:B:295:MET:HE3	2:B:375:ALA:CA	2.09	0.55
1:A:426:ALA:C	1:A:428:LEU:H	2.14	0.55
2:B:87:PHE:HE1	2:B:89:PRO:HG3	1.58	0.55
2:B:158:ARG:HH11	2:B:197:ASN:N	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:THR:OG1	2:B:226:ASP:CB	2.54	0.55
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.55
2:B:394:GLN:O	2:B:398:MET:CB	2.54	0.55
1:A:25:CYS:O	1:A:26:LEU:HD23	2.06	0.55
1:A:115:ILE:CD1	1:A:152:LEU:HD21	2.32	0.55
1:A:141:PHE:HB2	1:A:172:TYR:HA	1.87	0.55
1:A:157:LEU:HB2	1:A:166:LYS:NZ	2.21	0.55
1:A:208:ALA:HB2	1:A:303:VAL:CA	2.36	0.55
2:B:197:ASN:CG	2:B:197:ASN:O	2.50	0.55
1:A:66:VAL:HG21	1:A:125:LEU:HD12	1.87	0.55
2:B:414:ASP:HB3	3:K:253:GLU:OE2	2.05	0.55
1:A:105:ARG:HG3	1:A:411:GLU:CD	2.32	0.55
1:A:217:LEU:CD2	1:A:368:LEU:CD1	2.70	0.55
1:A:292:THR:CG2	1:A:319:TYR:OH	2.42	0.55
2:B:40:SER:O	2:B:41:ASP:CB	2.54	0.55
2:B:143:GLY:H	2:B:147:SER:HG	1.52	0.55
2:B:147:SER:HB3	2:B:189:LEU:HD11	0.56	0.55
2:B:174:SER:O	2:B:176:LYS:N	2.39	0.55
1:A:14:VAL:HG21	1:A:74:VAL:CG1	2.36	0.55
1:A:69:ASP:HB3	1:A:71:GLU:O	2.07	0.55
2:B:175:PRO:HD2	2:B:207:GLU:HG2	1.88	0.55
2:B:191:VAL:HG22	2:B:421:ALA:HA	1.79	0.55
2:B:222:PRO:C	2:B:223:THR:CG2	2.72	0.55
2:B:278:ARG:CB	2:B:278:ARG:C	2.79	0.55
2:B:296:PHE:CD1	2:B:335:VAL:HG11	2.40	0.55
1:A:209:ILE:HD11	1:A:231:ILE:CD1	2.17	0.55
2:B:181:VAL:C	2:B:398:MET:HE1	2.31	0.55
2:B:231:VAL:O	2:B:232:SER:C	2.46	0.55
1:A:9:VAL:CG1	1:A:150:THR:HG23	2.31	0.55
1:A:133:GLN:HE22	2:B:98:GLY:HA2	1.69	0.55
2:B:56:ALA:CB	2:B:62:VAL:CG2	2.69	0.55
2:B:103:TRP:HE3	2:B:413:MET:CE	1.90	0.55
2:B:296:PHE:CE1	2:B:335:VAL:CG1	2.83	0.55
2:B:313:LEU:N	2:B:381:SER:HA	2.22	0.55
1:A:224:TYR:CE1	4:A:500:GTP:C4	2.94	0.55
1:A:11:GLN:OE1	1:A:74:VAL:HB	2.07	0.55
1:A:26:LEU:O	1:A:27:GLU:HB2	2.06	0.55
1:A:70:LEU:HG	1:A:145:THR:HG21	1.87	0.55
1:A:137:VAL:CB	1:A:168:GLU:HG2	2.37	0.55
1:A:196:GLU:C	1:A:197:HIS:CG	2.83	0.55
1:A:274:PRO:C	1:A:275:VAL:HG23	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:C	2:B:399:PHE:CE2	2.85	0.55
2:B:265:LEU:HD23	2:B:267:PHE:HZ	1.67	0.55
1:A:103:TYR:CZ	1:A:151:SER:OG	2.59	0.54
1:A:289:ALA:HB1	1:A:331:ALA:HB1	1.89	0.54
2:B:287:THR:CA	2:B:290:GLU:HB3	2.36	0.54
2:B:295:MET:HE1	2:B:375:ALA:CA	2.29	0.54
1:A:68:VAL:CG1	1:A:149:PHE:HZ	2.07	0.54
1:A:108:TYR:CZ	1:A:417:GLU:CD	2.85	0.54
2:B:48:ARG:HH12	2:B:60:LYS:H	1.54	0.54
2:B:344:VAL:O	2:B:344:VAL:HG12	2.07	0.54
1:A:28:HIS:CD2	1:A:33:ASP:HB3	2.41	0.54
1:A:166:LYS:CD	1:A:197:HIS:HD2	2.20	0.54
1:A:166:LYS:HD2	1:A:197:HIS:HD2	1.73	0.54
2:B:102:ASN:CA	2:B:408:TYR:HE1	2.18	0.54
2:B:273:ALA:CB	2:B:294:GLN:CD	2.80	0.54
2:B:414:ASP:CG	3:K:253:GLU:CD	2.72	0.54
1:A:313:MET:N	1:A:380:ASN:O	2.40	0.54
2:B:129:CYS:O	2:B:130:ASP:OD1	2.24	0.54
2:B:136:GLN:NE2	2:B:243:ARG:HH12	2.05	0.54
2:B:140:SER:O	2:B:147:SER:OG	2.25	0.54
2:B:287:THR:CG2	2:B:290:GLU:N	2.68	0.54
2:B:308:ARG:HD3	2:B:342:TYR:HE2	1.66	0.54
1:A:148:GLY:HA2	1:A:151:SER:HG	1.71	0.54
1:A:179:THR:CG2	1:A:180:ALA:N	2.67	0.54
1:A:306:ASP:CG	1:A:308:ARG:HD2	2.31	0.54
1:A:313:MET:HE1	1:A:346:TRP:HZ2	1.60	0.54
2:B:6:HIS:HB2	2:B:65:ALA:CA	2.28	0.54
2:B:14:ASN:HD21	2:B:69:ASP:HA	1.72	0.54
2:B:23:VAL:O	2:B:26:ASP:HB3	2.08	0.54
2:B:49:ILE:O	2:B:50:ASN:ND2	2.40	0.54
2:B:416:MET:O	2:B:417:GLU:CB	2.55	0.54
1:A:5:ILE:HD13	1:A:135:PHE:CE1	2.42	0.54
1:A:20:CYS:C	1:A:24:TYR:CD2	2.80	0.54
1:A:53:PHE:HA	1:A:88:HIS:ND1	2.16	0.54
2:B:44:LEU:C	2:B:47:GLU:CG	2.56	0.54
1:A:108:TYR:HA	1:A:112:LYS:HE2	1.86	0.54
1:A:148:GLY:O	1:A:152:LEU:N	2.40	0.54
1:A:220:GLU:CG	1:A:220:GLU:N	2.70	0.54
1:A:416:GLY:O	1:A:417:GLU:CB	2.55	0.54
2:B:48:ARG:HH11	2:B:60:LYS:HG2	1.60	0.54
2:B:106:GLY:HA2	2:B:111:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:VAL:O	2:B:122:VAL:HG23	2.07	0.54
2:B:284:ARG:HD3	2:B:290:GLU:OE1	2.05	0.54
3:K:317:GLU:CD	3:K:322:ASN:H	2.15	0.54
1:A:146:GLY:HA2	1:A:150:THR:CG2	2.37	0.54
1:A:157:LEU:O	1:A:161:TYR:HB2	2.07	0.54
1:A:259:LEU:O	1:A:380:ASN:ND2	2.41	0.54
1:A:267:PHE:CD2	1:A:388:TRP:HZ2	2.25	0.54
2:B:105:LYS:CE	2:B:411:GLU:CG	2.86	0.54
2:B:309:HIS:HB3	2:B:386:GLU:OE2	2.07	0.54
1:A:200:CYS:SG	1:A:256:GLN:HA	2.48	0.54
1:A:209:ILE:HD12	1:A:227:LEU:HD21	1.90	0.54
2:B:35:SER:HA	2:B:60:LYS:CE	2.30	0.54
2:B:202:TYR:OH	2:B:238:VAL:HG11	2.08	0.54
2:B:206:ASN:O	2:B:210:TYR:HD2	1.86	0.54
2:B:244:PHE:O	2:B:245:PRO:C	2.51	0.54
2:B:360:PRO:HG2	2:B:374:SER:HB3	1.90	0.54
2:B:399:PHE:CZ	2:B:408:TYR:CZ	2.96	0.54
1:A:119:LEU:CA	1:A:122:ILE:HG22	2.38	0.54
1:A:252:LEU:CA	1:A:255:PHE:HD2	2.07	0.54
1:A:431:ASP:CA	3:K:303:PHE:HE1	2.16	0.54
1:A:81:GLY:O	1:A:83:TYR:N	2.41	0.53
1:A:151:SER:CB	1:A:192:HIS:CB	2.75	0.53
1:A:167:LEU:HD11	1:A:252:LEU:HD22	1.90	0.53
1:A:291:ILE:HD13	1:A:373:ARG:C	2.33	0.53
1:A:335:ILE:HG22	1:A:341:ILE:HG13	1.88	0.53
2:B:103:TRP:CD1	2:B:147:SER:C	2.85	0.53
2:B:139:HIS:C	2:B:139:HIS:ND1	2.67	0.53
2:B:158:ARG:HG3	2:B:197:ASN:ND2	2.22	0.53
2:B:321:GLY:HA2	2:B:359:PRO:HB3	1.90	0.53
2:B:426:ASN:C	2:B:428:LEU:H	2.17	0.53
1:A:9:VAL:CB	1:A:138:PHE:O	2.54	0.53
1:A:22:GLU:O	1:A:25:CYS:HB2	2.07	0.53
1:A:114:ILE:O	1:A:114:ILE:HG22	2.07	0.53
2:B:135:PHE:CD2	2:B:157:ILE:HG21	2.44	0.53
2:B:238:VAL:HG13	2:B:255:LEU:HD13	1.88	0.53
2:B:339:ASN:HA	2:B:342:TYR:CD1	2.43	0.53
3:K:215:SER:C	3:K:216:ARG:HD2	2.34	0.53
1:A:256:GLN:O	1:A:260:VAL:CB	2.55	0.53
1:A:363:VAL:HG12	1:A:364:PRO:CG	2.35	0.53
1:A:386:GLU:O	1:A:389:ALA:HB3	2.09	0.53
2:B:4:ILE:HD13	2:B:30:ILE:CA	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:H	2:B:32:PRO:CD	2.20	0.53
2:B:195:VAL:O	2:B:195:VAL:HG12	2.08	0.53
2:B:293:GLN:O	2:B:297:ASP:OD1	2.27	0.53
1:A:241:SER:HB2	1:A:356:ASN:CG	2.32	0.53
1:A:361:THR:C	1:A:362:VAL:CG2	2.81	0.53
1:A:424:ASP:CA	3:K:307:ARG:HH22	2.08	0.53
2:B:8:GLN:O	2:B:68:VAL:HB	2.08	0.53
2:B:94:PHE:HZ	2:B:110:GLU:O	1.92	0.53
2:B:172:VAL:HG21	2:B:205:ASP:OD1	2.09	0.53
2:B:201:THR:CG2	2:B:265:LEU:CD2	2.43	0.53
1:A:2:ARG:HG2	1:A:133:GLN:NE2	2.23	0.53
1:A:172:TYR:HB3	1:A:203:MET:HE2	1.89	0.53
1:A:194:THR:CG2	1:A:195:LEU:H	2.02	0.53
1:A:277:SER:H	1:A:280:LYS:HG2	1.60	0.53
1:A:311:LYS:O	1:A:312:TYR:C	2.51	0.53
1:A:313:MET:CG	1:A:380:ASN:O	2.57	0.53
2:B:102:ASN:CA	2:B:408:TYR:CE1	2.91	0.53
2:B:141:LEU:HD12	2:B:173:PRO:CD	2.37	0.53
1:A:191:THR:HG21	1:A:421:ALA:HA	1.88	0.53
1:A:219:ILE:CG2	1:A:219:ILE:CD1	2.86	0.53
2:B:7:ILE:HG21	2:B:137:LEU:HD22	1.91	0.53
2:B:42:LEU:O	2:B:43:GLN:CB	2.56	0.53
2:B:295:MET:HE2	2:B:375:ALA:C	2.34	0.53
2:B:301:MET:HE1	2:B:377:PHE:CE1	2.42	0.53
2:B:339:ASN:HB3	2:B:342:TYR:HB2	1.90	0.53
2:B:242:LEU:HB3	2:B:250:ALA:O	2.08	0.53
2:B:273:ALA:HB1	2:B:294:GLN:CD	2.32	0.53
3:K:321:GLY:O	3:K:356:ASN:HB3	2.08	0.53
1:A:103:TYR:O	1:A:148:GLY:HA3	2.08	0.53
1:A:207:GLU:HG3	1:A:207:GLU:O	2.08	0.53
1:A:220:GLU:CG	1:A:220:GLU:H	2.20	0.53
1:A:233:GLN:O	1:A:234:ILE:C	2.49	0.53
2:B:64:ARG:NH2	2:B:125:GLU:C	2.67	0.53
1:A:142:GLY:HA2	1:A:185:TYR:CE1	2.43	0.53
2:B:34:GLY:C	2:B:35:SER:HG	2.09	0.53
2:B:92:PHE:CE2	2:B:114:LEU:CD1	2.89	0.53
2:B:151:THR:C	2:B:192:HIS:HD2	2.12	0.53
1:A:191:THR:HG22	1:A:421:ALA:HA	1.91	0.53
2:B:6:HIS:ND1	2:B:21:TRP:HZ2	2.07	0.53
2:B:57:ALA:O	2:B:64:ARG:N	2.42	0.53
2:B:360:PRO:HD3	2:B:374:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CE1	2:B:21:TRP:CZ2	2.97	0.52
2:B:8:GLN:HE22	2:B:21:TRP:CD1	2.27	0.52
2:B:184:PRO:CA	2:B:395:PHE:HD1	2.22	0.52
2:B:342:TYR:O	2:B:343:PHE:CG	2.62	0.52
1:A:256:GLN:HB2	2:B:407:TRP:CZ3	2.44	0.52
2:B:6:HIS:HD2	2:B:64:ARG:O	1.90	0.52
2:B:126:SER:HA	2:B:132:LEU:HD11	1.88	0.52
2:B:184:PRO:CB	2:B:399:PHE:CE2	2.69	0.52
1:A:219:ILE:O	1:A:222:PRO:HD3	2.09	0.52
2:B:107:HIS:CD2	2:B:151:THR:OG1	2.62	0.52
2:B:190:SER:OG	2:B:191:VAL:N	2.42	0.52
2:B:206:ASN:O	2:B:210:TYR:HE2	1.85	0.52
2:B:259:MET:HE3	2:B:268:PHE:CD1	2.44	0.52
1:A:21:TRP:N	1:A:21:TRP:CD1	2.76	0.52
1:A:63:PRO:HB2	1:A:65:ALA:HB2	1.92	0.52
1:A:288:VAL:CG2	1:A:373:ARG:CD	2.44	0.52
1:A:325:PRO:HG2	2:B:223:THR:HA	1.91	0.52
2:B:135:PHE:CD2	2:B:157:ILE:HD13	2.45	0.52
2:B:251:ASP:O	2:B:254:LYS:N	2.33	0.52
2:B:286:LEU:HD13	2:B:373:MET:H	1.70	0.52
2:B:339:ASN:HA	2:B:342:TYR:HD1	1.73	0.52
1:A:13:GLY:O	1:A:16:ILE:CG2	2.56	0.52
1:A:101:ASN:ND2	4:A:500:GTP:O2G	2.42	0.52
2:B:22:GLU:HA	2:B:83:PHE:HE2	1.73	0.52
2:B:41:ASP:O	2:B:42:LEU:CB	2.56	0.52
2:B:192:HIS:HA	2:B:196:GLU:OE2	2.08	0.52
1:A:237:SER:HA	1:A:320:ARG:HH11	1.73	0.52
2:B:9:ALA:O	2:B:13:GLY:HA3	2.10	0.52
2:B:135:PHE:CG	2:B:166:MET:SD	3.02	0.52
3:K:216:ARG:HD2	3:K:216:ARG:N	2.24	0.52
1:A:97:GLU:HG3	1:A:110:ILE:HG23	1.92	0.52
1:A:301:GLN:NE2	1:A:305:CYS:HB2	2.24	0.52
2:B:319:PHE:HZ	2:B:332:MET:SD	2.31	0.52
1:A:83:TYR:O	1:A:84:ARG:HB2	2.09	0.52
1:A:126:ALA:C	1:A:132:LEU:HD11	2.32	0.52
2:B:319:PHE:CZ	2:B:332:MET:SD	3.03	0.52
2:B:320:ARG:HH22	6:B:502:TXL:H27	1.70	0.52
2:B:431:GLU:HA	2:B:434:GLN:CG	2.39	0.52
1:A:152:LEU:HD11	1:A:156:ARG:HE	1.75	0.52
1:A:179:THR:CG2	1:A:181:VAL:CA	2.88	0.52
1:A:362:VAL:CG1	1:A:363:VAL:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ALA:O	1:A:401:LYS:C	2.52	0.52
2:B:68:VAL:HG13	2:B:149:MET:HE1	1.92	0.52
2:B:151:THR:HG21	2:B:192:HIS:CG	2.36	0.52
2:B:212:ILE:HD11	2:B:302:MET:CA	2.40	0.52
2:B:389:LYS:O	2:B:393:GLU:HG2	2.09	0.52
6:B:502:TXL:H192	6:B:502:TXL:C5	2.39	0.52
2:B:27:GLU:OE1	2:B:36:TYR:HA	2.09	0.52
2:B:154:ILE:CG2	2:B:198:THR:HG22	2.37	0.52
2:B:208:ALA:HB2	2:B:303:ALA:O	2.05	0.52
2:B:212:ILE:HD11	2:B:302:MET:HA	1.91	0.52
1:A:7:ILE:HG22	1:A:8:HIS:O	2.10	0.51
1:A:108:TYR:CB	1:A:112:LYS:HE3	2.35	0.51
1:A:282:TYR:O	1:A:284:GLU:C	2.53	0.51
2:B:8:GLN:O	2:B:68:VAL:N	2.41	0.51
2:B:33:THR:CA	2:B:59:ASN:ND2	2.72	0.51
2:B:49:ILE:CA	2:B:61:TYR:CE2	2.93	0.51
2:B:57:ALA:CA	2:B:64:ARG:HB3	2.35	0.51
2:B:98:GLY:C	2:B:99:ALA:O	2.52	0.51
2:B:183:GLU:CD	2:B:394:GLN:HG3	2.35	0.51
2:B:313:LEU:CD2	2:B:344:VAL:CG2	2.71	0.51
1:A:172:TYR:CE2	1:A:388:TRP:HZ3	2.28	0.51
1:A:419:SER:OG	3:K:172:PRO:HD3	2.10	0.51
2:B:75:MET:HE2	2:B:79:ARG:CG	2.35	0.51
2:B:259:MET:CE	2:B:268:PHE:CD1	2.93	0.51
2:B:259:MET:HG3	2:B:378:ILE:HG21	1.92	0.51
2:B:343:PHE:CG	2:B:350:ASN:ND2	2.78	0.51
2:B:359:PRO:O	2:B:360:PRO:C	2.49	0.51
3:K:83[A]:GLN:O	3:K:87:GLU:HG3	2.10	0.51
1:A:132:LEU:O	1:A:133:GLN:C	2.54	0.51
1:A:205:ASP:HB2	1:A:208:ALA:HB3	1.91	0.51
1:A:306:ASP:OD1	1:A:308:ARG:CD	2.55	0.51
1:A:431:ASP:CB	3:K:303:PHE:CE1	2.86	0.51
2:B:194:LEU:CA	2:B:265:LEU:HB2	2.38	0.51
2:B:295:MET:HE1	2:B:375:ALA:HA	1.91	0.51
2:B:319:PHE:CD1	2:B:319:PHE:N	2.78	0.51
2:B:398:MET:CE	2:B:399:PHE:CE2	2.93	0.51
2:B:400:ARG:NH1	2:B:422:GLU:OE1	2.37	0.51
2:B:405:LEU:C	2:B:409:THR:HG1	2.09	0.51
1:A:70:LEU:HG	1:A:145:THR:CG2	2.32	0.51
1:A:288:VAL:HG22	1:A:373:ARG:HG2	1.88	0.51
1:A:340:THR:O	1:A:341:ILE:HD13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:O	1:A:342:GLN:C	2.52	0.51
2:B:140:SER:OG	2:B:143:GLY:HA3	2.10	0.51
2:B:250:ALA:HA	2:B:254:LYS:CD	2.17	0.51
2:B:320:ARG:HH21	6:B:502:TXL:H27	1.76	0.51
1:A:108:TYR:OH	1:A:417:GLU:CG	2.59	0.51
1:A:178:SER:O	1:A:179:THR:HB	2.10	0.51
1:A:405:VAL:HG23	1:A:409:VAL:HG23	1.90	0.51
2:B:295:MET:HE2	2:B:376:THR:N	2.25	0.51
2:B:335:VAL:C	2:B:339:ASN:ND2	2.59	0.51
2:B:378:ILE:HG22	2:B:379:GLY:N	2.24	0.51
3:K:33:SER:HB2	3:K:52:PHE:O	2.10	0.51
1:A:81:GLY:C	1:A:83:TYR:N	2.68	0.51
1:A:192:HIS:O	1:A:193:THR:C	2.53	0.51
1:A:209:ILE:CG2	1:A:230:LEU:HD23	2.29	0.51
1:A:267:PHE:CD1	1:A:388:TRP:CZ2	2.98	0.51
1:A:396:ASP:OD2	1:A:422:ARG:CZ	2.59	0.51
2:B:35:SER:HB3	2:B:60:LYS:CE	2.40	0.51
2:B:101:ASN:O	2:B:102:ASN:ND2	2.43	0.51
2:B:114:LEU:O	2:B:117:SER:N	2.44	0.51
2:B:192:HIS:CG	2:B:196:GLU:HG3	2.44	0.51
2:B:208:ALA:CB	2:B:303:ALA:C	2.81	0.51
2:B:229:HIS:HD1	6:B:502:TXL:H432	1.75	0.51
2:B:315:VAL:HG13	2:B:377:PHE:CE2	2.45	0.51
2:B:404:PHE:CD2	2:B:404:PHE:O	2.64	0.51
1:A:25:CYS:O	1:A:25:CYS:SG	2.69	0.51
1:A:269:LEU:O	1:A:377:MET:O	2.29	0.51
2:B:28:HIS:CD2	2:B:240:THR:HA	2.45	0.51
2:B:262:PHE:CB	2:B:263:PRO:CD	2.78	0.51
2:B:339:ASN:O	2:B:340:SER:O	2.29	0.51
2:B:369:ARG:O	6:B:502:TXL:C22	2.59	0.51
1:A:3:GLU:CA	1:A:31:GLN:CG	2.86	0.51
1:A:41:THR:O	1:A:41:THR:CG2	2.59	0.51
1:A:181:VAL:HG13	1:A:399:TYR:OH	2.11	0.51
1:A:212:ILE:HD13	1:A:230:LEU:CD2	2.14	0.51
1:A:219:ILE:CG2	1:A:219:ILE:HD13	2.39	0.51
2:B:33:THR:HG22	2:B:34:GLY:H	1.73	0.51
2:B:312:TYR:C	2:B:381:SER:HA	2.36	0.51
1:A:420:GLU:OE2	3:K:170:GLU:N	2.43	0.51
2:B:94:PHE:CE2	2:B:114:LEU:HB2	2.46	0.51
2:B:188:THR:CG2	2:B:417:GLU:O	2.59	0.51
2:B:229:HIS:ND1	6:B:502:TXL:H432	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:THR:C	2:B:290:GLU:HB3	2.36	0.51
2:B:384:ILE:HG22	2:B:388:PHE:CE2	2.45	0.51
1:A:40:LYS:C	1:A:42:ILE:N	2.65	0.50
1:A:141:PHE:CB	1:A:173:PRO:HD3	2.41	0.50
1:A:186:ASN:O	1:A:190:THR:N	2.44	0.50
1:A:250:VAL:HG11	1:A:352:LYS:NZ	2.26	0.50
2:B:270:PRO:HB3	2:B:378:ILE:HD13	1.93	0.50
2:B:316:ALA:O	2:B:378:ILE:N	2.38	0.50
2:B:318:VAL:O	2:B:376:THR:N	2.26	0.50
2:B:321:GLY:HA3	2:B:373:MET:CG	2.15	0.50
3:K:83[B]:GLN:O	3:K:87:GLU:HG3	2.10	0.50
3:K:171:HIS:CD2	3:K:173:LEU:H	2.28	0.50
1:A:142:GLY:O	1:A:185:TYR:CE1	2.63	0.50
1:A:205:ASP:O	1:A:209:ILE:HG13	2.11	0.50
2:B:14:ASN:OD1	2:B:69:ASP:OD1	2.29	0.50
2:B:34:GLY:HA2	2:B:37:HIS:NE2	2.26	0.50
2:B:194:LEU:CD2	2:B:265:LEU:HB3	2.38	0.50
2:B:194:LEU:HD23	2:B:267:PHE:HZ	1.72	0.50
2:B:201:THR:CG2	2:B:265:LEU:CG	2.87	0.50
6:B:502:TXL:C17	6:B:502:TXL:C13	2.89	0.50
1:A:405:VAL:CG2	1:A:405:VAL:CA	2.77	0.50
2:B:44:LEU:CD1	2:B:63:PRO:HG3	2.42	0.50
2:B:68:VAL:HG13	2:B:149:MET:CE	2.42	0.50
2:B:312:TYR:O	2:B:344:VAL:HG21	2.00	0.50
2:B:332:MET:O	2:B:336:GLN:HG3	2.11	0.50
3:K:138:MET:SD	3:K:229:ARG:HB2	2.52	0.50
1:A:78:VAL:HG13	1:A:87:PHE:CE1	2.42	0.50
1:A:103:TYR:HD2	1:A:189:LEU:HG	1.76	0.50
1:A:150:THR:O	1:A:154:MET:HG2	2.11	0.50
1:A:155:GLU:HA	1:A:196:GLU:HB3	1.94	0.50
1:A:277:SER:HB3	1:A:280:LYS:CE	2.36	0.50
1:A:301:GLN:HE21	1:A:305:CYS:HB2	1.76	0.50
2:B:7:ILE:HG13	2:B:66:ILE:CG2	2.36	0.50
2:B:64:ARG:HH22	2:B:132:LEU:HD11	1.76	0.50
2:B:213:CYS:SG	2:B:227:LEU:HD11	2.52	0.50
2:B:217:LEU:HD23	2:B:275:LEU:O	2.10	0.50
2:B:389:LYS:HG2	2:B:429:VAL:HG21	1.93	0.50
2:B:433:GLN:C	2:B:435:TYR:N	2.67	0.50
1:A:88:HIS:NE2	1:A:89:PRO:HD2	2.26	0.50
1:A:253:THR:O	1:A:253:THR:CG2	2.57	0.50
1:A:267:PHE:CZ	1:A:388:TRP:CZ2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLN:C	1:A:373:ARG:HG3	2.33	0.50
1:A:440:VAL:HB	2:B:402:LYS:NZ	2.27	0.50
2:B:35:SER:H	2:B:60:LYS:NZ	2.09	0.50
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.39	0.50
1:A:183:GLU:OE1	1:A:183:GLU:HA	2.10	0.50
1:A:230:LEU:CD2	1:A:302:MET:HE1	2.41	0.50
1:A:397:LEU:CA	1:A:401:LYS:HB2	2.37	0.50
2:B:19:LYS:HG3	2:B:228:ASN:HB3	1.30	0.50
1:A:242:LEU:HD12	1:A:255:PHE:HZ	1.62	0.50
1:A:382:THR:O	1:A:385:ALA:N	2.43	0.50
2:B:312:TYR:CG	2:B:381:SER:HB3	2.46	0.50
6:B:502:TXL:O11	6:B:502:TXL:H332	2.12	0.50
2:B:33:THR:CG2	2:B:34:GLY:N	2.73	0.50
2:B:280:SER:O	2:B:281:GLN:C	2.55	0.50
2:B:288:VAL:HB	2:B:289:PRO:CD	2.42	0.50
2:B:295:MET:CE	2:B:375:ALA:HA	2.40	0.50
2:B:416:MET:N	2:B:416:MET:SD	2.85	0.50
1:A:78:VAL:O	1:A:78:VAL:HG12	2.10	0.50
1:A:209:ILE:HG12	1:A:302:MET:CE	2.42	0.50
1:A:340:THR:O	1:A:341:ILE:CG1	2.59	0.50
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.77	0.50
1:A:423:GLU:HB3	3:K:170:GLU:HG2	1.94	0.50
2:B:12:CYS:SG	5:B:501:GDP:C1'	3.00	0.50
2:B:15:GLN:C	2:B:17:GLY:N	2.70	0.50
2:B:44:LEU:CD1	2:B:86:ILE:O	2.49	0.50
2:B:63:PRO:CG	2:B:86:ILE:O	2.60	0.50
2:B:346:TRP:C	2:B:347:ILE:HG13	2.37	0.50
2:B:384:ILE:HG23	2:B:388:PHE:CE2	2.45	0.50
1:A:14:VAL:HB	1:A:74:VAL:HG11	1.94	0.49
1:A:33:ASP:O	1:A:33:ASP:CG	2.49	0.49
1:A:190:THR:O	1:A:191:THR:C	2.52	0.49
1:A:220:GLU:CB	1:A:220:GLU:CD	2.74	0.49
1:A:229:ARG:O	1:A:233:GLN:CG	2.52	0.49
1:A:264:ARG:O	1:A:266:HIS:ND1	2.45	0.49
1:A:326:LYS:O	1:A:326:LYS:HG2	2.12	0.49
2:B:62:VAL:CG1	2:B:63:PRO:N	2.75	0.49
2:B:246:GLY:N	2:B:357:ASP:OD2	2.45	0.49
1:A:134:GLY:HA3	1:A:252:LEU:CD1	2.43	0.49
2:B:101:ASN:C	2:B:102:ASN:CG	2.78	0.49
2:B:233:ALA:CB	2:B:272:PHE:CD2	2.79	0.49
1:A:101:ASN:O	1:A:102:ASN:CB	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:C	1:A:118:VAL:N	2.68	0.49
1:A:261:PRO:HB2	1:A:346:TRP:HH2	1.77	0.49
1:A:6:SER:HB3	1:A:30:ILE:HD12	1.92	0.49
1:A:241:SER:HB2	1:A:356:ASN:CB	2.42	0.49
2:B:121:VAL:O	2:B:125:GLU:HG3	2.12	0.49
2:B:324:SER:CB	2:B:327:GLU:H	2.25	0.49
1:A:158:SER:HB2	1:A:196:GLU:O	2.11	0.49
1:A:205:ASP:HB2	1:A:208:ALA:CB	2.42	0.49
1:A:209:ILE:O	1:A:213:CYS:SG	2.63	0.49
1:A:119:LEU:HA	1:A:122:ILE:HG22	1.94	0.49
1:A:142:GLY:O	1:A:185:TYR:CZ	2.66	0.49
1:A:194:THR:CG2	1:A:195:LEU:N	2.59	0.49
1:A:359:PRO:HB2	1:A:360:PRO:HD2	1.94	0.49
2:B:29:GLY:O	2:B:58:GLY:O	2.30	0.49
2:B:308:ARG:CD	2:B:342:TYR:CZ	2.93	0.49
2:B:394:GLN:OE1	2:B:394:GLN:HA	2.12	0.49
6:B:502:TXL:H173	6:B:502:TXL:C13	2.37	0.49
1:A:2:ARG:C	1:A:31:GLN:HG3	2.34	0.49
1:A:11:GLN:HG2	4:A:500:GTP:O2A	2.13	0.49
1:A:121:ARG:O	1:A:125:LEU:CG	2.44	0.49
1:A:200:CYS:SG	1:A:260:VAL:CG2	3.01	0.49
1:A:217:LEU:C	1:A:218:ASP:OD1	2.55	0.49
1:A:272:TYR:CE1	1:A:274:PRO:C	2.70	0.49
2:B:108:TYR:OH	2:B:417:GLU:HG3	2.13	0.49
2:B:135:PHE:CE2	2:B:157:ILE:HD13	2.47	0.49
2:B:141:LEU:HB3	2:B:186:ASN:ND2	1.87	0.49
1:A:14:VAL:HG12	1:A:74:VAL:HG22	1.95	0.49
1:A:97:GLU:HG3	1:A:110:ILE:HG22	1.93	0.49
1:A:101:ASN:ND2	4:A:500:GTP:PG	2.85	0.49
1:A:306:ASP:OD1	1:A:308:ARG:N	2.46	0.49
1:A:312:TYR:C	1:A:313:MET:HG2	2.37	0.49
1:A:314:ALA:HB3	1:A:380:ASN:ND2	2.13	0.49
1:A:369:ALA:O	1:A:370:LYS:HG3	2.12	0.49
2:B:3:GLU:CG	2:B:4:ILE:H	2.09	0.49
2:B:56:ALA:C	2:B:62:VAL:HB	2.38	0.49
2:B:104:ALA:C	2:B:108:TYR:HD2	2.20	0.49
2:B:226:ASP:OD1	2:B:226:ASP:O	2.30	0.49
3:K:222:ASN:HD22	3:K:245[B]:SER:HA	1.78	0.49
1:A:5:ILE:CD1	1:A:135:PHE:CZ	2.93	0.49
1:A:7:ILE:HG21	1:A:153:LEU:CD2	2.43	0.49
1:A:15:GLN:O	1:A:18:ASN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HD11	1:A:361:THR:HG23	1.83	0.49
1:A:83:TYR:C	1:A:84:ARG:CG	2.73	0.49
1:A:217:LEU:HD13	1:A:368:LEU:CD2	2.27	0.49
2:B:79:ARG:HB2	2:B:86:ILE:HD11	1.95	0.49
2:B:183:GLU:OE1	2:B:183:GLU:HA	2.13	0.49
2:B:213:CYS:CB	2:B:219:LEU:CD1	2.86	0.49
2:B:342:TYR:C	2:B:343:PHE:CG	2.90	0.49
3:K:234:THR:HB	3:K:236:ILE:HD13	1.93	0.49
1:A:42:ILE:HD13	1:A:61:HIS:O	2.13	0.49
1:A:204:VAL:CG1	1:A:209:ILE:CG1	2.86	0.49
1:A:209:ILE:HD13	1:A:231:ILE:HG12	1.94	0.49
2:B:35:SER:O	2:B:36:TYR:C	2.39	0.49
1:A:3:GLU:HB3	1:A:64:ARG:NH1	2.28	0.48
1:A:34:GLY:O	1:A:35:GLN:HG3	2.13	0.48
1:A:107:HIS:ND1	1:A:108:TYR:CD2	2.80	0.48
1:A:282:TYR:CD2	1:A:285:GLN:CA	2.81	0.48
1:A:312:TYR:CE1	1:A:341:ILE:HD12	2.47	0.48
2:B:13:GLY:CA	2:B:138:THR:CB	2.85	0.48
2:B:39:ASP:O	2:B:40:SER:HB3	2.08	0.48
2:B:47:GLU:OE2	2:B:85:GLN:OE1	2.30	0.48
2:B:61:TYR:O	2:B:61:TYR:CD1	2.66	0.48
2:B:101:ASN:HD22	2:B:101:ASN:HA	1.47	0.48
2:B:230:LEU:HD21	2:B:302:MET:HB2	1.94	0.48
3:K:215:SER:OG	3:K:216:ARG:HD2	2.13	0.48
1:A:390:ARG:O	1:A:394:LYS:HG3	2.12	0.48
2:B:3:GLU:CD	2:B:64:ARG:NH1	2.71	0.48
2:B:30:ILE:HG21	2:B:136:GLN:NE2	2.23	0.48
2:B:143:GLY:O	2:B:185:TYR:OH	2.31	0.48
2:B:274:PRO:C	2:B:276:THR:CG2	2.85	0.48
1:A:9:VAL:HG11	1:A:146:GLY:HA2	1.95	0.48
1:A:14:VAL:HB	1:A:74:VAL:CG1	2.43	0.48
1:A:16:ILE:HG23	1:A:138:PHE:CD1	2.47	0.48
1:A:242:LEU:HD13	1:A:250:VAL:HB	1.94	0.48
1:A:248:LEU:CD2	5:B:501:GDP:C8	2.96	0.48
1:A:250:VAL:CB	1:A:254:GLU:HG2	2.43	0.48
2:B:2:ARG:NH2	2:B:243:ARG:O	2.46	0.48
2:B:102:ASN:CB	2:B:105:LYS:HG3	2.43	0.48
2:B:239:THR:O	2:B:243:ARG:CG	2.51	0.48
1:A:180:ALA:CB	1:A:398:MET:CE	2.92	0.48
1:A:228:ASN:O	1:A:232:GLY:N	2.39	0.48
2:B:12:CYS:O	2:B:16:ILE:HG13	1.98	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:HA	2:B:94:PHE:HB2	1.94	0.48
2:B:114:LEU:C	2:B:116:ASP:N	2.71	0.48
2:B:144:GLY:N	2:B:185:TYR:HE1	2.08	0.48
2:B:183:GLU:HB3	2:B:184:PRO:HD3	1.81	0.48
2:B:238:VAL:HG13	2:B:255:LEU:HD11	1.94	0.48
1:A:70:LEU:HD12	1:A:145:THR:CA	2.40	0.48
1:A:115:ILE:CB	1:A:152:LEU:HD21	2.43	0.48
2:B:52:TYR:N	2:B:52:TYR:CD1	2.81	0.48
2:B:192:HIS:O	2:B:196:GLU:HG2	2.05	0.48
1:A:107:HIS:HB2	1:A:149:PHE:N	2.17	0.48
1:A:155:GLU:CG	1:A:196:GLU:HG3	2.34	0.48
2:B:385:GLN:O	2:B:389:LYS:CG	2.62	0.48
1:A:108:TYR:OH	1:A:417:GLU:CD	2.56	0.48
1:A:109:THR:HG21	1:A:411:GLU:CB	2.44	0.48
1:A:291:ILE:O	1:A:375:VAL:HG21	2.13	0.48
2:B:64:ARG:HH22	2:B:132:LEU:HD21	1.79	0.48
2:B:272:PHE:O	2:B:275:LEU:HD21	2.13	0.48
2:B:347:ILE:N	2:B:348:PRO:HD3	2.27	0.48
2:B:386:GLU:O	2:B:387:LEU:C	2.57	0.48
2:B:433:GLN:O	2:B:435:TYR:N	2.46	0.48
1:A:212:ILE:HB	1:A:216:ASN:HD22	1.79	0.48
1:A:224:TYR:C	1:A:226:ASN:N	2.71	0.48
1:A:292:THR:N	1:A:375:VAL:HG21	2.28	0.48
2:B:23:VAL:O	2:B:23:VAL:HG12	2.14	0.48
1:A:174:ALA:CB	1:A:390:ARG:NH2	2.52	0.48
1:A:224:TYR:C	1:A:226:ASN:H	2.21	0.48
1:A:224:TYR:HD1	4:A:500:GTP:C2	2.31	0.48
1:A:252:LEU:HD23	1:A:255:PHE:HE2	1.78	0.48
1:A:429:GLU:O	1:A:433:GLU:CG	2.51	0.48
2:B:23:VAL:HG21	2:B:232:SER:HB2	1.95	0.48
2:B:70:LEU:C	2:B:71:GLU:HG3	2.38	0.48
2:B:191:VAL:CG2	2:B:421:ALA:CB	2.90	0.48
2:B:394:GLN:O	2:B:398:MET:HB2	2.14	0.48
1:A:35:GLN:O	1:A:36:MET:HG2	2.13	0.48
1:A:158:SER:N	1:A:166:LYS:CE	2.76	0.48
1:A:362:VAL:C	1:A:363:VAL:HG23	2.38	0.48
2:B:50:ASN:HD22	2:B:61:TYR:HB2	1.78	0.48
2:B:241:CYS:O	2:B:242:LEU:HG	2.14	0.48
2:B:311:ARG:O	2:B:381:SER:CA	2.62	0.48
2:B:328:VAL:HG12	2:B:353:THR:HG21	1.96	0.48
1:A:6:SER:O	1:A:66:VAL:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:CYS:SG	1:A:138:PHE:CE1	3.07	0.47
1:A:287:SER:O	1:A:291:ILE:HG13	2.13	0.47
2:B:4:ILE:HG21	2:B:30:ILE:HG21	1.93	0.47
2:B:102:ASN:CB	2:B:105:LYS:CD	2.79	0.47
2:B:192:HIS:CE1	2:B:193:GLN:HG2	2.48	0.47
2:B:211:ASP:O	2:B:215:ARG:HB2	2.14	0.47
2:B:435:TYR:O	2:B:436:GLN:OE1	2.29	0.47
1:A:137:VAL:HB	1:A:168:GLU:CG	2.40	0.47
1:A:346:TRP:CD1	1:A:346:TRP:N	2.82	0.47
1:A:420:GLU:OE1	1:A:420:GLU:HA	2.13	0.47
2:B:114:LEU:HA	2:B:117:SER:OG	2.14	0.47
2:B:142:GLY:HA2	2:B:185:TYR:CE1	2.37	0.47
3:K:234:THR:CB	3:K:236:ILE:CD1	2.88	0.47
2:B:35:SER:CB	2:B:60:LYS:HE3	2.44	0.47
2:B:87:PHE:CD1	2:B:88:ARG:N	2.82	0.47
2:B:109:THR:CG2	2:B:411:GLU:O	2.61	0.47
2:B:270:PRO:HA	2:B:377:PHE:O	2.14	0.47
2:B:292:THR:O	2:B:293:GLN:C	2.54	0.47
3:K:222:ASN:HD22	3:K:245[A]:SER:HA	1.78	0.47
1:A:48:SER:O	1:A:49:PHE:HB2	2.14	0.47
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.13	0.47
1:A:264:ARG:CZ	3:K:307:ARG:HB3	2.31	0.47
2:B:31:ASP:N	2:B:32:PRO:HD3	2.26	0.47
2:B:94:PHE:CZ	2:B:110:GLU:O	2.68	0.47
2:B:205:ASP:CG	2:B:304:ALA:N	2.72	0.47
1:A:3:GLU:OE1	1:A:132:LEU:CD2	2.62	0.47
1:A:122:ILE:HG23	1:A:123:ARG:N	2.29	0.47
1:A:152:LEU:HD11	1:A:156:ARG:HH21	1.78	0.47
1:A:275:VAL:O	1:A:275:VAL:CG1	2.62	0.47
1:A:307:PRO:C	1:A:309:HIS:N	2.68	0.47
1:A:424:ASP:CG	3:K:307:ARG:HH22	2.14	0.47
2:B:102:ASN:CG	2:B:408:TYR:HD1	2.18	0.47
2:B:209:LEU:HB3	2:B:227:LEU:HD21	1.96	0.47
2:B:294:GLN:HG2	2:B:294:GLN:O	2.14	0.47
2:B:435:TYR:O	2:B:436:GLN:CB	2.56	0.47
1:A:66:VAL:HG22	1:A:125:LEU:HD13	1.92	0.47
2:B:24:ILE:CA	2:B:26:ASP:H	2.25	0.47
2:B:62:VAL:HG12	2:B:63:PRO:O	2.14	0.47
2:B:74:THR:O	2:B:75:MET:O	2.33	0.47
2:B:103:TRP:HE1	2:B:148:GLY:HA2	1.72	0.47
2:B:151:THR:HG21	2:B:189:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:THR:HB	2:B:302:MET:HE1	1.89	0.47
2:B:311:ARG:H	2:B:382:THR:HB	1.79	0.47
2:B:414:ASP:C	2:B:416:MET:N	2.68	0.47
1:A:3:GLU:OE1	1:A:132:LEU:HD23	2.14	0.47
1:A:31:GLN:NE2	1:A:243:ARG:HB3	2.30	0.47
1:A:103:TYR:N	1:A:185:TYR:CE2	2.82	0.47
1:A:153:LEU:O	1:A:153:LEU:HG	2.14	0.47
1:A:169:PHE:CZ	1:A:235:VAL:CG2	2.78	0.47
1:A:175:PRO:HG3	1:A:304:LYS:NZ	2.29	0.47
1:A:209:ILE:CD1	1:A:231:ILE:CG1	2.90	0.47
1:A:256:GLN:O	1:A:260:VAL:HB	2.14	0.47
1:A:276:ILE:HB	1:A:369:ALA:HB2	1.95	0.47
1:A:289:ALA:C	1:A:291:ILE:N	2.69	0.47
1:A:335:ILE:C	1:A:337:THR:N	2.71	0.47
1:A:340:THR:O	1:A:341:ILE:CD1	2.63	0.47
2:B:14:ASN:HB3	2:B:74:THR:CB	2.43	0.47
2:B:33:THR:CG2	2:B:34:GLY:H	2.28	0.47
2:B:57:ALA:C	2:B:64:ARG:N	2.69	0.47
2:B:75:MET:CE	2:B:79:ARG:CB	2.90	0.47
2:B:119:LEU:HD21	2:B:156:LYS:HD3	1.96	0.47
2:B:135:PHE:CB	2:B:166:MET:HE3	2.13	0.47
2:B:174:SER:CB	2:B:175:PRO:CD	2.89	0.47
2:B:179:ASP:O	2:B:180:THR:HG23	2.15	0.47
2:B:248:LEU:HD23	2:B:353:THR:O	2.15	0.47
1:A:1:MET:CA	2:B:96:GLN:OE1	2.53	0.47
1:A:104:ALA:O	1:A:108:TYR:HD2	1.96	0.47
2:B:22:GLU:CD	2:B:83:PHE:CD1	2.88	0.47
2:B:196:GLU:HA	2:B:196:GLU:OE1	2.15	0.47
2:B:250:ALA:HB1	2:B:352:LYS:HZ3	1.80	0.47
3:K:83[A]:GLN:NE2	3:K:87:GLU:CD	2.73	0.47
1:A:23:LEU:CD2	1:A:233:GLN:HA	2.45	0.47
1:A:23:LEU:HD22	1:A:233:GLN:HA	1.96	0.47
1:A:196:GLU:HB3	1:A:197:HIS:CE1	2.50	0.47
1:A:209:ILE:CD1	1:A:231:ILE:HG12	2.45	0.47
1:A:305:CYS:O	1:A:307:PRO:CD	2.56	0.47
1:A:349:THR:O	1:A:351:PHE:N	2.48	0.47
2:B:27:GLU:CB	2:B:36:TYR:HB3	2.44	0.47
1:A:3:GLU:HB2	1:A:64:ARG:NH2	2.30	0.47
1:A:87:PHE:HZ	1:A:92:LEU:HD21	1.80	0.47
1:A:205:ASP:HB2	1:A:303:VAL:CA	2.31	0.47
1:A:259:LEU:CB	1:A:380:ASN:HD21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:GLY:CA	2:B:185:TYR:CE1	2.87	0.47
2:B:212:ILE:C	2:B:214:PHE:H	2.23	0.47
2:B:346:TRP:O	2:B:347:ILE:HG13	2.14	0.47
3:K:44:LYS:HE2	3:K:44:LYS:HB2	1.61	0.47
1:A:166:LYS:CE	1:A:197:HIS:CD2	2.63	0.46
1:A:277:SER:CB	1:A:279:GLU:H	2.23	0.46
1:A:297:GLU:O	1:A:298:PRO:C	2.52	0.46
1:A:389:ALA:O	1:A:393:HIS:ND1	2.47	0.46
2:B:23:VAL:HG22	6:B:502:TXL:C33	2.30	0.46
2:B:261:PRO:HG3	2:B:314:THR:HG23	1.97	0.46
2:B:112:ALA:HA	2:B:115:VAL:HB	1.96	0.46
2:B:313:LEU:CD1	2:B:435:TYR:HD2	2.27	0.46
2:B:338:LYS:C	2:B:339:ASN:CG	2.83	0.46
3:K:216:ARG:CG	3:K:216:ARG:NH1	2.67	0.46
1:A:3:GLU:CA	1:A:31:GLN:CB	2.61	0.46
1:A:3:GLU:CB	1:A:64:ARG:NH1	2.78	0.46
1:A:14:VAL:CB	1:A:74:VAL:CG1	2.94	0.46
1:A:31:GLN:OE1	1:A:243:ARG:HD3	2.01	0.46
1:A:146:GLY:C	1:A:189:LEU:HD13	2.41	0.46
1:A:261:PRO:HB2	1:A:346:TRP:CH2	2.50	0.46
1:A:289:ALA:CB	1:A:331:ALA:HB2	2.44	0.46
1:A:296:PHE:O	1:A:298:PRO:N	2.47	0.46
1:A:387:ALA:O	1:A:390:ARG:HB2	2.15	0.46
2:B:103:TRP:CD1	2:B:147:SER:O	2.59	0.46
2:B:313:LEU:H	2:B:381:SER:HA	1.81	0.46
1:A:267:PHE:CD1	1:A:388:TRP:HZ2	2.34	0.46
1:A:430:LYS:O	1:A:434:GLU:HG3	2.15	0.46
2:B:50:ASN:HB2	2:B:61:TYR:CB	2.45	0.46
2:B:56:ALA:HB1	2:B:62:VAL:N	2.31	0.46
2:B:103:TRP:CD1	2:B:148:GLY:N	2.83	0.46
2:B:249:ASN:O	2:B:249:ASN:OD1	2.34	0.46
2:B:273:ALA:CB	2:B:294:GLN:OE1	2.60	0.46
2:B:427:ASP:O	2:B:431:GLU:HG3	2.16	0.46
2:B:243:ARG:CZ	2:B:252:LEU:HD21	2.45	0.46
3:K:230:HIS:CG	3:K:231:ASP:N	2.83	0.46
1:A:8:HIS:HB2	1:A:67:PHE:HA	1.98	0.46
1:A:267:PHE:CE1	1:A:388:TRP:CH2	3.03	0.46
1:A:277:SER:C	1:A:368:LEU:HD22	2.40	0.46
1:A:312:TYR:HE1	1:A:341:ILE:HD12	1.81	0.46
2:B:102:ASN:CB	2:B:105:LYS:HE3	2.46	0.46
2:B:194:LEU:HD21	2:B:267:PHE:CZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:PHE:CE1	2:B:328:VAL:HG13	2.32	0.46
6:B:502:TXL:H13	6:B:502:TXL:C17	2.31	0.46
1:A:30:ILE:HB	1:A:64:ARG:HB3	1.90	0.46
1:A:187:SER:OG	1:A:188:ILE:N	2.49	0.46
2:B:97:SER:CB	2:B:110:GLU:CD	2.60	0.46
2:B:263:PRO:O	2:B:264:ARG:C	2.57	0.46
1:A:16:ILE:O	1:A:19:ALA:HB3	2.16	0.46
1:A:35:GLN:C	1:A:36:MET:CG	2.89	0.46
1:A:271:THR:OG1	1:A:377:MET:N	2.48	0.46
1:A:293:ASN:O	1:A:297:GLU:HG3	2.16	0.46
2:B:166:MET:HG2	2:B:197:ASN:O	2.16	0.46
2:B:273:ALA:HB1	2:B:294:GLN:HB3	1.97	0.46
1:A:10:GLY:O	1:A:11:GLN:C	2.59	0.46
1:A:104:ALA:CA	1:A:108:TYR:CD2	2.83	0.46
1:A:272:TYR:HD1	1:A:275:VAL:CG2	2.28	0.46
2:B:35:SER:CB	2:B:60:LYS:CE	2.94	0.46
2:B:86:ILE:HB	2:B:87:PHE:H	1.29	0.46
2:B:212:ILE:HD12	2:B:302:MET:HB2	1.98	0.46
2:B:237:GLY:C	2:B:241:CYS:HB2	2.28	0.46
1:A:35:GLN:N	1:A:60:LYS:HD3	2.31	0.46
1:A:141:PHE:CE1	1:A:170:SER:HB2	2.51	0.46
1:A:170:SER:OG	1:A:202:PHE:O	2.34	0.46
1:A:275:VAL:O	1:A:368:LEU:CD1	2.64	0.46
1:A:306:ASP:OD2	1:A:308:ARG:HB2	2.16	0.46
1:A:334:THR:HA	1:A:337:THR:HG21	1.98	0.46
2:B:103:TRP:HZ3	2:B:413:MET:HE2	1.56	0.46
2:B:273:ALA:CB	2:B:294:GLN:HB3	2.46	0.46
2:B:319:PHE:O	2:B:355:VAL:HG13	2.16	0.46
1:A:291:ILE:HD11	1:A:373:ARG:HB2	1.95	0.45
1:A:328:VAL:O	1:A:332:ILE:CG1	2.63	0.45
2:B:48:ARG:HD2	2:B:60:LYS:CA	2.38	0.45
2:B:210:TYR:O	2:B:211:ASP:C	2.59	0.45
2:B:275:LEU:CD1	2:B:300:ASN:ND2	2.67	0.45
2:B:417:GLU:OE1	2:B:417:GLU:HA	2.17	0.45
1:A:3:GLU:OE2	1:A:129:CYS:CB	2.59	0.45
1:A:123:ARG:O	1:A:127:ASP:OD1	2.34	0.45
1:A:177:VAL:CG1	1:A:178:SER:N	2.49	0.45
1:A:287:SER:O	1:A:288:VAL:C	2.57	0.45
1:A:344:VAL:HG12	1:A:345:ASP:H	1.81	0.45
2:B:30:ILE:CG2	2:B:243:ARG:HH11	2.23	0.45
2:B:141:LEU:CD1	2:B:173:PRO:CD	2.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:PRO:CA	2:B:395:PHE:CD1	2.98	0.45
2:B:318:VAL:HG22	2:B:354:ALA:HB3	1.98	0.45
3:K:203:ARG:CZ	3:K:219:ALA:HB2	2.47	0.45
3:K:216:ARG:HG3	3:K:216:ARG:NH1	2.15	0.45
1:A:152:LEU:CD1	1:A:156:ARG:NE	2.75	0.45
1:A:197:HIS:C	1:A:198:SER:OG	2.56	0.45
1:A:267:PHE:CE2	1:A:388:TRP:HZ2	2.35	0.45
2:B:275:LEU:CB	2:B:294:GLN:HE22	2.28	0.45
2:B:286:LEU:HD12	2:B:372:LYS:CB	2.29	0.45
1:A:197:HIS:O	1:A:198:SER:OG	2.34	0.45
1:A:384:ILE:O	1:A:386:GLU:N	2.49	0.45
1:A:437:VAL:O	1:A:437:VAL:CG1	2.64	0.45
2:B:3:GLU:HA	2:B:31:ASP:HB2	1.85	0.45
2:B:152:LEU:O	2:B:155:SER:OG	2.34	0.45
1:A:20:CYS:SG	1:A:138:PHE:CZ	3.06	0.45
1:A:31:GLN:CD	1:A:243:ARG:NE	2.70	0.45
1:A:175:PRO:HD3	1:A:390:ARG:CZ	2.44	0.45
1:A:278:ALA:N	1:A:368:LEU:HD22	2.32	0.45
2:B:68:VAL:HA	2:B:92:PHE:HB2	1.98	0.45
2:B:213:CYS:HB3	2:B:219:LEU:HD13	1.93	0.45
1:A:175:PRO:HD2	1:A:207:GLU:HG2	1.98	0.45
1:A:183:GLU:HB3	1:A:394:LYS:HB2	1.87	0.45
1:A:267:PHE:HA	1:A:268:PRO:HD2	1.57	0.45
1:A:409:VAL:O	1:A:412:GLY:N	2.40	0.45
3:K:216:ARG:NH1	3:K:272:ASN:OD1	2.49	0.45
1:A:3:GLU:HG3	1:A:131:GLY:O	2.16	0.45
1:A:248:LEU:HD21	5:B:501:GDP:C8	2.52	0.45
2:B:94:PHE:CD2	2:B:114:LEU:CD2	3.00	0.45
1:A:2:ARG:HH21	2:B:99:ALA:CB	2.24	0.45
1:A:26:LEU:HD13	1:A:361:THR:OG1	2.12	0.45
1:A:107:HIS:ND1	1:A:107:HIS:C	2.74	0.45
1:A:217:LEU:O	1:A:218:ASP:OD1	2.33	0.45
2:B:313:LEU:HD22	2:B:346:TRP:CH2	2.51	0.45
2:B:344:VAL:HB	2:B:347:ILE:HD12	1.99	0.45
2:B:389:LYS:HG2	2:B:429:VAL:HG11	1.75	0.45
1:A:97:GLU:OE2	1:A:114:ILE:HD11	2.16	0.45
1:A:103:TYR:CD2	1:A:148:GLY:N	2.85	0.45
2:B:241:CYS:O	2:B:242:LEU:CG	2.64	0.45
3:K:38:VAL:HG22	3:K:47:PRO:HG3	1.99	0.45
1:A:155:GLU:HG2	1:A:196:GLU:CB	2.46	0.45
1:A:157:LEU:HB2	1:A:166:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:O	1:A:184:PRO:C	2.58	0.45
1:A:258:ASN:CG	1:A:352:LYS:CD	2.77	0.45
1:A:306:ASP:C	1:A:308:ARG:N	2.72	0.45
1:A:409:VAL:O	1:A:412:GLY:O	2.35	0.45
2:B:312:TYR:N	2:B:381:SER:CB	2.80	0.45
1:A:5:ILE:HG13	1:A:64:ARG:NH2	2.31	0.44
1:A:35:GLN:C	1:A:36:MET:HG3	2.42	0.44
1:A:172:TYR:CD1	1:A:173:PRO:O	2.64	0.44
1:A:182:VAL:O	1:A:183:GLU:O	2.34	0.44
1:A:276:ILE:CD1	1:A:371:VAL:CG2	2.87	0.44
1:A:277:SER:OG	1:A:279:GLU:C	2.56	0.44
1:A:312:TYR:CG	1:A:381:THR:CG2	2.90	0.44
2:B:183:GLU:OE1	2:B:394:GLN:HB2	2.14	0.44
2:B:227:LEU:HD12	2:B:227:LEU:HA	1.74	0.44
2:B:289:PRO:CD	2:B:290:GLU:H	2.29	0.44
1:A:152:LEU:O	1:A:156:ARG:HG3	2.17	0.44
1:A:312:TYR:CD1	1:A:341:ILE:HG23	2.51	0.44
2:B:20:PHE:HB2	2:B:235:MET:HE1	1.15	0.44
2:B:184:PRO:CB	2:B:395:PHE:CD1	3.00	0.44
2:B:230:LEU:HD21	2:B:302:MET:HG3	1.99	0.44
2:B:250:ALA:HB2	2:B:352:LYS:HZ1	1.81	0.44
2:B:333:LEU:HG	2:B:337:ASN:HD21	1.81	0.44
3:K:189:TYR:O	3:K:192:ILE:HG22	2.16	0.44
1:A:103:TYR:CD2	1:A:188:ILE:HG22	2.50	0.44
1:A:147:SER:OG	1:A:148:GLY:N	2.50	0.44
1:A:184:PRO:HD2	1:A:398:MET:HB3	1.99	0.44
1:A:303:VAL:CG1	1:A:304:LYS:N	2.80	0.44
2:B:22:GLU:HB3	2:B:83:PHE:CE1	2.46	0.44
2:B:22:GLU:C	2:B:24:ILE:N	2.70	0.44
2:B:143:GLY:C	2:B:185:TYR:OH	2.59	0.44
2:B:265:LEU:HD21	2:B:267:PHE:CE1	2.52	0.44
2:B:411:GLU:OE1	2:B:411:GLU:HA	2.17	0.44
2:B:426:ASN:C	2:B:426:ASN:HD22	2.25	0.44
3:K:112:GLU:O	3:K:114:ASP:N	2.50	0.44
3:K:159:ASN:C	3:K:161:LYS:N	2.74	0.44
1:A:38:SER:C	1:A:39:ASP:CG	2.85	0.44
1:A:306:ASP:CG	1:A:308:ARG:CD	2.90	0.44
1:A:328:VAL:CG1	1:A:332:ILE:HD11	2.16	0.44
1:A:328:VAL:O	1:A:332:ILE:HB	2.17	0.44
2:B:75:MET:SD	2:B:93:VAL:HG21	2.57	0.44
2:B:102:ASN:CG	2:B:105:LYS:HE3	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:MET:HG3	2:B:197:ASN:O	2.18	0.44
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.51	0.44
3:K:216:ARG:HA	3:K:250:ALA:HB1	2.00	0.44
1:A:31:GLN:NE2	1:A:243:ARG:CB	2.57	0.44
1:A:53:PHE:CA	1:A:88:HIS:HE1	1.94	0.44
1:A:204:VAL:HG13	1:A:209:ILE:CD1	2.30	0.44
1:A:254:GLU:OE1	2:B:101:ASN:CG	2.55	0.44
1:A:312:TYR:HD1	1:A:341:ILE:O	2.01	0.44
2:B:259:MET:HB3	2:B:268:PHE:CD1	2.30	0.44
2:B:385:GLN:OE1	2:B:433:GLN:HB2	2.17	0.44
1:A:146:GLY:O	1:A:150:THR:OG1	2.25	0.44
1:A:289:ALA:C	1:A:291:ILE:H	2.25	0.44
1:A:309:HIS:CB	1:A:386:GLU:OE2	2.65	0.44
2:B:56:ALA:CB	2:B:62:VAL:N	2.80	0.44
2:B:129:CYS:C	2:B:130:ASP:OD1	2.61	0.44
2:B:146:GLY:O	2:B:150:GLY:N	2.48	0.44
2:B:157:ILE:O	2:B:161:TYR:HB2	2.18	0.44
2:B:250:ALA:HB1	2:B:352:LYS:NZ	2.32	0.44
1:A:122:ILE:HD13	1:A:122:ILE:HG21	1.83	0.44
1:A:154:MET:CE	1:A:166:LYS:CD	2.79	0.44
1:A:170:SER:OG	1:A:203:MET:CA	2.66	0.44
1:A:184:PRO:HG2	1:A:399:TYR:CD2	2.51	0.44
1:A:211:ASP:OD1	1:A:214:ARG:NH1	2.51	0.44
2:B:94:PHE:CE2	2:B:114:LEU:CB	3.01	0.44
2:B:115:VAL:HG11	2:B:152:LEU:HB3	2.00	0.44
2:B:217:LEU:CD2	2:B:275:LEU:O	2.65	0.44
1:A:7:ILE:HB	1:A:136:SER:O	2.18	0.44
1:A:184:PRO:HB3	1:A:187:SER:OG	2.18	0.44
1:A:432:TYR:O	1:A:435:VAL:HB	2.17	0.44
2:B:29:GLY:O	2:B:58:GLY:HA3	2.18	0.44
2:B:32:PRO:HB2	2:B:59:ASN:HD22	0.60	0.44
2:B:89:PRO:C	2:B:90:ASP:CG	2.84	0.44
2:B:191:VAL:HG23	2:B:421:ALA:HB1	2.00	0.44
1:A:38:SER:HB3	1:A:45:GLY:HA3	2.00	0.44
1:A:137:VAL:CG2	1:A:168:GLU:HG2	2.48	0.44
1:A:256:GLN:HB2	2:B:407:TRP:HZ3	1.81	0.44
1:A:298:PRO:O	1:A:301:GLN:HB2	2.18	0.44
1:A:307:PRO:O	1:A:308:ARG:C	2.61	0.44
2:B:22:GLU:CD	2:B:83:PHE:HB2	2.39	0.44
2:B:66:ILE:HG23	2:B:66:ILE:O	2.16	0.44
2:B:75:MET:HE3	2:B:75:MET:CA	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:O	1:A:185:TYR:HB2	2.18	0.43
1:A:205:ASP:CB	1:A:303:VAL:CA	2.78	0.43
1:A:241:SER:OG	1:A:242:LEU:N	2.51	0.43
1:A:341:ILE:C	1:A:342:GLN:HG3	2.42	0.43
2:B:64:ARG:HH12	2:B:132:LEU:HD21	1.83	0.43
2:B:133:GLN:NE2	2:B:253:ARG:HB2	2.33	0.43
2:B:142:GLY:N	2:B:186:ASN:CG	2.61	0.43
1:A:141:PHE:HB3	1:A:186:ASN:CG	2.43	0.43
1:A:238:ILE:CG2	1:A:255:PHE:CZ	2.99	0.43
1:A:397:LEU:CA	1:A:401:LYS:CB	2.84	0.43
2:B:118:VAL:O	2:B:118:VAL:CG1	2.62	0.43
2:B:212:ILE:O	2:B:216:THR:OG1	2.35	0.43
2:B:236:SER:O	2:B:240:THR:HB	2.18	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CE1	2.53	0.43
3:K:10:VAL:HG12	3:K:329:ALA:HB3	2.00	0.43
1:A:345:ASP:OD2	1:A:439:SER:HA	2.17	0.43
1:A:362:VAL:HG13	1:A:367:ASP:CB	2.48	0.43
1:A:363:VAL:HG12	1:A:364:PRO:HG3	1.99	0.43
3:K:100:GLY:N	8:K:503:ACP:H3B1	2.32	0.43
1:A:179:THR:HG22	1:A:180:ALA:C	2.28	0.43
2:B:313:LEU:HA	2:B:344:VAL:CG2	2.30	0.43
2:B:377:PHE:CD1	2:B:377:PHE:C	2.97	0.43
1:A:5:ILE:CB	1:A:135:PHE:CE1	3.01	0.43
1:A:297:GLU:C	1:A:299:ALA:H	2.25	0.43
1:A:325:PRO:HG3	2:B:223:THR:HA	1.98	0.43
2:B:21:TRP:CE3	2:B:24:ILE:HD12	2.53	0.43
2:B:32:PRO:CG	2:B:33:THR:H	2.19	0.43
2:B:186:ASN:HA	2:B:189:LEU:HD12	2.00	0.43
2:B:254:LYS:C	2:B:258:ASN:OD1	2.59	0.43
2:B:259:MET:SD	2:B:378:ILE:CG2	3.05	0.43
3:K:233:GLU:CG	3:K:234:THR:N	2.50	0.43
1:A:14:VAL:CG2	1:A:74:VAL:CG1	2.96	0.43
1:A:26:LEU:O	1:A:27:GLU:CB	2.66	0.43
2:B:4:ILE:HG21	2:B:30:ILE:HG22	1.99	0.43
1:A:71:GLU:HG2	1:A:99:ALA:HB2	1.01	0.43
1:A:154:MET:HB2	1:A:192:HIS:HE1	1.75	0.43
1:A:312:TYR:HA	1:A:381:THR:CB	2.48	0.43
1:A:340:THR:C	1:A:341:ILE:HD13	2.44	0.43
2:B:44:LEU:HG	2:B:85:GLN:CG	2.46	0.43
2:B:176:LYS:CD	2:B:207:GLU:OE2	2.67	0.43
2:B:219:LEU:O	2:B:220:THR:C	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:GLU:O	2:B:434:GLN:HB2	2.18	0.43
1:A:157:LEU:HB2	1:A:166:LYS:CE	2.49	0.43
1:A:341:ILE:H	1:A:342:GLN:HG3	1.84	0.43
1:A:346:TRP:O	1:A:346:TRP:HE3	2.01	0.43
2:B:56:ALA:CB	2:B:62:VAL:CB	2.70	0.43
2:B:96:GLN:OE1	2:B:96:GLN:HA	2.19	0.43
2:B:398:MET:SD	2:B:399:PHE:CD2	3.12	0.43
3:K:304:ILE:HA	3:K:305:PRO:HD3	1.90	0.43
1:A:105:ARG:HG2	1:A:109:THR:HG1	1.84	0.43
1:A:119:LEU:HA	1:A:122:ILE:CG2	2.48	0.43
1:A:343:PHE:CE2	1:A:351:PHE:CE1	3.01	0.43
2:B:196:GLU:O	2:B:197:ASN:HB3	2.19	0.43
2:B:319:PHE:CE1	2:B:353:THR:HG21	2.44	0.43
2:B:344:VAL:H	2:B:350:ASN:HD21	1.67	0.43
3:K:212:GLU:O	3:K:213:THR:C	2.61	0.43
1:A:137:VAL:HB	1:A:168:GLU:CB	2.49	0.43
1:A:147:SER:N	1:A:189:LEU:HD13	2.33	0.43
1:A:362:VAL:O	1:A:363:VAL:HG23	2.19	0.43
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.19	0.43
2:B:6:HIS:CD2	2:B:21:TRP:CZ2	3.03	0.43
2:B:260:VAL:HG13	2:B:262:PHE:O	2.13	0.43
2:B:301:MET:HG3	2:B:307:PRO:HG3	2.00	0.43
1:A:192:HIS:O	1:A:196:GLU:CB	2.67	0.42
1:A:259:LEU:CA	1:A:380:ASN:HD21	2.31	0.42
1:A:404:PHE:O	1:A:404:PHE:CG	2.72	0.42
1:A:414:GLU:O	1:A:415:GLU:HB2	2.19	0.42
2:B:48:ARG:O	2:B:61:TYR:CE2	2.72	0.42
1:A:21:TRP:CD1	1:A:21:TRP:H	2.38	0.42
1:A:76:ASP:O	1:A:76:ASP:OD1	2.37	0.42
1:A:114:ILE:HD13	1:A:114:ILE:HG21	1.84	0.42
1:A:437:VAL:HG12	1:A:438:ASP:OD1	2.19	0.42
2:B:102:ASN:HB2	2:B:105:LYS:HG3	1.98	0.42
2:B:102:ASN:O	2:B:105:LYS:HB2	2.19	0.42
2:B:292:THR:HG22	2:B:332:MET:SD	2.58	0.42
2:B:301:MET:CE	2:B:377:PHE:CE1	3.03	0.42
1:A:185:TYR:CD1	1:A:185:TYR:C	2.97	0.42
3:K:18[A]:ARG:HE	3:K:22[A]:ARG:HH22	1.66	0.42
1:A:12:ALA:HB1	1:A:171:ILE:HD12	2.00	0.42
1:A:20:CYS:C	1:A:24:TYR:HD2	2.17	0.42
1:A:206:ASN:HD22	1:A:206:ASN:HA	1.46	0.42
1:A:229:ARG:HH11	1:A:229:ARG:HD2	1.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:THR:O	1:A:383:ALA:C	2.61	0.42
2:B:114:LEU:O	2:B:118:VAL:HG23	2.20	0.42
2:B:234:THR:HG23	2:B:270:PRO:HB2	2.00	0.42
2:B:244:PHE:HE2	2:B:358:ILE:HD13	1.67	0.42
2:B:296:PHE:C	2:B:297:ASP:O	2.60	0.42
2:B:370:GLY:O	6:B:502:TXL:C18	2.38	0.42
2:B:385:GLN:NE2	2:B:433:GLN:HB2	2.34	0.42
3:K:122:LEU:C	3:K:122:LEU:HD23	2.44	0.42
1:A:273:ALA:HB2	1:A:294:ALA:HB3	1.98	0.42
1:A:342:GLN:O	1:A:343:PHE:C	2.58	0.42
2:B:27:GLU:HB2	2:B:36:TYR:CB	2.49	0.42
2:B:258:ASN:O	2:B:314:THR:HG21	2.19	0.42
2:B:339:ASN:C	2:B:342:TYR:HD1	2.28	0.42
2:B:346:TRP:CZ2	2:B:435:TYR:CD2	3.05	0.42
1:A:58:ALA:C	1:A:60:LYS:N	2.75	0.42
1:A:179:THR:HG21	1:A:181:VAL:CA	2.46	0.42
2:B:50:ASN:HB3	2:B:51:VAL:H	1.30	0.42
2:B:87:PHE:HD1	2:B:88:ARG:C	2.23	0.42
2:B:92:PHE:CD1	2:B:92:PHE:N	2.87	0.42
1:A:170:SER:OG	1:A:203:MET:CB	2.42	0.42
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.86	0.42
1:A:312:TYR:HD2	1:A:381:THR:HG23	1.84	0.42
2:B:48:ARG:CZ	2:B:60:LYS:HA	2.46	0.42
2:B:231:VAL:C	2:B:233:ALA:N	2.74	0.42
2:B:253:ARG:HH11	2:B:253:ARG:CB	2.29	0.42
2:B:313:LEU:HD22	2:B:346:TRP:CZ2	2.55	0.42
2:B:340:SER:OG	2:B:341:SER:N	2.38	0.42
2:B:397:ALA:C	2:B:401:ARG:CB	2.92	0.42
1:A:31:GLN:NE2	1:A:243:ARG:NE	2.59	0.42
1:A:66:VAL:CG2	1:A:125:LEU:HD12	2.44	0.42
1:A:79:ARG:O	1:A:79:ARG:HG3	2.18	0.42
1:A:109:THR:HG21	1:A:411:GLU:CD	2.41	0.42
1:A:115:ILE:HD12	1:A:152:LEU:HD23	1.87	0.42
1:A:122:ILE:HD11	1:A:157:LEU:HD22	1.97	0.42
1:A:252:LEU:HD23	1:A:255:PHE:CD2	2.54	0.42
1:A:256:GLN:CB	2:B:407:TRP:HZ3	2.27	0.42
1:A:294:ALA:O	1:A:295:CYS:C	2.61	0.42
1:A:409:VAL:HG22	1:A:414:GLU:CG	2.43	0.42
2:B:69:ASP:OD2	2:B:74:THR:HG22	2.15	0.42
2:B:103:TRP:HZ3	2:B:108:TYR:HH	0.67	0.42
2:B:241:CYS:C	2:B:243:ARG:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:SER:O	2:B:283:TYR:HD1	2.02	0.42
2:B:305:CYS:HG	2:B:387:LEU:HB2	1.84	0.42
1:A:67:PHE:CB	1:A:92:LEU:CD2	2.97	0.42
1:A:101:ASN:HD22	4:A:500:GTP:PG	2.42	0.42
1:A:306:ASP:CG	1:A:308:ARG:CB	2.73	0.42
2:B:62:VAL:HG12	2:B:63:PRO:C	2.45	0.42
2:B:151:THR:O	2:B:192:HIS:HD2	2.02	0.42
2:B:190:SER:O	2:B:192:HIS:C	2.56	0.42
2:B:296:PHE:CD1	2:B:335:VAL:CG1	3.02	0.42
2:B:324:SER:O	2:B:328:VAL:HG23	2.19	0.42
3:K:161:LYS:H	3:K:161:LYS:HG2	1.25	0.42
1:A:130:THR:O	1:A:131:GLY:O	2.38	0.42
1:A:143:GLY:C	1:A:185:TYR:OH	2.63	0.42
1:A:228:ASN:ND2	4:A:500:GTP:C6	2.72	0.42
1:A:292:THR:CG2	1:A:319:TYR:CE2	2.98	0.42
2:B:27:GLU:HG2	2:B:48:ARG:HH21	1.85	0.42
2:B:27:GLU:OE2	2:B:40:SER:O	2.37	0.42
2:B:157:ILE:HG21	2:B:166:MET:CE	2.49	0.42
2:B:183:GLU:HG3	2:B:398:MET:SD	2.59	0.42
2:B:431:GLU:CA	2:B:434:GLN:HG3	2.50	0.42
1:A:31:GLN:NE2	1:A:239:THR:HG23	2.35	0.41
1:A:34:GLY:O	1:A:35:GLN:CB	2.64	0.41
1:A:147:SER:HB3	1:A:189:LEU:HD11	0.97	0.41
1:A:264:ARG:O	1:A:265:ALA:C	2.62	0.41
1:A:434:GLU:HB2	3:K:303:PHE:CD1	2.55	0.41
2:B:31:ASP:OD1	2:B:31:ASP:C	2.63	0.41
2:B:102:ASN:HB2	2:B:105:LYS:CE	2.50	0.41
2:B:172:VAL:CG2	2:B:205:ASP:OD1	2.67	0.41
2:B:216:THR:HG21	2:B:275:LEU:HD13	2.00	0.41
2:B:320:ARG:CG	2:B:320:ARG:O	2.64	0.41
2:B:405:LEU:O	2:B:409:THR:CB	2.68	0.41
6:B:502:TXL:H162	6:B:502:TXL:O6	2.19	0.41
1:A:181:VAL:O	1:A:399:TYR:CE2	2.71	0.41
1:A:266:HIS:HD2	1:A:432:TYR:CZ	2.37	0.41
1:A:416:GLY:O	1:A:417:GLU:HB2	2.19	0.41
1:A:420:GLU:CD	3:K:169:ARG:HB3	2.45	0.41
2:B:259:MET:HG3	2:B:378:ILE:CG2	2.50	0.41
2:B:260:VAL:HG12	2:B:262:PHE:H	1.85	0.41
2:B:320:ARG:NH2	6:B:502:TXL:C27	2.78	0.41
2:B:388:PHE:O	2:B:391:ILE:N	2.54	0.41
1:A:9:VAL:HG13	1:A:150:THR:HG22	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:C	1:A:108:TYR:HD2	2.28	0.41
1:A:157:LEU:CB	1:A:166:LYS:HE2	2.51	0.41
1:A:181:VAL:HG12	1:A:185:TYR:HB2	2.01	0.41
1:A:276:ILE:HG22	1:A:277:SER:N	2.35	0.41
2:B:14:ASN:ND2	2:B:69:ASP:HA	2.35	0.41
3:K:347:TYR:CE2	3:K:350:ARG:NH1	2.89	0.41
1:A:77:GLU:CA	1:A:80:THR:CB	2.84	0.41
1:A:219:ILE:CG2	1:A:219:ILE:O	2.68	0.41
1:A:276:ILE:CD1	1:A:371:VAL:HG22	2.30	0.41
2:B:111:GLY:O	2:B:115:VAL:CA	2.66	0.41
2:B:339:ASN:CA	2:B:342:TYR:HD1	2.32	0.41
1:A:64:ARG:NH2	1:A:132:LEU:CB	2.83	0.41
1:A:107:HIS:HD1	1:A:108:TYR:N	2.18	0.41
1:A:191:THR:OG1	1:A:192:HIS:N	2.53	0.41
1:A:246:GLY:O	1:A:249:ASN:ND2	2.48	0.41
1:A:344:VAL:HG12	1:A:345:ASP:N	2.34	0.41
2:B:391:ILE:C	2:B:394:GLN:HB2	2.45	0.41
1:A:110:ILE:HG21	1:A:110:ILE:HD13	1.85	0.41
1:A:262:TYR:CB	1:A:263:PRO:HD3	2.24	0.41
1:A:416:GLY:C	1:A:418:PHE:H	2.06	0.41
2:B:259:MET:C	2:B:261:PRO:HD3	2.46	0.41
1:A:9:VAL:HG12	1:A:146:GLY:HA2	2.01	0.41
1:A:271:THR:CB	1:A:377:MET:HB3	2.50	0.41
1:A:282:TYR:CD2	1:A:284:GLU:O	2.74	0.41
2:B:6:HIS:CE1	2:B:30:ILE:CG1	3.00	0.41
2:B:174:SER:HB2	2:B:207:GLU:CG	2.51	0.41
2:B:191:VAL:HG23	2:B:421:ALA:HA	1.87	0.41
2:B:224:TYR:O	2:B:225:GLY:C	2.54	0.41
2:B:308:ARG:O	2:B:342:TYR:CE2	2.72	0.41
2:B:393:GLU:OE1	2:B:393:GLU:HA	2.20	0.41
3:K:98:GLN:HG2	3:K:99:THR:N	2.35	0.41
1:A:3:GLU:HB2	1:A:64:ARG:CZ	2.51	0.41
1:A:14:VAL:HG22	1:A:69:ASP:OD1	2.20	0.41
1:A:72:PRO:HA	1:A:94:THR:HG23	2.02	0.41
1:A:296:PHE:HD2	1:A:312:TYR:OH	2.03	0.41
1:A:397:LEU:HA	1:A:401:LYS:HD2	2.00	0.41
2:B:71:GLU:HG2	2:B:99:ALA:H	1.65	0.41
2:B:94:PHE:CE1	2:B:97:SER:HB3	2.52	0.41
2:B:115:VAL:HG12	2:B:156:LYS:HZ2	1.86	0.41
2:B:238:VAL:CG1	2:B:255:LEU:CD1	2.98	0.41
2:B:435:TYR:CB	2:B:436:GLN:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:168:VAL:HG21	3:K:310:VAL:CG1	2.48	0.41
1:A:4:CYS:CB	1:A:30:ILE:HG21	2.44	0.41
1:A:5:ILE:HB	1:A:135:PHE:CE1	2.55	0.41
1:A:82:THR:C	1:A:84:ARG:N	2.73	0.41
1:A:173:PRO:HG3	1:A:186:ASN:ND2	2.35	0.41
1:A:212:ILE:HD12	1:A:230:LEU:HD21	1.75	0.41
1:A:313:MET:HB2	1:A:380:ASN:HB2	2.03	0.41
1:A:397:LEU:CA	1:A:401:LYS:HB3	2.49	0.41
1:A:423:GLU:OE2	3:K:172:PRO:C	2.64	0.41
2:B:3:GLU:O	2:B:4:ILE:HG13	2.11	0.41
2:B:25:SER:O	2:B:27:GLU:CG	2.55	0.41
2:B:48:ARG:NH1	2:B:60:LYS:HG3	2.30	0.41
2:B:49:ILE:HG21	2:B:49:ILE:HD13	1.75	0.41
2:B:165:ILE:HD12	2:B:256:ALA:CB	2.51	0.41
2:B:172:VAL:HG12	2:B:173:PRO:O	2.20	0.41
2:B:212:ILE:CD1	2:B:302:MET:HA	2.51	0.41
2:B:259:MET:HE2	2:B:379:GLY:H	1.79	0.41
2:B:296:PHE:CE2	2:B:335:VAL:CG1	2.98	0.41
2:B:433:GLN:CD	2:B:437:ASP:OD2	2.64	0.41
3:K:41:LYS:C	3:K:43:PRO:HD3	2.46	0.41
1:A:34:GLY:C	1:A:60:LYS:HZ2	2.27	0.41
1:A:242:LEU:HD11	1:A:318:LEU:CD1	2.51	0.41
2:B:44:LEU:HD21	2:B:85:GLN:HB2	1.07	0.41
2:B:239:THR:O	2:B:243:ARG:NE	2.42	0.41
2:B:312:TYR:N	2:B:381:SER:HB2	2.36	0.41
6:B:502:TXL:C21	6:B:502:TXL:C18	2.91	0.41
1:A:14:VAL:CG2	1:A:74:VAL:HG11	2.51	0.40
1:A:102:ASN:HA	1:A:408:TYR:CE1	2.56	0.40
1:A:154:MET:HB2	1:A:192:HIS:HE2	1.82	0.40
1:A:434:GLU:CB	3:K:303:PHE:HB3	2.43	0.40
2:B:70:LEU:O	2:B:70:LEU:HG	2.20	0.40
2:B:242:LEU:HD13	2:B:250:ALA:O	2.20	0.40
2:B:286:LEU:HD13	2:B:372:LYS:C	2.45	0.40
1:A:12:ALA:O	1:A:16:ILE:HB	2.21	0.40
1:A:150:THR:O	1:A:192:HIS:NE2	2.53	0.40
1:A:242:LEU:HD22	1:A:250:VAL:HB	2.03	0.40
2:B:223:THR:HG1	2:B:226:ASP:HB2	1.85	0.40
1:A:33:ASP:O	1:A:34:GLY:C	2.48	0.40
1:A:116:ASP:O	1:A:119:LEU:HB2	2.22	0.40
1:A:311:LYS:O	1:A:382:THR:HG23	2.21	0.40
1:A:329:ASN:ND2	2:B:210:TYR:OH	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PHE:C	1:A:397:LEU:N	2.76	0.40
2:B:282:GLN:HA	2:B:282:GLN:OE1	2.21	0.40
3:K:83[A]:GLN:HE21	3:K:87:GLU:CD	2.28	0.40
1:A:2:ARG:HA	1:A:133:GLN:CD	2.46	0.40
1:A:103:TYR:CZ	1:A:148:GLY:HA2	2.56	0.40
1:A:210:TYR:CE2	1:A:227:LEU:HD23	2.40	0.40
1:A:248:LEU:HD21	5:B:501:GDP:H2'	2.03	0.40
1:A:316:CYS:C	1:A:317:LEU:HD23	2.46	0.40
2:B:35:SER:HB3	2:B:60:LYS:HE3	2.02	0.40
2:B:194:LEU:HD11	2:B:428:LEU:HD22	2.03	0.40
2:B:274:PRO:HB2	2:B:371:LEU:CD2	2.51	0.40
3:K:340[B]:GLU:OE1	3:K:340[B]:GLU:HA	2.21	0.40
1:A:21:TRP:HA	1:A:24:TYR:HD2	1.87	0.40
1:A:75:ILE:HG23	1:A:76:ASP:N	2.36	0.40
1:A:116:ASP:OD1	1:A:156:ARG:NH1	2.54	0.40
1:A:395:PHE:C	1:A:397:LEU:H	2.29	0.40
2:B:142:GLY:N	2:B:186:ASN:ND2	2.69	0.40
2:B:236:SER:OG	6:B:502:TXL:H27	2.21	0.40
2:B:238:VAL:CG1	2:B:255:LEU:HD13	2.52	0.40
2:B:287:THR:O	2:B:290:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	438/451 (97%)	322 (74%)	63 (14%)	53 (12%)	0	4
2	B	425/445 (96%)	298 (70%)	48 (11%)	79 (19%)	0	2
3	K	332/394 (84%)	319 (96%)	11 (3%)	2 (1%)	21	59
All	All	1195/1290 (93%)	939 (79%)	122 (10%)	134 (11%)	1	5

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	33	ASP
1	A	35	GLN
1	A	39	ASP
1	A	42	ILE
1	A	46	ASP
1	A	50	ASN
1	A	51	THR
1	A	73	THR
1	A	83	TYR
1	A	129	CYS
1	A	133	GLN
1	A	174	ALA
1	A	177	VAL
1	A	183	GLU
1	A	185	TYR
1	A	193	THR
1	A	197	HIS
1	A	198	SER
1	A	219	ILE
1	A	248	LEU
1	A	265	ALA
1	A	268	PRO
1	A	275	VAL
1	A	281	ALA
1	A	283	HIS
1	A	284	GLU
1	A	312	TYR
1	A	341	ILE
1	A	344	VAL
1	A	348	PRO
1	A	359	PRO
1	A	364	PRO
1	A	368	LEU
1	A	369	ALA
2	B	2	ARG
2	B	25	SER
2	B	33	THR
2	B	36	TYR
2	B	39	ASP
2	B	40	SER
2	B	41	ASP

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Mol	Chain	Res	Type
2	B	42	LEU
2	B	43	GLN
2	B	47	GLU
2	B	54	ASN
2	B	60	LYS
2	B	61	TYR
2	B	80	SER
2	B	81	GLY
2	B	83	PHE
2	B	86	ILE
2	B	89	PRO
2	B	90	ASP
2	B	97	SER
2	B	99	ALA
2	B	102	ASN
2	B	177	VAL
2	B	179	ASP
2	B	195	VAL
2	B	204	ILE
2	B	219	LEU
2	B	245	PRO
2	B	261	PRO
2	B	270	PRO
2	B	274	PRO
2	B	280	SER
2	B	284	ARG
2	B	322	ARG
2	B	344	VAL
2	B	345	GLU
2	B	385	GLN
2	B	401	ARG
2	B	415	GLU
3	K	233	GLU
1	A	25	CYS
1	A	81	GLY
1	A	102	ASN
1	A	131	GLY
1	A	350	GLY
1	A	384	ILE
1	A	417	GLU
1	A	427	ALA
2	B	30	ILE

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Mol	Chain	Res	Type
2	B	32	PRO
2	B	50	ASN
2	B	72	PRO
2	B	75	MET
2	B	129	CYS
2	B	176	LYS
2	B	276	THR
2	B	285	ALA
2	B	341	SER
2	B	387	LEU
2	B	427	ASP
3	K	113	LYS
1	A	66	VAL
1	A	82	THR
1	A	194	THR
2	B	27	GLU
2	B	28	HIS
2	B	57	ALA
2	B	144	GLY
2	B	173	PRO
2	B	248	LEU
2	B	262	PHE
2	B	281	GLN
2	B	339	ASN
2	B	347	ILE
2	B	348	PRO
2	B	412	GLY
1	A	65	ALA
1	A	175	PRO
1	A	261	PRO
2	B	29	GLY
2	B	31	ASP
2	B	48	ARG
2	B	53	TYR
2	B	87	PHE
2	B	183	GLU
2	B	242	LEU
2	B	340	SER
1	A	98	ASP
1	A	410	GLY
2	B	222	PRO
2	B	360	PRO

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Mol	Chain	Res	Type
2	B	389	LYS
2	B	403	ALA
2	B	277	SER
2	B	314	THR
1	A	142	GLY
2	B	175	PRO
2	B	63	PRO
1	A	221	ARG

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 PDB entries followed by that with respect to all EM entries.

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	369/377 (98%)	353 (96%)	16 (4%)	26	47
2	B	368/381 (97%)	354 (96%)	14 (4%)	29	50
3	K	300/345 (87%)	271 (90%)	29 (10%)	8	24
All	All	1037/1103 (94%)	978 (94%)	59 (6%)	21	40

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	101	ASN
1	A	139	HIS
1	A	172	TYR
1	A	192	HIS
1	A	206	ASN
1	A	212	ILE
1	A	214	ARG
1	A	219	ILE
1	A	264	ARG
1	A	313	MET
1	A	390	ARG
1	A	396	ASP
1	A	405	VAL

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Mol	Chain	Res	Type
1	A	422	ARG
1	A	425	MET
2	B	30	ILE
2	B	101	ASN
2	B	139	HIS
2	B	192	HIS
2	B	227	LEU
2	B	229	HIS
2	B	253	ARG
2	B	278	ARG
2	B	302	MET
2	B	308	ARG
2	B	319	PHE
2	B	390	ARG
2	B	416	MET
2	B	436	GLN
3	K	22[A]	ARG
3	K	22[B]	ARG
3	K	38	VAL
3	K	44	LYS
3	K	46	THR
3	K	83[A]	GLN
3	K	83[B]	GLN
3	K	111	GLN
3	K	112	GLU
3	K	115	GLN
3	K	132	ASP
3	K	141	SER
3	K	145[A]	SER
3	K	145[B]	SER
3	K	161	LYS
3	K	162	ASN
3	K	201	LYS
3	K	209	ASN
3	K	216	ARG
3	K	235	ASN
3	K	236	ILE
3	K	242[A]	SER
3	K	242[B]	SER
3	K	271	ILE
3	K	275	LEU
3	K	303	PHE

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Mol	Chain	Res	Type
3	K	304	ILE
3	K	323	SER
3	K	358	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	31	GLN
1	A	61	HIS
1	A	85	GLN
1	A	88	HIS
1	A	107	HIS
1	A	192	HIS
1	A	206	ASN
1	A	226	ASN
1	A	228	ASN
1	A	300	ASN
1	A	329	ASN
1	A	356	ASN
1	A	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	28	HIS
2	B	50	ASN
2	B	54	ASN
2	B	59	ASN
2	B	101	ASN
2	B	102	ASN
2	B	107	HIS
2	B	133	GLN
2	B	136	GLN
2	B	193	GLN
2	B	197	ASN
2	B	294	GLN
2	B	336	GLN
2	B	337	ASN
2	B	350	ASN
2	B	426	ASN
3	K	111	GLN
3	K	135	ASN

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Mol	Chain	Res	Type
3	K	137	ASN
3	K	159	ASN
3	K	171	HIS
3	K	193	GLN
3	K	222	ASN
3	K	322	ASN

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GTP	A	500	-	33,34,34	1.93	6 (18%)	50,54,54	1.45	5 (10%)
6	TXL	B	502	-	63,63,63	4.48	48 (76%)	100,100,100	3.47	55 (55%)
8	ACP	K	503	7	31,33,33	1.43	6 (19%)	47,52,52	2.01	9 (19%)
5	GDP	B	501	-	29,30,30	1.32	3 (10%)	45,47,47	0.96	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	500	-	-	1/22/38/38	0/3/3/3
6	TXL	B	502	-	-	0/38/124/124	0/6/6/6
8	ACP	K	503	7	-	0/19/38/38	0/3/3/3
5	GDP	B	501	-	-	4/16/32/32	0/3/3/3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TXL	O3-C4	-10.07	1.26	1.46
6	B	502	TXL	C41-C36	9.38	1.53	1.39
6	B	502	TXL	C37-C36	-8.72	1.26	1.39
6	B	502	TXL	C8-C3	-8.12	1.38	1.57
6	B	502	TXL	O6-C9	-8.01	1.08	1.21
6	B	502	TXL	C25-C24	-7.64	1.27	1.39
6	B	502	TXL	C13-C12	-7.17	1.37	1.51
6	B	502	TXL	C14-C13	7.16	1.66	1.52
4	A	500	GTP	PB-O3A	-7.05	1.51	1.59
6	B	502	TXL	O5-C7	-6.91	1.32	1.43
6	B	502	TXL	C16-C15	-6.78	1.41	1.53
6	B	502	TXL	C6-C7	6.01	1.63	1.53
6	B	502	TXL	C43-C42	-5.89	1.30	1.49
6	B	502	TXL	C12-C11	-5.87	1.26	1.34
6	B	502	TXL	C10-C11	-5.40	1.34	1.50
6	B	502	TXL	O8-C13	-5.34	1.36	1.45
6	B	502	TXL	C14-C1	-5.27	1.43	1.54
6	B	502	TXL	O4-C5	5.23	1.56	1.46
6	B	502	TXL	C20-C4	5.22	1.67	1.53
6	B	502	TXL	C17-C15	4.62	1.62	1.53
6	B	502	TXL	C40-C39	-4.59	1.28	1.38
6	B	502	TXL	C28-C27	-4.46	1.28	1.38
6	B	502	TXL	C4-C3	4.45	1.64	1.54
6	B	502	TXL	C40-C41	4.30	1.46	1.38
6	B	502	TXL	C8-C9	4.22	1.67	1.55
6	B	502	TXL	O12-C30	-4.12	1.26	1.34
6	B	502	TXL	C24-C23	-4.11	1.46	1.52
6	B	502	TXL	O11-C30	4.07	1.29	1.21
4	A	500	GTP	PA-O3A	-4.03	1.55	1.59
6	B	502	TXL	O10-C22	3.90	1.49	1.42
6	B	502	TXL	C30-N1	3.87	1.44	1.34
6	B	502	TXL	C22-C21	-3.54	1.43	1.52
6	B	502	TXL	O12-C31	3.48	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TXL	C36-C35	-3.28	1.42	1.50
6	B	502	TXL	C23-N1	-3.23	1.39	1.46
4	A	500	GTP	O2'-C2'	-3.10	1.35	1.43
8	K	503	ACP	C4-N9	-3.06	1.31	1.37
6	B	502	TXL	O2-C35	3.05	1.40	1.34
4	A	500	GTP	O4'-C1'	-3.02	1.35	1.42
6	B	502	TXL	C34-C31	-3.00	1.43	1.51
6	B	502	TXL	O4-C20	-2.87	1.38	1.45
6	B	502	TXL	C28-C29	-2.80	1.34	1.38
6	B	502	TXL	O8-C21	2.79	1.40	1.34
8	K	503	ACP	C5-N7	-2.78	1.34	1.39
6	B	502	TXL	C39-C38	-2.76	1.32	1.38
8	K	503	ACP	C4-N3	2.75	1.39	1.34
8	K	503	ACP	PG-O3G	-2.63	1.49	1.55
6	B	502	TXL	O13-C35	-2.63	1.15	1.22
8	K	503	ACP	PG-O2G	2.55	1.60	1.55
5	B	501	GDP	PB-O2B	-2.54	1.45	1.54
6	B	502	TXL	C6-C5	-2.52	1.47	1.52
6	B	502	TXL	C4-C5	-2.51	1.50	1.55
6	B	502	TXL	C10-C9	2.49	1.60	1.53
5	B	501	GDP	PB-O1B	-2.48	1.42	1.50
6	B	502	TXL	O3-C42	2.43	1.40	1.35
6	B	502	TXL	C32-C31	-2.35	1.45	1.51
6	B	502	TXL	O1-C1	-2.33	1.40	1.43
4	A	500	GTP	C3'-C4'	-2.32	1.47	1.53
6	B	502	TXL	C26-C25	-2.30	1.35	1.38
5	B	501	GDP	PA-O3A	-2.18	1.57	1.59
4	A	500	GTP	C5'-C4'	-2.16	1.45	1.51
8	K	503	ACP	C2-N1	2.08	1.37	1.33
6	B	502	TXL	C1-C2	2.03	1.64	1.57

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	502	TXL	C39-C38-C37	11.07	133.89	120.24
6	B	502	TXL	C15-C1-C2	10.90	123.90	111.93
6	B	502	TXL	C38-C37-C36	-9.75	110.78	120.36
6	B	502	TXL	O7-C10-C9	7.22	121.55	109.51
8	K	503	ACP	C5-C4-N3	-6.47	117.80	126.72
6	B	502	TXL	C39-C40-C41	-6.24	112.54	120.24
6	B	502	TXL	C8-C9-C10	6.23	131.97	122.69
8	K	503	ACP	N3-C2-N1	-6.15	119.27	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	GTP	O2B-PB-O3B	5.96	123.38	107.27
6	B	502	TXL	C13-C12-C11	-5.85	108.09	117.73
6	B	502	TXL	O11-C30-N1	5.77	134.31	124.86
6	B	502	TXL	C11-C10-C9	-5.62	107.58	114.05
6	B	502	TXL	O2-C2-C1	5.42	115.99	104.74
6	B	502	TXL	C6-C5-C4	-5.30	112.42	119.63
6	B	502	TXL	C17-C15-C1	5.25	122.23	111.13
6	B	502	TXL	O4-C5-C6	4.85	122.10	113.17
6	B	502	TXL	C18-C12-C11	4.72	130.95	125.32
6	B	502	TXL	C16-C15-C1	-4.63	101.36	111.13
6	B	502	TXL	O12-C30-N1	-4.51	102.64	110.03
6	B	502	TXL	C33-C31-C32	4.51	122.38	111.13
6	B	502	TXL	O10-C22-C23	4.45	122.21	109.69
6	B	502	TXL	C10-C11-C12	-4.41	113.97	120.65
8	K	503	ACP	C2-N3-C4	4.37	122.50	111.83
6	B	502	TXL	C14-C1-C15	-4.27	103.75	111.48
4	A	500	GTP	O3B-PB-O1B	-4.23	97.97	110.70
6	B	502	TXL	C2-O2-C35	4.14	125.37	117.80
6	B	502	TXL	O12-C31-C32	-4.06	91.19	107.21
8	K	503	ACP	C4-C5-N7	-4.05	105.96	110.58
6	B	502	TXL	O6-C9-C10	-3.97	112.83	117.37
6	B	502	TXL	O3-C42-O14	3.89	130.40	123.61
6	B	502	TXL	C31-O12-C30	-3.86	115.11	120.97
6	B	502	TXL	C19-C8-C9	3.86	116.55	106.56
6	B	502	TXL	C20-C4-C3	3.80	126.20	120.32
6	B	502	TXL	O7-C10-C11	-3.75	105.42	111.48
6	B	502	TXL	O2-C35-C36	3.72	117.88	111.90
6	B	502	TXL	C24-C23-N1	3.64	119.08	112.07
8	K	503	ACP	N3-C4-N9	3.56	133.22	127.17
6	B	502	TXL	C15-C11-C12	3.49	124.30	119.60
8	K	503	ACP	C5-N7-C8	3.28	108.60	103.45
6	B	502	TXL	C13-O8-C21	-3.24	110.76	116.58
4	A	500	GTP	O3G-PG-O3B	3.11	115.08	104.64
8	K	503	ACP	N9-C8-N7	-3.08	109.56	113.94
6	B	502	TXL	C24-C23-C22	-3.04	103.89	111.46
6	B	502	TXL	O5-C7-C6	3.02	115.26	109.12
6	B	502	TXL	C1-C2-C3	-2.98	113.73	118.19
6	B	502	TXL	C34-C31-C33	-2.92	103.85	111.13
8	K	503	ACP	C5-C4-N9	2.90	108.97	105.81
6	B	502	TXL	C20-C4-C5	-2.84	82.45	85.38
6	B	502	TXL	C37-C36-C35	-2.75	114.33	120.40
6	B	502	TXL	C18-C12-C13	2.68	120.88	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	502	TXL	O3-C42-C43	-2.66	106.17	110.67
6	B	502	TXL	C23-N1-C30	-2.64	116.22	121.69
6	B	502	TXL	O4-C5-C4	2.56	93.38	90.58
6	B	502	TXL	O8-C13-C12	-2.55	103.78	109.85
6	B	502	TXL	O8-C21-O9	2.54	128.53	123.95
6	B	502	TXL	O12-C31-C34	2.51	117.12	107.21
6	B	502	TXL	C19-C8-C3	-2.50	105.64	113.26
6	B	502	TXL	C41-C36-C35	2.48	125.87	120.40
8	K	503	ACP	C6-C5-C4	2.38	120.43	117.18
6	B	502	TXL	C14-C1-C2	-2.37	107.46	111.67
6	B	502	TXL	C27-C26-C25	2.37	123.16	120.24
4	A	500	GTP	O3A-PB-O1B	-2.36	103.61	110.70
5	B	501	GDP	C1'-N9-C8	2.36	133.43	126.73
6	B	502	TXL	O10-C22-C21	-2.33	103.76	110.33
6	B	502	TXL	C3-C4-C5	2.33	123.69	119.49
6	B	502	TXL	O1-C1-C2	-2.28	100.59	105.54
5	B	501	GDP	O2B-PB-O1B	2.26	119.64	110.83
6	B	502	TXL	O3-C4-C5	-2.25	107.07	112.26
4	A	500	GTP	O2G-PG-O3B	2.15	111.86	104.64
6	B	502	TXL	O2-C2-C3	-2.10	104.35	108.17
6	B	502	TXL	O6-C9-C8	-2.03	114.75	119.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

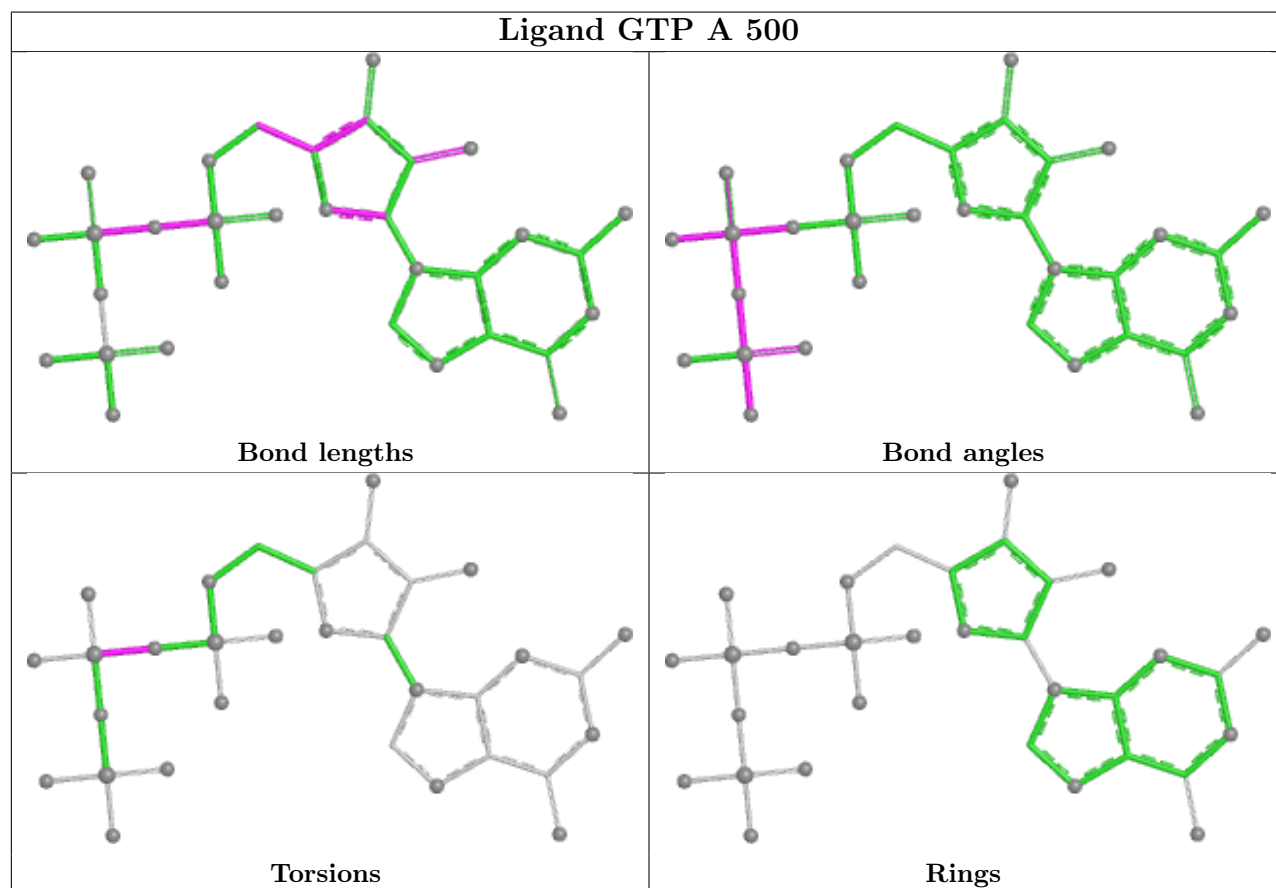
Mol	Chain	Res	Type	Atoms
5	B	501	GDP	PA-O3A-PB-O2B
5	B	501	GDP	C5'-O5'-PA-O1A
5	B	501	GDP	PA-O3A-PB-O1B
5	B	501	GDP	PA-O3A-PB-O3B
4	A	500	GTP	PA-O3A-PB-O2B

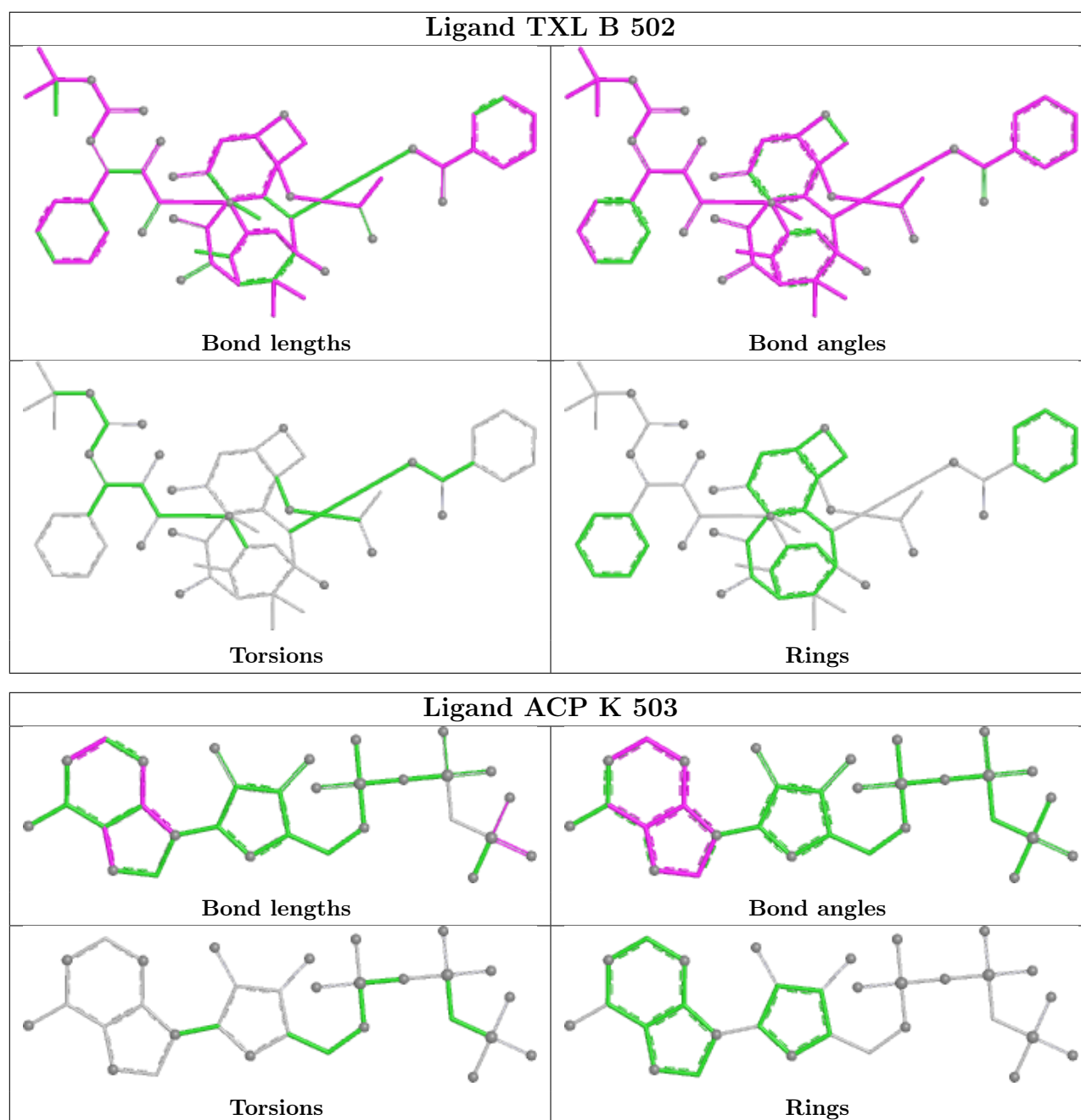
There are no ring outliers.

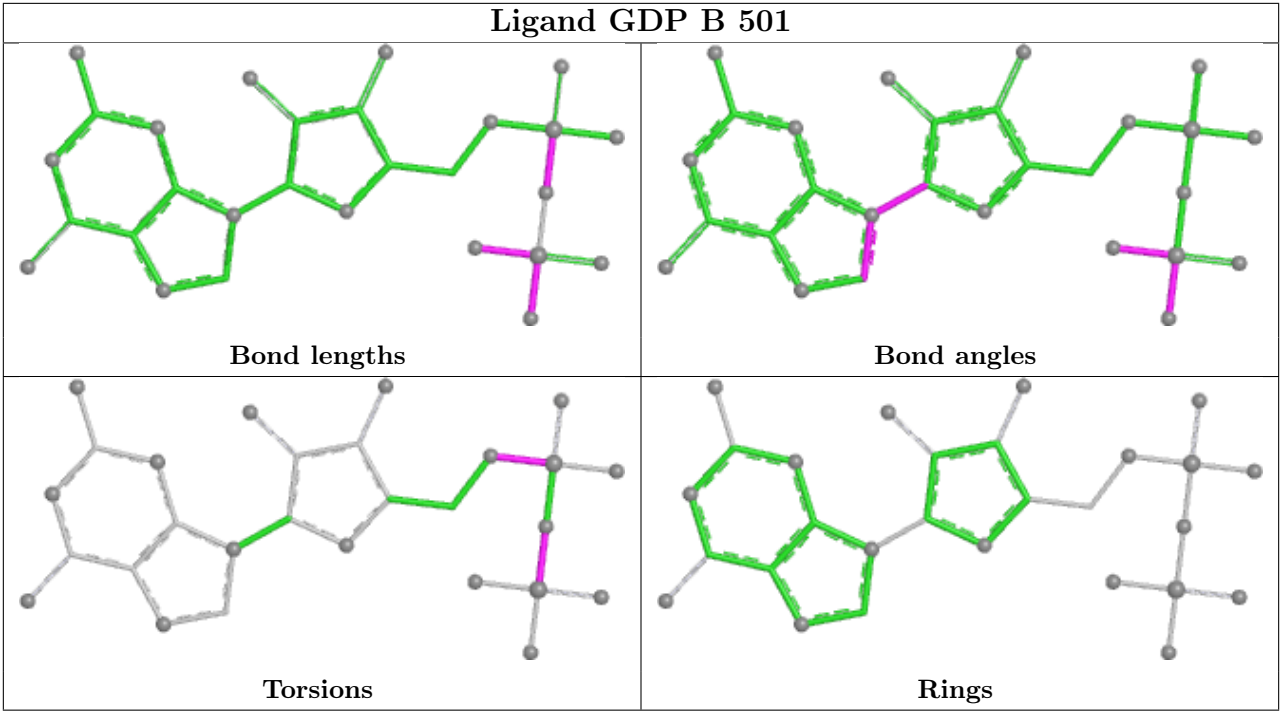
4 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	GTP	22	0
6	B	502	TXL	61	0
8	K	503	ACP	2	0
5	B	501	GDP	20	0

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







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	52
1	A	41

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	387:LEU	C	388:PHE	N	1.63
1	A	283:HIS	C	284:GLU	N	1.20
1	A	380:ASN	C	381:THR	N	1.20
1	A	437:VAL	C	438:ASP	N	1.20
1	B	52:TYR	C	53:TYR	N	1.20
1	A	111:GLY	C	112:LYS	N	1.19
1	A	137:VAL	C	138:PHE	N	1.19
1	A	140:SER	C	141:PHE	N	1.19
1	A	146:GLY	C	147:SER	N	1.19
1	A	149:PHE	C	150:THR	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	377:MET	C	378:LEU	N	1.19
1	A	383:ALA	C	384:ILE	N	1.19
1	B	72:PRO	C	73:GLY	N	1.19
1	B	111:GLY	C	112:ALA	N	1.19
1	B	178:SER	C	179:ASP	N	1.19
1	B	193:GLN	C	194:LEU	N	1.19
1	B	194:LEU	C	195:VAL	N	1.19
1	B	234:THR	C	235:MET	N	1.19
1	B	244:PHE	C	245:PRO	N	1.19
1	B	259:MET	C	260:VAL	N	1.19
1	B	347:ILE	C	348:PRO	N	1.19
1	B	348:PRO	C	349:ASN	N	1.19
1	A	34:GLY	C	35:GLN	N	1.18
1	A	433:GLU	C	434:GLU	N	1.18
1	B	130:ASP	C	131:CYS	N	1.18
1	A	259:LEU	C	260:VAL	N	1.17
1	A	346:TRP	C	347:CYS	N	1.17
1	A	367:ASP	C	368:LEU	N	1.17
1	B	53:TYR	C	54:ASN	N	1.17
1	B	299:LYS	C	300:ASN	N	1.17
1	A	204:VAL	C	205:ASP	N	1.16
1	A	233:GLN	C	234:ILE	N	1.16
1	A	274:PRO	C	275:VAL	N	1.16
1	B	70:LEU	C	71:GLU	N	1.16
1	B	89:PRO	C	90:ASP	N	1.16
1	B	171:VAL	C	172:VAL	N	1.16
1	B	243:ARG	C	244:PHE	N	1.16
1	A	24:TYR	C	25:CYS	N	1.15
1	A	379:SER	C	380:ASN	N	1.15
1	B	154:ILE	C	155:SER	N	1.15
1	B	173:PRO	C	174:SER	N	1.15
1	B	337:ASN	C	338:LYS	N	1.15
1	B	151:THR	C	152:LEU	N	1.14
1	B	436:GLN	C	437:ASP	N	1.14
1	A	90:GLU	C	91:GLN	N	1.13
1	B	292:THR	C	293:GLN	N	1.13
1	A	33:ASP	C	34:GLY	N	1.12
1	A	280:LYS	C	281:ALA	N	1.12
1	B	273:ALA	C	274:PRO	N	1.12
1	A	87:PHE	C	88:HIS	N	1.11
1	B	64:ARG	C	65:ALA	N	1.11
1	B	334:ASN	C	335:VAL	N	1.11

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	414:ASP	C	415:GLU	N	1.11
1	B	60:LYS	C	61:TYR	N	1.10
1	B	179:ASP	C	180:THR	N	1.10
1	B	371:LEU	C	372:LYS	N	1.10
1	A	216:ASN	C	217:LEU	N	1.09
1	A	402:ARG	C	403:ALA	N	1.09
1	B	344:VAL	C	345:GLU	N	1.09
1	A	221:ARG	C	222:PRO	N	1.08
1	A	190:THR	C	191:THR	N	1.07
1	B	22:GLU	C	23:VAL	N	1.07
1	B	331:GLN	C	332:MET	N	1.07
1	A	31:GLN	C	32:PRO	N	1.06
1	B	71:GLU	C	72:PRO	N	1.06
1	B	127:GLU	C	128:SER	N	1.05
1	B	400:ARG	C	401:ARG	N	1.05
1	B	380:ASN	C	381:SER	N	1.04
1	A	69:ASP	C	70:LEU	N	1.03
1	A	405:VAL	C	406:HIS	N	1.03
1	A	415:GLU	C	416:GLY	N	1.03
1	A	371:VAL	C	372:GLN	N	1.02
1	B	203:CYS	C	204:ILE	N	1.02
1	B	275:LEU	C	276:THR	N	1.02
1	B	309:HIS	C	310:GLY	N	1.00
1	B	346:TRP	C	347:ILE	N	0.99
1	B	417:GLU	C	418:PHE	N	0.98
1	A	358:GLU	C	359:PRO	N	0.97
1	B	247:GLN	C	248:LEU	N	0.96
1	A	193:THR	C	194:THR	N	0.95
1	A	350:GLY	C	351:PHE	N	0.95
1	A	416:GLY	C	417:GLU	N	0.95
1	B	340:SER	C	341:SER	N	0.92
1	A	53:PHE	C	54:SER	N	0.90
1	B	182:VAL	C	183:GLU	N	0.90
1	B	197:ASN	C	198:THR	N	0.90
1	B	200:GLU	C	201:THR	N	0.90
1	A	347:CYS	C	348:PRO	N	0.89
1	B	321:GLY	C	322:ARG	N	0.88
1	A	218:ASP	C	219:ILE	N	0.84
1	B	105:LYS	C	106:GLY	N	0.80
1	A	38:SER	C	39:ASP	N	0.70
1	B	73:GLY	C	74:THR	N	0.69