



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:08 AM UTC

PDB ID : 1TUB / pdb_00001tub
Title : TUBULIN ALPHA-BETA DIMER, ELECTRON DIFFRACTION
Authors : Nogales, E.; Downing, K.H.
Deposited on : 1997-09-23
Resolution : 3.70 Å(reported)

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)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

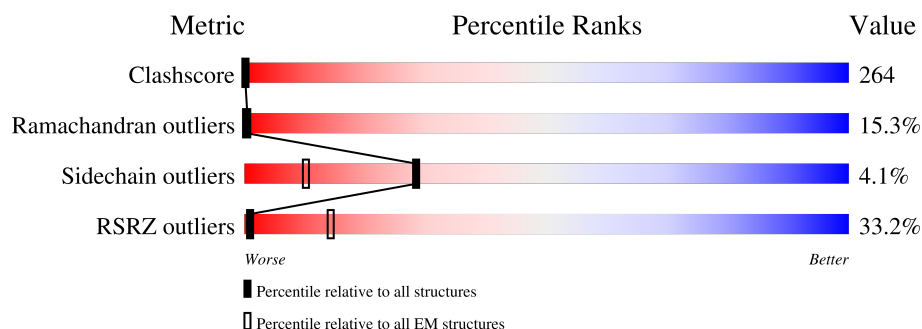
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.70 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
RSRZ outliers	180361	209

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	440	6% 32% 38% 38% 18%
2	B	427	• 35% 38% 37% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GTP	A	500	-	-	X	-
4	GDP	B	500	-	-	X	-
5	TXL	B	501	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6907 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.

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

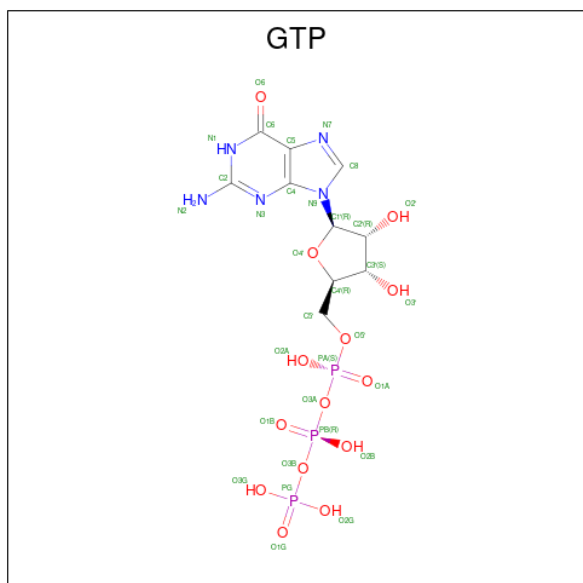
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called TUBULIN.

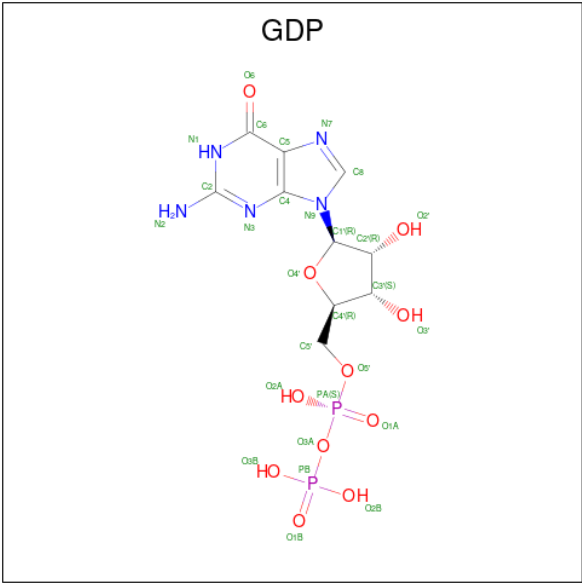
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	427	3359	2110	576	647	26	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

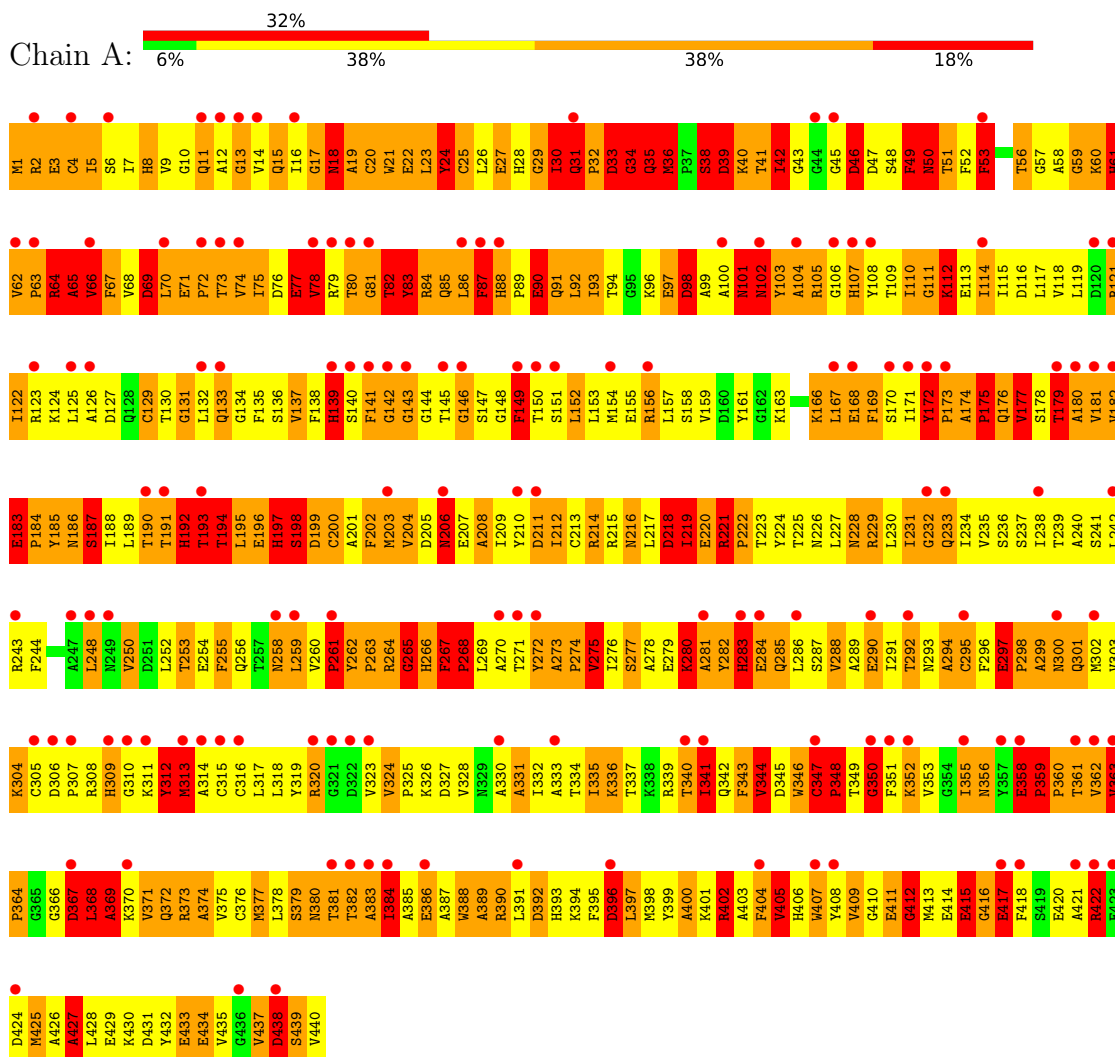


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	58	43	1	14	0

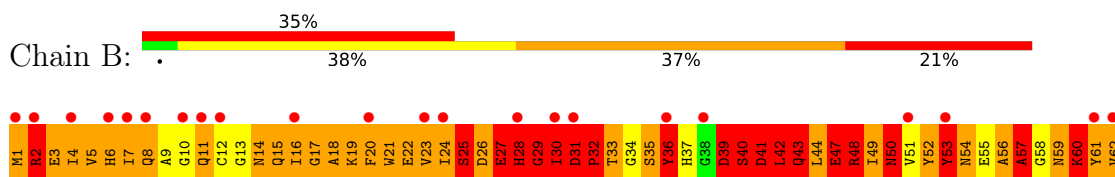
3 Residue-property plots

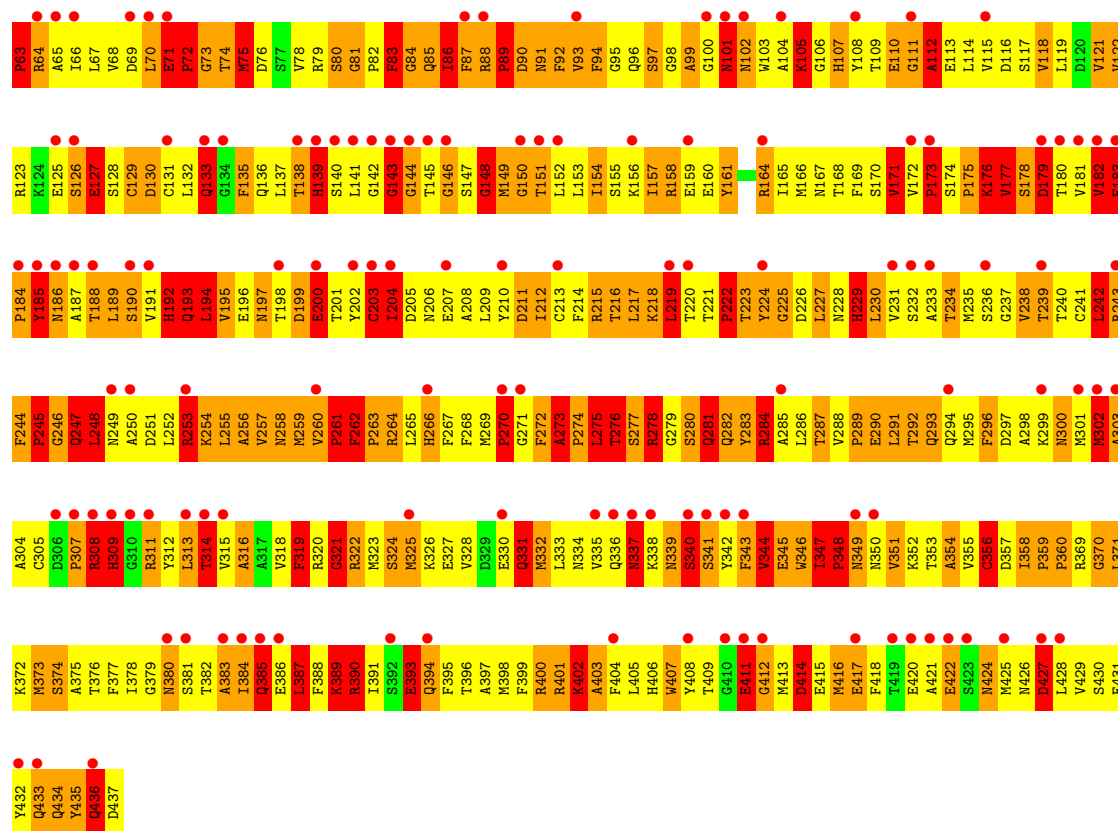
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• Molecule 2: TUBULIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.00Å 92.00Å 90.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.70 90.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.70) 84.4 (90.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.537 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	144.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 393.4	EDS
L-test for twinning ¹	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.006 for h,-k,-l	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	6907	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2123e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	244/3508 (7.0%)	3.46	307/4762 (6.4%)
2	B	3.61	240/3434 (7.0%)	3.81	361/4652 (7.8%)
All	All	3.48	484/6942 (7.0%)	3.64	668/9414 (7.1%)

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	56
2	B	0	59
All	All	0	115

All (484) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	278	ARG	CA-CB	48.85	2.30	1.53
1	A	38	SER	C-N	-44.88	0.70	1.33
2	B	73	GLY	C-N	-44.00	0.69	1.33
2	B	105	LYS	C-N	-37.83	0.80	1.33
1	A	218	ASP	C-N	-35.82	0.84	1.33
2	B	200	GLU	C-N	-33.93	0.90	1.33
1	A	53	PHE	C-N	-33.54	0.90	1.33
2	B	321	GLY	C-N	-32.27	0.88	1.33
2	B	197	ASN	C-N	-30.32	0.90	1.33
1	A	358	GLU	C-N	-30.14	0.97	1.33
2	B	346	TRP	C-N	-30.05	0.99	1.33
2	B	340	SER	C-N	-29.40	0.92	1.33
1	A	416	GLY	C-N	-27.67	0.94	1.33
1	A	193	THR	C-N	-27.42	0.95	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	GLY	C-N	-27.33	0.95	1.33
2	B	247	GLN	C-N	-26.47	0.96	1.33
2	B	417	GLU	C-N	-26.39	0.98	1.33
1	A	415	GLU	C-N	-26.04	1.03	1.33
1	A	219	ILE	CB-CG1	-24.35	1.04	1.53
2	B	203	CYS	C-N	-23.25	1.02	1.33
1	A	69	ASP	C-N	-22.83	1.03	1.33
2	B	309	HIS	C-N	-22.48	1.00	1.33
2	B	275	LEU	C-N	-22.30	1.02	1.33
1	A	405	VAL	C-N	-21.74	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	-20.54	1.08	1.33
2	B	127	GLU	C-N	-20.27	1.05	1.33
2	B	400	ARG	C-N	-20.12	1.05	1.33
2	B	270	PRO	C-N	20.08	1.58	1.33
1	A	371	VAL	C-N	-19.80	1.02	1.33
2	B	331	GLN	C-N	-19.67	1.07	1.33
2	B	22	GLU	C-N	-19.25	1.07	1.33
1	A	347	CYS	C-N	-18.85	0.89	1.33
1	A	190	THR	C-N	-18.50	1.07	1.33
1	A	219	ILE	CB-CG2	18.34	2.13	1.52
2	B	334	ASN	C-N	-18.09	1.11	1.33
2	B	64	ARG	C-N	-18.02	1.11	1.33
1	A	409	VAL	C-N	17.62	1.59	1.33
2	B	380	ASN	C-N	-17.61	1.04	1.33
1	A	216	ASN	C-N	-17.59	1.09	1.33
2	B	387	LEU	C-N	17.35	1.63	1.33
2	B	344	VAL	C-N	-17.08	1.09	1.33
1	A	402	ARG	C-N	-16.99	1.09	1.33
1	A	187	SER	C-N	16.64	1.54	1.33
2	B	292	THR	C-N	-16.57	1.13	1.33
2	B	60	LYS	C-N	-16.47	1.10	1.33
2	B	371	LEU	C-N	-16.33	1.10	1.33
2	B	414	ASP	C-N	-15.88	1.11	1.33
2	B	337	ASN	C-N	-15.51	1.15	1.33
2	B	179	ASP	C-N	-15.29	1.10	1.33
1	A	280	LYS	C-N	-15.14	1.12	1.33
2	B	151	THR	C-N	-15.11	1.14	1.33
1	A	21	TRP	C-O	14.82	1.42	1.24
2	B	171	VAL	C-N	-14.77	1.16	1.33
1	A	33	ASP	C-N	-14.70	1.12	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	GLY	N-CA	-14.52	1.24	1.45
2	B	146	GLY	C-N	14.46	1.53	1.33
1	A	233	GLN	C-N	-14.12	1.16	1.34
2	B	259	MET	C-N	-14.07	1.19	1.32
1	A	259	LEU	C-N	-14.01	1.17	1.33
2	B	71	GLU	C-O	-13.98	1.06	1.24
2	B	54	ASN	N-CA	-13.81	1.28	1.46
1	A	90	GLU	C-N	-13.73	1.13	1.33
2	B	154	ILE	C-N	-13.69	1.15	1.33
2	B	436	GLN	C-N	-13.37	1.14	1.33
1	A	346	TRP	C-N	-13.22	1.17	1.33
1	A	24	TYR	C-N	-12.99	1.15	1.33
1	A	43	GLY	C-N	12.97	1.50	1.33
1	A	231	ILE	C-O	12.85	1.39	1.24
1	A	181	VAL	C-N	12.57	1.47	1.34
1	A	438	ASP	C-O	12.48	1.38	1.23
2	B	193	GLN	C-O	12.43	1.40	1.24
2	B	89	PRO	C-N	-12.40	1.16	1.33
2	B	218	LYS	C-N	12.38	1.51	1.33
1	A	274	PRO	C-N	-12.36	1.16	1.33
2	B	299	LYS	C-N	-12.29	1.17	1.33
1	A	36	MET	C-N	-12.27	1.22	1.34
1	A	379	SER	C-N	-12.00	1.15	1.33
1	A	367	ASP	C-N	-11.94	1.17	1.33
2	B	72	PRO	C-N	-11.89	1.19	1.33
1	A	204	VAL	C-N	-11.85	1.16	1.33
2	B	71	GLU	C-N	-11.81	1.06	1.33
2	B	193	GLN	C-N	-11.78	1.19	1.33
1	A	31	GLN	C-N	-11.68	1.06	1.33
2	B	291	LEU	N-CA	-11.66	1.31	1.46
2	B	190	SER	C-N	11.65	1.49	1.33
2	B	53	TYR	C-N	-11.60	1.17	1.33
2	B	412	GLY	C-N	11.60	1.48	1.33
1	A	32	PRO	N-CD	-11.42	1.31	1.47
1	A	111	GLY	C-N	-11.41	1.19	1.33
2	B	111	GLY	C-N	-11.41	1.19	1.33
1	A	176	GLN	C-N	11.37	1.49	1.33
1	A	1	MET	C-N	11.36	1.47	1.33
2	B	243	ARG	C-N	-11.35	1.16	1.33
1	A	433	GLU	C-N	-11.15	1.18	1.33
1	A	87	PHE	C-N	-10.73	1.11	1.33
1	A	34	GLY	C-N	-10.68	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	167	ASN	C-N	10.53	1.47	1.33
2	B	2	ARG	CA-C	-10.51	1.38	1.52
2	B	130	ASP	C-N	-10.50	1.18	1.33
2	B	221	THR	N-CA	10.50	1.57	1.46
1	A	184	PRO	CA-CB	-10.49	1.39	1.53
1	A	384	ILE	C-O	-10.43	1.11	1.24
1	A	140	SER	C-N	-10.42	1.19	1.33
2	B	168	THR	C-N	10.41	1.47	1.33
2	B	139	HIS	C-N	10.39	1.47	1.33
1	A	2	ARG	N-CA	10.37	1.60	1.46
2	B	383	ALA	C-N	-10.35	1.21	1.33
1	A	43	GLY	C-O	-10.35	1.11	1.23
1	A	77	GLU	C-N	10.31	1.46	1.34
1	A	437	VAL	C-N	-10.30	1.20	1.33
2	B	348	PRO	C-N	-10.29	1.19	1.33
2	B	164	ARG	C-N	10.28	1.45	1.33
1	A	146	GLY	C-N	-10.26	1.19	1.33
2	B	234	THR	C-N	-10.26	1.19	1.33
1	A	383	ALA	C-N	-10.25	1.19	1.33
1	A	339	ARG	CA-C	-10.23	1.39	1.52
1	A	137	VAL	C-N	-10.18	1.19	1.33
1	A	91	GLN	C-N	10.05	1.48	1.33
1	A	46	ASP	C-N	10.02	1.47	1.33
1	A	221	ARG	CB-CG	-10.00	1.22	1.52
1	A	273	ALA	C-N	-9.99	1.25	1.33
2	B	92	PHE	C-N	-9.97	1.21	1.33
2	B	178	SER	C-N	-9.91	1.19	1.33
2	B	393	GLU	C-O	-9.89	1.11	1.24
1	A	149	PHE	C-N	-9.89	1.19	1.33
1	A	33	ASP	CA-C	-9.88	1.39	1.52
1	A	17	GLY	C-N	9.85	1.47	1.34
1	A	229	ARG	CA-CB	-9.83	1.37	1.53
2	B	194	LEU	C-N	-9.74	1.19	1.33
2	B	86	ILE	C-N	9.62	1.47	1.33
1	A	283	HIS	C-N	-9.61	1.20	1.33
2	B	192	HIS	C-O	9.60	1.36	1.24
1	A	362	VAL	CA-CB	-9.60	1.48	1.55
1	A	27	GLU	C-N	9.57	1.48	1.33
1	A	380	ASN	C-N	-9.55	1.20	1.33
2	B	52	TYR	C-N	-9.54	1.20	1.33
1	A	229	ARG	NE-CZ	-9.50	1.22	1.33
2	B	2	ARG	C-N	-9.49	1.21	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	149	MET	C-N	-9.47	1.22	1.33
1	A	22	GLU	C-O	9.40	1.35	1.24
1	A	114	ILE	C-N	-9.40	1.21	1.33
1	A	183	GLU	C-O	-9.30	1.12	1.24
2	B	349	ASN	N-CA	-9.25	1.34	1.46
1	A	94	THR	C-N	-9.24	1.29	1.33
2	B	346	TRP	N-CA	-9.22	1.34	1.45
1	A	258	ASN	C-N	-9.17	1.21	1.33
2	B	298	ALA	C-N	9.16	1.46	1.33
1	A	43	GLY	CA-C	9.11	1.61	1.52
1	A	19	ALA	C-N	-9.11	1.22	1.33
1	A	196	GLU	C-N	-9.10	1.21	1.33
1	A	20	CYS	C-N	9.09	1.46	1.34
2	B	40	SER	N-CA	-9.08	1.34	1.46
2	B	273	ALA	C-N	-9.05	1.12	1.33
2	B	52	TYR	N-CA	-9.04	1.35	1.45
2	B	278	ARG	CD-NE	-9.03	1.33	1.46
2	B	133	GLN	C-N	-9.00	1.22	1.33
2	B	222	PRO	C-N	-8.95	1.22	1.33
2	B	51	VAL	C-N	-8.92	1.21	1.33
1	A	107	HIS	C-O	8.82	1.34	1.24
2	B	107	HIS	C-O	8.82	1.34	1.24
1	A	183	GLU	C-N	-8.80	1.22	1.33
2	B	85	GLN	C-N	8.76	1.45	1.33
2	B	173	PRO	C-N	-8.73	1.15	1.33
1	A	285	GLN	C-N	-8.72	1.21	1.33
2	B	290	GLU	C-O	-8.70	1.13	1.24
1	A	141	PHE	N-CA	-8.69	1.34	1.46
2	B	76	ASP	C-O	8.68	1.34	1.24
1	A	222	PRO	N-CD	8.68	1.59	1.47
1	A	220	GLU	CB-CG	8.67	1.78	1.52
2	B	296	PHE	C-N	-8.63	1.21	1.33
2	B	27	GLU	C-N	-8.60	1.21	1.33
1	A	166	LYS	C-N	-8.59	1.21	1.33
1	A	200	CYS	C-N	-8.57	1.21	1.33
1	A	112	LYS	C-O	-8.53	1.14	1.24
2	B	112	ALA	C-O	-8.53	1.14	1.24
2	B	28	HIS	C-O	-8.53	1.13	1.24
1	A	80	THR	C-N	-8.52	1.21	1.33
2	B	143	GLY	C-N	-8.49	1.21	1.33
2	B	356	CYS	C-N	-8.46	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	242	LEU	C-N	-8.45	1.21	1.33
2	B	25	SER	C-N	8.39	1.45	1.33
1	A	292	THR	C-N	-8.37	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	-8.31	1.21	1.33
1	A	41	THR	C-N	-8.29	1.22	1.33
2	B	70	LEU	C-N	-8.27	1.16	1.33
1	A	277	SER	C-N	-8.26	1.22	1.33
1	A	85	GLN	CA-C	-8.25	1.43	1.53
2	B	244	PHE	N-CA	-8.25	1.33	1.45
1	A	377	MET	C-N	-8.24	1.20	1.33
2	B	248	LEU	C-N	-8.20	1.21	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
1	A	66	VAL	N-CA	8.15	1.56	1.46
2	B	238	VAL	C-N	8.10	1.45	1.33
2	B	346	TRP	CA-C	-8.08	1.41	1.53
2	B	225	GLY	C-N	-8.03	1.22	1.34
1	A	166	LYS	CA-C	-7.99	1.42	1.52
2	B	7	ILE	C-N	-7.97	1.23	1.33
1	A	102	ASN	C-N	-7.95	1.22	1.33
1	A	266	HIS	N-CA	-7.94	1.35	1.45
2	B	4	ILE	CA-CB	-7.86	1.44	1.54
2	B	407	TRP	CA-CB	-7.84	1.40	1.53
1	A	194	THR	C-N	-7.82	1.23	1.33
1	A	295	CYS	C-N	-7.81	1.23	1.34
1	A	184	PRO	CA-C	-7.76	1.42	1.52
2	B	53	TYR	N-CA	-7.71	1.36	1.46
2	B	5	VAL	CA-C	-7.68	1.43	1.52
2	B	1	MET	CA-C	-7.66	1.36	1.52
2	B	39	ASP	C-N	-7.65	1.23	1.33
2	B	118	VAL	C-N	-7.65	1.24	1.33
2	B	1	MET	C-N	7.63	1.44	1.33
1	A	19	ALA	C-O	-7.61	1.15	1.24
1	A	1	MET	CA-C	-7.58	1.37	1.52
1	A	265	GLY	CA-C	-7.57	1.41	1.51
1	A	374	ALA	C-N	7.57	1.43	1.33
2	B	344	VAL	N-CA	-7.56	1.36	1.46
2	B	343	PHE	CA-C	-7.54	1.44	1.52
1	A	24	TYR	C-O	7.53	1.32	1.24
1	A	98	ASP	N-CA	-7.51	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	ASP	C-N	-7.50	1.23	1.33
2	B	219	LEU	C-N	-7.50	1.23	1.33
1	A	23	LEU	C-N	-7.49	1.24	1.33
2	B	222	PRO	CA-C	-7.48	1.41	1.52
1	A	167	LEU	N-CA	-7.47	1.36	1.46
2	B	35	SER	C-N	-7.45	1.23	1.33
2	B	6	HIS	N-CA	-7.43	1.37	1.46
2	B	3	GLU	N-CA	-7.38	1.35	1.45
1	A	47	ASP	N-CA	-7.37	1.37	1.46
2	B	325	MET	C-N	-7.37	1.23	1.33
1	A	391	LEU	C-N	-7.35	1.24	1.33
1	A	263	PRO	CA-CB	-7.35	1.45	1.53
2	B	113	GLU	C-N	7.30	1.44	1.33
1	A	222	PRO	CB-CG	7.29	1.86	1.49
1	A	438	ASP	C-N	-7.28	1.24	1.34
1	A	228	ASN	C-N	-7.28	1.23	1.33
1	A	98	ASP	C-N	-7.25	1.24	1.33
2	B	276	THR	C-O	7.23	1.33	1.24
1	A	88	HIS	C-N	-7.21	1.24	1.33
2	B	256	ALA	C-N	-7.19	1.24	1.33
1	A	405	VAL	CB-CG2	7.18	1.76	1.52
1	A	32	PRO	CA-CB	-7.17	1.43	1.53
2	B	245	PRO	N-CD	-7.15	1.37	1.47
2	B	204	ILE	C-O	7.11	1.32	1.24
1	A	61	HIS	C-N	-7.09	1.25	1.33
1	A	267	PHE	N-CA	-7.07	1.36	1.45
2	B	138	THR	CA-C	-7.04	1.44	1.52
1	A	340	THR	C-N	-7.04	1.24	1.33
2	B	406	HIS	C-N	-7.03	1.24	1.33
1	A	111	GLY	CA-C	-7.03	1.44	1.52
2	B	111	GLY	CA-C	-7.03	1.44	1.52
2	B	345	GLU	CA-C	-7.00	1.43	1.52
2	B	223	THR	N-CA	-7.00	1.37	1.46
1	A	388	TRP	NE1-CE2	-7.00	1.29	1.37
2	B	261	PRO	CA-C	-6.99	1.42	1.52
2	B	53	TYR	CA-C	-6.98	1.43	1.52
2	B	44	LEU	C-N	6.97	1.43	1.33
2	B	300	ASN	C-O	-6.97	1.14	1.24
2	B	50	ASN	C-N	6.96	1.43	1.33
1	A	366	GLY	C-N	6.95	1.44	1.33
1	A	263	PRO	N-CA	-6.93	1.42	1.47
1	A	266	HIS	CA-C	-6.92	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	PHE	C-N	-6.92	1.24	1.33
1	A	93	ILE	C-N	-6.90	1.24	1.33
1	A	417	GLU	CA-C	-6.89	1.43	1.52
1	A	163	LYS	C-N	-6.88	1.21	1.33
2	B	43	GLN	C-N	-6.88	1.24	1.33
2	B	219	LEU	N-CA	6.86	1.55	1.46
2	B	20	PHE	C-N	-6.85	1.24	1.33
2	B	224	TYR	C-O	-6.85	1.16	1.24
2	B	62	VAL	CA-CB	-6.84	1.47	1.55
1	A	197	HIS	C-N	6.83	1.43	1.33
2	B	121	VAL	C-N	-6.80	1.25	1.33
1	A	64	ARG	C-N	-6.74	1.24	1.33
2	B	24	ILE	CA-CB	-6.67	1.47	1.55
1	A	272	TYR	CA-C	-6.66	1.44	1.52
2	B	192	HIS	C-N	-6.62	1.23	1.33
1	A	50	ASN	C-N	-6.62	1.24	1.33
2	B	435	TYR	CA-C	-6.60	1.44	1.52
2	B	332	MET	C-O	6.59	1.32	1.24
1	A	104	ALA	N-CA	-6.59	1.38	1.46
2	B	290	GLU	C-N	-6.57	1.24	1.33
1	A	232	GLY	C-N	-6.54	1.25	1.34
2	B	52	TYR	CA-C	-6.54	1.45	1.52
1	A	384	ILE	C-N	6.53	1.42	1.33
2	B	348	PRO	CA-C	-6.53	1.43	1.52
2	B	255	LEU	C-N	-6.50	1.23	1.33
1	A	407	TRP	CA-CB	-6.49	1.42	1.53
2	B	229	HIS	C-O	-6.49	1.15	1.24
1	A	202	PHE	C-N	-6.48	1.25	1.33
2	B	220	THR	C-N	6.46	1.39	1.33
1	A	268	PRO	C-N	-6.45	1.24	1.33
1	A	281	ALA	C-N	-6.45	1.24	1.33
2	B	219	LEU	CA-C	-6.44	1.44	1.52
2	B	436	GLN	N-CA	-6.42	1.38	1.46
1	A	181	VAL	C-O	6.41	1.32	1.24
2	B	40	SER	C-N	-6.39	1.24	1.33
1	A	434	GLU	C-O	6.39	1.32	1.24
2	B	244	PHE	C-N	-6.37	1.19	1.33
1	A	169	PHE	C-N	-6.37	1.24	1.33
1	A	85	GLN	C-N	-6.37	1.24	1.33
1	A	110	ILE	C-N	-6.35	1.25	1.33
2	B	185	TYR	N-CA	6.33	1.53	1.46
2	B	21	TRP	NE1-CE2	-6.32	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	358	ILE	C-N	-6.31	1.25	1.33
2	B	86	ILE	C-O	6.31	1.31	1.24
1	A	229	ARG	CD-NE	-6.31	1.37	1.46
1	A	40	LYS	CA-C	-6.29	1.47	1.53
2	B	110	GLU	C-N	-6.29	1.25	1.33
1	A	198	SER	C-N	-6.29	1.24	1.33
2	B	223	THR	CA-C	-6.27	1.44	1.52
2	B	51	VAL	CA-C	-6.26	1.45	1.52
1	A	42	ILE	C-N	-6.26	1.26	1.33
1	A	283	HIS	CE1-NE2	-6.23	1.26	1.32
1	A	324	VAL	CA-CB	-6.23	1.46	1.54
2	B	51	VAL	N-CA	-6.23	1.38	1.46
2	B	278	ARG	NE-CZ	-6.23	1.26	1.33
1	A	290	GLU	C-N	6.22	1.41	1.33
2	B	224	TYR	N-CA	-6.21	1.38	1.46
1	A	74	VAL	C-N	-6.21	1.26	1.33
1	A	300	ASN	CA-C	-6.21	1.44	1.52
1	A	2	ARG	C-N	-6.20	1.25	1.33
2	B	347	ILE	C-N	-6.17	1.19	1.33
1	A	21	TRP	NE1-CE2	-6.16	1.30	1.37
1	A	84	ARG	C-N	-6.13	1.25	1.33
2	B	29	GLY	C-N	-6.12	1.25	1.33
2	B	384	ILE	CA-CB	-6.09	1.46	1.54
2	B	230	LEU	N-CA	6.08	1.54	1.46
1	A	94	THR	CA-C	-6.08	1.45	1.53
1	A	348	PRO	CA-CB	-6.08	1.45	1.53
1	A	406	HIS	CE1-NE2	-6.06	1.26	1.32
2	B	229	HIS	CB-CG	6.04	1.58	1.50
1	A	97	GLU	C-N	-6.01	1.25	1.33
1	A	103	TYR	CA-C	-6.01	1.44	1.52
1	A	346	TRP	CA-CB	-5.97	1.45	1.53
2	B	217	LEU	C-N	-5.97	1.25	1.33
2	B	407	TRP	CA-C	-5.96	1.45	1.52
1	A	5	ILE	CA-CB	-5.96	1.47	1.54
1	A	35	GLN	C-N	-5.96	1.26	1.33
1	A	175	PRO	CA-CB	-5.94	1.45	1.53
1	A	389	ALA	C-N	-5.91	1.26	1.33
1	A	156	ARG	C-N	-5.90	1.25	1.33
1	A	65	ALA	C-O	-5.90	1.16	1.24
1	A	221	ARG	CA-C	-5.90	1.45	1.52
2	B	59	ASN	C-N	-5.89	1.25	1.33
1	A	416	GLY	CA-C	-5.89	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	351	VAL	CA-CB	-5.89	1.46	1.54
1	A	180	ALA	C-N	-5.87	1.26	1.34
2	B	303	ALA	C-N	5.85	1.42	1.33
1	A	411	GLU	C-O	5.84	1.31	1.24
1	A	405	VAL	CB-CG1	-5.80	1.33	1.52
1	A	39	ASP	N-CA	-5.79	1.38	1.46
2	B	173	PRO	CA-C	-5.78	1.44	1.52
1	A	386	GLU	C-N	5.75	1.41	1.34
2	B	422	GLU	C-N	-5.74	1.25	1.33
2	B	245	PRO	CA-CB	-5.73	1.45	1.53
2	B	17	GLY	C-N	-5.71	1.26	1.33
2	B	23	VAL	C-O	-5.69	1.17	1.24
2	B	385	GLN	C-O	-5.67	1.16	1.24
2	B	215	ARG	C-N	-5.66	1.26	1.33
1	A	346	TRP	NE1-CE2	-5.66	1.31	1.37
2	B	76	ASP	N-CA	-5.63	1.39	1.46
1	A	250	VAL	C-N	-5.63	1.25	1.33
2	B	122	VAL	C-N	-5.62	1.26	1.33
1	A	31	GLN	CA-C	5.61	1.59	1.52
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	347	CYS	C-O	-5.59	1.18	1.24
2	B	42	LEU	C-N	-5.58	1.25	1.33
1	A	359	PRO	C-O	-5.54	1.18	1.24
1	A	434	GLU	C-N	-5.54	1.27	1.34
2	B	246	GLY	N-CA	5.53	1.53	1.45
1	A	331	ALA	C-N	-5.52	1.27	1.34
2	B	100	GLY	CA-C	-5.51	1.46	1.51
1	A	97	GLU	CA-C	-5.51	1.45	1.52
2	B	148	GLY	C-N	5.50	1.42	1.33
2	B	262	PHE	C-N	-5.50	1.27	1.34
1	A	288	VAL	N-CA	-5.50	1.40	1.46
1	A	72	PRO	N-CD	-5.49	1.40	1.47
2	B	289	PRO	CA-CB	-5.48	1.46	1.53
2	B	84	GLY	C-N	-5.48	1.26	1.33
1	A	13	GLY	C-N	-5.48	1.27	1.34
2	B	139	HIS	CE1-NE2	-5.47	1.27	1.32
2	B	217	LEU	CA-C	-5.46	1.45	1.53
1	A	211	ASP	C-N	-5.46	1.27	1.34
1	A	313	MET	N-CA	-5.45	1.39	1.46
1	A	152	LEU	C-N	-5.45	1.25	1.33
1	A	262	TYR	C-N	-5.45	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	313	LEU	C-N	-5.44	1.26	1.33
1	A	261	PRO	CA-CB	-5.44	1.46	1.53
1	A	301	GLN	N-CA	-5.42	1.39	1.46
1	A	407	TRP	NE1-CE2	-5.42	1.31	1.37
2	B	257	VAL	C-N	-5.42	1.26	1.33
2	B	332	MET	C-N	-5.41	1.26	1.33
1	A	103	TYR	N-CA	-5.41	1.39	1.46
2	B	135	PHE	C-N	-5.41	1.26	1.33
1	A	360	PRO	N-CD	-5.41	1.40	1.47
1	A	422	ARG	C-N	-5.40	1.26	1.33
1	A	169	PHE	N-CA	-5.40	1.39	1.45
2	B	19	LYS	C-N	-5.39	1.27	1.33
1	A	312	TYR	C-N	-5.39	1.26	1.33
2	B	262	PHE	N-CA	-5.39	1.38	1.46
2	B	72	PRO	C-O	5.38	1.30	1.24
2	B	35	SER	CA-C	-5.38	1.47	1.52
2	B	189	LEU	C-N	-5.37	1.27	1.33
1	A	339	ARG	C-N	-5.36	1.24	1.33
1	A	32	PRO	C-O	5.36	1.30	1.24
1	A	283	HIS	C-O	5.35	1.30	1.24
2	B	346	TRP	NE1-CE2	-5.35	1.31	1.37
1	A	400	ALA	C-N	-5.35	1.26	1.33
1	A	282	TYR	N-CA	-5.34	1.39	1.46
1	A	201	ALA	C-N	-5.34	1.26	1.33
2	B	354	ALA	C-N	-5.33	1.26	1.33
2	B	346	TRP	CA-CB	-5.32	1.44	1.53
1	A	46	ASP	N-CA	-5.32	1.39	1.46
2	B	374	SER	C-N	-5.32	1.26	1.33
1	A	286	LEU	C-N	-5.31	1.26	1.33
2	B	18	ALA	N-CA	-5.31	1.40	1.46
1	A	177	VAL	C-N	-5.30	1.26	1.33
2	B	138	THR	C-N	-5.30	1.26	1.33
1	A	4	CYS	C-N	-5.29	1.26	1.33
1	A	253	THR	C-N	-5.29	1.25	1.33
2	B	345	GLU	C-N	-5.29	1.25	1.33
1	A	70	LEU	C-N	-5.28	1.27	1.33
2	B	261	PRO	CA-CB	-5.27	1.46	1.53
1	A	248	LEU	C-N	-5.26	1.26	1.33
2	B	32	PRO	C-N	-5.25	1.26	1.33
2	B	266	HIS	CE1-NE2	-5.25	1.27	1.32
2	B	92	PHE	C-O	-5.24	1.17	1.24
1	A	341	ILE	C-O	-5.23	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	139	HIS	N-CA	-5.22	1.40	1.46
2	B	212	ILE	CA-CB	-5.21	1.48	1.54
2	B	178	SER	C-O	5.21	1.30	1.23
2	B	32	PRO	N-CA	-5.20	1.40	1.47
2	B	216	THR	C-N	-5.20	1.25	1.33
1	A	274	PRO	CA-C	-5.18	1.47	1.52
2	B	39	ASP	CA-C	-5.18	1.45	1.52
1	A	122	ILE	C-N	-5.17	1.27	1.33
2	B	253	ARG	CD-NE	-5.17	1.39	1.46
2	B	26	ASP	C-N	5.16	1.41	1.33
1	A	86	LEU	N-CA	-5.15	1.39	1.46
2	B	21	TRP	N-CA	-5.15	1.39	1.46
2	B	63	PRO	CA-C	-5.15	1.45	1.52
2	B	101	ASN	N-CA	-5.14	1.39	1.46
1	A	33	ASP	CA-CB	-5.14	1.44	1.53
2	B	59	ASN	CA-C	5.13	1.58	1.52
2	B	74	THR	C-N	-5.13	1.26	1.33
2	B	184	PRO	N-CA	-5.13	1.40	1.47
2	B	57	ALA	C-N	-5.13	1.26	1.33
1	A	8	HIS	CD2-NE2	-5.10	1.32	1.37
1	A	199	ASP	C-N	-5.10	1.26	1.33
2	B	258	ASN	N-CA	-5.10	1.39	1.46
1	A	64	ARG	C-O	-5.09	1.17	1.24
1	A	105	ARG	C-N	-5.09	1.25	1.33
2	B	211	ASP	C-O	-5.09	1.18	1.24
2	B	343	PHE	CA-CB	-5.09	1.44	1.53
2	B	373	MET	C-N	5.09	1.40	1.33
1	A	3	GLU	C-N	-5.09	1.26	1.33
1	A	67	PHE	C-N	5.09	1.39	1.33
1	A	281	ALA	CA-C	-5.08	1.46	1.52
2	B	272	PHE	CA-C	-5.08	1.46	1.52
1	A	71	GLU	CA-C	5.08	1.58	1.52
1	A	192	HIS	CE1-NE2	-5.08	1.27	1.32
2	B	307	PRO	C-N	-5.08	1.27	1.33
2	B	407	TRP	NE1-CE2	-5.07	1.31	1.37
2	B	16	ILE	C-O	-5.07	1.17	1.24
1	A	392	ASP	C-O	-5.06	1.18	1.24
1	A	268	PRO	CA-C	-5.06	1.45	1.52
1	A	266	HIS	CE1-NE2	-5.06	1.27	1.32
1	A	363	VAL	C-N	5.06	1.45	1.33
1	A	168	GLU	CA-C	-5.05	1.46	1.52
2	B	309	HIS	CD2-NE2	-5.05	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	139	HIS	CG-CD2	-5.04	1.30	1.35
2	B	183	GLU	C-N	-5.04	1.27	1.34
2	B	14	ASN	CA-C	-5.04	1.46	1.52
1	A	382	THR	C-N	-5.01	1.27	1.33
1	A	301	GLN	C-N	-5.01	1.27	1.33
1	A	312	TYR	CA-C	-5.01	1.46	1.52
1	A	343	PHE	N-CA	-5.01	1.39	1.46
1	A	361	THR	C-N	-5.00	1.30	1.33

All (668) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	O-C-N	-65.10	36.00	122.59
2	B	105	LYS	O-C-N	-56.44	47.53	122.59
2	B	73	GLY	O-C-N	-47.20	76.40	122.19
1	A	283	HIS	O-C-N	-41.55	67.32	122.59
2	B	275	LEU	O-C-N	-39.64	79.28	122.09
1	A	369	ALA	O-C-N	-39.52	70.03	122.59
1	A	415	GLU	CA-C-N	30.99	145.47	121.61
1	A	415	GLU	C-N-CA	30.99	145.47	121.61
2	B	321	GLY	O-C-N	-30.02	83.67	122.70
1	A	24	TYR	O-C-N	-30.01	89.62	122.03
2	B	194	LEU	O-C-N	-29.23	87.62	122.11
2	B	143	GLY	O-C-N	-28.22	79.56	122.18
1	A	363	VAL	C-N-CD	-27.19	13.51	125.00
2	B	179	ASP	O-C-N	-26.90	86.81	122.59
2	B	344	VAL	O-C-N	-26.90	88.95	122.57
1	A	221	ARG	CA-C-N	26.45	149.49	120.66
1	A	221	ARG	C-N-CA	26.45	149.49	120.66
1	A	1	MET	O-C-N	26.05	164.69	123.00
2	B	273	ALA	C-N-CD	-26.01	18.35	125.00
1	A	53	PHE	O-C-N	-25.90	88.14	122.59
2	B	321	GLY	CA-C-N	25.83	170.87	121.54
2	B	321	GLY	C-N-CA	25.83	170.87	121.54
1	A	218	ASP	O-C-N	-25.64	93.52	123.27
2	B	86	ILE	O-C-N	25.59	154.55	122.57
2	B	60	LYS	CA-C-N	24.92	169.14	121.54
2	B	60	LYS	C-N-CA	24.92	169.14	121.54
2	B	179	ASP	CA-C-N	24.86	161.27	122.24
2	B	179	ASP	C-N-CA	24.86	161.27	122.24
2	B	88	ARG	C-N-CD	-24.72	23.65	125.00
1	A	402	ARG	O-C-N	-24.29	78.24	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	247	GLN	O-C-N	-24.17	95.13	123.16
2	B	402	LYS	CA-C-N	23.96	167.30	121.54
2	B	402	LYS	C-N-CA	23.96	167.30	121.54
2	B	85	GLN	O-C-N	23.93	157.13	122.20
2	B	203	CYS	CA-C-N	23.57	164.40	121.97
2	B	203	CYS	C-N-CA	23.57	164.40	121.97
2	B	194	LEU	CA-C-N	23.46	163.94	121.70
2	B	194	LEU	C-N-CA	23.46	163.94	121.70
2	B	348	PRO	O-C-N	23.21	153.98	122.64
2	B	278	ARG	N-CA-CB	23.08	148.96	109.72
2	B	52	TYR	O-C-N	22.75	152.45	123.10
2	B	105	LYS	CA-C-N	21.61	147.15	120.14
2	B	105	LYS	C-N-CA	21.61	147.15	120.14
1	A	34	GLY	O-C-N	-20.83	95.61	122.70
2	B	1	MET	O-C-N	20.78	156.25	123.00
1	A	405	VAL	CA-C-N	20.77	157.65	121.52
1	A	405	VAL	C-N-CA	20.77	157.65	121.52
1	A	36	MET	CA-C-N	20.66	142.58	120.47
1	A	36	MET	C-N-CA	20.66	142.58	120.47
1	A	183	GLU	O-C-N	-20.49	97.76	121.32
2	B	127	GLU	O-C-N	-20.36	95.93	122.39
2	B	21	TRP	O-C-N	-20.26	95.99	122.33
2	B	60	LYS	O-C-N	-20.15	95.79	122.59
2	B	359	PRO	O-C-N	19.89	144.93	121.46
2	B	92	PHE	CA-CB-CG	-19.78	94.02	113.80
2	B	73	GLY	CA-C-N	19.54	153.90	120.68
2	B	73	GLY	C-N-CA	19.54	153.90	120.68
2	B	411	GLU	CA-C-N	19.27	159.19	121.41
2	B	411	GLU	C-N-CA	19.27	159.19	121.41
1	A	347	CYS	O-C-N	-19.20	97.48	121.10
2	B	53	TYR	O-C-N	19.01	147.88	122.59
1	A	87	PHE	O-C-N	-18.95	97.59	122.42
1	A	358	GLU	CA-C-N	18.70	139.64	120.38
1	A	358	GLU	C-N-CA	18.70	139.64	120.38
1	A	415	GLU	O-C-N	-18.57	103.92	121.56
2	B	344	VAL	CA-C-N	18.52	156.91	121.54
2	B	344	VAL	C-N-CA	18.52	156.91	121.54
2	B	30	ILE	CB-CA-C	18.43	141.52	111.29
1	A	67	PHE	CA-CB-CG	-18.21	95.59	113.80
1	A	367	ASP	O-C-N	-18.07	93.33	122.42
1	A	283	HIS	CA-C-N	17.72	155.38	121.54
1	A	283	HIS	C-N-CA	17.72	155.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	CB-CA-C	17.67	143.67	110.10
1	A	38	SER	O-C-N	-17.57	102.12	122.68
1	A	38	SER	CA-C-N	17.39	154.75	121.54
1	A	38	SER	C-N-CA	17.39	154.75	121.54
1	A	221	ARG	O-C-N	-17.09	101.67	121.32
1	A	50	ASN	O-C-N	-16.89	100.12	122.59
2	B	343	PHE	O-C-N	16.78	146.33	123.34
1	A	409	VAL	O-C-N	16.68	138.62	121.94
2	B	370	GLY	O-C-N	-16.64	101.69	122.32
1	A	266	HIS	O-C-N	16.63	143.70	123.24
1	A	297	GLU	CA-C-N	-16.53	99.17	119.84
1	A	297	GLU	C-N-CA	-16.53	99.17	119.84
2	B	247	GLN	CA-C-N	16.52	153.09	121.54
2	B	247	GLN	C-N-CA	16.52	153.09	121.54
1	A	347	CYS	CA-C-N	16.41	140.35	119.84
1	A	347	CYS	C-N-CA	16.41	140.35	119.84
1	A	405	VAL	CA-CB-CG1	16.34	138.19	110.40
2	B	1	MET	CB-CA-C	16.08	140.65	110.10
2	B	49	ILE	O-C-N	-16.05	107.47	123.03
2	B	347	ILE	CA-C-N	15.94	139.77	119.84
2	B	347	ILE	C-N-CA	15.94	139.77	119.84
1	A	218	ASP	CA-C-N	15.94	150.66	121.97
1	A	218	ASP	C-N-CA	15.94	150.66	121.97
2	B	171	VAL	O-C-N	-15.87	106.02	123.00
2	B	331	GLN	O-C-N	-15.71	99.19	122.28
2	B	411	GLU	O-C-N	-15.70	101.29	122.33
2	B	224	TYR	O-C-N	-15.67	104.29	122.15
1	A	184	PRO	O-C-N	15.66	141.89	123.10
2	B	400	ARG	O-C-N	-15.58	101.45	122.33
2	B	91	ASN	CA-CB-CG	15.43	128.03	112.60
2	B	402	LYS	O-C-N	-15.37	101.47	122.06
2	B	203	CYS	O-C-N	-15.16	103.48	123.19
1	A	392	ASP	CA-C-O	-15.14	104.37	120.42
1	A	69	ASP	O-C-N	-15.11	105.74	123.27
1	A	358	GLU	C-N-CD	-15.04	63.33	125.00
1	A	1	MET	CA-C-N	14.71	149.48	122.27
1	A	1	MET	C-N-CA	14.71	149.48	122.27
1	A	139	HIS	CA-CB-CG	14.63	128.43	113.80
2	B	400	ARG	CA-C-N	14.62	149.46	121.54
2	B	400	ARG	C-N-CA	14.62	149.46	121.54
2	B	30	ILE	O-C-N	-14.44	104.52	122.57
2	B	47	GLU	CA-C-N	14.41	149.06	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	GLU	C-N-CA	14.41	149.06	121.54
1	A	107	HIS	O-C-N	-14.41	106.47	122.03
2	B	107	HIS	O-C-N	-14.41	106.47	122.03
2	B	24	ILE	O-C-N	-14.37	109.19	121.98
2	B	1	MET	N-CA-C	-14.27	71.04	111.00
2	B	89	PRO	O-C-N	-14.24	103.42	122.64
2	B	406	HIS	CA-CB-CG	-13.98	99.82	113.80
1	A	41	THR	O-C-N	13.89	141.63	122.46
1	A	219	ILE	CA-CB-CG2	-13.85	86.96	110.50
1	A	416	GLY	O-C-N	-13.82	111.21	123.37
1	A	355	ILE	CA-C-O	-13.82	105.83	120.48
1	A	280	LYS	O-C-N	-13.81	104.22	122.59
2	B	253	ARG	CD-NE-CZ	13.80	143.72	124.40
1	A	183	GLU	CA-C-N	-13.79	105.97	119.76
1	A	183	GLU	C-N-CA	-13.79	105.97	119.76
1	A	42	ILE	CA-C-N	13.69	134.86	119.94
1	A	42	ILE	C-N-CA	13.69	134.86	119.94
1	A	297	GLU	O-C-N	13.48	136.83	121.32
1	A	280	LYS	CA-C-N	13.47	147.26	121.54
1	A	280	LYS	C-N-CA	13.47	147.26	121.54
1	A	179	THR	O-C-N	-13.42	104.75	122.59
1	A	412	GLY	O-C-N	-13.42	109.12	124.15
2	B	177	VAL	CA-C-O	13.37	137.49	120.78
1	A	396	ASP	O-C-N	-13.30	105.03	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	13.06	145.48	121.97
2	B	85	GLN	C-N-CA	13.06	145.48	121.97
1	A	405	VAL	O-C-N	-13.00	106.65	122.77
2	B	200	GLU	CA-C-N	12.98	142.37	121.86
2	B	200	GLU	C-N-CA	12.98	142.37	121.86
2	B	182	VAL	CA-C-N	12.96	153.43	121.80
2	B	182	VAL	C-N-CA	12.96	153.43	121.80
1	A	21	TRP	CA-CB-CG	-12.90	89.08	113.60
2	B	113	GLU	CA-C-O	12.60	133.91	120.55
2	B	182	VAL	O-C-N	-12.59	106.83	122.57
1	A	1	MET	N-CA-C	-12.55	75.86	111.00
2	B	52	TYR	CA-C-N	12.49	145.40	121.54
2	B	52	TYR	C-N-CA	12.49	145.40	121.54
2	B	275	LEU	CA-C-N	12.30	145.04	121.54
2	B	275	LEU	C-N-CA	12.30	145.04	121.54
2	B	289	PRO	O-C-N	12.30	138.73	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	GLY	CA-C-N	12.30	145.03	121.54
1	A	416	GLY	C-N-CA	12.30	145.03	121.54
2	B	414	ASP	CA-C-N	12.30	145.03	121.54
2	B	414	ASP	C-N-CA	12.30	145.03	121.54
1	A	113	GLU	CA-C-O	12.22	133.91	120.10
2	B	192	HIS	O-C-N	-12.16	105.67	122.46
1	A	30	ILE	CA-C-N	12.14	151.43	121.80
1	A	30	ILE	C-N-CA	12.14	151.43	121.80
2	B	127	GLU	CA-C-N	12.12	145.17	121.18
2	B	127	GLU	C-N-CA	12.12	145.17	121.18
2	B	154	ILE	CA-C-N	12.09	136.88	120.44
2	B	154	ILE	C-N-CA	12.09	136.88	120.44
2	B	414	ASP	O-C-N	-12.01	109.01	123.30
1	A	43	GLY	O-C-N	11.97	133.68	122.19
2	B	29	GLY	O-C-N	11.94	138.22	122.70
1	A	15	GLN	OE1-CD-NE2	-11.93	110.67	122.60
1	A	369	ALA	CA-C-N	11.90	141.97	123.04
1	A	369	ALA	C-N-CA	11.90	141.97	123.04
2	B	193	GLN	CA-C-N	11.86	138.67	120.89
2	B	193	GLN	C-N-CA	11.86	138.67	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	-11.80	110.80	122.60
2	B	49	ILE	CA-C-N	11.80	144.07	121.54
2	B	49	ILE	C-N-CA	11.80	144.07	121.54
1	A	32	PRO	CA-N-CD	11.77	128.48	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
1	A	87	PHE	CA-C-N	11.69	150.33	121.80
1	A	87	PHE	C-N-CA	11.69	150.33	121.80
2	B	11	GLN	OE1-CD-NE2	-11.69	110.91	122.60
2	B	29	GLY	CA-C-N	11.67	142.97	121.97
2	B	29	GLY	C-N-CA	11.67	142.97	121.97
2	B	281	GLN	OE1-CD-NE2	-11.60	111.00	122.60
1	A	2	ARG	CB-CA-C	-11.59	96.56	111.50
1	A	61	HIS	CA-CB-CG	11.53	125.33	113.80
2	B	219	LEU	O-C-N	-11.50	107.29	122.59
1	A	193	THR	O-C-N	-11.43	107.39	122.59
2	B	4	ILE	N-CA-C	11.39	123.39	108.35
2	B	200	GLU	O-C-N	-11.37	108.37	123.15
1	A	111	GLY	CA-C-O	-11.29	109.12	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	111	GLY	CA-C-O	-11.29	109.12	120.75
1	A	21	TRP	O-C-N	-11.25	108.43	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	167	ASN	CA-C-N	-11.16	107.26	122.99
2	B	167	ASN	C-N-CA	-11.16	107.26	122.99
1	A	186	ASN	CA-C-N	11.14	134.92	120.44
1	A	186	ASN	C-N-CA	11.14	134.92	120.44
2	B	178	SER	CA-C-O	-11.13	108.52	120.99
2	B	412	GLY	CA-C-N	11.13	138.86	122.39
2	B	412	GLY	C-N-CA	11.13	138.86	122.39
2	B	21	TRP	CA-C-N	-11.02	102.44	122.38
2	B	21	TRP	C-N-CA	-11.02	102.44	122.38
2	B	359	PRO	CA-C-N	-10.99	106.11	119.84
2	B	359	PRO	C-N-CA	-10.99	106.11	119.84
2	B	433	GLN	OE1-CD-NE2	-10.98	111.62	122.60
2	B	278	ARG	CB-CA-C	-10.92	92.71	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	-10.76	111.84	122.60
2	B	193	GLN	O-C-N	-10.72	107.77	122.46
2	B	356	CYS	O-C-N	-10.65	107.42	122.76
2	B	15	GLN	OE1-CD-NE2	-10.52	112.08	122.60
2	B	385	GLN	OE1-CD-NE2	-10.51	112.09	122.60
2	B	89	PRO	CA-C-N	10.51	141.61	121.54
2	B	89	PRO	C-N-CA	10.51	141.61	121.54
1	A	17	GLY	O-C-N	10.49	133.71	122.28
2	B	290	GLU	O-C-N	10.48	134.10	122.15
1	A	113	GLU	O-C-N	-10.46	109.98	122.22
1	A	267	PHE	C-N-CD	-10.44	82.21	125.00
1	A	15	GLN	O-C-N	10.41	134.77	122.17
2	B	59	ASN	CA-C-N	10.41	141.43	121.54
2	B	59	ASN	C-N-CA	10.41	141.43	121.54
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	299	LYS	O-C-N	10.34	135.27	122.34
1	A	412	GLY	CA-C-N	10.33	137.15	120.94
1	A	412	GLY	C-N-CA	10.33	137.15	120.94
1	A	274	PRO	O-C-N	-10.32	112.92	122.93
2	B	394	GLN	OE1-CD-NE2	-10.28	112.32	122.60
1	A	172	TYR	CA-CB-CG	10.24	132.32	113.90
1	A	65	ALA	N-CA-C	10.18	132.48	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	85	GLN	OE1-CD-NE2	-10.13	112.47	122.60
1	A	92	LEU	CA-C-N	10.10	135.72	123.19
1	A	92	LEU	C-N-CA	10.10	135.72	123.19
2	B	161	TYR	CA-C-N	10.07	129.71	119.24
2	B	161	TYR	C-N-CA	10.07	129.71	119.24
1	A	18	ASN	O-C-N	10.05	134.64	122.27
2	B	47	GLU	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	9.99	134.93	123.05
2	B	229	HIS	O-C-N	-9.99	109.31	122.59
2	B	331	GLN	CA-C-N	9.96	136.67	120.63
2	B	331	GLN	C-N-CA	9.96	136.67	120.63
2	B	282	GLN	OE1-CD-NE2	-9.94	112.66	122.60
1	A	32	PRO	N-CA-CB	-9.88	92.87	103.25
2	B	94	PHE	CA-CB-CG	-9.88	103.92	113.80
1	A	61	HIS	CB-CA-C	9.83	129.54	110.67
1	A	31	GLN	N-CA-C	9.75	131.35	109.81
2	B	8	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	A	298	PRO	CA-C-N	9.71	133.64	120.44
1	A	298	PRO	C-N-CA	9.71	133.64	120.44
1	A	190	THR	O-C-N	-9.66	109.39	122.33
1	A	78	VAL	O-C-N	-9.64	112.16	121.90
1	A	34	GLY	CA-C-N	9.63	139.94	121.54
1	A	34	GLY	C-N-CA	9.63	139.94	121.54
1	A	222	PRO	N-CA-CB	9.54	113.63	102.85
2	B	157	ILE	CA-C-O	-9.47	110.24	120.47
1	A	339	ARG	O-C-N	9.43	134.50	122.23
1	A	396	ASP	N-CA-C	-9.42	100.09	112.34
2	B	185	TYR	CA-CB-CG	9.41	130.85	113.90
2	B	412	GLY	O-C-N	-9.39	110.49	122.70
2	B	299	LYS	CA-C-N	-9.37	107.95	122.37
2	B	299	LYS	C-N-CA	-9.37	107.95	122.37
1	A	35	GLN	OE1-CD-NE2	-9.35	113.25	122.60
1	A	42	ILE	CA-C-O	-9.31	109.14	120.78
2	B	151	THR	O-C-N	-9.31	110.82	122.27
1	A	91	GLN	OE1-CD-NE2	-9.29	113.31	122.60
2	B	71	GLU	O-C-N	-9.28	110.65	121.32
2	B	72	PRO	CA-C-N	9.24	130.16	120.00
2	B	72	PRO	C-N-CA	9.24	130.16	120.00
2	B	24	ILE	CA-C-N	-9.14	104.09	121.54
2	B	24	ILE	C-N-CA	-9.14	104.09	121.54
1	A	172	TYR	CB-CA-C	9.13	122.58	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	THR	CA-C-N	9.12	138.95	121.54
2	B	276	THR	C-N-CA	9.12	138.95	121.54
1	A	36	MET	O-C-N	-9.10	114.73	121.83
1	A	90	GLU	O-C-N	-9.10	107.38	122.03
1	A	405	VAL	N-CA-CB	-9.07	100.15	111.31
1	A	372	GLN	OE1-CD-NE2	-9.06	113.54	122.60
2	B	273	ALA	CA-C-N	9.06	131.17	119.84
2	B	273	ALA	C-N-CA	9.06	131.17	119.84
1	A	298	PRO	O-C-N	-9.04	110.43	122.64
1	A	417	GLU	O-C-N	8.99	134.55	122.59
1	A	368	LEU	CA-C-N	8.97	138.68	121.54
1	A	368	LEU	C-N-CA	8.97	138.68	121.54
1	A	62	VAL	O-C-N	8.92	131.27	121.10
2	B	2	ARG	O-C-N	8.92	134.45	122.59
2	B	417	GLU	CA-C-N	8.89	135.86	122.17
2	B	417	GLU	C-N-CA	8.89	135.86	122.17
2	B	340	SER	CA-C-N	-8.88	104.59	121.54
2	B	340	SER	C-N-CA	-8.88	104.59	121.54
2	B	53	TYR	N-CA-CB	8.86	125.47	110.49
2	B	270	PRO	CA-C-N	8.86	129.19	121.58
2	B	270	PRO	C-N-CA	8.86	129.19	121.58
2	B	1	MET	CA-C-N	8.82	138.38	121.54
2	B	1	MET	C-N-CA	8.82	138.38	121.54
1	A	56	THR	CA-C-N	-8.74	104.28	121.41
1	A	56	THR	C-N-CA	-8.74	104.28	121.41
2	B	133	GLN	OE1-CD-NE2	-8.71	113.89	122.60
1	A	203	MET	O-C-N	8.70	133.69	123.17
2	B	348	PRO	CA-C-N	8.68	138.13	121.54
2	B	348	PRO	C-N-CA	8.68	138.13	121.54
1	A	371	VAL	O-C-N	8.61	132.82	122.83
1	A	391	LEU	CA-C-N	8.57	132.46	120.29
1	A	391	LEU	C-N-CA	8.57	132.46	120.29
1	A	38	SER	CA-C-O	-8.55	111.89	121.89
2	B	433	GLN	O-C-N	8.53	132.20	122.22
2	B	434	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	A	275	VAL	O-C-N	8.39	133.06	122.57
1	A	195	LEU	CA-C-O	-8.34	109.12	119.38
1	A	72	PRO	O-C-N	8.33	133.51	122.27
2	B	272	PHE	CA-C-O	-8.33	111.41	120.24
1	A	31	GLN	O-C-N	8.30	130.87	121.32
2	B	234	THR	CA-C-O	-8.30	110.42	119.97
2	B	183	GLU	CA-C-N	8.26	128.22	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	183	GLU	C-N-CA	8.26	128.22	119.05
1	A	347	CYS	C-N-CD	-8.23	91.24	125.00
1	A	182	VAL	CA-C-O	-8.23	109.64	119.85
2	B	143	GLY	CA-C-N	8.21	137.51	121.41
2	B	143	GLY	C-N-CA	8.21	137.51	121.41
1	A	18	ASN	CA-C-O	-8.21	110.53	119.97
2	B	32	PRO	O-C-N	8.17	133.67	122.64
1	A	290	GLU	O-C-N	8.16	133.37	122.43
1	A	56	THR	O-C-N	8.15	131.75	122.22
1	A	295	CYS	N-CA-C	8.03	120.82	111.02
2	B	59	ASN	O-C-N	-8.02	112.72	123.15
2	B	436	GLN	O-C-N	-8.01	111.94	122.59
1	A	31	GLN	CA-C-N	7.99	129.83	119.84
1	A	31	GLN	C-N-CA	7.99	129.83	119.84
1	A	197	HIS	O-C-N	7.98	133.21	122.59
2	B	289	PRO	CA-C-N	-7.97	108.97	120.29
2	B	289	PRO	C-N-CA	-7.97	108.97	120.29
2	B	247	GLN	OE1-CD-NE2	-7.94	114.66	122.60
2	B	50	ASN	CA-C-O	7.93	131.84	120.51
2	B	281	GLN	O-C-N	-7.92	112.06	122.59
2	B	113	GLU	O-C-N	-7.90	113.75	122.12
2	B	343	PHE	CA-CB-CG	-7.84	105.96	113.80
2	B	266	HIS	CA-CB-CG	-7.83	105.97	113.80
1	A	33	ASP	CA-C-N	-7.81	106.09	121.41
1	A	33	ASP	C-N-CA	-7.81	106.09	121.41
1	A	82	THR	CA-C-N	7.80	136.44	121.54
1	A	82	THR	C-N-CA	7.80	136.44	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	177	VAL	O-C-N	-7.78	112.85	122.57
2	B	299	LYS	CA-C-O	-7.74	110.30	119.35
1	A	90	GLU	CA-C-N	7.73	135.64	122.26
1	A	90	GLU	C-N-CA	7.73	135.64	122.26
2	B	154	ILE	O-C-N	-7.73	113.87	121.83
2	B	245	PRO	CA-N-CD	7.70	122.78	112.00
2	B	283	TYR	CA-C-N	7.68	136.22	121.54
2	B	283	TYR	C-N-CA	7.68	136.22	121.54
2	B	346	TRP	O-C-N	7.68	131.54	122.94
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
1	A	11	GLN	CG-CD-NE2	7.63	127.85	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	TYR	O-C-N	-7.62	112.45	122.59
1	A	50	ASN	CA-C-N	7.59	136.04	121.54
1	A	50	ASN	C-N-CA	7.59	136.04	121.54
2	B	281	GLN	CG-CD-NE2	7.55	127.73	116.40
2	B	85	GLN	CG-CD-NE2	7.55	127.73	116.40
1	A	402	ARG	CA-C-N	7.54	133.89	122.65
1	A	402	ARG	C-N-CA	7.54	133.89	122.65
2	B	260	VAL	O-C-N	7.53	128.46	121.61
1	A	21	TRP	CA-C-N	7.51	130.96	120.29
1	A	21	TRP	C-N-CA	7.51	130.96	120.29
2	B	407	TRP	CA-CB-CG	-7.50	99.35	113.60
1	A	184	PRO	N-CA-C	7.48	122.94	111.19
2	B	324	SER	O-C-N	7.47	132.22	122.95
1	A	17	GLY	CA-C-N	-7.45	108.98	120.31
1	A	17	GLY	C-N-CA	-7.45	108.98	120.31
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	-7.34	98.65	108.11
2	B	5	VAL	N-CA-C	7.34	118.23	107.37
2	B	385	GLN	CG-CD-NE2	7.33	127.40	116.40
1	A	15	GLN	CG-CD-NE2	7.33	127.39	116.40
1	A	62	VAL	CA-C-N	7.30	128.96	119.84
1	A	62	VAL	C-N-CA	7.30	128.96	119.84
2	B	224	TYR	N-CA-C	-7.29	103.41	111.36
1	A	232	GLY	O-C-N	7.27	129.17	122.19
2	B	60	LYS	CA-C-O	7.27	130.90	120.51
2	B	284	ARG	NE-CZ-NH2	7.26	125.73	119.20
1	A	91	GLN	CG-CD-NE2	7.24	127.26	116.40
1	A	343	PHE	O-C-N	7.18	131.65	122.81
1	A	32	PRO	N-CD-CG	-7.18	92.43	103.20
1	A	83	TYR	CA-CB-CG	-7.16	101.01	113.90
2	B	86	ILE	CA-C-N	7.16	135.22	121.54
2	B	86	ILE	C-N-CA	7.16	135.22	121.54
2	B	263	PRO	CB-CA-C	-7.15	101.82	112.55
1	A	82	THR	O-C-N	7.14	132.09	122.59
2	B	346	TRP	N-CA-CB	7.14	121.88	110.46
2	B	31	ASP	O-C-N	-7.14	113.11	121.32
2	B	373	MET	O-C-N	-7.11	115.09	123.41
1	A	267	PHE	O-C-N	-7.10	112.11	121.34
2	B	433	GLN	CG-CD-NE2	7.08	127.03	116.40
1	A	65	ALA	CB-CA-C	-7.08	96.32	110.42
2	B	282	GLN	CG-CD-NE2	7.08	127.02	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	SER	O-C-N	7.06	133.04	122.94
1	A	97	GLU	O-C-N	7.05	131.16	122.34
2	B	243	ARG	O-C-N	7.04	132.63	122.28
2	B	4	ILE	O-C-N	7.03	131.25	123.09
2	B	271	GLY	O-C-N	6.98	129.77	123.42
1	A	71	GLU	O-C-N	-6.97	116.39	121.83
2	B	293	GLN	CG-CD-NE2	6.97	126.85	116.40
2	B	347	ILE	C-N-CD	-6.95	96.50	125.00
1	A	438	ASP	O-C-N	-6.94	114.80	122.92
1	A	373	ARG	CD-NE-CZ	6.94	134.11	124.40
2	B	349	ASN	N-CA-C	-6.93	96.03	110.80
1	A	92	LEU	O-C-N	-6.92	115.14	123.16
1	A	88	HIS	CA-CB-CG	-6.89	106.91	113.80
1	A	379	SER	O-C-N	6.89	131.26	123.27
2	B	349	ASN	CB-CA-C	6.89	124.12	110.42
2	B	264	ARG	NE-CZ-NH2	6.88	125.40	119.20
2	B	269	MET	C-N-CD	-6.88	96.80	125.00
2	B	17	GLY	O-C-N	6.87	129.77	122.28
2	B	30	ILE	N-CA-CB	-6.82	99.99	111.23
1	A	85	GLN	CA-C-N	-6.81	110.50	122.07
1	A	85	GLN	C-N-CA	-6.81	110.50	122.07
2	B	75	MET	CA-C-N	6.80	129.40	120.28
2	B	75	MET	C-N-CA	6.80	129.40	120.28
2	B	43	GLN	O-C-N	6.80	131.64	122.59
2	B	356	CYS	CA-C-O	-6.75	112.62	121.73
1	A	112	LYS	CA-C-O	6.72	128.10	120.90
2	B	112	ALA	CA-C-O	6.72	128.10	120.90
2	B	269	MET	CA-C-O	-6.72	111.97	120.04
1	A	229	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	A	360	PRO	CA-C-N	-6.72	108.43	121.06
1	A	360	PRO	C-N-CA	-6.72	108.43	121.06
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	311	ARG	NE-CZ-NH2	6.70	125.23	119.20
1	A	438	ASP	CA-C-O	-6.68	114.28	121.36
2	B	190	SER	CA-C-N	-6.68	109.94	121.97
2	B	190	SER	C-N-CA	-6.68	109.94	121.97
2	B	314	THR	N-CA-CB	6.68	121.77	110.49
2	B	433	GLN	CA-C-N	-6.68	108.79	121.54
2	B	433	GLN	C-N-CA	-6.68	108.79	121.54
2	B	53	TYR	CA-C-N	6.67	134.28	121.54
2	B	53	TYR	C-N-CA	6.67	134.28	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	LYS	N-CA-C	-6.61	99.54	110.17
2	B	158	ARG	NE-CZ-NH2	6.60	125.14	119.20
2	B	243	ARG	CA-C-N	-6.60	111.36	121.92
2	B	243	ARG	C-N-CA	-6.60	111.36	121.92
2	B	59	ASN	N-CA-C	-6.57	99.34	109.52
1	A	372	GLN	CG-CD-NE2	6.54	126.20	116.40
2	B	184	PRO	CA-C-N	6.53	129.36	120.54
2	B	184	PRO	C-N-CA	6.53	129.36	120.54
1	A	121	ARG	NE-CZ-NH2	6.53	125.08	119.20
1	A	208	ALA	CA-C-N	6.52	128.91	120.56
1	A	208	ALA	C-N-CA	6.52	128.91	120.56
1	A	172	TYR	CB-CG-CD1	6.50	130.54	120.80
2	B	337	ASN	O-C-N	-6.49	114.63	122.48
2	B	8	GLN	CG-CD-NE2	6.48	126.12	116.40
1	A	336	LYS	O-C-N	6.48	131.21	122.59
1	A	36	MET	CA-C-O	-6.46	113.50	119.76
2	B	296	PHE	CA-C-N	-6.45	109.22	121.54
2	B	296	PHE	C-N-CA	-6.45	109.22	121.54
1	A	32	PRO	CB-CA-C	-6.45	100.92	111.56
1	A	2	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	A	404	PHE	CA-C-N	-6.44	114.31	122.43
1	A	404	PHE	C-N-CA	-6.44	114.31	122.43
1	A	266	HIS	CA-CB-CG	-6.42	107.38	113.80
1	A	65	ALA	O-C-N	-6.41	114.06	122.59
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	110.30	122.13
2	B	287	THR	C-N-CA	-6.40	110.30	122.13
2	B	272	PHE	CA-CB-CG	6.38	120.18	113.80
2	B	41	ASP	O-C-N	6.38	131.07	122.59
1	A	320	ARG	NE-CZ-NH2	6.37	124.93	119.20
2	B	28	HIS	O-C-N	6.37	131.06	122.59
2	B	76	ASP	CA-C-O	-6.36	113.81	120.55
2	B	26	ASP	CA-C-N	6.36	133.69	121.54
2	B	26	ASP	C-N-CA	6.36	133.69	121.54
1	A	101	ASN	CA-CB-CG	6.36	118.96	112.60
2	B	219	LEU	CB-CA-C	-6.35	97.78	110.42
2	B	380	ASN	O-C-N	-6.35	115.84	123.27
2	B	72	PRO	O-C-N	-6.35	114.07	122.64
2	B	247	GLN	CG-CD-NE2	6.33	125.89	116.40
2	B	7	ILE	CA-C-O	-6.33	114.11	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	PRO	N-CA-CB	-6.32	96.61	103.25
1	A	407	TRP	CA-CB-CG	-6.32	101.59	113.60
2	B	39	ASP	CA-CB-CG	-6.29	106.31	112.60
2	B	133	GLN	CG-CD-NE2	6.29	125.83	116.40
1	A	411	GLU	CA-C-O	-6.27	112.00	119.15
2	B	48	ARG	NE-CZ-NH2	6.25	124.83	119.20
1	A	439	SER	CA-C-N	6.22	132.90	121.70
1	A	439	SER	C-N-CA	6.22	132.90	121.70
1	A	299	ALA	O-C-N	-6.22	115.38	122.09
1	A	35	GLN	CG-CD-NE2	6.21	125.72	116.40
1	A	356	ASN	CA-C-O	-6.21	114.17	121.44
2	B	264	ARG	CB-CA-C	6.21	120.73	109.62
1	A	219	ILE	CG1-CB-CG2	-6.20	92.11	110.70
2	B	188	THR	CA-C-O	6.19	127.10	119.79
2	B	131	CYS	CA-C-N	6.19	129.62	120.95
2	B	131	CYS	C-N-CA	6.19	129.62	120.95
2	B	176	LYS	O-C-N	-6.19	114.36	122.59
2	B	255	LEU	O-C-N	-6.18	115.57	122.12
1	A	187	SER	CA-C-N	-6.17	112.78	120.56
1	A	187	SER	C-N-CA	-6.17	112.78	120.56
1	A	427	ALA	O-C-N	6.17	130.80	122.59
1	A	29	GLY	O-C-N	-6.17	117.82	123.56
2	B	356	CYS	CA-C-N	6.17	131.88	122.08
2	B	356	CYS	C-N-CA	6.17	131.88	122.08
1	A	72	PRO	CB-CA-C	-6.17	103.11	112.11
2	B	220	THR	CA-C-N	6.16	131.12	122.74
2	B	220	THR	C-N-CA	6.16	131.12	122.74
2	B	269	MET	O-C-N	6.16	127.45	121.66
2	B	173	PRO	O-C-N	-6.15	114.34	122.64
2	B	15	GLN	CG-CD-NE2	6.14	125.61	116.40
2	B	84	GLY	O-C-N	6.12	130.66	122.70
2	B	290	GLU	CA-C-N	-6.12	110.28	120.68
2	B	290	GLU	C-N-CA	-6.12	110.28	120.68
1	A	22	GLU	O-C-N	6.11	129.11	122.15
1	A	71	GLU	CA-C-N	6.10	125.66	119.19
1	A	71	GLU	C-N-CA	6.10	125.66	119.19
1	A	32	PRO	N-CA-C	6.08	124.99	112.47
2	B	182	VAL	CA-C-O	-6.08	113.18	120.78
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
1	A	381	THR	CA-C-O	6.04	128.87	121.56
2	B	394	GLN	CG-CD-NE2	6.04	125.46	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	O-C-N	6.04	130.62	122.59
2	B	200	GLU	CA-C-O	-6.03	114.39	121.44
1	A	373	ARG	CB-CA-C	5.99	120.02	109.89
1	A	335	ILE	O-C-N	5.99	127.68	121.87
2	B	264	ARG	NH1-CZ-NH2	-5.97	111.54	119.30
1	A	211	ASP	CA-CB-CG	-5.97	106.63	112.60
1	A	363	VAL	O-C-N	-5.96	114.30	121.10
1	A	262	TYR	O-C-N	-5.95	114.48	121.32
2	B	139	HIS	N-CA-CB	-5.95	101.58	111.57
1	A	438	ASP	CA-C-N	5.94	129.34	120.31
1	A	438	ASP	C-N-CA	5.94	129.34	120.31
1	A	344	VAL	N-CA-CB	-5.93	101.44	111.23
2	B	26	ASP	CA-C-O	5.92	126.66	119.49
2	B	185	TYR	N-CA-CB	-5.90	101.14	109.94
2	B	281	GLN	CA-C-N	5.90	133.03	122.06
2	B	281	GLN	C-N-CA	5.90	133.03	122.06
1	A	229	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	A	374	ALA	O-C-N	-5.88	116.01	123.24
2	B	244	PHE	N-CA-C	-5.87	101.50	110.07
1	A	63	PRO	N-CA-C	5.87	124.56	112.47
1	A	124	LYS	O-C-N	5.87	128.34	122.12
1	A	63	PRO	O-C-N	5.86	130.55	122.64
1	A	139	HIS	N-CA-CB	-5.86	100.64	111.53
2	B	400	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	13	GLY	O-C-N	-5.84	115.11	122.70
1	A	233	GLN	O-C-N	-5.82	115.11	122.27
1	A	366	GLY	N-CA-C	-5.80	107.14	114.16
2	B	270	PRO	O-C-N	-5.80	114.80	122.64
1	A	265	GLY	CA-C-N	-5.80	113.57	122.62
1	A	265	GLY	C-N-CA	-5.80	113.57	122.62
2	B	345	GLU	CA-C-N	-5.79	110.44	122.07
2	B	345	GLU	C-N-CA	-5.79	110.44	122.07
2	B	23	VAL	CA-C-N	-5.76	117.27	123.08
2	B	23	VAL	C-N-CA	-5.76	117.27	123.08
2	B	434	GLN	CG-CD-NE2	5.76	125.03	116.40
2	B	261	PRO	O-C-N	5.74	130.39	122.64
1	A	434	GLU	CA-C-O	-5.73	111.60	119.05
1	A	187	SER	O-C-N	5.72	127.96	122.07
1	A	413	MET	CA-C-O	-5.70	115.34	121.56
2	B	215	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	31	GLN	C-N-CD	-5.70	101.62	125.00
1	A	215	ARG	NE-CZ-NH2	5.69	124.32	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	42	LEU	O-C-N	5.69	130.16	122.59
1	A	222	PRO	CA-CB-CG	-5.68	93.70	104.50
1	A	422	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	A	105	ARG	CD-NE-CZ	5.68	132.35	124.40
1	A	273	ALA	CA-C-N	5.66	128.78	120.46
1	A	273	ALA	C-N-CA	5.66	128.78	120.46
1	A	352	LYS	CA-C-O	-5.66	114.09	120.32
1	A	350	GLY	O-C-N	5.65	130.05	122.70
2	B	424	ASN	CA-C-N	5.64	131.01	121.14
2	B	424	ASN	C-N-CA	5.64	131.01	121.14
2	B	256	ALA	CA-C-N	5.63	129.55	121.55
2	B	256	ALA	C-N-CA	5.63	129.55	121.55
1	A	221	ARG	CA-CB-CG	5.63	125.35	114.10
1	A	396	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	107	HIS	CA-C-O	5.62	126.69	120.90
2	B	107	HIS	CA-C-O	5.62	126.69	120.90
1	A	294	ALA	CA-C-N	-5.61	113.00	120.79
1	A	294	ALA	C-N-CA	-5.61	113.00	120.79
1	A	255	PHE	CA-CB-CG	5.60	119.40	113.80
2	B	244	PHE	CB-CA-C	5.59	122.13	110.50
2	B	23	VAL	O-C-N	5.58	129.54	122.57
2	B	389	LYS	CB-CA-C	5.57	121.51	110.42
2	B	4	ILE	N-CA-CB	-5.57	102.23	111.36
2	B	164	ARG	NE-CZ-NH2	5.57	124.21	119.20
2	B	224	TYR	CA-C-N	-5.56	113.15	120.22
2	B	224	TYR	C-N-CA	-5.56	113.15	120.22
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	179	THR	CA-C-N	5.54	131.85	122.26
1	A	179	THR	C-N-CA	5.54	131.85	122.26
1	A	206	ASN	CA-CB-CG	-5.53	107.07	112.60
1	A	437	VAL	CA-C-O	-5.53	113.87	120.78
1	A	309	HIS	O-C-N	5.52	129.48	123.13
1	A	374	ALA	CA-C-O	5.52	127.57	121.11
1	A	411	GLU	N-CA-C	-5.52	106.59	113.38
2	B	384	ILE	CA-C-N	-5.49	111.05	121.54
2	B	384	ILE	C-N-CA	-5.49	111.05	121.54
1	A	415	GLU	CA-C-O	-5.49	113.51	119.00
2	B	390	ARG	CB-CA-C	5.48	117.84	109.34
1	A	262	TYR	CA-CB-CG	5.46	123.73	113.90
2	B	224	TYR	CA-C-O	5.45	126.19	120.42
2	B	93	VAL	O-C-N	5.40	128.92	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	254	LYS	N-CA-C	-5.38	105.58	111.82
2	B	278	ARG	CA-CB-CG	5.38	124.86	114.10
2	B	302	MET	CG-SD-CE	5.38	112.74	100.90
1	A	229	ARG	CD-NE-CZ	-5.38	116.87	124.40
2	B	64	ARG	NE-CZ-NH2	5.37	124.04	119.20
2	B	253	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	33	ASP	CA-C-O	5.37	128.18	120.51
2	B	150	GLY	CA-C-O	-5.36	114.40	120.30
1	A	60	LYS	CB-CA-C	-5.36	102.24	110.81
2	B	83	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	59	GLY	O-C-N	5.34	127.69	122.19
1	A	299	ALA	CA-C-O	-5.33	115.21	120.70
1	A	103	TYR	O-C-N	5.33	129.47	122.33
2	B	246	GLY	N-CA-C	5.30	125.75	113.18
1	A	304	LYS	O-C-N	5.30	130.01	121.53
1	A	191	THR	CA-C-N	5.29	129.60	121.19
1	A	191	THR	C-N-CA	5.29	129.60	121.19
2	B	22	GLU	CA-C-O	5.27	125.66	119.28
2	B	291	LEU	CA-C-N	5.25	127.58	120.44
2	B	291	LEU	C-N-CA	5.25	127.58	120.44
2	B	126	SER	O-C-N	5.25	127.68	122.12
2	B	308	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	B	247	GLN	CA-C-O	-5.23	114.90	120.92
1	A	114	ILE	O-C-N	-5.23	116.04	122.57
1	A	86	LEU	N-CA-C	5.22	116.99	108.63
2	B	407	TRP	CB-CA-C	5.21	119.71	110.85
1	A	221	ARG	C-N-CD	-5.21	103.65	125.00
2	B	319	PHE	N-CA-C	5.20	116.87	108.34
2	B	186	ASN	CA-C-O	-5.20	112.46	119.11
1	A	85	GLN	O-C-N	-5.20	112.07	121.63
2	B	220	THR	O-C-N	5.17	129.25	122.33
1	A	172	TYR	CA-C-N	5.16	125.13	120.03
1	A	172	TYR	C-N-CA	5.16	125.13	120.03
1	A	101	ASN	CB-CA-C	-5.15	102.32	110.81
1	A	262	TYR	N-CA-CB	5.12	119.49	110.37
1	A	283	HIS	CA-C-O	-5.12	113.19	120.51
2	B	19	LYS	CD-CE-NZ	5.11	128.26	111.90
1	A	200	CYS	O-C-N	5.11	128.89	122.86
2	B	160	GLU	O-C-N	5.10	129.32	122.49
2	B	40	SER	O-C-N	5.09	129.36	122.59
2	B	264	ARG	N-CA-C	-5.08	103.44	110.35
2	B	71	GLU	CA-C-N	5.08	126.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	GLU	C-N-CA	5.08	126.19	119.84
1	A	53	PHE	CA-C-N	5.07	129.91	122.77
1	A	53	PHE	C-N-CA	5.07	129.91	122.77
1	A	93	ILE	O-C-N	5.03	128.47	123.18
1	A	339	ARG	N-CA-C	-5.02	105.52	111.69
1	A	173	PRO	CB-CA-C	-5.01	104.39	110.95
1	A	320	ARG	O-C-N	5.00	129.46	123.36
2	B	259	MET	O-C-N	-5.00	115.26	122.36

There are no chirality outliers.

All (115) 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	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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3277	1691	34
2	B	3359	0	3182	1957	15
3	A	32	0	11	30	0
4	B	28	0	12	17	0
5	B	58	0	51	60	0
All	All	6907	0	6533	3549	35

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 264.

All (3549) 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:229:HIS:CE1	5:B:501:TXL:H343	1.28	1.68
2:B:346:TRP:CE3	2:B:347:ILE:HG13	1.25	1.66
1:A:212:ILE:HD11	1:A:230:LEU:CD2	1.25	1.65
2:B:151:THR:CB	2:B:192:HIS:CD2	1.75	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:CD1	1:A:152:LEU:HG	1.15	1.62
2:B:405:LEU:HD22	2:B:418:PHE:CZ	1.17	1.62
2:B:147:SER:HB3	2:B:189:LEU:CD1	1.19	1.62
2:B:287:THR:HB	2:B:290:GLU:CB	1.26	1.62
2:B:158:ARG:CB	2:B:197:ASN:CB	1.76	1.61
2:B:184:PRO:HG2	2:B:399:PHE:CE2	1.12	1.60
1:A:210:TYR:CE1	2:B:326:LYS:CG	1.78	1.60
2:B:295:MET:HE3	2:B:375:ALA:CB	1.18	1.60
1:A:407:TRP:CH2	2:B:165:ILE:CD1	1.81	1.59
2:B:158:ARG:HB2	2:B:197:ASN:CB	1.14	1.59
1:A:217:LEU:HD13	1:A:368:LEU:CD1	1.25	1.59
1:A:53:PHE:N	1:A:88:HIS:CE1	1.68	1.58
2:B:103:TRP:CE3	2:B:413:MET:HE1	1.30	1.58
2:B:229:HIS:CD2	5:B:501:TXL:C38	1.86	1.58
1:A:220:GLU:CB	1:A:220:GLU:CG	1.78	1.58
1:A:405:VAL:CG2	1:A:405:VAL:CB	1.76	1.58
2:B:151:THR:HG22	2:B:192:HIS:CE1	1.39	1.57
2:B:181:VAL:HG13	2:B:399:PHE:CZ	1.40	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	1.56
2:B:346:TRP:CZ3	2:B:347:ILE:HD11	1.34	1.56
2:B:405:LEU:CD1	2:B:408:TYR:CB	1.76	1.56
2:B:70:LEU:HD12	2:B:94:PHE:CD2	1.40	1.56
2:B:151:THR:CA	2:B:192:HIS:CD2	1.89	1.55
1:A:115:ILE:HD12	1:A:152:LEU:CG	1.26	1.55
1:A:296:PHE:CE1	1:A:335:ILE:HD13	1.38	1.55
1:A:31:GLN:HE22	1:A:243:ARG:CG	1.15	1.54
2:B:158:ARG:CD	2:B:197:ASN:HB2	1.30	1.54
1:A:407:TRP:HH2	2:B:165:ILE:CD1	1.07	1.53
2:B:405:LEU:CD2	2:B:418:PHE:CZ	1.91	1.53
2:B:181:VAL:CG1	2:B:399:PHE:HZ	1.18	1.53
2:B:399:PHE:CE1	2:B:408:TYR:HE2	1.22	1.53
2:B:295:MET:CE	2:B:375:ALA:HB1	1.08	1.53
2:B:158:ARG:CG	2:B:197:ASN:HB2	1.13	1.52
1:A:210:TYR:CD1	2:B:326:LYS:HG2	1.43	1.52
2:B:107:HIS:C	2:B:152:LEU:HD11	1.35	1.52
1:A:103:TYR:CE2	1:A:189:LEU:HD23	1.41	1.52
2:B:158:ARG:CA	2:B:197:ASN:HD22	0.89	1.52
1:A:62:VAL:CG1	1:A:63:PRO:HD2	1.39	1.51
1:A:407:TRP:CH2	2:B:165:ILE:HD11	1.39	1.51
2:B:184:PRO:CG	2:B:399:PHE:CG	1.92	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD12	1:A:145:THR:CG2	1.07	1.51
1:A:100:ALA:CB	1:A:105:ARG:HD3	1.38	1.51
1:A:158:SER:CB	1:A:197:HIS:CB	1.84	1.51
1:A:103:TYR:CD2	1:A:189:LEU:HD23	1.44	1.50
2:B:151:THR:HG22	2:B:192:HIS:ND1	1.24	1.50
1:A:64:ARG:HH22	1:A:132:LEU:CD2	1.22	1.50
1:A:31:GLN:CD	1:A:243:ARG:HD2	1.08	1.50
1:A:210:TYR:CE2	1:A:227:LEU:HD22	1.45	1.50
2:B:169:PHE:CE1	2:B:235:MET:HG2	1.46	1.50
2:B:346:TRP:CE3	2:B:347:ILE:CG1	1.90	1.49
2:B:192:HIS:CA	2:B:196:GLU:HG3	1.42	1.48
1:A:272:TYR:CE1	1:A:274:PRO:O	1.64	1.48
1:A:107:HIS:HB2	1:A:148:GLY:CA	1.42	1.46
2:B:405:LEU:HD13	2:B:408:TYR:CD2	1.48	1.46
2:B:19:LYS:CB	2:B:228:ASN:HB3	1.45	1.46
2:B:259:MET:HB3	2:B:268:PHE:CE1	1.47	1.46
2:B:399:PHE:HE1	2:B:408:TYR:CE2	1.30	1.45
1:A:31:GLN:N	1:A:32:PRO:CD	1.76	1.44
1:A:70:LEU:CD1	1:A:145:THR:HG22	0.98	1.44
2:B:70:LEU:CD1	2:B:94:PHE:CD2	1.99	1.44
1:A:107:HIS:CB	1:A:148:GLY:HA3	1.47	1.44
2:B:87:PHE:CE1	2:B:89:PRO:HG2	1.52	1.44
2:B:135:PHE:HB3	2:B:166:MET:CE	1.47	1.44
2:B:147:SER:CB	2:B:189:LEU:CD1	1.79	1.44
2:B:158:ARG:HD2	2:B:197:ASN:CA	1.44	1.44
2:B:239:THR:O	2:B:243:ARG:CD	1.65	1.44
2:B:405:LEU:CD1	2:B:408:TYR:HB2	0.96	1.44
1:A:250:VAL:HG13	1:A:254:GLU:CB	1.48	1.43
1:A:212:ILE:CD1	1:A:230:LEU:HD21	1.45	1.43
2:B:172:VAL:CG1	2:B:173:PRO:HD2	1.46	1.43
2:B:405:LEU:CD2	2:B:418:PHE:CE2	1.99	1.43
1:A:172:TYR:OH	1:A:387:ALA:CB	1.64	1.43
2:B:286:LEU:CD1	2:B:372:LYS:HB2	1.47	1.43
1:A:397:LEU:CD2	1:A:401:LYS:HD2	1.47	1.42
2:B:405:LEU:HD11	2:B:408:TYR:CB	1.34	1.42
2:B:147:SER:CB	2:B:189:LEU:HD11	0.95	1.41
2:B:19:LYS:HG3	2:B:228:ASN:CB	1.46	1.41
2:B:151:THR:CA	2:B:192:HIS:NE2	1.82	1.41
2:B:184:PRO:HG2	2:B:399:PHE:CG	1.55	1.40
1:A:53:PHE:CA	1:A:88:HIS:CE1	2.01	1.40
2:B:7:ILE:HB	2:B:137:LEU:CD2	1.51	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:CG	2:B:197:ASN:CB	1.95	1.40
2:B:151:THR:HB	2:B:192:HIS:CD2	1.39	1.40
2:B:229:HIS:CD2	5:B:501:TXL:C37	2.03	1.40
1:A:64:ARG:NH2	1:A:132:LEU:HD22	1.31	1.40
1:A:222:PRO:CB	1:A:222:PRO:CG	1.86	1.40
1:A:277:SER:OG	1:A:280:LYS:CG	1.68	1.40
2:B:175:PRO:O	2:B:176:LYS:CE	1.70	1.40
1:A:210:TYR:CE1	2:B:326:LYS:HG2	0.86	1.39
2:B:57:ALA:HA	2:B:64:ARG:CB	1.52	1.39
2:B:399:PHE:CE1	2:B:408:TYR:CE2	2.03	1.39
1:A:103:TYR:CD2	1:A:147:SER:HB2	1.50	1.39
2:B:151:THR:HA	2:B:192:HIS:CD2	1.49	1.39
1:A:176:GLN:O	1:A:177:VAL:CG2	1.70	1.38
2:B:19:LYS:CG	2:B:228:ASN:HB3	1.50	1.38
2:B:184:PRO:CB	2:B:399:PHE:CD2	2.05	1.38
2:B:435:TYR:O	2:B:436:GLN:CG	1.72	1.38
1:A:250:VAL:HG13	1:A:254:GLU:CG	1.53	1.37
2:B:103:TRP:CD1	2:B:189:LEU:HD23	1.57	1.37
2:B:405:LEU:HD22	2:B:418:PHE:CE2	1.56	1.37
1:A:210:TYR:HE1	2:B:326:LYS:CG	1.20	1.37
2:B:20:PHE:HE2	2:B:235:MET:CB	1.24	1.37
2:B:435:TYR:C	2:B:436:GLN:HG3	1.17	1.37
2:B:20:PHE:CE2	2:B:235:MET:HB3	1.50	1.36
2:B:87:PHE:CD1	2:B:88:ARG:O	1.76	1.36
1:A:204:VAL:CG2	1:A:231:ILE:HG23	1.50	1.36
1:A:68:VAL:HG11	1:A:149:PHE:CZ	1.57	1.36
2:B:175:PRO:O	2:B:176:LYS:CD	1.74	1.36
1:A:288:VAL:CG2	1:A:373:ARG:HD3	1.52	1.35
2:B:192:HIS:HA	2:B:196:GLU:CG	1.55	1.35
2:B:184:PRO:CD	2:B:399:PHE:CD2	2.08	1.35
1:A:212:ILE:CD1	1:A:230:LEU:CD2	2.02	1.35
2:B:311:ARG:HG2	2:B:341:SER:O	1.21	1.35
1:A:369:ALA:CB	1:A:371:VAL:HG23	1.56	1.34
2:B:151:THR:HA	2:B:192:HIS:NE2	1.04	1.34
2:B:158:ARG:HA	2:B:197:ASN:ND2	1.04	1.34
1:A:31:GLN:CD	1:A:243:ARG:CD	1.99	1.34
1:A:217:LEU:CD1	1:A:368:LEU:HD11	1.55	1.34
2:B:19:LYS:CG	2:B:228:ASN:CB	2.02	1.34
1:A:108:TYR:O	1:A:112:LYS:CD	1.76	1.34
1:A:182:VAL:HG13	1:A:186:ASN:ND2	1.40	1.34
2:B:44:LEU:HD23	2:B:85:GLN:CG	1.34	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ILE:O	2:B:26:ASP:N	1.60	1.33
2:B:405:LEU:CD1	2:B:408:TYR:CD2	2.06	1.33
2:B:97:SER:HB2	2:B:110:GLU:OE1	1.19	1.33
2:B:12:CYS:O	2:B:16:ILE:HG12	1.25	1.33
1:A:184:PRO:HG3	1:A:395:PHE:CB	1.57	1.33
2:B:32:PRO:CB	2:B:59:ASN:HD22	1.25	1.33
2:B:96:GLN:O	2:B:98:GLY:N	1.59	1.33
2:B:229:HIS:CD2	5:B:501:TXL:H38	1.54	1.33
2:B:305:CYS:SG	2:B:384:ILE:HD13	1.67	1.33
2:B:4:ILE:HD12	2:B:30:ILE:C	1.53	1.32
2:B:22:GLU:HG2	2:B:83:PHE:CD2	1.63	1.32
2:B:142:GLY:C	2:B:185:TYR:CE1	2.07	1.32
1:A:272:TYR:CZ	1:A:274:PRO:HG2	1.62	1.32
2:B:183:GLU:HB2	2:B:184:PRO:CD	1.59	1.32
2:B:294:GLN:CG	2:B:300:ASN:OD1	1.77	1.32
1:A:30:ILE:O	1:A:32:PRO:HG2	1.27	1.32
2:B:201:THR:CG2	2:B:265:LEU:HD21	1.58	1.32
2:B:346:TRP:CZ3	2:B:347:ILE:CD1	2.10	1.32
1:A:30:ILE:O	1:A:32:PRO:CG	1.78	1.31
1:A:250:VAL:CG2	1:A:352:LYS:HE2	1.60	1.31
1:A:306:ASP:OD1	1:A:308:ARG:CG	1.76	1.31
2:B:335:VAL:O	2:B:339:ASN:ND2	1.60	1.31
1:A:31:GLN:NE2	1:A:243:ARG:CG	1.93	1.31
1:A:179:THR:HG22	1:A:181:VAL:N	1.42	1.31
1:A:31:GLN:NE2	1:A:243:ARG:CD	1.92	1.31
2:B:114:LEU:HD12	2:B:117:SER:OG	1.24	1.31
2:B:435:TYR:O	2:B:436:GLN:HG3	1.20	1.31
2:B:175:PRO:O	2:B:176:LYS:HE2	1.22	1.31
1:A:101:ASN:O	1:A:102:ASN:CG	1.72	1.31
1:A:179:THR:CG2	1:A:181:VAL:H	1.42	1.31
1:A:250:VAL:CG1	1:A:254:GLU:HB3	1.61	1.30
1:A:53:PHE:N	1:A:88:HIS:NE2	1.75	1.30
2:B:20:PHE:CE2	2:B:235:MET:CB	2.00	1.30
2:B:75:MET:CE	2:B:79:ARG:HD2	1.60	1.30
2:B:145:THR:O	2:B:149:MET:HB3	1.19	1.30
2:B:158:ARG:HD2	2:B:197:ASN:CB	1.59	1.30
1:A:103:TYR:CD2	1:A:189:LEU:CD2	2.13	1.30
1:A:277:SER:CB	1:A:280:LYS:HG2	1.59	1.30
1:A:115:ILE:CD1	1:A:152:LEU:CG	1.92	1.30
1:A:225:THR:CG2	2:B:247:GLN:HE22	1.43	1.30
2:B:151:THR:HG22	2:B:192:HIS:CG	1.67	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:THR:O	2:B:398:MET:CE	1.78	1.29
2:B:229:HIS:CG	5:B:501:TXL:H38	1.67	1.29
2:B:244:PHE:CD2	2:B:245:PRO:HD2	1.65	1.29
2:B:319:PHE:CE1	2:B:353:THR:HG23	1.67	1.29
2:B:201:THR:HG21	2:B:265:LEU:CD2	1.60	1.29
2:B:268:PHE:CE1	2:B:380:ASN:ND2	1.99	1.29
2:B:32:PRO:CB	2:B:59:ASN:ND2	1.80	1.28
2:B:69:ASP:OD2	2:B:74:THR:HB	1.32	1.28
1:A:107:HIS:HB2	1:A:148:GLY:C	1.59	1.28
1:A:291:ILE:HG22	1:A:375:VAL:CG2	1.62	1.28
2:B:107:HIS:CA	2:B:152:LEU:HD11	1.63	1.28
1:A:38:SER:C	1:A:39:ASP:CA	2.04	1.28
1:A:184:PRO:CG	1:A:395:PHE:CD2	2.17	1.28
2:B:107:HIS:CD2	2:B:152:LEU:HG	1.66	1.28
2:B:181:VAL:CG1	2:B:399:PHE:CZ	2.03	1.28
1:A:172:TYR:OH	1:A:387:ALA:HB3	1.11	1.28
2:B:158:ARG:CB	2:B:197:ASN:HB2	1.44	1.28
2:B:192:HIS:O	2:B:196:GLU:HB2	1.17	1.28
1:A:38:SER:O	1:A:39:ASP:N	1.58	1.27
1:A:266:HIS:CD2	1:A:432:TYR:HE1	1.50	1.27
2:B:192:HIS:CA	2:B:196:GLU:CG	2.12	1.27
2:B:192:HIS:O	2:B:196:GLU:CB	1.80	1.27
2:B:287:THR:O	2:B:291:LEU:CG	1.81	1.27
1:A:97:GLU:CB	1:A:110:ILE:HG21	1.65	1.27
2:B:193:GLN:O	2:B:265:LEU:CD2	1.82	1.27
2:B:151:THR:CG2	2:B:192:HIS:CG	2.16	1.27
2:B:259:MET:HE1	2:B:379:GLY:CA	1.64	1.26
2:B:92:PHE:CD2	2:B:114:LEU:HD11	1.70	1.26
2:B:312:TYR:HA	2:B:381:SER:CB	1.63	1.26
1:A:2:ARG:CG	1:A:133:GLN:OE1	1.82	1.26
1:A:272:TYR:HE1	1:A:274:PRO:O	0.94	1.26
2:B:94:PHE:HD1	2:B:94:PHE:O	1.16	1.26
1:A:220:GLU:C	1:A:222:PRO:HD3	1.61	1.26
2:B:12:CYS:O	2:B:16:ILE:CG1	1.82	1.26
1:A:204:VAL:CG1	1:A:209:ILE:CD1	2.13	1.25
2:B:102:ASN:HD22	2:B:105:LYS:CE	1.49	1.25
2:B:183:GLU:CB	2:B:184:PRO:HD3	1.63	1.25
1:A:108:TYR:C	1:A:112:LYS:HE3	1.59	1.25
1:A:219:ILE:CB	1:A:219:ILE:CG2	2.13	1.25
2:B:107:HIS:O	2:B:152:LEU:HD11	1.28	1.25
1:A:77:GLU:HA	1:A:80:THR:OG1	1.09	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TRP:CD1	2:B:189:LEU:CD2	2.18	1.25
2:B:111:GLY:O	2:B:115:VAL:HG23	1.32	1.25
2:B:3:GLU:OE1	2:B:130:ASP:CB	1.84	1.25
2:B:287:THR:CG2	2:B:289:PRO:HD2	1.67	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
1:A:108:TYR:CA	1:A:112:LYS:HE3	1.67	1.24
1:A:306:ASP:OD1	1:A:308:ARG:HG3	1.16	1.24
2:B:87:PHE:CE1	2:B:88:ARG:O	1.87	1.24
2:B:312:TYR:O	2:B:344:VAL:CG2	1.84	1.24
1:A:9:VAL:HG11	1:A:150:THR:CG2	1.67	1.24
2:B:4:ILE:HD13	2:B:30:ILE:CG2	1.68	1.24
2:B:107:HIS:HA	2:B:152:LEU:CD1	1.67	1.24
2:B:182:VAL:HG13	2:B:186:ASN:ND2	1.48	1.24
1:A:53:PHE:HA	1:A:88:HIS:CE1	1.64	1.24
2:B:237:GLY:HA2	2:B:241:CYS:SG	1.74	1.24
1:A:433:GLU:O	1:A:437:VAL:HG23	1.32	1.24
2:B:143:GLY:N	2:B:185:TYR:CE1	2.06	1.24
2:B:143:GLY:N	2:B:185:TYR:HE1	1.35	1.24
1:A:291:ILE:CG2	1:A:375:VAL:HG23	1.65	1.24
1:A:383:ALA:O	1:A:385:ALA:N	1.69	1.24
1:A:242:LEU:HD12	1:A:255:PHE:CZ	1.73	1.23
2:B:237:GLY:O	2:B:241:CYS:HB2	1.33	1.23
1:A:20:CYS:O	1:A:24:TYR:CD2	1.91	1.23
1:A:276:ILE:O	1:A:368:LEU:HB3	1.31	1.23
1:A:4:CYS:HB2	1:A:30:ILE:CG2	1.68	1.23
1:A:30:ILE:CG2	1:A:64:ARG:HG2	1.68	1.23
1:A:206:ASN:ND2	1:A:227:LEU:CD2	2.00	1.23
1:A:210:TYR:CE2	1:A:227:LEU:CD2	2.21	1.23
2:B:35:SER:O	2:B:37:HIS:N	1.71	1.23
2:B:103:TRP:CE3	2:B:413:MET:CE	2.20	1.23
1:A:185:TYR:HD2	1:A:408:TYR:OH	0.92	1.23
2:B:87:PHE:HE1	2:B:89:PRO:CG	1.51	1.23
1:A:77:GLU:CA	1:A:80:THR:OG1	1.86	1.23
1:A:360:PRO:CG	1:A:371:VAL:O	1.86	1.23
2:B:287:THR:CB	2:B:290:GLU:HB2	1.67	1.23
1:A:312:TYR:O	1:A:344:VAL:CG2	1.87	1.22
2:B:244:PHE:CE2	2:B:358:ILE:HD12	1.73	1.22
1:A:108:TYR:O	1:A:112:LYS:CE	1.85	1.22
2:B:184:PRO:CD	2:B:399:PHE:HD2	1.49	1.22
2:B:103:TRP:HD1	2:B:189:LEU:CD2	1.49	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:LEU:O	2:B:193:GLN:HG3	1.31	1.22
2:B:319:PHE:HE1	2:B:353:THR:CG2	1.50	1.22
2:B:405:LEU:CD1	2:B:408:TYR:CG	2.20	1.22
1:A:3:GLU:HA	1:A:31:GLN:CB	1.70	1.22
1:A:28:HIS:CE1	1:A:29:GLY:O	1.93	1.22
1:A:93:ILE:CD1	1:A:118:VAL:HG22	1.70	1.22
1:A:16:ILE:HD13	1:A:138:PHE:CD1	1.75	1.22
1:A:108:TYR:O	1:A:112:LYS:HE3	1.40	1.22
1:A:206:ASN:ND2	1:A:227:LEU:HD21	1.51	1.22
2:B:75:MET:CE	2:B:79:ARG:CD	2.17	1.22
1:A:78:VAL:CG1	1:A:87:PHE:HE1	1.53	1.21
2:B:97:SER:CB	2:B:110:GLU:OE1	1.89	1.21
1:A:31:GLN:OE1	1:A:243:ARG:CD	1.85	1.21
1:A:48:SER:O	1:A:56:THR:CG2	1.87	1.21
1:A:158:SER:CB	1:A:197:HIS:HB3	1.49	1.21
1:A:220:GLU:O	1:A:222:PRO:CD	1.89	1.21
1:A:259:LEU:O	1:A:261:PRO:HD3	1.38	1.21
2:B:175:PRO:O	2:B:176:LYS:CG	1.88	1.21
1:A:30:ILE:C	1:A:32:PRO:CD	2.11	1.21
2:B:319:PHE:CE1	2:B:328:VAL:CG1	2.24	1.21
1:A:344:VAL:HB	1:A:347:CYS:SG	1.80	1.21
1:A:396:ASP:O	1:A:401:LYS:HB2	1.40	1.21
2:B:183:GLU:CD	2:B:394:GLN:HB3	1.66	1.21
1:A:2:ARG:HG2	1:A:133:GLN:OE1	1.05	1.21
1:A:26:LEU:HD11	1:A:361:THR:CG2	1.69	1.21
1:A:3:GLU:O	1:A:132:LEU:O	1.59	1.20
1:A:31:GLN:OE1	1:A:243:ARG:HD2	1.02	1.20
2:B:229:HIS:CE1	5:B:501:TXL:C34	2.23	1.20
1:A:183:GLU:HB3	1:A:394:LYS:HB3	1.24	1.20
1:A:272:TYR:CE1	1:A:274:PRO:HG2	1.75	1.20
1:A:343:PHE:CE2	1:A:351:PHE:CZ	2.30	1.20
2:B:75:MET:HE2	2:B:79:ARG:CD	1.70	1.20
2:B:435:TYR:C	2:B:436:GLN:CG	2.06	1.20
1:A:31:GLN:N	1:A:32:PRO:HD3	1.05	1.20
1:A:176:GLN:O	1:A:177:VAL:HG23	1.03	1.20
1:A:184:PRO:HG3	1:A:395:PHE:CD2	1.74	1.20
1:A:332:ILE:CD1	1:A:353:VAL:HG21	1.70	1.20
2:B:6:HIS:HE1	2:B:30:ILE:CD1	1.53	1.20
1:A:177:VAL:HG12	1:A:178:SER:H	1.04	1.19
2:B:36:TYR:CE2	2:B:244:PHE:CE1	1.94	1.19
2:B:107:HIS:O	2:B:152:LEU:CD1	1.89	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PHE:CE1	2:B:235:MET:CG	2.25	1.19
1:A:222:PRO:O	2:B:324:SER:HB2	1.40	1.19
1:A:103:TYR:CD1	1:A:188:ILE:CG2	2.26	1.19
2:B:44:LEU:O	2:B:47:GLU:CG	1.91	1.19
1:A:30:ILE:HB	1:A:64:ARG:HB2	1.24	1.19
1:A:224:TYR:CD2	2:B:325:MET:HB3	1.77	1.19
1:A:231:ILE:HD13	1:A:302:MET:HE2	1.25	1.19
2:B:151:THR:CG2	2:B:192:HIS:CE1	2.26	1.19
2:B:259:MET:CE	2:B:379:GLY:HA2	1.72	1.19
2:B:312:TYR:HA	2:B:381:SER:CA	1.71	1.19
1:A:48:SER:O	1:A:56:THR:HG21	1.02	1.18
2:B:175:PRO:HD3	2:B:390:ARG:NH2	1.57	1.18
1:A:4:CYS:SG	1:A:252:LEU:HD11	1.83	1.18
2:B:370:GLY:O	5:B:501:TXL:H183	1.43	1.18
1:A:184:PRO:CB	1:A:395:PHE:HD2	1.55	1.18
2:B:135:PHE:CB	2:B:166:MET:CE	2.20	1.18
2:B:250:ALA:HA	2:B:254:LYS:HD2	1.25	1.18
2:B:346:TRP:HE3	2:B:347:ILE:CG1	1.35	1.18
1:A:100:ALA:HB2	1:A:105:ARG:HD3	1.19	1.18
2:B:44:LEU:O	2:B:47:GLU:HG3	1.01	1.18
2:B:174:SER:CB	2:B:207:GLU:HB3	1.73	1.18
1:A:62:VAL:CG1	1:A:63:PRO:CD	2.22	1.17
1:A:437:VAL:O	1:A:438:ASP:OD1	1.62	1.17
2:B:294:GLN:HG2	2:B:300:ASN:OD1	1.01	1.17
1:A:397:LEU:HD22	1:A:401:LYS:HD2	1.27	1.17
2:B:175:PRO:C	2:B:176:LYS:HG2	1.54	1.17
1:A:115:ILE:HD13	1:A:156:ARG:CZ	1.74	1.17
1:A:174:ALA:HB1	1:A:175:PRO:CD	1.75	1.17
1:A:312:TYR:CE2	1:A:377:MET:HE1	1.79	1.17
1:A:100:ALA:CB	1:A:105:ARG:CD	2.23	1.17
1:A:177:VAL:HB	2:B:349:ASN:ND2	1.60	1.17
2:B:382:THR:CG2	2:B:436:GLN:OE1	1.78	1.17
1:A:220:GLU:O	1:A:222:PRO:HD2	1.45	1.16
2:B:7:ILE:CA	2:B:66:ILE:HG23	1.75	1.16
2:B:87:PHE:CE1	2:B:89:PRO:CG	2.23	1.16
2:B:80:SER:C	2:B:82:PRO:HD2	1.70	1.16
2:B:183:GLU:HB2	2:B:398:MET:SD	1.85	1.16
2:B:405:LEU:HD12	2:B:408:TYR:CB	1.56	1.16
1:A:176:GLN:HE21	2:B:333:LEU:CD2	1.58	1.16
1:A:217:LEU:CD1	1:A:368:LEU:CD1	2.14	1.16
2:B:154:ILE:HG21	2:B:198:THR:HG23	1.21	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HG3	1:A:395:PHE:CG	1.80	1.16
2:B:103:TRP:CZ3	2:B:413:MET:CE	2.28	1.16
2:B:191:VAL:CG2	2:B:421:ALA:HA	1.75	1.16
2:B:234:THR:OG1	2:B:302:MET:HE1	1.44	1.16
2:B:287:THR:HG22	2:B:289:PRO:HD2	1.20	1.16
1:A:59:GLY:O	1:A:62:VAL:O	1.63	1.16
1:A:115:ILE:HD12	1:A:152:LEU:CD2	1.75	1.15
1:A:185:TYR:CD2	1:A:408:TYR:OH	1.85	1.15
1:A:210:TYR:CD1	2:B:326:LYS:CG	2.10	1.15
1:A:103:TYR:HD2	1:A:147:SER:CB	1.59	1.15
1:A:137:VAL:HG21	1:A:154:MET:SD	1.85	1.15
2:B:151:THR:CG2	2:B:192:HIS:CD2	2.27	1.15
1:A:176:GLN:NE2	2:B:333:LEU:HD22	1.60	1.15
1:A:204:VAL:HG21	1:A:231:ILE:CG2	1.47	1.15
2:B:7:ILE:HA	2:B:66:ILE:CG2	1.75	1.15
2:B:313:LEU:CD2	2:B:344:VAL:HG11	1.75	1.15
2:B:7:ILE:CG1	2:B:66:ILE:HG21	1.77	1.15
2:B:103:TRP:CZ3	2:B:413:MET:HE1	1.81	1.15
1:A:31:GLN:NE2	1:A:243:ARG:HD2	1.51	1.15
2:B:320:ARG:HG2	2:B:374:SER:OG	1.47	1.15
2:B:22:GLU:HB3	2:B:83:PHE:CZ	1.82	1.14
1:A:155:GLU:HG3	1:A:192:HIS:CD2	1.82	1.14
1:A:62:VAL:HG13	1:A:63:PRO:CD	1.77	1.14
1:A:176:GLN:C	1:A:177:VAL:HG23	1.71	1.14
2:B:22:GLU:CG	2:B:83:PHE:CD2	2.30	1.14
2:B:111:GLY:C	2:B:115:VAL:HG23	1.70	1.14
2:B:151:THR:CB	2:B:192:HIS:CG	2.31	1.14
2:B:158:ARG:CB	2:B:197:ASN:HD22	1.60	1.14
2:B:312:TYR:HA	2:B:381:SER:HB3	1.30	1.14
2:B:22:GLU:HB3	2:B:83:PHE:CE2	1.81	1.14
2:B:33:THR:N	2:B:59:ASN:HD22	1.42	1.14
2:B:50:ASN:N	2:B:61:TYR:CD2	2.15	1.14
2:B:172:VAL:CG1	2:B:173:PRO:CD	2.25	1.14
2:B:234:THR:OG1	2:B:302:MET:SD	2.05	1.14
2:B:241:CYS:SG	2:B:320:ARG:NH1	2.20	1.14
2:B:244:PHE:HE2	2:B:358:ILE:CD1	1.60	1.14
1:A:312:TYR:HA	1:A:381:THR:HG22	1.26	1.14
2:B:56:ALA:HB3	2:B:62:VAL:CB	1.78	1.14
2:B:97:SER:HB2	2:B:110:GLU:CD	1.71	1.14
2:B:104:ALA:HA	2:B:108:TYR:CD2	1.83	1.14
2:B:151:THR:HB	2:B:192:HIS:CG	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:THR:OG1	2:B:302:MET:CE	1.95	1.14
2:B:296:PHE:CZ	2:B:335:VAL:HG11	1.83	1.14
2:B:158:ARG:CB	2:B:197:ASN:CG	2.19	1.13
2:B:193:GLN:O	2:B:265:LEU:HD22	0.96	1.13
1:A:174:ALA:CB	1:A:175:PRO:CD	2.20	1.13
1:A:296:PHE:CE1	1:A:335:ILE:CD1	2.31	1.13
1:A:57:GLY:HA3	1:A:61:HIS:CE1	1.83	1.13
1:A:184:PRO:CG	1:A:395:PHE:HD2	1.56	1.13
1:A:217:LEU:HD13	1:A:368:LEU:HD13	1.21	1.13
1:A:217:LEU:CG	1:A:368:LEU:HD11	1.79	1.13
2:B:158:ARG:HB2	2:B:197:ASN:CG	1.72	1.13
2:B:48:ARG:HH11	2:B:60:LYS:CA	1.62	1.13
2:B:105:LYS:HE2	2:B:411:GLU:OE2	1.48	1.13
1:A:217:LEU:HG	1:A:218:ASP:H	0.96	1.13
1:A:312:TYR:CE2	1:A:377:MET:CE	2.32	1.13
2:B:107:HIS:CD2	2:B:152:LEU:CG	2.32	1.13
2:B:44:LEU:CD2	2:B:85:GLN:HG3	1.78	1.12
2:B:176:LYS:HE3	2:B:207:GLU:OE2	1.49	1.12
2:B:390:ARG:O	2:B:394:GLN:HG2	1.46	1.13
1:A:100:ALA:HB1	1:A:105:ARG:HD3	1.13	1.12
1:A:182:VAL:CG1	1:A:186:ASN:ND2	2.12	1.12
1:A:224:TYR:OH	3:A:500:GTP:O2'	1.65	1.12
1:A:266:HIS:CD2	1:A:432:TYR:CE1	2.38	1.12
2:B:24:ILE:C	2:B:26:ASP:N	2.01	1.12
2:B:141:LEU:HD22	2:B:186:ASN:HB3	1.21	1.12
2:B:154:ILE:HG21	2:B:198:THR:CG2	1.79	1.12
1:A:105:ARG:HH21	1:A:110:ILE:HD11	1.03	1.12
1:A:313:MET:HE1	1:A:346:TRP:CZ2	1.85	1.12
2:B:107:HIS:CE1	2:B:152:LEU:HD21	1.84	1.12
2:B:135:PHE:CG	2:B:166:MET:HE1	1.85	1.12
1:A:38:SER:CA	1:A:39:ASP:N	2.11	1.12
2:B:102:ASN:HD22	2:B:105:LYS:NZ	1.45	1.12
2:B:158:ARG:CB	2:B:197:ASN:ND2	2.10	1.12
2:B:192:HIS:C	2:B:196:GLU:HG3	1.73	1.12
1:A:26:LEU:HD11	1:A:361:THR:HG21	1.23	1.12
2:B:41:ASP:O	2:B:42:LEU:HG	1.45	1.12
2:B:154:ILE:CG2	2:B:198:THR:HG23	1.79	1.12
1:A:48:SER:OG	1:A:56:THR:HB	1.51	1.11
2:B:107:HIS:NE2	2:B:152:LEU:HD23	1.64	1.11
2:B:135:PHE:HB3	2:B:166:MET:HE1	1.27	1.11
2:B:242:LEU:HD13	2:B:250:ALA:HB3	1.28	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:13:GLY:N	1.83	1.11
1:A:97:GLU:CB	1:A:110:ILE:CG2	2.27	1.11
1:A:407:TRP:CZ2	2:B:256:ALA:HB1	1.84	1.11
2:B:201:THR:CG2	2:B:265:LEU:HD11	1.79	1.11
2:B:209:LEU:HD13	2:B:227:LEU:HG	1.21	1.11
2:B:287:THR:CB	2:B:290:GLU:CB	2.23	1.11
2:B:312:TYR:O	2:B:344:VAL:HG23	1.47	1.11
2:B:313:LEU:HD23	2:B:344:VAL:CG2	1.79	1.11
2:B:385:GLN:CG	2:B:389:LYS:HE3	1.79	1.11
2:B:192:HIS:O	2:B:196:GLU:CG	1.98	1.11
2:B:287:THR:HB	2:B:290:GLU:HB3	1.21	1.11
2:B:319:PHE:CD1	2:B:328:VAL:HG11	1.85	1.11
1:A:22:GLU:HG2	1:A:85:GLN:HE22	0.95	1.11
1:A:174:ALA:HB1	1:A:390:ARG:HH22	1.03	1.10
2:B:6:HIS:CE1	2:B:30:ILE:CD1	2.32	1.10
2:B:192:HIS:C	2:B:196:GLU:CG	2.24	1.10
2:B:287:THR:HG22	2:B:289:PRO:CD	1.79	1.10
1:A:103:TYR:CD1	1:A:188:ILE:HG21	1.86	1.10
2:B:70:LEU:CD1	2:B:94:PHE:HD2	1.47	1.10
2:B:184:PRO:CG	2:B:399:PHE:CE2	1.90	1.10
2:B:346:TRP:O	2:B:347:ILE:HB	1.49	1.10
2:B:405:LEU:HD21	2:B:418:PHE:CE2	1.82	1.10
1:A:107:HIS:CB	1:A:148:GLY:CA	2.17	1.10
1:A:169:PHE:CZ	1:A:235:VAL:HG22	1.85	1.10
2:B:107:HIS:CA	2:B:152:LEU:CD1	2.25	1.10
2:B:181:VAL:HG12	2:B:399:PHE:HZ	1.06	1.10
1:A:93:ILE:HD13	1:A:118:VAL:HG22	1.11	1.10
2:B:80:SER:O	2:B:82:PRO:HD2	1.52	1.10
2:B:103:TRP:HZ3	2:B:108:TYR:OH	1.33	1.10
1:A:100:ALA:HB2	1:A:105:ARG:CD	1.80	1.10
1:A:177:VAL:HB	2:B:349:ASN:HD21	1.05	1.10
2:B:3:GLU:HB3	2:B:132:LEU:HD23	1.33	1.10
2:B:66:ILE:HG13	2:B:121:VAL:CG1	1.82	1.10
2:B:94:PHE:O	2:B:94:PHE:CD1	2.05	1.10
2:B:259:MET:CE	2:B:379:GLY:CA	2.29	1.10
2:B:286:LEU:HD11	2:B:372:LYS:HB2	1.12	1.10
2:B:321:GLY:HA3	2:B:373:MET:HG3	1.22	1.10
1:A:174:ALA:HB1	1:A:175:PRO:HD3	1.27	1.09
2:B:48:ARG:HB2	2:B:61:TYR:HA	1.33	1.09
2:B:135:PHE:CD2	2:B:166:MET:HE1	1.86	1.09
2:B:242:LEU:N	2:B:356:CYS:SG	2.25	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:385:GLN:HG3	2:B:389:LYS:HE3	1.21	1.09
1:A:45:GLY:O	1:A:46:ASP:CB	1.98	1.09
1:A:266:HIS:NE2	1:A:432:TYR:HE1	1.48	1.09
2:B:41:ASP:C	2:B:42:LEU:HG	1.76	1.09
2:B:147:SER:OG	2:B:189:LEU:HD11	1.50	1.09
2:B:175:PRO:CD	2:B:390:ARG:HH21	1.66	1.09
2:B:260:VAL:HG22	2:B:266:HIS:HB2	1.21	1.09
1:A:62:VAL:HG12	1:A:63:PRO:HD2	1.24	1.09
1:A:70:LEU:CG	1:A:145:THR:HG22	1.82	1.09
1:A:210:TYR:CZ	1:A:227:LEU:HD22	1.87	1.09
2:B:4:ILE:CD1	2:B:30:ILE:HA	1.83	1.09
2:B:69:ASP:CG	2:B:74:THR:HB	1.77	1.09
2:B:107:HIS:CD2	2:B:152:LEU:CD2	2.34	1.09
2:B:150:GLY:O	2:B:154:ILE:HG13	1.52	1.09
2:B:384:ILE:C	2:B:386:GLU:H	1.52	1.09
1:A:59:GLY:C	1:A:62:VAL:O	1.95	1.09
1:A:237:SER:O	1:A:241:SER:OG	1.69	1.09
1:A:407:TRP:HH2	2:B:165:ILE:HD12	1.02	1.09
2:B:7:ILE:HG12	2:B:66:ILE:HD13	1.09	1.09
2:B:56:ALA:HB3	2:B:62:VAL:CG2	1.81	1.09
1:A:97:GLU:HB3	1:A:110:ILE:CG2	1.81	1.09
2:B:3:GLU:OE1	2:B:130:ASP:HB2	0.91	1.09
2:B:435:TYR:O	2:B:436:GLN:CD	1.95	1.09
1:A:2:ARG:O	1:A:31:GLN:HG3	1.51	1.08
1:A:191:THR:HG21	1:A:421:ALA:CB	1.81	1.08
2:B:24:ILE:O	2:B:25:SER:C	1.80	1.08
2:B:313:LEU:N	2:B:380:ASN:O	1.86	1.08
1:A:277:SER:OG	1:A:280:LYS:HG2	0.93	1.08
2:B:180:THR:O	2:B:398:MET:HE3	1.44	1.08
2:B:313:LEU:CD2	2:B:344:VAL:CG1	2.32	1.08
2:B:3:GLU:HA	2:B:31:ASP:CB	1.83	1.08
2:B:44:LEU:HD23	2:B:85:GLN:HG3	1.12	1.08
2:B:244:PHE:CG	2:B:245:PRO:HD2	1.89	1.08
2:B:313:LEU:HD22	2:B:344:VAL:HG11	1.13	1.08
1:A:252:LEU:HA	1:A:255:PHE:HD2	1.18	1.08
1:A:277:SER:OG	1:A:280:LYS:N	1.87	1.08
1:A:360:PRO:HG3	1:A:371:VAL:O	0.91	1.08
2:B:102:ASN:HB2	2:B:105:LYS:HD2	1.33	1.08
2:B:305:CYS:SG	2:B:384:ILE:CD1	2.41	1.08
1:A:3:GLU:CA	1:A:31:GLN:HB2	1.82	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLY:O	1:A:46:ASP:CG	1.96	1.08
1:A:204:VAL:HG12	1:A:209:ILE:HD11	1.10	1.08
1:A:332:ILE:HD13	1:A:353:VAL:HG21	1.35	1.08
2:B:44:LEU:C	2:B:47:GLU:HG3	1.79	1.08
1:A:31:GLN:NE2	1:A:243:ARG:HG3	1.56	1.07
1:A:103:TYR:HD2	1:A:189:LEU:CD2	1.59	1.07
1:A:108:TYR:CE2	1:A:417:GLU:OE2	2.06	1.07
1:A:171:ILE:N	1:A:203:MET:HE1	1.69	1.07
1:A:179:THR:HG21	1:A:181:VAL:HB	1.13	1.07
1:A:217:LEU:HD11	1:A:368:LEU:HD21	1.15	1.07
1:A:328:VAL:HG13	1:A:332:ILE:HD11	1.31	1.07
2:B:19:LYS:CD	2:B:228:ASN:HB2	1.84	1.07
2:B:49:ILE:C	2:B:61:TYR:CD2	2.32	1.07
2:B:107:HIS:C	2:B:152:LEU:CD1	2.27	1.07
2:B:135:PHE:HB3	2:B:166:MET:HE3	1.24	1.07
2:B:174:SER:OG	2:B:207:GLU:CB	2.02	1.07
2:B:243:ARG:HH21	2:B:252:LEU:HD21	1.17	1.07
2:B:233:ALA:HB1	2:B:272:PHE:CD2	1.87	1.07
2:B:244:PHE:HE2	2:B:358:ILE:HD12	1.06	1.07
1:A:184:PRO:CG	1:A:395:PHE:HA	1.84	1.07
1:A:397:LEU:HD23	1:A:401:LYS:HD2	1.19	1.07
2:B:33:THR:O	2:B:59:ASN:ND2	1.87	1.07
1:A:78:VAL:HG11	1:A:87:PHE:HE1	1.19	1.07
2:B:319:PHE:CE1	2:B:328:VAL:HG11	1.87	1.07
2:B:33:THR:H	2:B:59:ASN:ND2	1.47	1.07
2:B:107:HIS:NE2	2:B:152:LEU:CD2	2.18	1.07
2:B:178:SER:CB	4:B:500:GDP:O3'	2.03	1.07
2:B:277:SER:HB2	2:B:280:SER:HB2	1.30	1.07
1:A:30:ILE:HG21	1:A:64:ARG:HG2	1.15	1.06
1:A:192:HIS:ND1	1:A:193:THR:N	2.03	1.06
1:A:250:VAL:HG21	1:A:352:LYS:HE2	1.13	1.06
1:A:262:TYR:HB3	1:A:263:PRO:CD	1.84	1.06
2:B:49:ILE:C	2:B:61:TYR:HD2	1.63	1.06
2:B:107:HIS:HA	2:B:152:LEU:HD12	1.35	1.06
2:B:44:LEU:HD21	2:B:86:ILE:N	1.67	1.06
1:A:32:PRO:O	1:A:34:GLY:N	1.89	1.06
1:A:224:TYR:H	2:B:325:MET:HB2	1.19	1.06
2:B:36:TYR:CD2	2:B:244:PHE:CE1	2.22	1.06
2:B:382:THR:HG21	2:B:436:GLN:OE1	1.51	1.06
1:A:24:TYR:O	1:A:26:LEU:N	1.87	1.06
2:B:53:TYR:CD1	2:B:87:PHE:CZ	2.44	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:C	2:B:4:ILE:HG13	1.77	1.06
2:B:75:MET:HE1	2:B:79:ARG:HD2	1.06	1.06
2:B:135:PHE:CB	2:B:166:MET:HE1	1.80	1.06
2:B:154:ILE:HD12	2:B:192:HIS:CE1	1.90	1.06
2:B:370:GLY:C	5:B:501:TXL:H183	1.81	1.06
1:A:105:ARG:NH2	1:A:110:ILE:HD11	1.67	1.05
1:A:204:VAL:HG11	1:A:209:ILE:HD11	1.10	1.05
1:A:206:ASN:HD22	1:A:227:LEU:HD21	0.97	1.05
1:A:250:VAL:HG13	1:A:254:GLU:HB3	1.08	1.05
1:A:292:THR:HG22	1:A:319:TYR:OH	1.53	1.05
2:B:7:ILE:HG12	2:B:66:ILE:HG21	1.34	1.05
2:B:22:GLU:CB	2:B:83:PHE:CE2	2.39	1.05
2:B:36:TYR:CE2	2:B:244:PHE:HE1	1.46	1.05
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.10	1.05
2:B:275:LEU:HG	2:B:294:GLN:HE22	1.21	1.05
1:A:97:GLU:HB2	1:A:110:ILE:HG21	1.38	1.05
2:B:35:SER:N	2:B:60:LYS:HE3	1.71	1.05
2:B:70:LEU:HD11	2:B:94:PHE:CD2	1.92	1.05
2:B:141:LEU:CD1	2:B:172:VAL:HA	1.86	1.05
2:B:265:LEU:HD23	2:B:267:PHE:CZ	1.92	1.05
1:A:70:LEU:HD12	1:A:145:THR:CB	1.86	1.05
1:A:174:ALA:CB	1:A:175:PRO:HD2	1.86	1.05
2:B:19:LYS:CG	2:B:228:ASN:HB2	1.86	1.05
2:B:104:ALA:HA	2:B:413:MET:HE3	1.38	1.05
2:B:158:ARG:HD2	2:B:197:ASN:N	1.70	1.05
2:B:279:GLY:C	2:B:281:GLN:H	1.63	1.05
1:A:31:GLN:HE22	1:A:243:ARG:HG3	0.94	1.05
1:A:103:TYR:CD1	1:A:188:ILE:HG22	1.89	1.05
2:B:75:MET:HE2	2:B:79:ARG:HD3	1.35	1.05
2:B:103:TRP:NE1	2:B:189:LEU:HD23	1.70	1.05
2:B:141:LEU:HD12	2:B:172:VAL:CA	1.86	1.05
1:A:121:ARG:O	1:A:125:LEU:HG	1.56	1.05
1:A:217:LEU:HD11	1:A:368:LEU:CD2	1.86	1.04
2:B:308:ARG:HD3	2:B:342:TYR:CE2	1.92	1.04
2:B:405:LEU:HD12	2:B:408:TYR:CG	1.88	1.04
1:A:184:PRO:HG3	1:A:395:PHE:HB2	1.33	1.04
2:B:24:ILE:C	2:B:26:ASP:H	1.55	1.04
1:A:103:TYR:OH	1:A:151:SER:CB	2.04	1.04
1:A:205:ASP:OD1	1:A:303:VAL:CG2	1.98	1.04
2:B:7:ILE:CB	2:B:137:LEU:CD2	2.34	1.04
2:B:172:VAL:HG12	2:B:173:PRO:CD	1.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:MET:CB	2:B:268:PHE:CE1	2.38	1.04
1:A:126:ALA:O	1:A:132:LEU:HD11	1.57	1.04
1:A:312:TYR:CD2	1:A:381:THR:CG2	2.40	1.04
2:B:69:ASP:OD2	2:B:74:THR:CB	2.06	1.04
2:B:145:THR:O	2:B:149:MET:CB	2.05	1.04
2:B:180:THR:O	2:B:398:MET:HE1	1.48	1.04
2:B:194:LEU:HA	2:B:265:LEU:CB	1.88	1.04
2:B:200:GLU:OE2	2:B:256:ALA:HA	1.56	1.04
1:A:266:HIS:NE2	1:A:432:TYR:CE1	2.26	1.04
1:A:306:ASP:OD1	1:A:308:ARG:CB	2.05	1.04
2:B:4:ILE:HD12	2:B:30:ILE:O	1.57	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	1.03
1:A:405:VAL:HG22	1:A:409:VAL:HG23	1.39	1.03
2:B:56:ALA:O	2:B:59:ASN:O	1.73	1.03
2:B:102:ASN:OD1	2:B:408:TYR:CE1	2.09	1.03
2:B:151:THR:CG2	2:B:192:HIS:ND1	2.14	1.03
2:B:242:LEU:HD22	2:B:250:ALA:H	1.23	1.03
2:B:295:MET:CE	2:B:375:ALA:CB	1.93	1.03
1:A:183:GLU:HB3	1:A:394:LYS:CB	1.87	1.03
2:B:48:ARG:HH11	2:B:60:LYS:HA	1.17	1.03
1:A:16:ILE:HD13	1:A:138:PHE:HD1	0.88	1.03
1:A:155:GLU:CG	1:A:192:HIS:CD2	2.41	1.03
1:A:193:THR:O	1:A:194:THR:O	1.77	1.03
2:B:56:ALA:HB3	2:B:62:VAL:HB	1.35	1.03
2:B:78:VAL:O	2:B:82:PRO:HG2	1.59	1.03
2:B:311:ARG:CG	2:B:341:SER:O	2.04	1.03
1:A:191:THR:O	1:A:194:THR:HB	1.56	1.03
1:A:324:VAL:HB	1:A:327:ASP:CG	1.82	1.03
2:B:4:ILE:CD1	2:B:30:ILE:HG22	1.88	1.03
2:B:102:ASN:HD22	2:B:105:LYS:HE3	1.17	1.03
2:B:147:SER:CA	2:B:189:LEU:CD1	2.36	1.03
2:B:287:THR:O	2:B:291:LEU:HG	0.85	1.03
2:B:397:ALA:HA	2:B:401:ARG:HD3	1.33	1.03
1:A:179:THR:HG21	1:A:181:VAL:CB	1.87	1.03
1:A:407:TRP:CH2	2:B:165:ILE:HD13	1.91	1.03
2:B:66:ILE:HG13	2:B:121:VAL:HG11	1.04	1.03
2:B:32:PRO:HB2	2:B:59:ASN:ND2	1.00	1.02
2:B:44:LEU:CD2	2:B:85:GLN:CG	2.15	1.02
2:B:384:ILE:C	2:B:386:GLU:N	2.11	1.02
2:B:19:LYS:HD2	2:B:228:ASN:HB2	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:PHE:CD1	2:B:380:ASN:ND2	2.28	1.02
1:A:210:TYR:CD1	2:B:326:LYS:CD	2.43	1.02
1:A:276:ILE:HD12	1:A:371:VAL:HG22	1.41	1.02
2:B:103:TRP:HD1	2:B:189:LEU:HD21	1.17	1.02
1:A:97:GLU:HB3	1:A:110:ILE:HG21	1.35	1.02
1:A:217:LEU:CD2	1:A:368:LEU:HD11	1.88	1.02
2:B:70:LEU:HD23	2:B:145:THR:HG22	1.05	1.02
2:B:326:LYS:O	2:B:330:GLU:HG3	1.56	1.02
1:A:30:ILE:O	1:A:32:PRO:CD	2.08	1.02
1:A:70:LEU:CG	1:A:145:THR:CG2	2.36	1.01
1:A:204:VAL:HG23	1:A:231:ILE:HG23	1.41	1.01
1:A:206:ASN:O	1:A:210:TYR:HD2	1.41	1.01
2:B:80:SER:O	2:B:82:PRO:CD	2.07	1.01
2:B:107:HIS:CE1	2:B:152:LEU:CD2	2.42	1.01
2:B:172:VAL:HG13	2:B:173:PRO:HD2	1.05	1.01
2:B:190:SER:O	2:B:193:GLN:N	1.93	1.01
2:B:275:LEU:HG	2:B:294:GLN:NE2	1.73	1.01
2:B:287:THR:CG2	2:B:289:PRO:CD	2.38	1.01
1:A:4:CYS:HB2	1:A:30:ILE:HG23	1.03	1.01
2:B:422:GLU:O	2:B:426:ASN:HB2	1.60	1.01
1:A:62:VAL:HG13	1:A:63:PRO:HD2	1.07	1.01
1:A:73:THR:HG21	2:B:249:ASN:ND2	1.74	1.01
1:A:115:ILE:HD11	1:A:152:LEU:HG	1.40	1.01
1:A:224:TYR:HD2	2:B:325:MET:HB3	0.87	1.01
1:A:225:THR:CG2	2:B:247:GLN:NE2	2.23	1.01
2:B:296:PHE:CE1	2:B:335:VAL:HG11	1.96	1.01
2:B:343:PHE:HD1	2:B:350:ASN:CG	1.67	1.01
2:B:384:ILE:O	2:B:386:GLU:N	1.93	1.01
2:B:405:LEU:CD1	2:B:408:TYR:HD2	1.53	1.01
1:A:103:TYR:CE1	1:A:188:ILE:HG22	1.96	1.01
2:B:286:LEU:CD1	2:B:372:LYS:CB	2.39	1.01
1:A:296:PHE:HE1	1:A:335:ILE:CD1	1.67	1.00
2:B:103:TRP:NE1	2:B:148:GLY:HA2	1.75	1.00
2:B:192:HIS:CB	2:B:196:GLU:HG3	1.90	1.00
1:A:88:HIS:CG	1:A:89:PRO:HD2	1.95	1.00
1:A:103:TYR:CD2	1:A:147:SER:CB	2.36	1.00
1:A:184:PRO:CD	1:A:395:PHE:HA	1.91	1.00
1:A:296:PHE:CZ	1:A:335:ILE:HG21	1.95	1.00
1:A:328:VAL:HG13	1:A:332:ILE:CD1	1.90	1.00
2:B:75:MET:HA	2:B:75:MET:HE3	1.38	1.00
2:B:262:PHE:HB3	2:B:263:PRO:HD2	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:CB	1:A:390:ARG:HH22	1.75	1.00
2:B:33:THR:N	2:B:59:ASN:ND2	2.04	1.00
2:B:191:VAL:HG21	2:B:421:ALA:HA	1.42	1.00
2:B:201:THR:HG23	2:B:265:LEU:CD1	1.91	1.00
2:B:260:VAL:CG1	2:B:262:PHE:O	2.08	1.00
2:B:396:THR:OG1	2:B:422:GLU:OE2	1.79	1.00
1:A:103:TYR:CE2	1:A:189:LEU:CD2	2.38	1.00
1:A:108:TYR:O	1:A:112:LYS:HD2	1.61	1.00
1:A:256:GLN:O	1:A:260:VAL:HG23	1.61	1.00
2:B:405:LEU:HD12	2:B:408:TYR:HB2	1.03	1.00
1:A:2:ARG:HG2	1:A:133:GLN:CD	1.85	1.00
1:A:104:ALA:HA	1:A:108:TYR:CD2	1.97	1.00
1:A:145:THR:O	1:A:149:PHE:HB3	1.62	1.00
2:B:184:PRO:CD	2:B:399:PHE:CE2	2.37	1.00
2:B:343:PHE:HB3	2:B:350:ASN:HD22	1.26	1.00
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.42	1.00
2:B:102:ASN:HB2	2:B:105:LYS:CD	1.92	1.00
2:B:111:GLY:O	2:B:115:VAL:N	1.95	1.00
1:A:143:GLY:O	1:A:146:GLY:N	1.95	1.00
1:A:51:THR:HG22	1:A:52:PHE:N	1.74	0.99
2:B:173:PRO:CG	2:B:391:ILE:HD11	1.92	0.99
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.07	0.99
2:B:44:LEU:CD2	2:B:86:ILE:H	1.61	0.99
2:B:147:SER:HB3	2:B:189:LEU:CG	1.77	0.99
1:A:269:LEU:O	1:A:378:LEU:HA	1.61	0.99
1:A:397:LEU:CD2	1:A:401:LYS:CD	2.40	0.99
2:B:158:ARG:CA	2:B:197:ASN:ND2	1.74	0.99
1:A:312:TYR:O	1:A:344:VAL:HG23	1.58	0.99
2:B:22:GLU:CD	2:B:83:PHE:CG	2.39	0.99
2:B:181:VAL:HG13	2:B:399:PHE:CE1	1.97	0.99
2:B:243:ARG:NH2	2:B:252:LEU:HD11	1.77	0.99
1:A:36:MET:SD	1:A:61:HIS:N	2.33	0.99
1:A:407:TRP:CH2	2:B:256:ALA:HB3	1.96	0.99
2:B:260:VAL:HG13	2:B:266:HIS:ND1	1.78	0.99
2:B:313:LEU:HA	2:B:344:VAL:HG21	1.43	0.99
2:B:101:ASN:O	2:B:102:ASN:CG	2.05	0.99
1:A:433:GLU:O	1:A:437:VAL:CG2	2.10	0.99
2:B:181:VAL:HG22	2:B:404:PHE:CE2	1.97	0.99
1:A:30:ILE:C	1:A:32:PRO:HD3	1.81	0.98
1:A:103:TYR:CE2	1:A:189:LEU:HA	1.98	0.98
1:A:115:ILE:HG21	1:A:152:LEU:HD21	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HG2	2:B:326:LYS:CD	1.93	0.98
1:A:250:VAL:HG13	1:A:254:GLU:HG2	1.44	0.98
1:A:422:ARG:O	1:A:426:ALA:HB2	1.63	0.98
2:B:155:SER:O	2:B:159:GLU:HG3	1.63	0.98
2:B:174:SER:OG	2:B:207:GLU:HB2	1.63	0.98
2:B:286:LEU:HD11	2:B:371:LEU:O	1.62	0.98
2:B:405:LEU:HD11	2:B:408:TYR:HB3	1.44	0.98
1:A:45:GLY:O	1:A:46:ASP:HB2	1.61	0.98
2:B:173:PRO:HG3	2:B:391:ILE:HD11	1.45	0.98
1:A:171:ILE:N	1:A:203:MET:CE	2.24	0.98
1:A:343:PHE:CZ	1:A:351:PHE:CZ	2.50	0.98
2:B:194:LEU:HA	2:B:265:LEU:HB3	1.44	0.98
2:B:320:ARG:HG2	2:B:374:SER:HG	1.24	0.98
2:B:405:LEU:HD22	2:B:418:PHE:CE1	1.98	0.98
1:A:219:ILE:CG2	1:A:219:ILE:CG1	2.40	0.98
1:A:313:MET:HE1	1:A:346:TRP:CH2	1.97	0.98
2:B:23:VAL:HG22	5:B:501:TXL:H333	1.41	0.98
1:A:174:ALA:HB3	1:A:175:PRO:HD2	1.44	0.98
1:A:184:PRO:CB	1:A:395:PHE:CD2	2.45	0.98
1:A:76:ASP:O	1:A:80:THR:N	1.97	0.98
1:A:194:THR:HG22	1:A:195:LEU:HG	1.43	0.98
2:B:275:LEU:HD11	2:B:300:ASN:ND2	1.78	0.98
1:A:72:PRO:O	1:A:76:ASP:N	1.96	0.98
1:A:242:LEU:HB3	1:A:250:VAL:O	1.63	0.98
1:A:270:ALA:O	1:A:302:MET:HG2	1.63	0.98
2:B:199:ASP:OD2	2:B:256:ALA:HB2	1.62	0.98
1:A:68:VAL:CG1	1:A:149:PHE:CZ	2.47	0.98
2:B:275:LEU:CD1	2:B:294:GLN:HE21	1.74	0.98
1:A:32:PRO:C	1:A:34:GLY:H	1.69	0.98
1:A:141:PHE:O	1:A:186:ASN:ND2	1.58	0.98
2:B:7:ILE:HB	2:B:137:LEU:HD23	1.01	0.98
1:A:22:GLU:HG2	1:A:85:GLN:NE2	1.78	0.98
1:A:158:SER:HB3	1:A:197:HIS:CB	1.34	0.98
2:B:36:TYR:CD2	2:B:244:PHE:HE1	1.43	0.98
2:B:70:LEU:HD23	2:B:145:THR:CG2	1.93	0.98
1:A:217:LEU:HD13	1:A:368:LEU:HD11	1.02	0.97
1:A:429:GLU:O	1:A:433:GLU:HG3	1.64	0.97
2:B:111:GLY:O	2:B:115:VAL:CG2	2.12	0.97
2:B:142:GLY:CA	2:B:182:VAL:HG22	1.94	0.97
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.30	0.97
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.58	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASP:CB	1:A:303:VAL:HA	1.92	0.97
1:A:397:LEU:HD22	1:A:401:LYS:CD	1.93	0.97
2:B:102:ASN:ND2	2:B:105:LYS:NZ	2.12	0.97
2:B:243:ARG:HH21	2:B:252:LEU:CD2	1.78	0.97
1:A:78:VAL:CG1	1:A:87:PHE:CE1	2.46	0.97
1:A:312:TYR:O	1:A:344:VAL:HG22	1.62	0.97
1:A:369:ALA:HB2	1:A:371:VAL:HG23	1.46	0.97
2:B:385:GLN:CG	2:B:389:LYS:CE	2.37	0.97
2:B:287:THR:HG22	2:B:290:GLU:H	1.29	0.97
1:A:100:ALA:HB1	1:A:105:ARG:CD	1.91	0.97
1:A:372:GLN:O	1:A:373:ARG:HG3	1.65	0.97
2:B:44:LEU:HD11	2:B:86:ILE:O	1.63	0.97
2:B:175:PRO:O	2:B:176:LYS:HG2	1.49	0.97
2:B:284:ARG:HD2	2:B:290:GLU:OE1	1.62	0.97
2:B:154:ILE:CG2	2:B:198:THR:CG2	2.40	0.97
1:A:42:ILE:O	1:A:42:ILE:HG22	1.60	0.97
1:A:78:VAL:HG11	1:A:87:PHE:CE1	2.00	0.97
1:A:217:LEU:CD1	1:A:368:LEU:HD21	1.95	0.97
2:B:19:LYS:HB2	2:B:228:ASN:HB3	1.42	0.97
1:A:241:SER:HB2	1:A:356:ASN:ND2	1.78	0.97
2:B:3:GLU:HA	2:B:31:ASP:HB3	1.47	0.97
2:B:53:TYR:HE1	2:B:89:PRO:HG3	1.29	0.97
2:B:103:TRP:CD1	2:B:148:GLY:CA	2.47	0.97
2:B:147:SER:HA	2:B:189:LEU:HD13	1.47	0.97
2:B:206:ASN:O	2:B:210:TYR:CE2	2.18	0.97
1:A:119:LEU:O	1:A:122:ILE:HG22	1.65	0.96
1:A:310:GLY:O	1:A:342:GLN:OE1	1.82	0.96
2:B:151:THR:HG22	2:B:192:HIS:CD2	1.96	0.96
2:B:68:VAL:HG11	2:B:149:MET:HE2	1.47	0.96
1:A:9:VAL:CG1	1:A:150:THR:CG2	2.42	0.96
1:A:313:MET:CE	1:A:346:TRP:CH2	2.47	0.96
2:B:206:ASN:O	2:B:210:TYR:CD2	2.18	0.96
1:A:16:ILE:CD1	1:A:138:PHE:HD1	1.78	0.96
1:A:206:ASN:ND2	1:A:227:LEU:HD23	1.79	0.96
1:A:383:ALA:O	1:A:384:ILE:C	2.07	0.96
1:A:407:TRP:CH2	2:B:256:ALA:CB	2.48	0.96
2:B:7:ILE:CA	2:B:66:ILE:CG2	2.38	0.96
2:B:201:THR:HG23	2:B:265:LEU:HD11	0.97	0.96
2:B:346:TRP:O	2:B:347:ILE:CB	2.09	0.96
2:B:3:GLU:HG2	2:B:4:ILE:H	1.27	0.96
2:B:6:HIS:HB2	2:B:65:ALA:HA	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HD13	1:A:156:ARG:NE	1.80	0.96
2:B:4:ILE:CD1	2:B:30:ILE:O	2.14	0.96
1:A:224:TYR:HD2	2:B:325:MET:CB	1.78	0.96
1:A:309:HIS:CG	1:A:386:GLU:OE2	2.19	0.96
2:B:208:ALA:CB	2:B:303:ALA:O	2.13	0.96
2:B:229:HIS:CD2	5:B:501:TXL:H37	1.98	0.96
1:A:53:PHE:CA	1:A:88:HIS:NE2	2.20	0.96
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.46	0.96
2:B:175:PRO:C	2:B:176:LYS:CG	2.32	0.96
1:A:3:GLU:O	1:A:132:LEU:C	2.09	0.95
1:A:241:SER:HB2	1:A:356:ASN:HD22	1.27	0.95
2:B:70:LEU:HD11	2:B:94:PHE:CE2	2.01	0.95
2:B:78:VAL:C	2:B:82:PRO:HG2	1.91	0.95
2:B:104:ALA:HA	2:B:108:TYR:HD2	1.20	0.95
1:A:101:ASN:O	1:A:102:ASN:ND2	1.97	0.95
2:B:39:ASP:O	2:B:40:SER:OG	1.82	0.95
2:B:312:TYR:HA	2:B:381:SER:HA	1.43	0.95
2:B:158:ARG:CG	2:B:197:ASN:CG	2.38	0.95
2:B:343:PHE:HD1	2:B:350:ASN:ND2	1.62	0.95
1:A:217:LEU:HD22	1:A:368:LEU:HD11	1.47	0.95
2:B:20:PHE:HE2	2:B:235:MET:HB3	0.80	0.95
2:B:79:ARG:O	2:B:80:SER:CB	2.10	0.95
1:A:31:GLN:N	1:A:32:PRO:HD2	1.81	0.95
1:A:141:PHE:O	1:A:182:VAL:HG13	1.66	0.95
1:A:158:SER:HB2	1:A:197:HIS:CB	1.67	0.95
1:A:314:ALA:HB3	1:A:380:ASN:HD22	1.31	0.95
2:B:97:SER:O	2:B:110:GLU:OE2	1.84	0.95
1:A:68:VAL:HG11	1:A:149:PHE:CE1	2.01	0.95
1:A:397:LEU:HA	1:A:401:LYS:CB	1.96	0.95
2:B:433:GLN:HG2	2:B:437:ASP:OD2	1.65	0.95
1:A:20:CYS:O	1:A:24:TYR:HD2	1.46	0.95
1:A:103:TYR:HE2	1:A:189:LEU:HD23	1.29	0.95
1:A:221:ARG:O	2:B:324:SER:HB3	1.67	0.95
2:B:398:MET:O	2:B:401:ARG:HB3	1.66	0.95
1:A:229:ARG:O	1:A:233:GLN:HG3	1.66	0.94
1:A:333:ALA:O	1:A:337:THR:HG23	1.66	0.94
2:B:4:ILE:CD1	2:B:30:ILE:C	2.40	0.94
1:A:212:ILE:HD13	1:A:230:LEU:HD21	1.49	0.94
1:A:250:VAL:CG2	1:A:352:LYS:CE	2.43	0.94
1:A:294:ALA:O	1:A:300:ASN:ND2	1.99	0.94
2:B:7:ILE:CB	2:B:137:LEU:HD23	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:GLN:OE1	4:B:500:GDP:O6	1.84	0.94
2:B:287:THR:HG21	2:B:289:PRO:HG2	1.49	0.94
1:A:108:TYR:HA	1:A:112:LYS:HE3	1.47	0.94
1:A:183:GLU:OE2	1:A:394:LYS:NZ	1.76	0.94
1:A:250:VAL:HG22	1:A:352:LYS:HE2	1.49	0.94
2:B:158:ARG:CD	2:B:197:ASN:CA	2.39	0.94
2:B:181:VAL:O	2:B:399:PHE:CE2	2.19	0.94
2:B:382:THR:HG23	2:B:436:GLN:OE1	1.64	0.94
1:A:405:VAL:CG2	1:A:405:VAL:CG1	2.44	0.94
2:B:79:ARG:O	2:B:80:SER:HB3	1.66	0.94
2:B:142:GLY:HA2	2:B:182:VAL:HG22	1.50	0.94
1:A:36:MET:SD	1:A:61:HIS:CA	2.56	0.94
2:B:183:GLU:CD	2:B:394:GLN:CB	2.41	0.94
2:B:229:HIS:HD2	5:B:501:TXL:C38	1.47	0.94
2:B:319:PHE:HE1	2:B:353:THR:HG23	0.78	0.94
1:A:210:TYR:HE1	2:B:326:LYS:HG3	1.28	0.94
1:A:250:VAL:HG13	1:A:352:LYS:HZ3	1.12	0.94
1:A:212:ILE:HD11	1:A:230:LEU:HD22	0.96	0.94
1:A:258:ASN:CG	1:A:352:LYS:HD2	1.93	0.94
2:B:48:ARG:NH1	2:B:60:LYS:CA	2.31	0.94
2:B:229:HIS:NE2	5:B:501:TXL:H343	1.82	0.94
2:B:259:MET:HB3	2:B:268:PHE:CZ	2.02	0.94
1:A:59:GLY:CA	1:A:62:VAL:O	2.15	0.94
1:A:107:HIS:CB	1:A:148:GLY:C	2.36	0.94
1:A:107:HIS:HD2	1:A:148:GLY:O	1.51	0.94
1:A:191:THR:O	1:A:194:THR:CB	2.14	0.94
1:A:225:THR:HG22	2:B:247:GLN:HE22	1.32	0.94
1:A:252:LEU:HA	1:A:255:PHE:CD2	2.02	0.94
2:B:172:VAL:HG12	2:B:173:PRO:HD2	1.43	0.94
1:A:250:VAL:HG22	1:A:254:GLU:HG2	1.50	0.94
2:B:44:LEU:HD21	2:B:86:ILE:H	1.00	0.94
1:A:65:ALA:CB	1:A:91:GLN:OE1	2.16	0.94
1:A:220:GLU:C	1:A:222:PRO:CD	2.37	0.94
2:B:182:VAL:CG1	2:B:186:ASN:ND2	2.30	0.94
2:B:295:MET:CE	2:B:375:ALA:CA	2.45	0.94
2:B:346:TRP:CZ3	2:B:347:ILE:CG1	2.45	0.94
1:A:204:VAL:CG2	1:A:231:ILE:CG2	2.24	0.93
2:B:71:GLU:O	2:B:73:GLY:N	2.01	0.93
2:B:275:LEU:HD12	2:B:294:GLN:HE21	1.29	0.93
2:B:39:ASP:O	2:B:40:SER:CB	2.16	0.93
2:B:158:ARG:HG3	2:B:197:ASN:CG	1.93	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:HB3	2:B:371:LEU:HD21	1.50	0.93
2:B:274:PRO:O	2:B:276:THR:HG23	1.67	0.93
2:B:142:GLY:HA2	2:B:185:TYR:CD1	2.03	0.93
1:A:51:THR:HG22	1:A:52:PHE:H	1.26	0.93
1:A:53:PHE:N	1:A:88:HIS:HE2	1.53	0.93
1:A:181:VAL:O	1:A:184:PRO:O	1.87	0.93
1:A:217:LEU:HG	1:A:218:ASP:N	1.77	0.93
2:B:154:ILE:HD12	2:B:192:HIS:NE2	1.83	0.93
2:B:241:CYS:SG	2:B:320:ARG:HD3	2.08	0.93
1:A:426:ALA:O	1:A:429:GLU:N	2.00	0.93
2:B:56:ALA:HB1	2:B:60:LYS:O	1.68	0.93
1:A:343:PHE:HE2	1:A:351:PHE:HZ	1.08	0.93
2:B:181:VAL:O	2:B:399:PHE:HE2	1.50	0.93
2:B:386:GLU:O	2:B:388:PHE:N	2.01	0.93
1:A:31:GLN:HE22	1:A:243:ARG:CB	1.81	0.93
1:A:184:PRO:CG	1:A:395:PHE:CB	2.45	0.93
1:A:272:TYR:CD1	1:A:274:PRO:O	2.22	0.93
2:B:435:TYR:N	2:B:435:TYR:HD1	1.66	0.93
1:A:59:GLY:O	1:A:62:VAL:C	2.12	0.93
2:B:86:ILE:HD12	2:B:91:ASN:HD21	1.33	0.93
2:B:103:TRP:CZ3	2:B:413:MET:HE2	2.02	0.93
2:B:275:LEU:CG	2:B:294:GLN:NE2	2.32	0.93
2:B:346:TRP:CE3	2:B:347:ILE:CD1	2.43	0.93
1:A:15:GLN:HA	1:A:18:ASN:ND2	1.83	0.93
1:A:405:VAL:CG2	1:A:409:VAL:HG23	1.98	0.93
2:B:19:LYS:HG3	2:B:228:ASN:CG	1.92	0.93
1:A:184:PRO:CG	1:A:395:PHE:CA	2.47	0.93
1:A:250:VAL:CG1	1:A:254:GLU:CG	2.46	0.93
2:B:49:ILE:CA	2:B:61:TYR:HD2	1.82	0.93
2:B:343:PHE:HB3	2:B:350:ASN:ND2	1.83	0.93
1:A:83:TYR:CD2	1:A:83:TYR:O	2.22	0.92
1:A:119:LEU:HD11	1:A:156:ARG:HD3	1.48	0.92
1:A:225:THR:HG22	2:B:247:GLN:NE2	1.84	0.92
1:A:277:SER:H	1:A:280:LYS:CG	1.82	0.92
1:A:64:ARG:NH2	1:A:132:LEU:CD2	2.05	0.92
2:B:107:HIS:ND1	2:B:152:LEU:HD21	1.85	0.92
2:B:184:PRO:CD	2:B:398:MET:SD	2.57	0.92
1:A:177:VAL:CG1	1:A:178:SER:H	1.78	0.92
1:A:193:THR:O	1:A:194:THR:C	2.05	0.92
1:A:204:VAL:HG12	1:A:209:ILE:CD1	1.87	0.92
2:B:8:GLN:HE21	2:B:21:TRP:NE1	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:TYR:N	2:B:435:TYR:CD1	2.32	0.92
1:A:68:VAL:HG11	1:A:149:PHE:HZ	1.30	0.92
1:A:158:SER:HB3	1:A:197:HIS:HB2	1.51	0.92
1:A:217:LEU:CD1	1:A:368:LEU:CD2	2.46	0.92
1:A:230:LEU:HG	1:A:302:MET:HE1	1.51	0.92
2:B:343:PHE:CD1	2:B:350:ASN:ND2	2.37	0.92
1:A:332:ILE:HD13	1:A:353:VAL:CG2	1.99	0.92
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.05	0.92
2:B:184:PRO:CB	2:B:399:PHE:CG	2.41	0.92
2:B:241:CYS:O	2:B:242:LEU:HB2	1.69	0.92
2:B:369:ARG:O	5:B:501:TXL:O9	1.88	0.92
2:B:426:ASN:O	2:B:429:VAL:N	2.00	0.92
2:B:151:THR:HG22	2:B:192:HIS:NE2	1.83	0.92
1:A:103:TYR:HE2	1:A:189:LEU:HA	1.32	0.92
2:B:346:TRP:HE3	2:B:347:ILE:HG12	1.33	0.92
1:A:103:TYR:H	1:A:408:TYR:HE1	0.96	0.92
1:A:176:GLN:HE21	2:B:333:LEU:HD22	0.76	0.92
1:A:256:GLN:O	1:A:260:VAL:CG2	2.16	0.92
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.52	0.92
2:B:126:SER:HA	2:B:132:LEU:HD12	1.50	0.92
2:B:433:GLN:HG2	2:B:437:ASP:CG	1.95	0.92
1:A:250:VAL:HG22	1:A:352:LYS:CE	2.00	0.92
1:A:64:ARG:HH22	1:A:132:LEU:HD22	0.76	0.91
1:A:155:GLU:HG2	1:A:196:GLU:HG3	1.51	0.91
1:A:258:ASN:OD1	1:A:352:LYS:HD2	1.69	0.91
1:A:277:SER:H	1:A:280:LYS:HG3	1.34	0.91
2:B:102:ASN:ND2	2:B:105:LYS:CE	2.33	0.91
2:B:229:HIS:CB	5:B:501:TXL:H38	2.01	0.91
1:A:5:ILE:HG21	1:A:135:PHE:HE1	1.35	0.91
1:A:105:ARG:NH1	2:B:253:ARG:CZ	2.33	0.91
1:A:180:ALA:HB1	1:A:398:MET:HE3	1.51	0.91
2:B:192:HIS:HA	2:B:196:GLU:HG2	1.53	0.91
1:A:154:MET:HE3	1:A:166:LYS:HD3	1.50	0.91
2:B:29:GLY:O	2:B:58:GLY:C	2.14	0.91
2:B:405:LEU:CD2	2:B:418:PHE:HZ	1.84	0.91
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.49	0.91
1:A:312:TYR:CA	1:A:381:THR:HG22	1.99	0.91
2:B:48:ARG:NH1	2:B:60:LYS:HA	1.83	0.91
1:A:108:TYR:O	1:A:112:LYS:CG	2.17	0.91
1:A:210:TYR:CE1	2:B:326:LYS:CD	2.54	0.91
2:B:103:TRP:HE3	2:B:413:MET:HE1	1.08	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:SER:HA	2:B:132:LEU:CD1	2.01	0.91
2:B:313:LEU:HD23	2:B:344:VAL:HG21	1.52	0.91
1:A:3:GLU:HA	1:A:31:GLN:HB2	0.94	0.91
1:A:103:TYR:CG	1:A:188:ILE:CG2	2.54	0.91
1:A:369:ALA:HB3	1:A:371:VAL:HG23	1.50	0.91
1:A:428:LEU:O	1:A:432:TYR:HB2	1.70	0.91
2:B:33:THR:C	2:B:59:ASN:HD21	1.76	0.91
2:B:87:PHE:HD1	2:B:88:ARG:O	1.47	0.91
2:B:101:ASN:O	2:B:102:ASN:CB	2.17	0.91
1:A:59:GLY:HA2	1:A:62:VAL:O	1.70	0.91
1:A:382:THR:O	1:A:385:ALA:HB3	1.71	0.91
2:B:4:ILE:HD13	2:B:30:ILE:HG22	0.93	0.91
2:B:158:ARG:HD2	2:B:197:ASN:HA	1.51	0.91
2:B:239:THR:C	2:B:243:ARG:HD2	1.95	0.91
2:B:24:ILE:O	2:B:27:GLU:N	2.04	0.91
2:B:189:LEU:O	2:B:193:GLN:CG	2.19	0.91
1:A:288:VAL:HG22	1:A:373:ARG:HD3	0.93	0.91
1:A:405:VAL:HG22	1:A:409:VAL:CG2	2.01	0.91
2:B:151:THR:HB	2:B:192:HIS:HD2	1.31	0.91
2:B:268:PHE:HE1	2:B:380:ASN:ND2	1.65	0.91
1:A:177:VAL:HG12	1:A:178:SER:N	1.79	0.90
1:A:328:VAL:CG1	1:A:332:ILE:CD1	2.49	0.90
1:A:328:VAL:CG1	1:A:353:VAL:HG11	2.00	0.90
1:A:26:LEU:CD1	1:A:361:THR:OG1	2.19	0.90
1:A:107:HIS:CD2	1:A:148:GLY:O	2.23	0.90
1:A:107:HIS:HB2	1:A:148:GLY:HA3	1.01	0.90
1:A:222:PRO:CG	2:B:326:LYS:HD2	2.01	0.90
2:B:11:GLN:HB3	4:B:500:GDP:PA	2.11	0.90
2:B:102:ASN:ND2	2:B:105:LYS:HE3	1.85	0.90
2:B:405:LEU:HD12	2:B:408:TYR:CD2	2.00	0.90
2:B:80:SER:O	2:B:82:PRO:N	2.05	0.90
2:B:92:PHE:HD2	2:B:114:LEU:HD11	1.04	0.90
2:B:94:PHE:CD1	2:B:97:SER:HB3	2.06	0.90
2:B:278:ARG:O	2:B:281:GLN:HB3	1.71	0.90
2:B:312:TYR:CA	2:B:381:SER:HB3	2.02	0.90
1:A:31:GLN:HE22	1:A:243:ARG:CD	1.67	0.90
1:A:107:HIS:CG	1:A:148:GLY:CA	2.54	0.90
1:A:407:TRP:CZ2	2:B:256:ALA:CB	2.54	0.90
2:B:20:PHE:CE2	2:B:235:MET:HB2	2.06	0.90
2:B:259:MET:CB	2:B:268:PHE:CZ	2.55	0.90
1:A:106:GLY:O	1:A:111:GLY:HA3	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ASN:HB3	2:B:74:THR:CG2	2.01	0.90
2:B:106:GLY:O	2:B:111:GLY:HA3	1.70	0.90
2:B:118:VAL:HG11	2:B:153:LEU:HD22	1.54	0.90
2:B:275:LEU:CD1	2:B:294:GLN:NE2	2.35	0.90
2:B:312:TYR:CA	2:B:381:SER:CB	2.49	0.90
1:A:312:TYR:CD2	1:A:381:THR:HG21	2.06	0.90
2:B:70:LEU:CD1	2:B:94:PHE:CE2	2.53	0.90
2:B:143:GLY:O	4:B:500:GDP:O3B	1.89	0.90
2:B:260:VAL:HG12	2:B:262:PHE:O	1.69	0.90
1:A:238:ILE:HG23	1:A:255:PHE:CE1	2.05	0.90
1:A:328:VAL:HG12	1:A:332:ILE:HD12	1.53	0.90
2:B:11:GLN:CB	4:B:500:GDP:O2A	2.20	0.90
1:A:166:LYS:O	1:A:199:ASP:HB2	1.72	0.90
1:A:250:VAL:HG13	1:A:352:LYS:NZ	1.86	0.90
2:B:319:PHE:CZ	2:B:328:VAL:CG1	2.54	0.90
2:B:70:LEU:CD2	2:B:145:THR:HG22	1.98	0.89
2:B:295:MET:HE1	2:B:375:ALA:CB	2.02	0.89
1:A:72:PRO:O	1:A:75:ILE:CG2	2.19	0.89
2:B:25:SER:O	2:B:27:GLU:HG3	1.73	0.89
2:B:239:THR:O	2:B:243:ARG:HD2	0.72	0.89
2:B:302:MET:O	2:B:302:MET:HG2	1.72	0.89
2:B:151:THR:CG2	2:B:192:HIS:NE2	2.35	0.89
1:A:53:PHE:N	1:A:88:HIS:HE1	1.41	0.89
1:A:276:ILE:HG21	1:A:282:TYR:CD1	2.08	0.89
2:B:98:GLY:O	2:B:99:ALA:O	1.91	0.89
2:B:229:HIS:HE1	5:B:501:TXL:H343	1.30	0.89
1:A:155:GLU:O	1:A:159:VAL:HG23	1.72	0.89
2:B:385:GLN:HE22	2:B:433:GLN:CD	1.79	0.89
1:A:72:PRO:HA	1:A:75:ILE:CG2	2.03	0.89
1:A:291:ILE:CD1	1:A:373:ARG:HB3	2.03	0.89
2:B:158:ARG:HA	2:B:197:ASN:HD21	1.35	0.89
2:B:104:ALA:CA	2:B:108:TYR:HD2	1.85	0.89
2:B:295:MET:HE1	2:B:375:ALA:HB1	1.50	0.89
2:B:56:ALA:HB3	2:B:62:VAL:HG23	1.54	0.89
2:B:184:PRO:HD2	2:B:399:PHE:CE2	2.06	0.89
2:B:87:PHE:HE1	2:B:89:PRO:HG2	0.84	0.89
2:B:182:VAL:HG13	2:B:186:ASN:HD22	1.29	0.89
2:B:8:GLN:HE21	2:B:21:TRP:HE1	1.21	0.89
1:A:184:PRO:HB3	1:A:395:PHE:HD2	1.33	0.88
1:A:231:ILE:HD13	1:A:302:MET:CE	2.03	0.88
2:B:173:PRO:HG3	2:B:391:ILE:CD1	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:GLU:HB2	2:B:184:PRO:HD3	0.90	0.88
1:A:239:THR:HG23	1:A:243:ARG:HG3	1.54	0.88
1:A:191:THR:CG2	1:A:421:ALA:HB1	2.03	0.88
2:B:7:ILE:HD12	2:B:137:LEU:HD21	1.55	0.88
2:B:44:LEU:CG	2:B:85:GLN:HG3	2.02	0.88
2:B:66:ILE:CG1	2:B:121:VAL:HG11	1.99	0.88
1:A:425:MET:O	1:A:428:LEU:HB3	1.74	0.88
2:B:158:ARG:CD	2:B:197:ASN:CB	2.09	0.88
1:A:65:ALA:HB1	1:A:91:GLN:OE1	1.73	0.88
1:A:67:PHE:HB2	1:A:92:LEU:HD23	1.53	0.88
1:A:206:ASN:O	1:A:210:TYR:CD2	2.25	0.88
1:A:222:PRO:O	2:B:326:LYS:HB2	1.73	0.88
1:A:328:VAL:CG1	1:A:332:ILE:HD12	2.03	0.88
2:B:22:GLU:OE2	2:B:83:PHE:HB2	1.74	0.88
2:B:275:LEU:CG	2:B:294:GLN:HE22	1.85	0.88
1:A:9:VAL:HG11	1:A:150:THR:HG21	1.53	0.88
1:A:93:ILE:HD13	1:A:118:VAL:CG2	2.01	0.88
2:B:53:TYR:CE1	2:B:87:PHE:CE1	2.62	0.88
2:B:142:GLY:HA3	2:B:182:VAL:CG2	2.04	0.88
2:B:243:ARG:NH2	2:B:252:LEU:HD21	1.86	0.88
1:A:183:GLU:CB	1:A:394:LYS:HB3	2.04	0.88
2:B:42:LEU:O	2:B:43:GLN:HG3	1.74	0.88
2:B:183:GLU:OE1	2:B:394:GLN:CB	2.21	0.88
2:B:385:GLN:NE2	2:B:433:GLN:OE1	2.07	0.88
2:B:405:LEU:HD13	2:B:408:TYR:HD2	0.74	0.88
1:A:23:LEU:CD2	1:A:236:SER:HB3	2.04	0.88
2:B:4:ILE:HD12	2:B:30:ILE:CA	2.03	0.88
2:B:234:THR:CB	2:B:302:MET:HE1	2.03	0.88
2:B:284:ARG:CD	2:B:290:GLU:OE1	2.22	0.88
2:B:405:LEU:CD1	2:B:418:PHE:HZ	1.85	0.88
1:A:72:PRO:C	1:A:75:ILE:HG22	1.99	0.88
1:A:88:HIS:ND1	1:A:89:PRO:HD2	1.88	0.88
2:B:57:ALA:CA	2:B:64:ARG:CB	2.38	0.88
2:B:184:PRO:HD3	2:B:398:MET:SD	2.14	0.88
1:A:305:CYS:O	1:A:307:PRO:HD3	1.71	0.87
2:B:49:ILE:CA	2:B:61:TYR:CD2	2.57	0.87
2:B:53:TYR:CE1	2:B:87:PHE:CZ	2.62	0.87
2:B:311:ARG:O	2:B:382:THR:N	2.05	0.87
1:A:81:GLY:O	1:A:82:THR:C	2.18	0.87
2:B:6:HIS:CD2	2:B:21:TRP:HH2	1.92	0.87
2:B:185:TYR:O	2:B:189:LEU:HG	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:O	1:A:252:LEU:HD12	1.73	0.87
1:A:276:ILE:O	1:A:368:LEU:CB	2.21	0.87
2:B:48:ARG:HD2	2:B:60:LYS:HA	1.55	0.87
2:B:172:VAL:HG12	2:B:173:PRO:N	1.89	0.87
2:B:274:PRO:CB	2:B:371:LEU:HD21	2.04	0.87
2:B:194:LEU:CD2	2:B:267:PHE:CE2	2.58	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:382:THR:O	1:A:385:ALA:CB	2.22	0.87
2:B:174:SER:OG	2:B:207:GLU:HB3	1.65	0.87
1:A:196:GLU:O	1:A:197:HIS:ND1	2.08	0.87
2:B:19:LYS:HG3	2:B:228:ASN:HB2	1.43	0.87
2:B:200:GLU:HB3	2:B:268:PHE:HE2	1.37	0.87
1:A:115:ILE:CD1	1:A:152:LEU:CD2	2.45	0.87
1:A:210:TYR:HD1	2:B:326:LYS:CG	1.87	0.87
2:B:96:GLN:C	2:B:98:GLY:N	2.31	0.87
1:A:208:ALA:O	1:A:212:ILE:HG23	1.75	0.87
1:A:222:PRO:HG2	2:B:326:LYS:HD2	1.56	0.87
1:A:277:SER:HB3	1:A:280:LYS:HE2	1.56	0.87
2:B:184:PRO:HG3	2:B:399:PHE:CG	1.84	0.87
2:B:279:GLY:O	2:B:281:GLN:N	2.08	0.87
2:B:320:ARG:CG	2:B:374:SER:OG	2.23	0.87
1:A:30:ILE:C	1:A:32:PRO:HD2	1.98	0.86
1:A:194:THR:HG22	1:A:195:LEU:H	1.38	0.86
2:B:154:ILE:HD13	2:B:198:THR:HG21	1.56	0.86
2:B:172:VAL:HG11	2:B:387:LEU:HD11	1.54	0.86
1:A:76:ASP:O	1:A:80:THR:OG1	1.91	0.86
1:A:174:ALA:HB1	1:A:390:ARG:NH2	1.81	0.86
2:B:200:GLU:OE2	2:B:256:ALA:CA	2.15	0.86
2:B:276:THR:OG1	5:B:501:TXL:H62	1.74	0.86
2:B:384:ILE:CG2	2:B:388:PHE:HE2	1.88	0.86
2:B:33:THR:H	2:B:59:ASN:HD22	0.93	0.86
5:B:501:TXL:H173	5:B:501:TXL:H13	1.57	0.86
1:A:154:MET:HE3	1:A:166:LYS:CD	2.04	0.86
1:A:191:THR:CG2	1:A:421:ALA:CB	2.53	0.86
1:A:303:VAL:CG1	1:A:305:CYS:SG	2.64	0.86
2:B:7:ILE:HA	2:B:66:ILE:HG23	0.89	0.86
2:B:244:PHE:CG	2:B:245:PRO:CD	2.56	0.86
1:A:104:ALA:HA	1:A:108:TYR:HD2	1.39	0.86
2:B:7:ILE:HG13	2:B:66:ILE:HG21	1.58	0.86
2:B:169:PHE:CE1	2:B:235:MET:SD	2.67	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:GLU:O	2:B:331:GLN:HG2	1.75	0.86
1:A:100:ALA:HB1	1:A:105:ARG:HB3	1.55	0.86
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.56	0.86
2:B:178:SER:HB3	4:B:500:GDP:O3'	1.74	0.86
2:B:301:MET:HE1	2:B:377:PHE:CD1	2.09	0.86
2:B:405:LEU:HD21	2:B:418:PHE:HE2	1.41	0.86
1:A:115:ILE:HD13	1:A:152:LEU:CG	2.02	0.86
1:A:231:ILE:CD1	1:A:302:MET:HE2	2.05	0.86
1:A:313:MET:HB2	1:A:380:ASN:O	1.75	0.86
2:B:181:VAL:HA	2:B:398:MET:CE	2.06	0.86
2:B:184:PRO:CG	2:B:399:PHE:CD2	0.91	0.86
2:B:273:ALA:N	2:B:274:PRO:HD2	1.45	0.86
1:A:108:TYR:HA	1:A:112:LYS:CE	2.05	0.86
2:B:107:HIS:CG	2:B:152:LEU:HD21	2.11	0.86
2:B:226:ASP:CG	5:B:501:TXL:C39	2.49	0.86
1:A:276:ILE:HD13	1:A:282:TYR:CD1	2.11	0.86
2:B:144:GLY:N	2:B:185:TYR:CE1	2.44	0.86
2:B:313:LEU:HD23	2:B:344:VAL:HG22	1.58	0.86
1:A:4:CYS:CB	1:A:30:ILE:HG23	1.99	0.86
1:A:109:THR:HG21	1:A:411:GLU:OE1	1.75	0.86
1:A:175:PRO:HD3	1:A:390:ARG:NH2	1.91	0.86
1:A:179:THR:CG2	1:A:181:VAL:HB	2.04	0.86
1:A:224:TYR:HE1	3:A:500:GTP:N3	1.73	0.86
1:A:282:TYR:CD2	1:A:285:GLN:HA	2.11	0.86
1:A:312:TYR:HE2	1:A:377:MET:CE	1.80	0.86
1:A:397:LEU:HA	1:A:401:LYS:HB2	1.57	0.86
2:B:147:SER:CA	2:B:189:LEU:HD13	2.04	0.86
2:B:226:ASP:CG	5:B:501:TXL:H39	2.00	0.86
2:B:241:CYS:HG	2:B:320:ARG:NH1	1.72	0.86
2:B:254:LYS:O	2:B:258:ASN:OD1	1.94	0.86
1:A:271:THR:OG1	1:A:377:MET:HB3	1.76	0.85
2:B:13:GLY:CA	2:B:138:THR:OG1	2.24	0.85
2:B:80:SER:C	2:B:82:PRO:CD	2.48	0.85
1:A:154:MET:HB2	1:A:192:HIS:CE1	2.11	0.85
1:A:306:ASP:OD2	1:A:308:ARG:HD2	1.76	0.85
2:B:158:ARG:CB	2:B:197:ASN:HB3	1.71	0.85
2:B:174:SER:CB	2:B:207:GLU:CB	2.52	0.85
1:A:250:VAL:HG12	1:A:254:GLU:HB3	1.55	0.85
2:B:312:TYR:CA	2:B:381:SER:HA	2.06	0.85
1:A:23:LEU:HD23	1:A:236:SER:HB3	1.57	0.85
1:A:103:TYR:HA	1:A:147:SER:OG	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:GTP:PA	2:B:248:LEU:CD1	2.64	0.85
2:B:169:PHE:HE1	2:B:235:MET:HG2	0.82	0.85
1:A:83:TYR:O	1:A:84:ARG:HG3	1.76	0.85
1:A:158:SER:HB2	1:A:197:HIS:HB3	0.87	0.85
2:B:14:ASN:CG	2:B:69:ASP:OD1	2.20	0.85
2:B:41:ASP:O	2:B:42:LEU:CG	2.25	0.85
2:B:401:ARG:HG3	2:B:402:LYS:H	1.41	0.85
2:B:430:SER:O	2:B:434:GLN:HG3	1.76	0.85
1:A:1:MET:O	1:A:130:THR:O	1.94	0.85
1:A:184:PRO:HG3	1:A:395:PHE:CA	2.06	0.85
1:A:205:ASP:OD1	1:A:303:VAL:HG22	1.18	0.85
2:B:53:TYR:CD1	2:B:87:PHE:CE1	2.63	0.85
2:B:275:LEU:HD12	2:B:294:GLN:NE2	1.92	0.85
1:A:115:ILE:O	1:A:119:LEU:HG	1.75	0.85
1:A:276:ILE:HD12	1:A:371:VAL:CG2	2.06	0.85
2:B:339:ASN:O	2:B:342:TYR:N	2.09	0.85
1:A:88:HIS:CE1	1:A:89:PRO:HD2	2.12	0.85
1:A:407:TRP:CZ2	2:B:165:ILE:CD1	2.58	0.85
2:B:184:PRO:HG3	2:B:399:PHE:CB	2.07	0.85
2:B:127:GLU:O	2:B:129:CYS:N	2.09	0.85
2:B:151:THR:CA	2:B:192:HIS:HD2	1.82	0.85
2:B:114:LEU:CD1	2:B:117:SER:OG	2.19	0.84
2:B:369:ARG:O	5:B:501:TXL:O10	1.93	0.84
1:A:41:THR:O	1:A:42:ILE:HB	1.73	0.84
2:B:287:THR:HB	2:B:290:GLU:HB2	0.86	0.84
1:A:108:TYR:CA	1:A:112:LYS:CE	2.54	0.84
1:A:221:ARG:O	2:B:324:SER:CB	2.26	0.84
2:B:19:LYS:CB	2:B:228:ASN:CB	2.41	0.84
2:B:343:PHE:CD1	2:B:350:ASN:CG	2.55	0.84
2:B:388:PHE:C	2:B:390:ARG:H	1.80	0.84
2:B:226:ASP:OD1	5:B:501:TXL:C39	2.25	0.84
2:B:4:ILE:HD12	2:B:30:ILE:HA	1.48	0.84
2:B:14:ASN:HB3	2:B:74:THR:HG21	1.59	0.84
2:B:233:ALA:HB1	2:B:272:PHE:CG	2.12	0.84
2:B:288:VAL:N	2:B:289:PRO:HD2	1.92	0.84
2:B:428:LEU:O	2:B:432:TYR:HB2	1.77	0.84
1:A:48:SER:HG	1:A:56:THR:HB	1.43	0.84
2:B:175:PRO:HD3	2:B:390:ARG:HH21	0.74	0.84
1:A:184:PRO:HB2	1:A:399:TYR:CD2	2.12	0.84
1:A:217:LEU:CG	1:A:218:ASP:H	1.86	0.84
1:A:220:GLU:O	1:A:222:PRO:HD3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:SER:HB2	2:B:175:PRO:HD2	1.59	0.84
2:B:405:LEU:CG	2:B:408:TYR:HB2	2.07	0.84
1:A:292:THR:HG22	1:A:319:TYR:CZ	2.12	0.84
2:B:229:HIS:CG	5:B:501:TXL:C38	2.41	0.84
2:B:96:GLN:O	2:B:97:SER:C	2.21	0.84
2:B:142:GLY:C	2:B:185:TYR:CZ	2.56	0.84
2:B:433:GLN:HG2	2:B:437:ASP:OD1	1.78	0.84
1:A:193:THR:O	1:A:197:HIS:O	1.94	0.84
1:A:217:LEU:HD22	1:A:368:LEU:CD1	2.08	0.84
1:A:272:TYR:CZ	1:A:274:PRO:CG	2.56	0.84
1:A:277:SER:OG	1:A:280:LYS:CB	2.25	0.84
2:B:87:PHE:CD1	2:B:89:PRO:HG2	2.03	0.84
2:B:102:ASN:HA	2:B:408:TYR:HE1	1.42	0.84
2:B:158:ARG:HB2	2:B:197:ASN:HB3	0.85	0.84
1:A:272:TYR:CE1	1:A:274:PRO:CG	2.59	0.83
1:A:273:ALA:HB1	1:A:294:ALA:CB	2.07	0.83
2:B:183:GLU:CB	2:B:398:MET:SD	2.65	0.83
1:A:9:VAL:HG11	1:A:150:THR:HG22	1.57	0.83
1:A:18:ASN:O	1:A:22:GLU:HG3	1.78	0.83
1:A:206:ASN:HD21	1:A:227:LEU:CD2	1.87	0.83
1:A:273:ALA:HB1	1:A:294:ALA:HB3	1.60	0.83
1:A:64:ARG:HH22	1:A:132:LEU:HD23	1.41	0.83
1:A:313:MET:HA	1:A:344:VAL:HG21	1.60	0.83
2:B:105:LYS:HE2	2:B:411:GLU:CD	2.03	0.83
2:B:182:VAL:HG13	2:B:186:ASN:HD21	1.41	0.83
2:B:199:ASP:OD2	2:B:256:ALA:CB	2.26	0.83
1:A:264:ARG:O	1:A:266:HIS:CE1	2.32	0.83
2:B:48:ARG:NH1	2:B:60:LYS:CG	2.42	0.83
1:A:80:THR:O	1:A:81:GLY:C	2.19	0.83
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.10	0.83
2:B:229:HIS:NE2	5:B:501:TXL:C37	2.40	0.83
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.58	0.83
1:A:204:VAL:HG11	1:A:209:ILE:CD1	1.92	0.83
2:B:6:HIS:NE2	2:B:21:TRP:HH2	1.77	0.83
2:B:49:ILE:N	2:B:61:TYR:HD2	1.75	0.83
2:B:53:TYR:CD1	2:B:87:PHE:HZ	1.96	0.83
2:B:68:VAL:CG1	2:B:149:MET:HE2	2.09	0.83
2:B:241:CYS:O	2:B:242:LEU:CB	2.27	0.83
2:B:289:PRO:O	2:B:293:GLN:HB2	1.78	0.83
1:A:73:THR:CG2	2:B:249:ASN:ND2	2.42	0.83
1:A:320:ARG:HG2	1:A:374:ALA:HB3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ASP:OD2	5:B:501:TXL:H40	1.77	0.83
1:A:70:LEU:CD1	1:A:145:THR:CG2	1.89	0.83
2:B:279:GLY:C	2:B:281:GLN:N	2.35	0.83
1:A:77:GLU:HA	1:A:80:THR:CB	2.08	0.82
1:A:202:PHE:CE1	1:A:378:LEU:HD13	2.14	0.82
1:A:222:PRO:CB	2:B:326:LYS:HD2	2.08	0.82
1:A:288:VAL:HG22	1:A:373:ARG:CG	2.08	0.82
1:A:332:ILE:CD1	1:A:353:VAL:CG2	2.54	0.82
1:A:383:ALA:C	1:A:385:ALA:H	1.84	0.82
2:B:250:ALA:CA	2:B:254:LYS:HD2	2.09	0.82
2:B:405:LEU:O	2:B:405:LEU:HG	1.75	0.82
1:A:33:ASP:OD2	1:A:244:PHE:HD2	1.62	0.82
1:A:76:ASP:O	1:A:80:THR:CA	2.27	0.82
2:B:23:VAL:CG2	5:B:501:TXL:H333	2.09	0.82
2:B:339:ASN:O	2:B:342:TYR:HB2	1.79	0.82
2:B:385:GLN:HG2	2:B:389:LYS:HD2	1.59	0.82
1:A:107:HIS:HB3	1:A:148:GLY:HA3	1.59	0.82
2:B:75:MET:HE1	2:B:79:ARG:CD	1.93	0.82
1:A:51:THR:CG2	1:A:52:PHE:H	1.92	0.82
1:A:383:ALA:C	1:A:385:ALA:N	2.23	0.82
1:A:407:TRP:CD2	2:B:257:VAL:HG22	2.15	0.82
2:B:48:ARG:NH1	2:B:60:LYS:HG2	1.95	0.82
2:B:68:VAL:CG1	2:B:149:MET:CE	2.58	0.82
2:B:75:MET:CE	2:B:79:ARG:HD3	1.99	0.82
1:A:107:HIS:CG	1:A:148:GLY:HA3	2.13	0.82
2:B:13:GLY:HA2	2:B:138:THR:HB	1.62	0.82
2:B:35:SER:N	2:B:60:LYS:CE	2.42	0.82
2:B:143:GLY:N	2:B:147:SER:OG	2.12	0.82
1:A:219:ILE:CG2	1:A:219:ILE:CA	2.57	0.82
2:B:178:SER:CB	4:B:500:GDP:HO3'	1.92	0.82
2:B:287:THR:CG2	2:B:290:GLU:H	1.92	0.82
2:B:319:PHE:CE1	2:B:353:THR:CG2	2.42	0.82
1:A:179:THR:CG2	1:A:181:VAL:CB	2.58	0.82
2:B:105:LYS:HG2	2:B:411:GLU:CG	2.09	0.82
2:B:222:PRO:O	2:B:223:THR:HG23	1.79	0.82
2:B:14:ASN:CB	2:B:74:THR:OG1	2.27	0.82
2:B:151:THR:CA	2:B:192:HIS:HE2	1.68	0.82
2:B:169:PHE:CZ	2:B:235:MET:SD	2.73	0.82
1:A:30:ILE:CG2	1:A:64:ARG:CG	2.55	0.81
1:A:108:TYR:O	1:A:112:LYS:HG3	1.80	0.81
2:B:7:ILE:CG1	2:B:66:ILE:CG2	2.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:THR:OG1	2:B:267:PHE:HA	1.78	0.81
1:A:312:TYR:HA	1:A:381:THR:CG2	2.09	0.81
1:A:407:TRP:CZ2	2:B:165:ILE:HD13	2.15	0.81
2:B:6:HIS:CD2	2:B:21:TRP:CH2	2.68	0.81
2:B:10:GLY:O	2:B:14:ASN:ND2	2.14	0.81
2:B:165:ILE:HD13	2:B:199:ASP:OD2	1.79	0.81
2:B:287:THR:CB	2:B:290:GLU:HB3	1.99	0.81
1:A:13:GLY:O	1:A:16:ILE:HG22	1.80	0.81
1:A:83:TYR:C	1:A:84:ARG:HG3	2.05	0.81
1:A:209:ILE:CD1	1:A:227:LEU:HD11	1.93	0.81
1:A:212:ILE:CD1	1:A:230:LEU:HD22	1.89	0.81
1:A:250:VAL:CG1	1:A:352:LYS:NZ	2.43	0.81
2:B:22:GLU:OE2	2:B:83:PHE:CB	2.27	0.81
2:B:287:THR:HG22	2:B:288:VAL:N	1.95	0.81
2:B:346:TRP:CE3	2:B:347:ILE:HG12	2.06	0.81
2:B:4:ILE:CD1	2:B:30:ILE:CA	2.58	0.81
1:A:2:ARG:CB	1:A:133:GLN:OE1	2.27	0.81
1:A:194:THR:HG22	1:A:195:LEU:N	1.95	0.81
2:B:7:ILE:HB	2:B:137:LEU:HD21	1.62	0.81
2:B:174:SER:HB2	2:B:207:GLU:HB3	1.59	0.81
2:B:30:ILE:CG2	2:B:243:ARG:NH1	2.44	0.81
2:B:286:LEU:HD13	2:B:373:MET:N	1.96	0.81
1:A:312:TYR:HE2	1:A:377:MET:HE1	1.33	0.81
1:A:407:TRP:CZ3	2:B:165:ILE:HD11	2.13	0.81
2:B:194:LEU:HD23	2:B:265:LEU:HB3	1.62	0.81
1:A:106:GLY:O	1:A:111:GLY:CA	2.29	0.81
3:A:500:GTP:O1A	2:B:248:LEU:HD11	1.80	0.81
2:B:13:GLY:HA2	2:B:138:THR:CB	2.10	0.81
2:B:106:GLY:O	2:B:111:GLY:CA	2.29	0.81
1:A:70:LEU:HB2	1:A:145:THR:HG21	1.62	0.81
2:B:184:PRO:HB3	2:B:395:PHE:CE1	2.16	0.81
2:B:385:GLN:HG2	2:B:389:LYS:CE	2.09	0.81
1:A:144:GLY:HA2	1:A:185:TYR:OH	1.81	0.81
2:B:105:LYS:CE	2:B:411:GLU:OE2	2.27	0.81
2:B:166:MET:HB2	2:B:198:THR:HA	1.61	0.81
1:A:101:ASN:HA	3:A:500:GTP:O2G	1.81	0.80
1:A:177:VAL:CB	2:B:349:ASN:HD21	1.91	0.80
1:A:184:PRO:CD	1:A:395:PHE:CA	2.58	0.80
1:A:306:ASP:CG	1:A:308:ARG:HB2	2.06	0.80
2:B:95:GLY:O	2:B:96:GLN:HB2	1.81	0.80
1:A:15:GLN:O	1:A:18:ASN:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASN:CG	2:B:408:TYR:CD1	2.59	0.80
2:B:103:TRP:CZ3	2:B:108:TYR:OH	2.18	0.80
2:B:105:LYS:HG2	2:B:411:GLU:CD	2.06	0.80
2:B:385:GLN:HG2	2:B:389:LYS:CD	2.11	0.80
1:A:72:PRO:O	1:A:75:ILE:HG23	1.82	0.80
1:A:271:THR:OG1	1:A:377:MET:CB	2.30	0.80
2:B:64:ARG:NH2	2:B:125:GLU:O	2.13	0.80
2:B:194:LEU:HA	2:B:265:LEU:HB2	1.60	0.80
2:B:218:LYS:O	2:B:219:LEU:O	2.00	0.80
2:B:229:HIS:CG	5:B:501:TXL:C37	2.62	0.80
1:A:20:CYS:O	1:A:24:TYR:CE2	2.33	0.80
1:A:97:GLU:HB3	1:A:110:ILE:HG23	1.61	0.80
1:A:103:TYR:CG	1:A:188:ILE:HG22	2.16	0.80
1:A:276:ILE:HG21	1:A:282:TYR:HD1	1.44	0.80
2:B:319:PHE:CD1	2:B:328:VAL:CG1	2.58	0.80
1:A:9:VAL:CG1	1:A:150:THR:HG22	2.08	0.80
1:A:38:SER:C	1:A:39:ASP:N	0.70	0.80
1:A:206:ASN:HD21	1:A:227:LEU:HD23	1.42	0.80
1:A:210:TYR:HD1	2:B:326:LYS:HD3	1.46	0.80
1:A:223:THR:HG22	2:B:324:SER:HA	1.62	0.80
2:B:11:GLN:HB3	4:B:500:GDP:O2A	1.79	0.80
2:B:35:SER:HA	2:B:60:LYS:HE2	1.62	0.80
2:B:119:LEU:O	2:B:123:ARG:HG3	1.80	0.80
2:B:142:GLY:CA	2:B:185:TYR:CD1	2.65	0.80
2:B:311:ARG:O	2:B:381:SER:HB2	1.80	0.80
1:A:3:GLU:HA	1:A:31:GLN:CG	2.11	0.80
1:A:17:GLY:O	1:A:21:TRP:N	2.11	0.80
1:A:291:ILE:HG22	1:A:375:VAL:HG23	0.84	0.80
1:A:343:PHE:HZ	1:A:351:PHE:CE2	1.99	0.80
2:B:42:LEU:C	2:B:43:GLN:HG3	2.07	0.80
2:B:268:PHE:CD1	2:B:380:ASN:CG	2.59	0.80
1:A:105:ARG:HH21	1:A:110:ILE:CD1	1.92	0.80
1:A:119:LEU:O	1:A:122:ILE:CG2	2.29	0.80
2:B:102:ASN:OD1	2:B:408:TYR:HE1	1.62	0.80
1:A:88:HIS:CG	1:A:89:PRO:CD	2.63	0.80
1:A:224:TYR:N	2:B:325:MET:HB2	1.96	0.80
1:A:306:ASP:OD1	1:A:308:ARG:HB2	1.79	0.80
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.62	0.80
1:A:4:CYS:CB	1:A:30:ILE:CG2	2.57	0.80
1:A:108:TYR:HE2	1:A:417:GLU:OE2	1.63	0.80
1:A:191:THR:HG21	1:A:421:ALA:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:CYS:O	2:B:16:ILE:CB	2.29	0.80
1:A:64:ARG:CZ	1:A:132:LEU:HD22	2.10	0.79
1:A:343:PHE:CZ	1:A:351:PHE:CE2	2.69	0.79
2:B:70:LEU:HD12	2:B:94:PHE:HD2	0.68	0.79
2:B:192:HIS:HA	2:B:196:GLU:CD	2.08	0.79
2:B:244:PHE:CB	2:B:245:PRO:HD2	2.05	0.79
2:B:313:LEU:HD23	2:B:344:VAL:CG1	2.08	0.79
1:A:309:HIS:CD2	1:A:386:GLU:OE2	2.36	0.79
1:A:361:THR:HG22	1:A:362:VAL:N	1.97	0.79
2:B:102:ASN:HB3	2:B:408:TYR:HD1	1.45	0.79
2:B:142:GLY:CA	2:B:185:TYR:CE1	2.64	0.79
2:B:53:TYR:CE1	2:B:89:PRO:HG3	2.17	0.79
2:B:265:LEU:HD23	2:B:267:PHE:CE1	2.18	0.79
1:A:115:ILE:CG2	1:A:152:LEU:HD21	2.12	0.79
1:A:154:MET:CE	1:A:166:LYS:HD3	2.11	0.79
1:A:301:GLN:NE2	1:A:305:CYS:O	2.12	0.79
2:B:4:ILE:HG21	2:B:30:ILE:CG2	2.12	0.79
2:B:102:ASN:CG	2:B:408:TYR:CE1	2.60	0.79
2:B:175:PRO:HB2	2:B:176:LYS:HE2	1.65	0.79
2:B:35:SER:CA	2:B:60:LYS:CE	2.60	0.79
2:B:48:ARG:NH1	2:B:60:LYS:H	1.81	0.79
2:B:56:ALA:CB	2:B:62:VAL:HB	2.11	0.79
2:B:141:LEU:HD22	2:B:186:ASN:CB	2.09	0.79
1:A:6:SER:HA	1:A:136:SER:OG	1.81	0.79
1:A:258:ASN:OD1	1:A:352:LYS:CD	2.30	0.79
1:A:409:VAL:HG22	1:A:414:GLU:HG2	1.64	0.79
2:B:190:SER:O	2:B:192:HIS:N	2.14	0.79
2:B:192:HIS:CA	2:B:196:GLU:HG2	2.11	0.79
2:B:259:MET:HE2	2:B:379:GLY:N	1.97	0.79
1:A:16:ILE:CD1	1:A:138:PHE:CD1	2.59	0.79
1:A:176:GLN:O	1:A:177:VAL:HG22	1.78	0.79
2:B:287:THR:CG2	2:B:289:PRO:HG2	2.12	0.79
2:B:34:GLY:O	2:B:35:SER:OG	2.01	0.79
1:A:3:GLU:OE2	1:A:129:CYS:HB3	1.82	0.79
1:A:116:ASP:O	1:A:119:LEU:N	2.15	0.79
1:A:221:ARG:N	1:A:222:PRO:HD3	1.97	0.79
2:B:4:ILE:HD13	2:B:30:ILE:CB	2.13	0.79
2:B:19:LYS:HB3	2:B:228:ASN:HB3	1.61	0.79
2:B:107:HIS:HD2	2:B:152:LEU:HG	1.48	0.79
2:B:305:CYS:SG	2:B:387:LEU:HB2	2.23	0.79
1:A:5:ILE:HG21	1:A:135:PHE:CE1	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD11	1:A:156:ARG:CZ	2.13	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:48:ARG:CD	2:B:60:LYS:HA	2.13	0.78
2:B:102:ASN:HA	2:B:408:TYR:CE1	2.18	0.78
2:B:323:MET:HG2	2:B:324:SER:N	1.98	0.78
2:B:405:LEU:HD21	2:B:418:PHE:CZ	2.03	0.78
1:A:51:THR:CG2	1:A:52:PHE:N	2.45	0.78
1:A:396:ASP:OD2	1:A:422:ARG:NH1	2.15	0.78
1:A:407:TRP:HZ2	2:B:256:ALA:HB1	1.43	0.78
2:B:284:ARG:HD2	2:B:290:GLU:CD	2.08	0.78
2:B:300:ASN:ND2	2:B:300:ASN:O	2.16	0.78
1:A:109:THR:CG2	1:A:411:GLU:HB3	2.12	0.78
1:A:303:VAL:HG11	1:A:305:CYS:SG	2.22	0.78
2:B:19:LYS:CD	2:B:228:ASN:CB	2.53	0.78
2:B:128:SER:O	2:B:129:CYS:HB2	1.84	0.78
2:B:184:PRO:HG3	2:B:399:PHE:CD2	1.33	0.78
1:A:65:ALA:O	1:A:66:VAL:HG23	1.83	0.78
1:A:155:GLU:HG3	1:A:192:HIS:NE2	1.98	0.78
1:A:173:PRO:HG3	1:A:182:VAL:HG12	1.66	0.78
1:A:210:TYR:HD1	2:B:326:LYS:CD	1.94	0.78
2:B:49:ILE:N	2:B:61:TYR:CD2	2.51	0.78
2:B:107:HIS:CG	2:B:152:LEU:HG	2.19	0.78
1:A:196:GLU:O	1:A:197:HIS:CB	2.31	0.78
2:B:48:ARG:NH1	2:B:60:LYS:N	2.32	0.78
2:B:194:LEU:HD23	2:B:267:PHE:CZ	2.19	0.78
2:B:213:CYS:HB3	2:B:219:LEU:HD11	1.64	0.78
2:B:405:LEU:HD13	2:B:418:PHE:HZ	1.47	0.78
1:A:155:GLU:OE2	1:A:192:HIS:HD2	1.65	0.78
2:B:30:ILE:HG21	2:B:136:GLN:HE22	1.47	0.78
2:B:277:SER:CB	2:B:280:SER:HB2	2.13	0.78
1:A:206:ASN:HD21	3:A:500:GTP:N2	1.82	0.78
1:A:210:TYR:CZ	1:A:227:LEU:CD2	2.60	0.78
2:B:104:ALA:HA	2:B:108:TYR:CE2	2.19	0.78
2:B:105:LYS:CG	2:B:411:GLU:HG3	2.14	0.78
2:B:169:PHE:CZ	2:B:235:MET:HG2	2.17	0.78
1:A:142:GLY:C	1:A:185:TYR:CE1	2.62	0.78
1:A:217:LEU:HD13	1:A:368:LEU:CG	2.12	0.78
2:B:44:LEU:HD11	2:B:86:ILE:C	2.09	0.78
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.11	0.78
2:B:286:LEU:CD1	2:B:371:LEU:O	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:HD12	2:B:372:LYS:HB2	1.61	0.78
2:B:399:PHE:CZ	2:B:408:TYR:OH	2.37	0.78
1:A:105:ARG:HH12	2:B:253:ARG:CZ	1.94	0.78
2:B:135:PHE:CG	2:B:166:MET:CE	2.63	0.78
2:B:244:PHE:CD2	2:B:358:ILE:HD12	2.18	0.78
2:B:320:ARG:NH2	5:B:501:TXL:H27	1.98	0.78
2:B:346:TRP:CD2	2:B:347:ILE:HG13	2.14	0.78
1:A:105:ARG:NH2	1:A:110:ILE:CD1	2.46	0.77
1:A:72:PRO:O	1:A:75:ILE:HG22	1.83	0.77
1:A:277:SER:OG	1:A:280:LYS:CA	2.32	0.77
2:B:181:VAL:HA	2:B:398:MET:HE2	1.65	0.77
2:B:229:HIS:ND1	5:B:501:TXL:O11	2.18	0.77
1:A:153:LEU:O	1:A:157:LEU:HG	1.84	0.77
1:A:155:GLU:OE2	1:A:192:HIS:CD2	2.37	0.77
2:B:86:ILE:HD12	2:B:91:ASN:ND2	1.99	0.77
2:B:176:LYS:CE	2:B:207:GLU:OE2	2.29	0.77
2:B:222:PRO:O	2:B:223:THR:CG2	2.32	0.77
1:A:227:LEU:HB2	2:B:326:LYS:HE2	1.64	0.77
1:A:296:PHE:HE1	1:A:335:ILE:HD13	0.98	0.77
2:B:273:ALA:HB1	2:B:294:GLN:OE1	1.83	0.77
2:B:425:MET:O	2:B:428:LEU:HB3	1.84	0.77
2:B:7:ILE:CD1	2:B:137:LEU:HD21	2.14	0.77
2:B:8:GLN:NE2	2:B:21:TRP:NE1	2.31	0.77
1:A:103:TYR:O	1:A:107:HIS:HB3	1.85	0.77
2:B:383:ALA:O	2:B:386:GLU:HG3	1.84	0.77
1:A:97:GLU:O	1:A:98:ASP:HB3	1.85	0.77
1:A:115:ILE:CD1	1:A:152:LEU:CD1	2.63	0.77
2:B:191:VAL:CG2	2:B:421:ALA:CA	2.61	0.77
1:A:70:LEU:HB2	1:A:145:THR:CG2	2.14	0.77
1:A:148:GLY:HA2	1:A:151:SER:OG	1.85	0.77
1:A:294:ALA:C	1:A:300:ASN:ND2	2.43	0.77
1:A:369:ALA:CB	1:A:371:VAL:CG2	2.51	0.77
2:B:154:ILE:HG22	2:B:196:GLU:O	1.85	0.77
1:A:151:SER:HB2	1:A:192:HIS:CB	2.15	0.77
1:A:158:SER:OG	1:A:196:GLU:O	2.02	0.77
1:A:192:HIS:O	1:A:196:GLU:HG2	1.85	0.77
2:B:66:ILE:HB	2:B:125:GLU:OE2	1.84	0.77
2:B:107:HIS:CG	2:B:152:LEU:CD2	2.67	0.77
2:B:184:PRO:HD2	2:B:399:PHE:HE2	1.47	0.77
2:B:208:ALA:HB1	2:B:303:ALA:O	1.82	0.77
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:PHE:CE2	2:B:114:LEU:HD11	2.20	0.76
2:B:107:HIS:O	2:B:152:LEU:HD13	1.82	0.76
2:B:144:GLY:N	2:B:185:TYR:CZ	2.52	0.76
2:B:254:LYS:O	2:B:258:ASN:CG	2.28	0.76
2:B:319:PHE:CZ	2:B:328:VAL:HG13	2.19	0.76
1:A:313:MET:CB	1:A:380:ASN:O	2.34	0.76
5:B:501:TXL:C9	5:B:501:TXL:H162	2.15	0.76
2:B:194:LEU:CD2	2:B:267:PHE:HE2	1.93	0.76
2:B:249:ASN:O	2:B:254:LYS:NZ	2.16	0.76
2:B:384:ILE:CG2	2:B:388:PHE:CE2	2.69	0.76
1:A:93:ILE:HD11	1:A:121:ARG:HD2	1.66	0.76
1:A:288:VAL:HG23	1:A:373:ARG:HD3	1.62	0.76
1:A:291:ILE:C	1:A:375:VAL:HG21	2.10	0.76
1:A:383:ALA:O	1:A:386:GLU:N	2.18	0.76
2:B:7:ILE:HG12	2:B:66:ILE:CD1	2.04	0.76
2:B:103:TRP:CZ3	2:B:108:TYR:CZ	2.73	0.76
2:B:107:HIS:CG	2:B:152:LEU:CG	2.69	0.76
2:B:192:HIS:C	2:B:196:GLU:HG2	2.09	0.76
1:A:70:LEU:CG	1:A:145:THR:HG21	2.14	0.76
1:A:252:LEU:HD23	1:A:255:PHE:CE2	2.19	0.76
2:B:262:PHE:HB3	2:B:263:PRO:CD	2.14	0.76
2:B:308:ARG:HD3	2:B:342:TYR:CZ	2.21	0.76
2:B:319:PHE:CE1	2:B:328:VAL:HG12	2.18	0.76
2:B:141:LEU:CD1	2:B:173:PRO:HD3	2.16	0.76
2:B:229:HIS:CE1	5:B:501:TXL:O11	2.38	0.76
1:A:97:GLU:CG	1:A:110:ILE:CG2	2.63	0.76
1:A:119:LEU:C	1:A:122:ILE:HG22	2.11	0.76
1:A:369:ALA:HB1	1:A:371:VAL:HG23	1.67	0.76
2:B:12:CYS:SG	4:B:500:GDP:C4	2.79	0.76
2:B:184:PRO:CG	2:B:399:PHE:HD2	0.66	0.76
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.65	0.76
1:A:97:GLU:HG3	1:A:110:ILE:CG2	2.16	0.76
1:A:311:LYS:CB	1:A:342:GLN:O	2.34	0.76
2:B:183:GLU:OE1	2:B:394:GLN:HB3	1.83	0.76
2:B:399:PHE:O	2:B:403:ALA:HA	1.86	0.76
2:B:400:ARG:HD3	2:B:422:GLU:OE1	1.85	0.76
1:A:344:VAL:CB	1:A:347:CYS:SG	2.69	0.76
2:B:75:MET:HE2	2:B:79:ARG:CB	2.16	0.76
2:B:147:SER:CB	2:B:189:LEU:HD13	2.08	0.76
2:B:15:GLN:CD	4:B:500:GDP:O6	2.29	0.76
2:B:27:GLU:O	2:B:36:TYR:HB3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:LYS:HG2	2:B:411:GLU:HG3	1.67	0.76
2:B:135:PHE:CB	2:B:166:MET:SD	2.74	0.76
2:B:147:SER:OG	2:B:189:LEU:CD1	2.21	0.76
2:B:201:THR:CG2	2:B:265:LEU:CD1	2.59	0.76
2:B:213:CYS:HB3	2:B:219:LEU:CD1	2.16	0.76
1:A:76:ASP:C	1:A:80:THR:HG1	1.93	0.75
1:A:179:THR:CG2	1:A:181:VAL:N	2.21	0.75
2:B:48:ARG:HH11	2:B:60:LYS:CG	1.97	0.75
1:A:101:ASN:OD1	2:B:254:LYS:HG2	1.86	0.75
1:A:179:THR:HG22	1:A:180:ALA:N	1.95	0.75
2:B:7:ILE:CG1	2:B:66:ILE:HD13	2.05	0.75
2:B:35:SER:CA	2:B:60:LYS:HE3	2.16	0.75
2:B:222:PRO:C	2:B:223:THR:HG23	2.11	0.75
2:B:243:ARG:HH21	2:B:252:LEU:CD1	1.98	0.75
2:B:252:LEU:O	2:B:255:LEU:HB2	1.85	0.75
2:B:313:LEU:HD22	2:B:344:VAL:CG1	1.98	0.75
1:A:179:THR:HG22	1:A:181:VAL:H	0.63	0.75
2:B:275:LEU:HD11	2:B:300:ASN:HD21	1.49	0.75
2:B:343:PHE:CB	2:B:350:ASN:ND2	2.50	0.75
1:A:53:PHE:HA	1:A:88:HIS:NE2	1.92	0.75
1:A:183:GLU:HB2	1:A:398:MET:SD	2.26	0.75
1:A:262:TYR:HB3	1:A:263:PRO:HD3	1.65	0.75
2:B:200:GLU:HB3	2:B:268:PHE:CE2	2.21	0.75
2:B:386:GLU:C	2:B:388:PHE:N	2.44	0.75
2:B:399:PHE:HZ	2:B:408:TYR:OH	1.68	0.75
1:A:66:VAL:CG2	1:A:125:LEU:CD1	2.64	0.75
2:B:170:SER:OG	2:B:203:CYS:HA	1.86	0.75
2:B:184:PRO:HG2	2:B:399:PHE:CD2	0.29	0.75
2:B:398:MET:HG2	2:B:399:PHE:N	2.00	0.75
1:A:26:LEU:HD11	1:A:361:THR:CB	2.17	0.75
1:A:210:TYR:CD1	2:B:326:LYS:HD3	2.15	0.75
1:A:228:ASN:ND2	3:A:500:GTP:HN1	1.84	0.75
2:B:6:HIS:NE2	2:B:21:TRP:CH2	2.55	0.75
2:B:87:PHE:CD1	2:B:89:PRO:HD2	2.20	0.75
2:B:188:THR:HG22	2:B:417:GLU:O	1.87	0.75
2:B:259:MET:HE1	2:B:379:GLY:HA2	0.83	0.75
1:A:219:ILE:CG2	1:A:219:ILE:HG12	2.16	0.75
2:B:154:ILE:HD13	2:B:198:THR:CG2	2.17	0.75
1:A:115:ILE:HD13	1:A:152:LEU:CD1	2.16	0.75
1:A:287:SER:OG	1:A:290:GLU:HB2	1.87	0.75
1:A:326:LYS:O	1:A:330:ALA:HB3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:PRO:O	2:B:90:ASP:OD1	2.05	0.75
2:B:296:PHE:CE2	2:B:335:VAL:HG11	2.22	0.75
1:A:88:HIS:CD2	1:A:89:PRO:CD	2.70	0.74
1:A:184:PRO:HD3	1:A:395:PHE:N	2.01	0.74
2:B:53:TYR:HE1	2:B:89:PRO:CG	1.98	0.74
2:B:123:ARG:O	2:B:127:GLU:HG3	1.87	0.74
2:B:175:PRO:C	2:B:176:LYS:HE2	2.12	0.74
2:B:181:VAL:CG2	2:B:404:PHE:CE2	2.70	0.74
2:B:184:PRO:HA	2:B:395:PHE:HD1	1.52	0.74
2:B:190:SER:O	2:B:191:VAL:C	2.30	0.74
2:B:259:MET:HB3	2:B:268:PHE:HE1	1.45	0.74
1:A:57:GLY:HA3	1:A:61:HIS:NE2	2.01	0.74
1:A:184:PRO:HB3	1:A:395:PHE:CD2	2.19	0.74
2:B:6:HIS:CG	2:B:21:TRP:HZ2	2.05	0.74
2:B:9:ALA:HA	2:B:68:VAL:O	1.86	0.74
1:A:42:ILE:O	1:A:42:ILE:CG2	2.30	0.74
2:B:22:GLU:HG2	2:B:83:PHE:HD2	1.47	0.74
1:A:33:ASP:OD2	1:A:244:PHE:CD2	2.39	0.74
1:A:76:ASP:C	1:A:80:THR:OG1	2.29	0.74
2:B:287:THR:CG2	2:B:289:PRO:CG	2.65	0.74
2:B:338:LYS:O	2:B:339:ASN:CG	2.29	0.74
1:A:62:VAL:HG12	1:A:63:PRO:CD	2.06	0.74
1:A:196:GLU:O	1:A:197:HIS:HB3	1.87	0.74
1:A:222:PRO:CG	2:B:326:LYS:CD	2.61	0.74
2:B:213:CYS:SG	2:B:227:LEU:CD1	2.75	0.74
2:B:405:LEU:HD11	2:B:408:TYR:HB2	0.78	0.74
1:A:30:ILE:CB	1:A:64:ARG:CB	2.66	0.74
1:A:80:THR:O	1:A:83:TYR:N	2.19	0.74
1:A:172:TYR:CZ	1:A:387:ALA:HB1	2.22	0.74
1:A:273:ALA:CB	1:A:294:ALA:HB3	2.16	0.74
1:A:224:TYR:CE1	3:A:500:GTP:N3	2.55	0.74
1:A:361:THR:O	1:A:362:VAL:HG23	1.87	0.74
2:B:35:SER:H	2:B:60:LYS:HE3	1.53	0.74
2:B:181:VAL:HG12	2:B:399:PHE:CZ	1.95	0.74
2:B:226:ASP:OD1	5:B:501:TXL:H39	1.87	0.74
2:B:243:ARG:HH21	2:B:252:LEU:HD11	1.47	0.74
2:B:311:ARG:C	2:B:381:SER:HB2	2.11	0.74
2:B:22:GLU:CG	2:B:83:PHE:CE2	2.70	0.74
2:B:229:HIS:NE2	5:B:501:TXL:H37	2.02	0.74
1:A:206:ASN:ND2	3:A:500:GTP:HN22	1.85	0.74
2:B:92:PHE:CE1	2:B:121:VAL:HG21	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CD2	1:A:227:LEU:HD22	2.20	0.74
1:A:282:TYR:HD2	1:A:285:GLN:CA	2.01	0.73
2:B:259:MET:CE	2:B:379:GLY:N	2.51	0.73
2:B:336:GLN:NE2	2:B:351:VAL:HB	2.03	0.73
1:A:3:GLU:HB3	1:A:64:ARG:CZ	2.18	0.73
1:A:103:TYR:OH	1:A:151:SER:HB3	1.87	0.73
1:A:179:THR:HG23	1:A:181:VAL:HG23	1.70	0.73
2:B:105:LYS:HE2	2:B:411:GLU:CG	2.18	0.73
1:A:65:ALA:HB2	1:A:91:GLN:OE1	1.87	0.73
1:A:137:VAL:HB	1:A:168:GLU:HG2	1.70	0.73
1:A:397:LEU:HD23	1:A:401:LYS:CD	2.11	0.73
2:B:169:PHE:HE1	2:B:235:MET:CG	1.76	0.73
2:B:239:THR:HA	2:B:243:ARG:CZ	2.18	0.73
2:B:346:TRP:HZ3	2:B:347:ILE:HD11	0.95	0.73
2:B:397:ALA:O	2:B:401:ARG:HG2	1.87	0.73
1:A:6:SER:HB3	1:A:30:ILE:CD1	2.19	0.73
1:A:319:TYR:O	1:A:355:ILE:HA	1.87	0.73
2:B:8:GLN:NE2	2:B:21:TRP:CD1	2.56	0.73
2:B:244:PHE:CE2	2:B:358:ILE:CD1	2.48	0.73
2:B:3:GLU:CB	2:B:132:LEU:HD23	2.14	0.73
2:B:101:ASN:O	2:B:102:ASN:HB2	1.88	0.73
2:B:141:LEU:HD12	2:B:172:VAL:HA	0.91	0.73
2:B:143:GLY:O	4:B:500:GDP:PB	2.41	0.73
1:A:152:LEU:HD11	1:A:156:ARG:NE	2.04	0.73
1:A:184:PRO:HD3	1:A:395:PHE:CA	2.19	0.73
1:A:405:VAL:CG2	1:A:409:VAL:CG2	2.65	0.73
1:A:431:ASP:O	1:A:435:VAL:HG23	1.88	0.73
2:B:229:HIS:HB2	5:B:501:TXL:H38	1.68	0.73
1:A:97:GLU:O	1:A:110:ILE:HD13	1.88	0.73
1:A:107:HIS:CD2	1:A:148:GLY:CA	2.71	0.73
1:A:341:ILE:CG2	1:A:343:PHE:CE2	2.72	0.73
2:B:56:ALA:CB	2:B:62:VAL:HG23	2.18	0.73
2:B:128:SER:O	2:B:129:CYS:CB	2.37	0.73
2:B:401:ARG:HG3	2:B:402:LYS:N	1.99	0.73
1:A:103:TYR:HD2	1:A:189:LEU:CG	2.00	0.73
2:B:286:LEU:HB3	2:B:373:MET:HB3	1.71	0.73
1:A:179:THR:CG2	1:A:181:VAL:HG23	2.18	0.73
1:A:209:ILE:HG23	1:A:230:LEU:CD2	2.17	0.73
1:A:314:ALA:O	1:A:379:SER:HA	1.89	0.73
2:B:237:GLY:O	2:B:241:CYS:CB	2.26	0.73
2:B:313:LEU:CD2	2:B:344:VAL:HG13	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.18	0.73
1:A:70:LEU:CB	1:A:145:THR:CG2	2.65	0.72
1:A:153:LEU:O	1:A:157:LEU:CD1	2.37	0.72
1:A:250:VAL:HG21	1:A:352:LYS:CE	2.07	0.72
1:A:277:SER:HB2	1:A:279:GLU:H	1.53	0.72
2:B:226:ASP:OD2	5:B:501:TXL:C40	2.37	0.72
2:B:259:MET:HB2	2:B:268:PHE:CZ	2.23	0.72
2:B:265:LEU:CD2	2:B:267:PHE:CE1	2.71	0.72
1:A:145:THR:C	1:A:149:PHE:HB3	2.13	0.72
1:A:262:TYR:CB	1:A:263:PRO:CD	2.57	0.72
2:B:6:HIS:CG	2:B:21:TRP:CZ2	2.77	0.72
2:B:244:PHE:HD2	2:B:245:PRO:HD2	1.45	0.72
1:A:277:SER:CA	1:A:280:LYS:HG2	2.18	0.72
1:A:404:PHE:HZ	2:B:257:VAL:O	1.73	0.72
1:A:407:TRP:CE3	2:B:257:VAL:CG2	2.72	0.72
2:B:103:TRP:CZ3	2:B:108:TYR:CE2	2.75	0.72
1:A:36:MET:SD	1:A:60:LYS:HB2	2.29	0.72
1:A:158:SER:H	1:A:166:LYS:NZ	1.86	0.72
1:A:206:ASN:HD21	3:A:500:GTP:HN22	1.35	0.72
1:A:222:PRO:O	2:B:324:SER:CB	2.29	0.72
2:B:231:VAL:HG12	2:B:235:MET:HE2	1.71	0.72
2:B:242:LEU:HD22	2:B:250:ALA:N	2.01	0.72
2:B:288:VAL:H	2:B:289:PRO:HD2	1.53	0.72
2:B:326:LYS:O	2:B:330:GLU:CG	2.35	0.72
1:A:70:LEU:CB	1:A:145:THR:HG21	2.20	0.72
1:A:144:GLY:N	3:A:500:GTP:O2G	2.19	0.72
2:B:7:ILE:CG2	2:B:137:LEU:HD22	2.19	0.72
2:B:14:ASN:HB2	2:B:74:THR:OG1	1.89	0.72
2:B:194:LEU:HD21	2:B:267:PHE:CE2	2.23	0.72
2:B:204:ILE:O	2:B:204:ILE:HG22	1.90	0.72
2:B:265:LEU:O	2:B:267:PHE:CE2	2.41	0.72
1:A:100:ALA:HB2	1:A:105:ARG:NE	2.04	0.72
1:A:292:THR:HG22	1:A:319:TYR:CE2	2.25	0.72
1:A:336:LYS:HG2	1:A:336:LYS:O	1.88	0.72
2:B:35:SER:H	2:B:60:LYS:CE	2.02	0.72
2:B:111:GLY:C	2:B:115:VAL:CG2	2.56	0.72
1:A:225:THR:HG23	2:B:247:GLN:HE22	1.52	0.72
1:A:250:VAL:CG2	1:A:254:GLU:HG2	2.19	0.72
1:A:289:ALA:HB1	1:A:331:ALA:CB	2.20	0.72
1:A:184:PRO:CB	1:A:399:TYR:CD2	2.73	0.72
1:A:184:PRO:HG2	1:A:395:PHE:CD2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASN:CB	2:B:408:TYR:CD1	2.73	0.72
2:B:280:SER:O	2:B:282:GLN:N	2.21	0.72
2:B:284:ARG:HB3	2:B:287:THR:OG1	1.90	0.72
2:B:383:ALA:O	2:B:386:GLU:CG	2.37	0.72
2:B:104:ALA:CA	2:B:413:MET:HE3	2.19	0.72
2:B:360:PRO:CD	2:B:374:SER:HB3	2.20	0.72
2:B:405:LEU:HD13	2:B:418:PHE:CZ	2.25	0.72
1:A:5:ILE:CD1	1:A:135:PHE:CE1	2.73	0.71
1:A:184:PRO:HG2	1:A:395:PHE:HA	1.72	0.71
1:A:210:TYR:HE2	1:A:227:LEU:CD2	2.01	0.71
1:A:253:THR:O	1:A:253:THR:HG22	1.90	0.71
1:A:397:LEU:HD22	1:A:401:LYS:CE	2.20	0.71
2:B:20:PHE:CZ	2:B:235:MET:HB3	2.22	0.71
2:B:288:VAL:O	2:B:292:THR:N	2.19	0.71
1:A:225:THR:HG21	2:B:247:GLN:HE22	1.47	0.71
1:A:266:HIS:HD2	1:A:432:TYR:CE1	2.04	0.71
1:A:311:LYS:C	1:A:312:TYR:O	2.31	0.71
2:B:133:GLN:NE2	2:B:253:ARG:NH1	2.38	0.71
2:B:142:GLY:HA3	2:B:182:VAL:HG21	1.71	0.71
1:A:4:CYS:SG	1:A:252:LEU:CD1	2.72	0.71
1:A:152:LEU:HD11	1:A:156:ARG:NH2	2.05	0.71
2:B:2:ARG:CG	2:B:2:ARG:O	2.36	0.71
2:B:184:PRO:HG3	2:B:399:PHE:HB2	1.70	0.71
2:B:431:GLU:HA	2:B:434:GLN:CD	2.15	0.71
1:A:9:VAL:HB	1:A:138:PHE:O	1.89	0.71
2:B:3:GLU:HG2	2:B:4:ILE:N	2.04	0.71
2:B:111:GLY:CA	2:B:115:VAL:HG23	2.20	0.71
2:B:340:SER:HG	2:B:341:SER:N	1.85	0.71
1:A:102:ASN:C	1:A:185:TYR:HE2	1.98	0.71
1:A:241:SER:CB	1:A:356:ASN:HD22	2.04	0.71
2:B:7:ILE:CG2	2:B:137:LEU:CD2	2.69	0.71
2:B:95:GLY:O	2:B:96:GLN:CB	2.39	0.71
1:A:30:ILE:HD12	1:A:64:ARG:HB3	1.72	0.71
2:B:237:GLY:CA	2:B:241:CYS:SG	2.68	0.71
2:B:259:MET:SD	2:B:378:ILE:HG22	2.31	0.71
2:B:272:PHE:CD1	2:B:274:PRO:HG2	2.24	0.71
2:B:390:ARG:O	2:B:394:GLN:CG	2.33	0.71
2:B:397:ALA:CA	2:B:401:ARG:HD3	2.19	0.71
1:A:72:PRO:C	1:A:75:ILE:CG2	2.64	0.71
1:A:234:ILE:HD12	1:A:270:ALA:HB1	1.71	0.71
1:A:319:TYR:CE2	1:A:375:VAL:HG22	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:TYR:O	2:B:344:VAL:HG22	1.84	0.71
1:A:101:ASN:O	1:A:102:ASN:OD1	2.07	0.71
1:A:202:PHE:HE1	1:A:378:LEU:HD13	1.55	0.71
1:A:222:PRO:HG2	2:B:326:LYS:HD3	1.72	0.71
2:B:104:ALA:CA	2:B:108:TYR:CD2	2.63	0.71
1:A:155:GLU:HG2	1:A:196:GLU:CG	2.21	0.71
1:A:291:ILE:HD11	1:A:373:ARG:HB3	1.72	0.71
1:A:312:TYR:CD2	1:A:381:THR:HG22	2.23	0.71
1:A:312:TYR:CB	1:A:381:THR:HG22	2.21	0.71
1:A:16:ILE:HG21	1:A:138:PHE:CD1	2.26	0.70
1:A:228:ASN:ND2	3:A:500:GTP:O6	2.23	0.70
1:A:407:TRP:CG	2:B:257:VAL:HG22	2.26	0.70
2:B:213:CYS:SG	2:B:227:LEU:HD12	2.31	0.70
1:A:30:ILE:HG22	1:A:64:ARG:HG2	1.70	0.70
2:B:143:GLY:CA	2:B:185:TYR:HE1	2.03	0.70
2:B:286:LEU:HD13	2:B:372:LYS:HB2	1.68	0.70
5:B:501:TXL:H181	5:B:501:TXL:C21	2.20	0.70
1:A:104:ALA:HA	1:A:108:TYR:CE2	2.25	0.70
1:A:239:THR:O	1:A:243:ARG:HB2	1.91	0.70
1:A:242:LEU:HD22	1:A:250:VAL:H	1.56	0.70
1:A:437:VAL:C	1:A:438:ASP:OD1	2.33	0.70
2:B:53:TYR:HD1	2:B:87:PHE:CZ	2.05	0.70
2:B:142:GLY:HA3	2:B:182:VAL:HG22	1.65	0.70
1:A:36:MET:SD	1:A:61:HIS:HA	2.30	0.70
1:A:100:ALA:O	1:A:144:GLY:HA3	1.90	0.70
1:A:294:ALA:C	1:A:300:ASN:HD22	2.00	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	1.73	0.70
1:A:100:ALA:HB1	1:A:105:ARG:CB	2.22	0.70
1:A:108:TYR:OH	1:A:417:GLU:HG3	1.91	0.70
2:B:48:ARG:HH11	2:B:60:LYS:CB	2.04	0.70
2:B:165:ILE:CD1	2:B:199:ASP:OD2	2.39	0.70
1:A:103:TYR:CE1	1:A:188:ILE:CG2	2.67	0.70
2:B:3:GLU:OE2	2:B:64:ARG:NH1	2.25	0.70
2:B:21:TRP:HA	2:B:24:ILE:HD12	1.71	0.70
2:B:97:SER:OG	2:B:110:GLU:OE1	2.10	0.70
1:A:167:LEU:CD1	1:A:252:LEU:HD22	2.21	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:HD2	0.76	0.70
2:B:53:TYR:CE1	2:B:87:PHE:HZ	2.07	0.70
2:B:242:LEU:CA	2:B:356:CYS:SG	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:THR:CG2	2:B:288:VAL:N	2.55	0.70
1:A:103:TYR:OH	1:A:151:SER:OG	2.08	0.70
1:A:103:TYR:CG	1:A:188:ILE:HG21	2.22	0.70
1:A:220:GLU:CG	1:A:220:GLU:CA	2.67	0.70
1:A:395:PHE:CE1	1:A:422:ARG:HG3	2.26	0.70
2:B:102:ASN:HD22	2:B:105:LYS:HZ1	1.40	0.70
2:B:183:GLU:CG	2:B:394:GLN:HB3	2.21	0.70
2:B:194:LEU:CD2	2:B:267:PHE:CZ	2.75	0.70
2:B:397:ALA:C	2:B:401:ARG:HB2	2.17	0.70
1:A:158:SER:N	1:A:166:LYS:NZ	2.40	0.69
1:A:271:THR:O	1:A:376:CYS:HA	1.92	0.69
1:A:273:ALA:N	1:A:274:PRO:HD2	2.07	0.69
2:B:132:LEU:HB2	2:B:164:ARG:NH1	2.06	0.69
2:B:141:LEU:CD2	2:B:186:ASN:HB3	2.12	0.69
2:B:259:MET:CE	2:B:378:ILE:HG22	2.22	0.69
2:B:265:LEU:CD2	2:B:267:PHE:CZ	2.71	0.69
1:A:312:TYR:CE2	1:A:377:MET:HE2	2.26	0.69
2:B:435:TYR:CA	2:B:436:GLN:HG3	2.18	0.69
1:A:72:PRO:CA	1:A:75:ILE:CG2	2.70	0.69
1:A:200:CYS:SG	1:A:259:LEU:HB2	2.32	0.69
2:B:44:LEU:CG	2:B:85:GLN:CG	2.67	0.69
2:B:142:GLY:CA	2:B:182:VAL:CG2	2.65	0.69
2:B:158:ARG:CD	2:B:197:ASN:N	2.51	0.69
2:B:183:GLU:CD	2:B:394:GLN:CG	2.65	0.69
1:A:241:SER:CB	1:A:356:ASN:ND2	2.53	0.69
1:A:282:TYR:HD2	1:A:285:GLN:HA	1.52	0.69
2:B:246:GLY:HA2	2:B:357:ASP:CG	2.18	0.69
2:B:259:MET:HE2	2:B:379:GLY:CA	2.22	0.69
2:B:265:LEU:O	2:B:267:PHE:CD2	2.45	0.69
2:B:369:ARG:O	5:B:501:TXL:C21	2.41	0.69
1:A:291:ILE:HD11	1:A:373:ARG:CB	2.22	0.69
1:A:361:THR:C	1:A:362:VAL:HG23	2.18	0.69
1:A:5:ILE:HD12	1:A:135:PHE:CE1	2.28	0.69
1:A:115:ILE:CD1	1:A:156:ARG:HD2	2.23	0.69
1:A:231:ILE:CD1	1:A:302:MET:CE	2.69	0.69
2:B:2:ARG:O	2:B:2:ARG:HG2	1.91	0.69
2:B:53:TYR:CE1	2:B:87:PHE:HE1	2.07	0.69
2:B:371:LEU:O	2:B:372:LYS:HB2	1.93	0.69
1:A:28:HIS:CG	1:A:29:GLY:H	2.10	0.69
1:A:115:ILE:CD1	1:A:156:ARG:CZ	2.62	0.69
1:A:122:ILE:CD1	1:A:157:LEU:HD22	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:C	1:A:177:VAL:CG2	2.42	0.69
1:A:200:CYS:SG	1:A:260:VAL:HG23	2.33	0.69
1:A:288:VAL:O	1:A:291:ILE:HG13	1.92	0.69
2:B:229:HIS:CE1	5:B:501:TXL:H37	2.28	0.69
2:B:242:LEU:HD13	2:B:250:ALA:CB	2.15	0.69
2:B:242:LEU:HD23	2:B:356:CYS:SG	2.33	0.69
2:B:416:MET:O	2:B:417:GLU:HB2	1.90	0.69
1:A:13:GLY:C	1:A:16:ILE:HG22	2.18	0.69
1:A:17:GLY:O	1:A:21:TRP:HD1	1.76	0.69
1:A:17:GLY:O	1:A:21:TRP:CD1	2.46	0.69
1:A:184:PRO:CG	1:A:399:TYR:HD2	2.05	0.69
1:A:219:ILE:CG2	1:A:219:ILE:C	2.65	0.69
1:A:230:LEU:CG	1:A:302:MET:HE1	2.23	0.69
1:A:341:ILE:HG21	1:A:343:PHE:CE2	2.27	0.69
1:A:369:ALA:HB2	1:A:371:VAL:CG2	2.21	0.69
1:A:397:LEU:HD22	1:A:401:LYS:NZ	2.08	0.69
2:B:7:ILE:HG12	2:B:66:ILE:CG2	2.16	0.69
2:B:80:SER:O	2:B:81:GLY:C	2.35	0.69
2:B:133:GLN:HE21	2:B:253:ARG:HH11	1.39	0.69
2:B:169:PHE:CZ	2:B:235:MET:CG	2.75	0.69
2:B:184:PRO:HD2	2:B:398:MET:SD	2.32	0.69
2:B:296:PHE:O	2:B:297:ASP:C	2.34	0.69
2:B:342:TYR:C	2:B:343:PHE:CD2	2.71	0.69
2:B:407:TRP:N	2:B:407:TRP:CD1	2.58	0.69
1:A:57:GLY:HA3	1:A:61:HIS:ND1	2.08	0.69
2:B:3:GLU:C	2:B:4:ILE:CG1	2.58	0.69
2:B:14:ASN:ND2	2:B:69:ASP:OD1	2.25	0.69
2:B:33:THR:C	2:B:59:ASN:ND2	2.44	0.69
2:B:253:ARG:HH11	2:B:253:ARG:HB2	1.58	0.69
2:B:433:GLN:O	2:B:434:GLN:C	2.34	0.69
2:B:35:SER:CA	2:B:60:LYS:HE2	2.21	0.69
2:B:191:VAL:HG21	2:B:421:ALA:CA	2.21	0.69
1:A:97:GLU:HB3	1:A:110:ILE:HD13	1.74	0.68
1:A:401:LYS:HG2	1:A:402:ARG:HG3	1.75	0.68
2:B:158:ARG:HH11	2:B:197:ASN:H	1.40	0.68
1:A:258:ASN:O	1:A:314:ALA:HB1	1.92	0.68
2:B:44:LEU:O	2:B:44:LEU:HG	1.93	0.68
2:B:320:ARG:HE	2:B:360:PRO:HG3	1.58	0.68
1:A:172:TYR:CZ	1:A:387:ALA:CB	2.74	0.68
1:A:250:VAL:CG1	1:A:254:GLU:HG2	2.15	0.68
1:A:315:CYS:HG	1:A:343:PHE:HE1	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:HB3	2:B:60:LYS:CG	2.22	0.68
2:B:57:ALA:C	2:B:64:ARG:H	2.00	0.68
2:B:184:PRO:HB2	2:B:399:PHE:CD2	2.22	0.68
2:B:259:MET:O	2:B:261:PRO:HD3	1.93	0.68
2:B:323:MET:HG2	2:B:324:SER:H	1.55	0.68
1:A:66:VAL:HG22	1:A:125:LEU:CD1	2.23	0.68
1:A:158:SER:CB	1:A:196:GLU:O	2.41	0.68
1:A:312:TYR:CG	1:A:381:THR:HG22	2.28	0.68
2:B:92:PHE:CD2	2:B:114:LEU:CD1	2.64	0.68
2:B:339:ASN:O	2:B:342:TYR:CB	2.40	0.68
1:A:13:GLY:HA2	1:A:16:ILE:HG22	1.75	0.68
1:A:296:PHE:CE1	1:A:335:ILE:HG21	2.28	0.68
1:A:395:PHE:CD1	1:A:422:ARG:HG3	2.28	0.68
2:B:244:PHE:O	2:B:245:PRO:O	2.12	0.68
2:B:286:LEU:HD11	2:B:372:LYS:CB	2.07	0.68
1:A:5:ILE:HD12	1:A:135:PHE:CZ	2.28	0.68
1:A:234:ILE:O	1:A:237:SER:OG	2.11	0.68
2:B:44:LEU:HB3	2:B:85:GLN:HG3	1.76	0.68
2:B:194:LEU:HD23	2:B:267:PHE:CE2	2.28	0.68
1:A:5:ILE:HD11	1:A:132:LEU:HD13	1.76	0.68
1:A:26:LEU:HD11	1:A:361:THR:OG1	1.94	0.68
1:A:184:PRO:CG	1:A:395:PHE:HB2	2.19	0.68
1:A:317:LEU:HA	1:A:376:CYS:O	1.94	0.68
1:A:361:THR:O	1:A:362:VAL:CG2	2.41	0.68
2:B:102:ASN:ND2	2:B:105:LYS:HZ1	1.90	0.68
2:B:144:GLY:N	2:B:185:TYR:OH	2.27	0.68
2:B:201:THR:HG21	2:B:265:LEU:CG	2.24	0.68
1:A:107:HIS:CD2	1:A:148:GLY:HA2	2.29	0.68
1:A:242:LEU:CD1	1:A:255:PHE:CZ	2.67	0.68
1:A:311:LYS:O	1:A:312:TYR:O	2.12	0.68
1:A:315:CYS:SG	1:A:343:PHE:CE1	2.87	0.68
2:B:175:PRO:O	2:B:176:LYS:HD3	1.88	0.68
2:B:352:LYS:HG2	2:B:353:THR:N	2.09	0.68
1:A:45:GLY:C	1:A:46:ASP:CG	2.58	0.68
1:A:57:GLY:CA	1:A:61:HIS:CE1	2.71	0.68
1:A:66:VAL:CG2	1:A:125:LEU:HD13	2.24	0.68
1:A:48:SER:O	1:A:50:ASN:ND2	2.22	0.68
1:A:115:ILE:HD13	1:A:152:LEU:HD11	1.73	0.68
2:B:75:MET:HE2	2:B:79:ARG:HB3	1.76	0.68
1:A:107:HIS:CD2	1:A:148:GLY:C	2.72	0.67
1:A:191:THR:HG21	1:A:421:ALA:CA	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:HB2	2:B:84:GLY:HA2	1.74	0.67
2:B:183:GLU:OE2	2:B:394:GLN:CD	2.36	0.67
2:B:289:PRO:HA	2:B:292:THR:OG1	1.93	0.67
1:A:77:GLU:C	1:A:80:THR:H	2.01	0.67
2:B:178:SER:HB2	4:B:500:GDP:O3'	1.89	0.67
2:B:183:GLU:CG	2:B:398:MET:SD	2.82	0.67
1:A:83:TYR:O	1:A:84:ARG:CG	2.41	0.67
1:A:153:LEU:O	1:A:157:LEU:CG	2.42	0.67
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.76	0.67
2:B:242:LEU:HD21	2:B:354:ALA:HB1	1.77	0.67
2:B:244:PHE:CB	2:B:245:PRO:CD	2.71	0.67
1:A:38:SER:C	1:A:39:ASP:CB	2.68	0.67
1:A:75:ILE:HD12	1:A:93:ILE:O	1.95	0.67
1:A:155:GLU:CD	1:A:192:HIS:CD2	2.68	0.67
1:A:155:GLU:CD	1:A:192:HIS:HD2	1.88	0.67
1:A:209:ILE:HD13	1:A:227:LEU:CD1	2.24	0.67
1:A:222:PRO:HB2	2:B:326:LYS:HD2	1.75	0.67
1:A:399:TYR:O	1:A:403:ALA:HA	1.94	0.67
1:A:422:ARG:O	1:A:426:ALA:CB	2.41	0.67
2:B:53:TYR:HD1	2:B:87:PHE:CE1	2.11	0.67
2:B:87:PHE:CE1	2:B:89:PRO:HG3	2.28	0.67
2:B:102:ASN:CB	2:B:408:TYR:HD1	2.07	0.67
2:B:104:ALA:HA	2:B:413:MET:CE	2.22	0.67
2:B:151:THR:HA	2:B:192:HIS:HE2	0.84	0.67
1:A:58:ALA:HB3	1:A:60:LYS:HG3	1.75	0.67
1:A:204:VAL:HG13	1:A:302:MET:HE3	1.75	0.67
1:A:239:THR:CG2	1:A:243:ARG:HG3	2.23	0.67
2:B:96:GLN:O	2:B:98:GLY:CA	2.42	0.67
1:A:16:ILE:CG2	1:A:138:PHE:CD1	2.77	0.67
1:A:103:TYR:N	1:A:408:TYR:HE1	1.81	0.67
1:A:277:SER:CA	1:A:368:LEU:HD22	2.24	0.67
2:B:399:PHE:CE1	2:B:408:TYR:CZ	2.80	0.67
1:A:172:TYR:HE2	1:A:388:TRP:CZ3	2.12	0.67
2:B:284:ARG:O	2:B:286:LEU:N	2.28	0.67
2:B:328:VAL:O	2:B:332:MET:HG2	1.93	0.67
2:B:336:GLN:HE21	2:B:351:VAL:HB	1.60	0.67
1:A:88:HIS:CG	1:A:89:PRO:N	2.62	0.67
2:B:30:ILE:HG23	2:B:243:ARG:NH1	2.08	0.67
2:B:31:ASP:H	2:B:32:PRO:HD3	1.59	0.67
2:B:44:LEU:CB	2:B:85:GLN:HG3	2.24	0.67
2:B:190:SER:C	2:B:192:HIS:N	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:O	1:A:80:THR:HB	1.95	0.67
1:A:176:GLN:NE2	2:B:333:LEU:CD2	2.36	0.67
1:A:312:TYR:HD2	1:A:381:THR:CG2	2.04	0.67
1:A:65:ALA:O	1:A:66:VAL:CG2	2.42	0.67
1:A:146:GLY:HA2	1:A:150:THR:HG23	1.76	0.67
2:B:107:HIS:CE1	2:B:152:LEU:HD23	2.22	0.67
2:B:181:VAL:CG2	2:B:404:PHE:HE2	2.09	0.67
2:B:197:ASN:OD1	2:B:197:ASN:O	2.13	0.67
1:A:196:GLU:O	1:A:197:HIS:CG	2.48	0.66
1:A:210:TYR:CE1	2:B:326:LYS:HE2	2.30	0.66
2:B:135:PHE:HB2	2:B:166:MET:SD	2.34	0.66
2:B:201:THR:HG21	2:B:265:LEU:HD21	0.74	0.66
2:B:230:LEU:HG	2:B:302:MET:HE3	1.76	0.66
1:A:22:GLU:O	1:A:25:CYS:CB	2.43	0.66
1:A:103:TYR:CE2	1:A:189:LEU:CA	2.75	0.66
1:A:143:GLY:O	1:A:144:GLY:C	2.35	0.66
1:A:220:GLU:H	1:A:220:GLU:HG3	1.58	0.66
1:A:291:ILE:HD12	1:A:373:ARG:HB3	1.77	0.66
1:A:407:TRP:CH2	2:B:256:ALA:HB1	2.21	0.66
2:B:11:GLN:HB2	4:B:500:GDP:O2A	1.95	0.66
2:B:19:LYS:HD2	2:B:228:ASN:CB	2.18	0.66
2:B:107:HIS:CD2	2:B:152:LEU:HD23	2.19	0.66
1:A:328:VAL:HG13	1:A:353:VAL:HG11	1.77	0.66
2:B:69:ASP:CG	2:B:74:THR:CB	2.60	0.66
2:B:141:LEU:HD12	2:B:173:PRO:HD3	1.77	0.66
2:B:359:PRO:CB	2:B:372:LYS:O	2.43	0.66
2:B:384:ILE:O	2:B:385:GLN:C	2.33	0.66
1:A:88:HIS:CD2	1:A:89:PRO:N	2.63	0.66
1:A:210:TYR:CE1	2:B:326:LYS:CE	2.78	0.66
1:A:239:THR:O	1:A:243:ARG:CG	2.43	0.66
3:A:500:GTP:O2A	2:B:248:LEU:HD12	1.95	0.66
1:A:14:VAL:HB	1:A:74:VAL:HG21	1.78	0.66
1:A:28:HIS:CG	1:A:29:GLY:N	2.64	0.66
1:A:104:ALA:CA	1:A:108:TYR:HD2	2.08	0.66
1:A:288:VAL:O	1:A:291:ILE:CG1	2.44	0.66
2:B:154:ILE:HG23	2:B:198:THR:CG2	2.26	0.66
2:B:272:PHE:CE1	2:B:274:PRO:HG2	2.30	0.66
2:B:391:ILE:O	2:B:394:GLN:HB2	1.95	0.66
1:A:262:TYR:CE1	1:A:435:VAL:HG13	2.31	0.66
2:B:153:LEU:O	2:B:157:ILE:HG13	1.95	0.66
2:B:154:ILE:HD12	2:B:192:HIS:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:PRO:HB3	2:B:395:PHE:CD1	2.30	0.66
1:A:32:PRO:C	1:A:34:GLY:N	2.32	0.66
2:B:405:LEU:O	2:B:409:THR:OG1	2.07	0.66
1:A:5:ILE:HG13	1:A:64:ARG:HH21	1.61	0.66
2:B:40:SER:O	2:B:41:ASP:CG	2.38	0.66
2:B:42:LEU:O	2:B:43:GLN:CG	2.42	0.66
2:B:103:TRP:HZ3	2:B:108:TYR:HH	1.00	0.66
1:A:179:THR:CG2	1:A:181:VAL:CG2	2.74	0.66
1:A:313:MET:HE3	1:A:346:TRP:CH2	2.27	0.66
1:A:73:THR:CB	2:B:249:ASN:ND2	2.59	0.66
1:A:107:HIS:CD2	1:A:151:SER:OG	2.49	0.66
1:A:109:THR:HG21	1:A:411:GLU:HB3	1.78	0.66
1:A:176:GLN:NE2	2:B:333:LEU:HB2	2.11	0.66
1:A:209:ILE:HG12	1:A:302:MET:HE3	1.78	0.66
1:A:272:TYR:CE2	1:A:274:PRO:HG2	2.26	0.66
1:A:277:SER:N	1:A:280:LYS:CG	2.58	0.66
1:A:313:MET:HA	1:A:344:VAL:CG2	2.25	0.66
2:B:35:SER:O	2:B:36:TYR:C	2.39	0.66
1:A:210:TYR:CD1	2:B:326:LYS:CB	2.78	0.65
2:B:103:TRP:CD1	2:B:148:GLY:HA3	2.31	0.65
2:B:229:HIS:CG	5:B:501:TXL:H37	2.28	0.65
2:B:386:GLU:C	2:B:388:PHE:H	2.01	0.65
1:A:172:TYR:HD1	1:A:173:PRO:O	1.79	0.65
1:A:239:THR:O	1:A:243:ARG:CB	2.44	0.65
1:A:291:ILE:CD1	1:A:373:ARG:CB	2.74	0.65
1:A:361:THR:CG2	1:A:362:VAL:N	2.59	0.65
2:B:23:VAL:HG21	2:B:232:SER:CB	2.26	0.65
2:B:133:GLN:NE2	2:B:253:ARG:HH11	1.94	0.65
2:B:268:PHE:CD1	2:B:380:ASN:OD1	2.49	0.65
2:B:422:GLU:O	2:B:426:ASN:CB	2.41	0.65
1:A:5:ILE:HB	1:A:135:PHE:CD1	2.32	0.65
1:A:154:MET:HE1	1:A:166:LYS:HB3	1.78	0.65
1:A:205:ASP:HB2	1:A:302:MET:O	1.96	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:433:GLN:CG	2:B:437:ASP:OD2	2.43	0.65
2:B:181:VAL:CA	2:B:398:MET:HE1	2.27	0.65
1:A:22:GLU:O	1:A:25:CYS:HB3	1.96	0.65
1:A:331:ALA:O	1:A:334:THR:OG1	2.12	0.65
2:B:158:ARG:HA	2:B:197:ASN:HD22	0.52	0.65
1:A:197:HIS:O	1:A:198:SER:CB	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:PRO:HA	2:B:395:PHE:CD1	2.30	0.65
1:A:202:PHE:CD1	1:A:378:LEU:HD22	2.30	0.65
1:A:217:LEU:CD1	1:A:277:SER:HA	2.27	0.65
1:A:275:VAL:O	1:A:275:VAL:HG12	1.94	0.65
2:B:22:GLU:CA	2:B:83:PHE:CE2	2.79	0.65
2:B:33:THR:HG22	2:B:34:GLY:N	2.11	0.65
2:B:34:GLY:O	2:B:36:TYR:CD2	2.49	0.65
2:B:75:MET:CE	2:B:75:MET:HA	2.21	0.65
2:B:274:PRO:C	2:B:276:THR:HG23	2.21	0.65
2:B:313:LEU:CA	2:B:344:VAL:HG21	2.22	0.65
1:A:30:ILE:HG21	1:A:64:ARG:CG	2.09	0.65
1:A:83:TYR:O	1:A:84:ARG:CB	2.44	0.65
2:B:101:ASN:O	2:B:105:LYS:HD2	1.97	0.65
2:B:241:CYS:SG	2:B:320:ARG:CD	2.84	0.65
1:A:98:ASP:OD2	2:B:133:GLN:CD	2.40	0.65
1:A:296:PHE:O	1:A:297:GLU:C	2.31	0.65
1:A:313:MET:CE	1:A:346:TRP:CZ2	2.70	0.65
2:B:165:ILE:HD13	2:B:256:ALA:CB	2.26	0.65
2:B:398:MET:HE2	2:B:399:PHE:CE2	2.31	0.65
2:B:405:LEU:O	2:B:409:THR:N	2.26	0.65
1:A:77:GLU:N	1:A:80:THR:OG1	2.30	0.65
2:B:22:GLU:CD	2:B:83:PHE:CD2	2.69	0.65
2:B:53:TYR:CE1	2:B:89:PRO:CG	2.78	0.65
2:B:103:TRP:HE1	2:B:189:LEU:HD23	1.59	0.65
2:B:142:GLY:O	2:B:185:TYR:CZ	2.49	0.64
2:B:226:ASP:CG	5:B:501:TXL:C40	2.70	0.64
2:B:296:PHE:CE1	2:B:335:VAL:HG21	2.32	0.64
1:A:13:GLY:CA	1:A:16:ILE:HG22	2.26	0.64
1:A:73:THR:HG21	2:B:249:ASN:HD21	1.59	0.64
1:A:142:GLY:HA2	1:A:185:TYR:CD1	2.32	0.64
2:B:8:GLN:HB2	2:B:67:LEU:HD12	1.78	0.64
2:B:111:GLY:O	2:B:115:VAL:CB	2.45	0.64
2:B:426:ASN:C	2:B:428:LEU:N	2.51	0.64
1:A:2:ARG:O	1:A:31:GLN:CG	2.39	0.64
1:A:175:PRO:HD3	1:A:390:ARG:HH22	1.62	0.64
1:A:224:TYR:HB2	2:B:325:MET:CB	2.28	0.64
1:A:312:TYR:CZ	1:A:377:MET:HE1	2.29	0.64
2:B:103:TRP:CD1	2:B:189:LEU:HD21	2.08	0.64
2:B:183:GLU:HB2	2:B:184:PRO:HD2	1.70	0.64
2:B:319:PHE:CE2	2:B:328:VAL:HG13	2.32	0.64
2:B:401:ARG:CG	2:B:402:LYS:H	2.03	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASP:C	1:A:33:ASP:OD1	2.40	0.64
1:A:151:SER:HB2	1:A:192:HIS:HB2	1.79	0.64
1:A:223:THR:H	1:A:226:ASN:HD22	1.44	0.64
1:A:270:ALA:O	1:A:302:MET:CG	2.43	0.64
2:B:12:CYS:SG	4:B:500:GDP:O4'	2.55	0.64
2:B:30:ILE:CG2	2:B:136:GLN:HE22	2.09	0.64
2:B:32:PRO:CA	2:B:59:ASN:HD22	2.05	0.64
2:B:92:PHE:CE1	2:B:121:VAL:CG2	2.80	0.64
2:B:94:PHE:CD2	2:B:114:LEU:HD22	2.32	0.64
1:A:80:THR:O	1:A:82:THR:N	2.30	0.64
2:B:48:ARG:C	2:B:61:TYR:CD2	2.76	0.64
1:A:103:TYR:CE2	1:A:147:SER:C	2.76	0.64
1:A:115:ILE:HD11	1:A:156:ARG:HD2	1.79	0.64
1:A:179:THR:HB	1:A:182:VAL:HG23	1.79	0.64
1:A:287:SER:OG	1:A:290:GLU:CB	2.45	0.64
2:B:11:GLN:HB3	4:B:500:GDP:O1A	1.97	0.64
2:B:12:CYS:SG	4:B:500:GDP:N9	2.71	0.64
2:B:231:VAL:HA	2:B:302:MET:CE	2.28	0.64
1:A:238:ILE:O	1:A:255:PHE:HZ	1.80	0.64
1:A:426:ALA:C	1:A:428:LEU:N	2.51	0.64
2:B:47:GLU:HG2	2:B:63:PRO:HD3	1.80	0.64
2:B:166:MET:O	2:B:199:ASP:HB3	1.97	0.64
1:A:30:ILE:CB	1:A:64:ARG:HB2	2.15	0.64
1:A:48:SER:OG	1:A:56:THR:CB	2.37	0.64
1:A:224:TYR:CE1	3:A:500:GTP:C2	2.86	0.64
1:A:348:PRO:O	1:A:349:THR:OG1	2.13	0.64
2:B:6:HIS:CE1	2:B:21:TRP:CH2	2.86	0.64
2:B:13:GLY:HA3	2:B:138:THR:OG1	1.98	0.64
2:B:173:PRO:HG2	2:B:391:ILE:HD11	1.78	0.64
1:A:41:THR:O	1:A:41:THR:HG22	1.97	0.64
1:A:191:THR:CG2	1:A:421:ALA:HA	2.28	0.64
1:A:426:ALA:O	1:A:428:LEU:N	2.31	0.64
2:B:3:GLU:HA	2:B:31:ASP:CG	2.19	0.64
2:B:30:ILE:HG22	2:B:243:ARG:NH1	2.13	0.64
2:B:272:PHE:CZ	5:B:501:TXL:H28	2.33	0.64
1:A:26:LEU:CD1	1:A:361:THR:HG21	2.15	0.64
1:A:132:LEU:O	1:A:134:GLY:N	2.30	0.64
1:A:206:ASN:CG	3:A:500:GTP:HN22	2.06	0.64
1:A:397:LEU:HA	1:A:401:LYS:HB3	1.78	0.64
2:B:12:CYS:O	2:B:16:ILE:HB	1.98	0.64
2:B:13:GLY:HA2	2:B:138:THR:OG1	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:PRO:HB2	2:B:399:PHE:CG	2.33	0.64
2:B:405:LEU:CG	2:B:418:PHE:CZ	2.77	0.64
1:A:102:ASN:CA	1:A:185:TYR:HE2	2.11	0.63
1:A:303:VAL:HG12	1:A:305:CYS:SG	2.38	0.63
1:A:306:ASP:CG	1:A:308:ARG:CG	2.69	0.63
2:B:49:ILE:O	2:B:50:ASN:CG	2.40	0.63
2:B:55:GLU:C	2:B:57:ALA:N	2.56	0.63
2:B:101:ASN:ND2	2:B:185:TYR:OH	2.31	0.63
2:B:398:MET:O	2:B:401:ARG:CB	2.45	0.63
1:A:238:ILE:HG23	1:A:255:PHE:CZ	2.32	0.63
1:A:324:VAL:O	1:A:327:ASP:HB2	1.97	0.63
2:B:183:GLU:OE1	2:B:394:GLN:HG3	1.98	0.63
1:A:65:ALA:CB	1:A:91:GLN:CD	2.71	0.63
1:A:115:ILE:CD1	1:A:156:ARG:NE	2.59	0.63
1:A:315:CYS:SG	1:A:343:PHE:HE1	2.21	0.63
2:B:92:PHE:HE1	2:B:121:VAL:CG2	2.10	0.63
2:B:229:HIS:NE2	5:B:501:TXL:C34	2.50	0.63
2:B:295:MET:CE	2:B:375:ALA:C	2.72	0.63
1:A:97:GLU:CB	1:A:110:ILE:HG23	2.21	0.63
1:A:204:VAL:HG13	1:A:302:MET:CE	2.28	0.63
1:A:267:PHE:O	1:A:380:ASN:OD1	2.15	0.63
1:A:282:TYR:CE2	1:A:285:GLN:HA	2.33	0.63
1:A:405:VAL:CG2	1:A:405:VAL:HG11	2.25	0.63
1:A:196:GLU:C	1:A:197:HIS:ND1	2.56	0.63
1:A:297:GLU:C	1:A:299:ALA:N	2.55	0.63
2:B:92:PHE:HE1	2:B:121:VAL:HG21	1.62	0.63
2:B:165:ILE:HD13	2:B:256:ALA:HB1	1.80	0.63
2:B:288:VAL:N	2:B:289:PRO:CD	2.59	0.63
2:B:118:VAL:O	2:B:118:VAL:HG12	1.98	0.63
2:B:287:THR:HG22	2:B:289:PRO:N	2.14	0.63
2:B:426:ASN:O	2:B:428:LEU:N	2.32	0.63
1:A:67:PHE:HB2	1:A:92:LEU:CD2	2.28	0.63
1:A:70:LEU:CD1	1:A:145:THR:CB	2.60	0.63
1:A:97:GLU:HA	1:A:97:GLU:OE1	1.97	0.63
1:A:192:HIS:O	1:A:196:GLU:CG	2.46	0.63
1:A:277:SER:CB	1:A:280:LYS:CG	2.51	0.63
1:A:282:TYR:O	1:A:284:GLU:N	2.31	0.63
1:A:296:PHE:CZ	1:A:335:ILE:HD13	2.22	0.63
2:B:5:VAL:HG11	2:B:135:PHE:CE2	2.33	0.63
2:B:250:ALA:HB2	2:B:352:LYS:NZ	2.13	0.63
1:A:14:VAL:HA	1:A:67:PHE:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:HB1	1:A:91:GLN:CD	2.23	0.63
1:A:154:MET:HB2	1:A:192:HIS:NE2	2.14	0.63
2:B:55:GLU:C	2:B:57:ALA:H	2.07	0.63
2:B:102:ASN:HB2	2:B:105:LYS:CG	2.29	0.63
2:B:103:TRP:CG	2:B:188:THR:HG1	2.16	0.63
1:A:57:GLY:HA3	1:A:61:HIS:CD2	2.34	0.62
1:A:103:TYR:CD2	1:A:189:LEU:CG	2.78	0.62
1:A:106:GLY:O	1:A:111:GLY:N	2.32	0.62
1:A:193:THR:HG1	1:A:194:THR:N	1.96	0.62
1:A:237:SER:HA	1:A:320:ARG:NH1	2.13	0.62
1:A:282:TYR:CE2	1:A:284:GLU:O	2.51	0.62
1:A:317:LEU:O	1:A:353:VAL:HA	1.98	0.62
2:B:200:GLU:CB	2:B:268:PHE:HE2	2.09	0.62
1:A:82:THR:C	1:A:84:ARG:H	2.07	0.62
1:A:103:TYR:OH	1:A:151:SER:HB2	1.98	0.62
1:A:361:THR:HG22	1:A:362:VAL:H	1.63	0.62
2:B:23:VAL:O	2:B:26:ASP:CB	2.47	0.62
2:B:106:GLY:O	2:B:111:GLY:N	2.33	0.62
2:B:166:MET:CG	2:B:197:ASN:O	2.46	0.62
2:B:223:THR:OG1	2:B:226:ASP:HB2	1.99	0.62
2:B:388:PHE:C	2:B:390:ARG:N	2.49	0.62
1:A:202:PHE:CE1	1:A:378:LEU:HD22	2.34	0.62
1:A:404:PHE:CD2	1:A:404:PHE:O	2.52	0.62
5:B:501:TXL:H192	5:B:501:TXL:C20	2.29	0.62
1:A:264:ARG:NH1	1:A:424:ASP:O	2.32	0.62
1:A:343:PHE:CE2	1:A:351:PHE:HZ	1.81	0.62
2:B:4:ILE:CD1	2:B:30:ILE:CB	2.77	0.62
2:B:192:HIS:ND1	2:B:192:HIS:C	2.57	0.62
2:B:238:VAL:HG13	2:B:255:LEU:CD1	2.30	0.62
2:B:22:GLU:C	2:B:24:ILE:H	2.06	0.62
2:B:274:PRO:HB2	2:B:371:LEU:HD11	1.81	0.62
2:B:342:TYR:O	2:B:343:PHE:CD2	2.52	0.62
1:A:2:ARG:O	1:A:243:ARG:NH1	2.32	0.62
1:A:139:HIS:HB3	1:A:169:PHE:O	2.00	0.62
1:A:224:TYR:CD1	3:A:500:GTP:C2	2.88	0.62
2:B:35:SER:HB3	2:B:60:LYS:HG3	1.81	0.62
2:B:57:ALA:O	2:B:62:VAL:O	2.16	0.62
2:B:216:THR:HG21	2:B:275:LEU:CD1	2.29	0.62
1:A:73:THR:CG2	2:B:249:ASN:HD22	2.10	0.62
1:A:103:TYR:CZ	1:A:188:ILE:HG22	2.34	0.62
1:A:115:ILE:HD12	1:A:152:LEU:HG	0.67	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PRO:C	2:B:59:ASN:HD22	2.05	0.62
2:B:41:ASP:C	2:B:42:LEU:CG	2.54	0.62
2:B:70:LEU:O	2:B:71:GLU:CG	2.47	0.62
2:B:133:GLN:O	2:B:133:GLN:HG2	1.99	0.62
2:B:246:GLY:CA	2:B:357:ASP:OD2	2.48	0.62
1:A:8:HIS:HE1	1:A:17:GLY:HA3	1.65	0.62
1:A:148:GLY:HA2	1:A:151:SER:HG	1.62	0.62
1:A:341:ILE:HG22	1:A:343:PHE:CE2	2.35	0.62
2:B:22:GLU:HG2	2:B:83:PHE:CE2	2.26	0.62
2:B:183:GLU:OE1	2:B:394:GLN:CG	2.48	0.62
1:A:142:GLY:CA	1:A:185:TYR:CE1	2.82	0.62
1:A:224:TYR:CD2	2:B:325:MET:CB	2.64	0.62
2:B:181:VAL:CA	2:B:398:MET:CE	2.77	0.62
2:B:243:ARG:NH2	2:B:252:LEU:CD1	2.52	0.62
1:A:122:ILE:CD1	1:A:157:LEU:CD2	2.77	0.62
1:A:276:ILE:HD13	1:A:282:TYR:CG	2.35	0.62
2:B:89:PRO:O	2:B:90:ASP:CG	2.43	0.62
2:B:141:LEU:HD13	2:B:173:PRO:HD3	1.81	0.62
2:B:246:GLY:HA2	2:B:357:ASP:OD2	2.00	0.62
2:B:250:ALA:CB	2:B:352:LYS:NZ	2.63	0.62
1:A:103:TYR:N	1:A:408:TYR:CE1	2.61	0.61
2:B:169:PHE:HA	2:B:202:TYR:HB2	1.81	0.61
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.35	0.61
1:A:151:SER:CB	1:A:192:HIS:CB	2.75	0.61
1:A:154:MET:HE3	1:A:166:LYS:HD2	1.82	0.61
1:A:242:LEU:HD12	1:A:255:PHE:CE2	2.34	0.61
1:A:304:LYS:HG2	1:A:304:LYS:O	1.98	0.61
1:A:335:ILE:C	1:A:337:THR:H	2.06	0.61
2:B:3:GLU:CG	2:B:4:ILE:H	2.09	0.61
2:B:288:VAL:O	2:B:291:LEU:N	2.33	0.61
2:B:313:LEU:HD13	2:B:435:TYR:HD2	1.65	0.61
1:A:64:ARG:HH22	1:A:132:LEU:CG	2.09	0.61
1:A:78:VAL:HG13	1:A:87:PHE:HE1	1.61	0.61
2:B:4:ILE:HG21	2:B:30:ILE:HB	1.82	0.61
2:B:71:GLU:O	2:B:72:PRO:C	2.38	0.61
2:B:78:VAL:CA	2:B:82:PRO:HG2	2.30	0.61
1:A:172:TYR:CE1	1:A:387:ALA:HB1	2.34	0.61
1:A:209:ILE:HD11	1:A:231:ILE:CD1	2.17	0.61
2:B:40:SER:C	2:B:41:ASP:CG	2.67	0.61
2:B:250:ALA:HA	2:B:254:LYS:CD	2.17	0.61
2:B:360:PRO:CG	2:B:374:SER:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:CB	1:A:64:ARG:CZ	2.77	0.61
1:A:72:PRO:HA	1:A:75:ILE:HG21	1.80	0.61
1:A:102:ASN:C	1:A:185:TYR:CE2	2.78	0.61
2:B:22:GLU:HA	2:B:83:PHE:CE2	2.35	0.61
2:B:78:VAL:O	2:B:82:PRO:CG	2.43	0.61
2:B:222:PRO:C	2:B:223:THR:CG2	2.72	0.61
1:A:6:SER:OG	1:A:65:ALA:N	2.34	0.61
1:A:209:ILE:CD1	1:A:227:LEU:CD1	2.67	0.61
1:A:269:LEU:HD21	1:A:384:ILE:HD11	1.83	0.61
1:A:288:VAL:O	1:A:291:ILE:HB	2.00	0.61
2:B:201:THR:CG2	2:B:265:LEU:CD2	2.43	0.61
2:B:385:GLN:CD	2:B:433:GLN:HB2	2.26	0.61
2:B:433:GLN:CG	2:B:437:ASP:OD1	2.48	0.61
1:A:219:ILE:C	1:A:219:ILE:HG22	2.26	0.61
1:A:313:MET:CE	1:A:346:TRP:HH2	2.12	0.61
2:B:31:ASP:N	2:B:32:PRO:CD	2.64	0.61
2:B:115:VAL:HG12	2:B:156:LYS:NZ	2.16	0.61
1:A:5:ILE:CG2	1:A:135:PHE:CE1	2.83	0.61
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.83	0.61
1:A:97:GLU:O	1:A:110:ILE:CD1	2.48	0.61
1:A:194:THR:CG2	1:A:195:LEU:H	2.02	0.61
2:B:216:THR:HG21	2:B:275:LEU:HD12	1.83	0.61
2:B:346:TRP:HZ3	2:B:347:ILE:CD1	1.79	0.61
2:B:399:PHE:CZ	2:B:408:TYR:CE2	2.80	0.61
1:A:9:VAL:CG1	1:A:146:GLY:HA2	2.31	0.61
1:A:277:SER:H	1:A:280:LYS:HG2	1.60	0.61
1:A:289:ALA:HB1	1:A:331:ALA:HB2	1.82	0.61
2:B:325:MET:HE1	2:B:355:VAL:HB	1.83	0.61
1:A:109:THR:HG23	1:A:411:GLU:HB3	1.81	0.61
1:A:151:SER:HB2	1:A:155:GLU:OE2	2.01	0.61
1:A:259:LEU:HB3	1:A:380:ASN:HD21	1.64	0.61
1:A:14:VAL:HB	1:A:74:VAL:CG2	2.30	0.60
1:A:96:LYS:O	2:B:1:MET:HE2	2.01	0.60
1:A:122:ILE:HD13	1:A:157:LEU:CD2	2.31	0.60
1:A:217:LEU:CD1	1:A:368:LEU:CG	2.75	0.60
1:A:437:VAL:O	1:A:437:VAL:HG12	2.01	0.60
2:B:3:GLU:CD	2:B:64:ARG:HH12	2.09	0.60
2:B:18:ALA:O	2:B:22:GLU:HG3	2.00	0.60
2:B:22:GLU:CD	2:B:83:PHE:CB	2.72	0.60
2:B:68:VAL:CG1	2:B:149:MET:HE1	2.31	0.60
2:B:398:MET:CG	2:B:399:PHE:H	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ILE:CD1	2:B:256:ALA:CB	2.79	0.60
1:A:34:GLY:O	1:A:60:LYS:NZ	2.34	0.60
1:A:242:LEU:HD13	1:A:250:VAL:O	2.00	0.60
2:B:15:GLN:O	2:B:18:ALA:HB3	2.00	0.60
2:B:34:GLY:HA2	2:B:37:HIS:CD2	2.36	0.60
2:B:94:PHE:CD1	2:B:94:PHE:C	2.68	0.60
2:B:102:ASN:ND2	2:B:105:LYS:HZ2	2.00	0.60
2:B:280:SER:C	2:B:282:GLN:H	2.07	0.60
2:B:414:ASP:C	2:B:416:MET:H	2.05	0.60
1:A:83:TYR:O	1:A:83:TYR:CG	2.54	0.60
1:A:158:SER:CB	1:A:197:HIS:HB2	2.14	0.60
1:A:191:THR:O	1:A:194:THR:OG1	2.19	0.60
1:A:228:ASN:ND2	3:A:500:GTP:N1	2.49	0.60
1:A:358:GLU:O	1:A:359:PRO:O	2.19	0.60
2:B:57:ALA:HA	2:B:64:ARG:HB2	0.69	0.60
1:A:101:ASN:C	1:A:102:ASN:CG	2.59	0.60
1:A:107:HIS:CG	1:A:148:GLY:C	2.77	0.60
1:A:219:ILE:HG22	1:A:219:ILE:O	2.01	0.60
1:A:227:LEU:HB2	2:B:326:LYS:CE	2.31	0.60
1:A:327:ASP:O	1:A:331:ALA:HB3	2.01	0.60
3:A:500:GTP:PA	2:B:248:LEU:HD12	2.41	0.60
2:B:48:ARG:HH11	2:B:60:LYS:HG2	1.60	0.60
2:B:141:LEU:HG	2:B:171:VAL:O	2.01	0.60
2:B:182:VAL:CG1	2:B:186:ASN:HD22	2.01	0.60
1:A:108:TYR:CZ	1:A:417:GLU:OE2	2.53	0.60
1:A:117:LEU:O	1:A:121:ARG:HG3	2.01	0.60
1:A:153:LEU:O	1:A:157:LEU:HD12	2.01	0.60
1:A:209:ILE:O	1:A:212:ILE:HG12	2.02	0.60
2:B:104:ALA:O	2:B:108:TYR:HB2	2.01	0.60
2:B:219:LEU:CD2	2:B:226:ASP:OD2	2.50	0.60
2:B:229:HIS:O	2:B:230:LEU:C	2.43	0.60
2:B:323:MET:CG	2:B:324:SER:H	2.13	0.60
2:B:323:MET:CG	2:B:324:SER:N	2.65	0.60
2:B:397:ALA:O	2:B:401:ARG:CG	2.50	0.60
1:A:100:ALA:HB1	1:A:105:ARG:CG	2.31	0.60
2:B:78:VAL:HA	2:B:82:PRO:CG	2.32	0.60
2:B:139:HIS:NE2	2:B:193:GLN:NE2	2.49	0.60
2:B:178:SER:O	2:B:179:ASP:HB2	2.01	0.60
2:B:424:ASN:O	2:B:424:ASN:ND2	2.32	0.60
1:A:237:SER:HB2	1:A:376:CYS:SG	2.41	0.60
2:B:289:PRO:O	2:B:293:GLN:CB	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:LEU:CD2	2:B:344:VAL:HG21	2.28	0.60
1:A:9:VAL:CG1	1:A:150:THR:HG23	2.31	0.60
1:A:14:VAL:HG11	1:A:74:VAL:HG13	1.83	0.60
2:B:79:ARG:O	2:B:80:SER:OG	2.19	0.60
1:A:115:ILE:CD1	1:A:152:LEU:HD21	2.32	0.60
1:A:141:PHE:HB3	1:A:173:PRO:HD3	1.84	0.60
1:A:171:ILE:N	1:A:203:MET:HE3	2.03	0.60
1:A:237:SER:CB	1:A:376:CYS:SG	2.90	0.60
1:A:262:TYR:HE1	1:A:435:VAL:HG13	1.65	0.60
2:B:136:GLN:HE22	2:B:243:ARG:HH12	1.49	0.60
2:B:274:PRO:O	2:B:276:THR:CG2	2.46	0.60
2:B:320:ARG:HG3	2:B:320:ARG:O	2.00	0.60
2:B:339:ASN:O	2:B:342:TYR:CA	2.50	0.60
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.02	0.59
1:A:62:VAL:HG13	1:A:63:PRO:HD3	1.79	0.59
1:A:126:ALA:O	1:A:132:LEU:CD1	2.41	0.59
2:B:20:PHE:HZ	2:B:239:THR:HG21	1.67	0.59
2:B:22:GLU:OE1	2:B:83:PHE:CD1	2.55	0.59
2:B:30:ILE:CG2	2:B:243:ARG:HH12	2.13	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
1:A:122:ILE:O	1:A:126:ALA:N	2.35	0.59
1:A:192:HIS:ND1	1:A:192:HIS:C	2.57	0.59
1:A:277:SER:OG	1:A:280:LYS:CD	2.47	0.59
2:B:66:ILE:CG1	2:B:121:VAL:CG1	2.69	0.59
2:B:176:LYS:C	2:B:177:VAL:HG13	2.25	0.59
1:A:144:GLY:CA	1:A:185:TYR:OH	2.50	0.59
1:A:173:PRO:HG3	1:A:182:VAL:CG1	2.32	0.59
2:B:23:VAL:O	2:B:26:ASP:HB2	2.02	0.59
2:B:27:GLU:HB2	2:B:36:TYR:HB3	1.84	0.59
2:B:180:THR:C	2:B:398:MET:HE1	2.27	0.59
2:B:198:THR:O	2:B:265:LEU:HD13	2.02	0.59
1:A:36:MET:SD	1:A:60:LYS:CB	2.90	0.59
1:A:57:GLY:HA3	1:A:61:HIS:CG	2.37	0.59
1:A:105:ARG:NH1	2:B:253:ARG:NH2	2.51	0.59
1:A:177:VAL:CB	2:B:349:ASN:ND2	2.52	0.59
1:A:191:THR:CG2	1:A:421:ALA:CA	2.79	0.59
2:B:62:VAL:HG12	2:B:63:PRO:N	2.18	0.59
2:B:103:TRP:O	2:B:107:HIS:HB3	2.02	0.59
2:B:174:SER:HB2	2:B:175:PRO:CD	2.29	0.59
2:B:398:MET:HG2	2:B:399:PHE:H	1.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:CB	1:A:399:TYR:HD2	2.15	0.59
2:B:383:ALA:O	2:B:386:GLU:CB	2.51	0.59
1:A:264:ARG:O	1:A:265:GLY:O	2.19	0.59
1:A:362:VAL:HG12	1:A:363:VAL:N	2.18	0.59
2:B:14:ASN:HB3	2:B:74:THR:OG1	2.01	0.59
2:B:19:LYS:HG3	2:B:228:ASN:ND2	2.16	0.59
2:B:97:SER:CB	2:B:110:GLU:CD	2.60	0.59
2:B:175:PRO:CB	2:B:176:LYS:HE2	2.32	0.59
2:B:340:SER:O	2:B:343:PHE:N	2.35	0.59
1:A:288:VAL:CG2	1:A:373:ARG:CD	2.44	0.59
1:A:312:TYR:CE1	1:A:341:ILE:HG23	2.38	0.59
2:B:4:ILE:HD11	2:B:30:ILE:O	1.98	0.59
2:B:56:ALA:CB	2:B:62:VAL:CG2	2.69	0.59
2:B:143:GLY:C	2:B:185:TYR:CE1	2.80	0.59
2:B:182:VAL:CG1	2:B:186:ASN:HD21	2.05	0.59
2:B:288:VAL:C	2:B:291:LEU:H	2.10	0.59
1:A:143:GLY:O	1:A:145:THR:N	2.36	0.59
1:A:282:TYR:O	1:A:284:GLU:CA	2.50	0.59
2:B:6:HIS:HB2	2:B:65:ALA:CA	2.28	0.59
2:B:143:GLY:C	2:B:185:TYR:HE1	2.11	0.59
2:B:371:LEU:O	2:B:372:LYS:CB	2.50	0.59
2:B:383:ALA:O	2:B:386:GLU:HB2	2.03	0.59
1:A:182:VAL:HG12	1:A:186:ASN:ND2	2.14	0.59
1:A:184:PRO:HG2	1:A:399:TYR:HD2	1.67	0.59
1:A:202:PHE:HA	1:A:268:PRO:HG2	1.85	0.59
2:B:30:ILE:HG23	2:B:243:ARG:HH11	1.65	0.59
2:B:346:TRP:HZ2	2:B:435:TYR:CD2	2.21	0.59
1:A:224:TYR:HB2	2:B:325:MET:HG3	1.84	0.59
1:A:303:VAL:HG12	1:A:304:LYS:N	2.17	0.59
2:B:133:GLN:HE21	2:B:253:ARG:HB2	1.68	0.59
2:B:142:GLY:HA2	2:B:185:TYR:CG	2.37	0.59
2:B:405:LEU:CD1	2:B:418:PHE:CZ	2.71	0.59
1:A:18:ASN:O	1:A:22:GLU:CG	2.50	0.58
1:A:190:THR:OG1	1:A:425:MET:HE1	2.02	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.03	0.58
1:A:361:THR:CG2	1:A:362:VAL:H	2.15	0.58
1:A:362:VAL:HG13	1:A:367:ASP:HB3	1.83	0.58
2:B:87:PHE:HE1	2:B:89:PRO:HG3	1.58	0.58
1:A:70:LEU:HG	1:A:145:THR:CG2	2.32	0.58
1:A:185:TYR:CE1	1:A:189:LEU:HD11	2.39	0.58
1:A:194:THR:CG2	1:A:195:LEU:HG	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:HB	1:A:327:ASP:OD2	2.03	0.58
1:A:346:TRP:CE3	1:A:346:TRP:O	2.56	0.58
1:A:397:LEU:HA	1:A:401:LYS:CD	2.32	0.58
2:B:272:PHE:CE2	5:B:501:TXL:H28	2.38	0.58
1:A:4:CYS:HB2	1:A:30:ILE:HG21	1.76	0.58
1:A:28:HIS:ND1	1:A:29:GLY:O	2.32	0.58
1:A:217:LEU:HD13	1:A:368:LEU:CD2	2.27	0.58
1:A:236:SER:O	1:A:240:ALA:HB3	2.02	0.58
1:A:324:VAL:CG1	1:A:325:PRO:HD2	2.33	0.58
1:A:332:ILE:HD11	1:A:353:VAL:HG21	1.78	0.58
2:B:29:GLY:O	2:B:58:GLY:CA	2.52	0.58
2:B:103:TRP:HE3	2:B:413:MET:CE	1.90	0.58
2:B:191:VAL:HG22	2:B:421:ALA:HA	1.79	0.58
2:B:294:GLN:CD	2:B:300:ASN:OD1	2.45	0.58
2:B:308:ARG:O	2:B:342:TYR:HE2	1.86	0.58
1:A:100:ALA:CB	1:A:105:ARG:CG	2.81	0.58
1:A:115:ILE:CD1	1:A:156:ARG:CD	2.82	0.58
2:B:29:GLY:HA2	2:B:30:ILE:HG12	1.85	0.58
2:B:92:PHE:HD2	2:B:114:LEU:CD1	1.97	0.58
1:A:291:ILE:O	1:A:294:ALA:HB3	2.03	0.58
1:A:310:GLY:HA3	1:A:382:THR:OG1	2.03	0.58
2:B:104:ALA:HB2	2:B:413:MET:SD	2.44	0.58
1:A:3:GLU:CA	1:A:31:GLN:CB	2.61	0.58
1:A:108:TYR:C	1:A:112:LYS:HG3	2.29	0.58
1:A:2:ARG:HB3	1:A:243:ARG:HH12	1.67	0.58
1:A:89:PRO:O	1:A:90:GLU:HB2	2.04	0.58
1:A:197:HIS:O	1:A:198:SER:HB3	2.03	0.58
1:A:273:ALA:CB	1:A:294:ALA:CB	2.78	0.58
2:B:123:ARG:O	2:B:126:SER:OG	2.20	0.58
2:B:346:TRP:O	2:B:347:ILE:CG1	2.51	0.58
1:A:97:GLU:CG	1:A:110:ILE:HG23	2.33	0.58
1:A:273:ALA:N	1:A:274:PRO:CD	2.66	0.58
1:A:313:MET:HE1	1:A:346:TRP:HZ2	1.60	0.58
2:B:12:CYS:C	2:B:16:ILE:HG12	2.20	0.58
2:B:70:LEU:O	2:B:71:GLU:HG3	2.03	0.58
2:B:274:PRO:HB2	2:B:371:LEU:CD1	2.34	0.58
2:B:295:MET:SD	2:B:375:ALA:HB1	2.36	0.58
5:B:501:TXL:C9	5:B:501:TXL:C16	2.79	0.58
1:A:328:VAL:O	1:A:332:ILE:HG13	2.04	0.58
2:B:105:LYS:CE	2:B:411:GLU:HG3	2.34	0.58
2:B:251:ASP:O	2:B:254:LYS:N	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:GLU:HA	2:B:434:GLN:NE2	2.17	0.58
1:A:74:VAL:O	1:A:77:GLU:HB2	2.03	0.58
1:A:324:VAL:HB	1:A:327:ASP:OD1	2.03	0.58
1:A:385:ALA:HB2	1:A:432:TYR:HD2	1.68	0.58
2:B:6:HIS:CD2	2:B:64:ARG:O	2.56	0.58
2:B:174:SER:HB2	2:B:207:GLU:CB	2.26	0.58
2:B:338:LYS:O	2:B:339:ASN:OD1	2.22	0.58
1:A:340:THR:O	1:A:341:ILE:HG12	2.04	0.57
1:A:208:ALA:HB2	1:A:303:VAL:HA	1.85	0.57
2:B:64:ARG:HH21	2:B:125:GLU:HB3	1.69	0.57
2:B:242:LEU:HA	2:B:356:CYS:SG	2.45	0.57
1:A:107:HIS:HB2	1:A:149:PHE:N	2.17	0.57
1:A:108:TYR:CB	1:A:112:LYS:HE3	2.34	0.57
1:A:8:HIS:CE1	1:A:17:GLY:HA3	2.39	0.57
1:A:14:VAL:CG1	1:A:74:VAL:HG22	2.35	0.57
1:A:271:THR:CG2	1:A:377:MET:HB3	2.35	0.57
1:A:407:TRP:CE3	2:B:257:VAL:HG22	2.36	0.57
2:B:4:ILE:HG21	2:B:30:ILE:CB	2.34	0.57
2:B:241:CYS:SG	2:B:320:ARG:CZ	2.89	0.57
2:B:268:PHE:HA	2:B:380:ASN:OD1	2.03	0.57
2:B:388:PHE:O	2:B:390:ARG:N	2.38	0.57
1:A:17:GLY:C	1:A:21:TRP:HD1	2.13	0.57
1:A:23:LEU:CD2	1:A:236:SER:CB	2.81	0.57
1:A:407:TRP:CE3	2:B:257:VAL:HG23	2.39	0.57
2:B:6:HIS:O	2:B:66:ILE:N	2.23	0.57
2:B:158:ARG:CG	2:B:197:ASN:ND2	2.61	0.57
2:B:181:VAL:C	2:B:399:PHE:HE2	2.12	0.57
2:B:385:GLN:O	2:B:389:LYS:HG3	2.04	0.57
2:B:427:ASP:O	2:B:431:GLU:N	2.18	0.57
1:A:76:ASP:O	1:A:80:THR:CB	2.51	0.57
2:B:158:ARG:HH11	2:B:197:ASN:N	2.03	0.57
1:A:23:LEU:HD21	1:A:236:SER:CB	2.34	0.57
1:A:34:GLY:C	1:A:35:GLN:HG3	2.29	0.57
1:A:77:GLU:O	1:A:83:TYR:HB2	2.05	0.57
1:A:242:LEU:CB	1:A:250:VAL:O	2.47	0.57
1:A:250:VAL:CG1	1:A:254:GLU:CB	2.34	0.57
2:B:141:LEU:C	2:B:186:ASN:ND2	2.63	0.57
2:B:274:PRO:CB	2:B:371:LEU:CD2	2.80	0.57
1:A:196:GLU:C	1:A:197:HIS:CG	2.83	0.57
2:B:21:TRP:HA	2:B:24:ILE:CD1	2.34	0.57
2:B:64:ARG:HH21	2:B:125:GLU:C	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:HG22	2:B:404:PHE:HE2	1.60	0.57
2:B:234:THR:CB	2:B:302:MET:CE	2.75	0.57
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.87	0.57
1:A:175:PRO:HG2	1:A:207:GLU:HG2	1.86	0.57
1:A:177:VAL:CG1	1:A:178:SER:N	2.49	0.57
1:A:191:THR:HG23	1:A:421:ALA:HB1	1.86	0.57
1:A:258:ASN:OD1	1:A:352:LYS:CE	2.53	0.57
1:A:267:PHE:CG	1:A:388:TRP:HZ2	2.23	0.57
1:A:14:VAL:CG2	1:A:69:ASP:OD1	2.52	0.57
1:A:222:PRO:HG2	2:B:326:LYS:CB	2.35	0.57
1:A:275:VAL:O	1:A:368:LEU:HD13	2.04	0.57
1:A:327:ASP:O	1:A:331:ALA:CB	2.53	0.57
1:A:341:ILE:HG22	1:A:343:PHE:CD2	2.40	0.57
2:B:181:VAL:HG22	2:B:404:PHE:CD2	2.39	0.57
2:B:259:MET:CE	2:B:379:GLY:C	2.78	0.57
2:B:320:ARG:HH22	5:B:501:TXL:H27	1.70	0.57
2:B:400:ARG:CD	2:B:422:GLU:OE1	2.51	0.57
1:A:23:LEU:HD21	1:A:236:SER:HB3	1.86	0.56
1:A:106:GLY:HA2	1:A:111:GLY:H	1.69	0.56
1:A:405:VAL:CG2	1:A:405:VAL:CA	2.77	0.56
2:B:158:ARG:HG3	2:B:197:ASN:CB	2.08	0.56
2:B:158:ARG:NH1	2:B:197:ASN:H	2.03	0.56
1:A:70:LEU:HG	1:A:145:THR:HG21	1.87	0.56
1:A:407:TRP:CH2	2:B:165:ILE:HD12	1.94	0.56
2:B:4:ILE:HD13	2:B:30:ILE:HA	1.66	0.56
2:B:7:ILE:O	2:B:137:LEU:HA	2.04	0.56
1:A:9:VAL:CG2	1:A:138:PHE:O	2.54	0.56
1:A:85:GLN:O	1:A:87:PHE:N	2.37	0.56
1:A:239:THR:O	1:A:243:ARG:HG2	2.05	0.56
1:A:254:GLU:OE2	1:A:352:LYS:HE3	2.05	0.56
1:A:267:PHE:CE1	1:A:388:TRP:CZ2	2.93	0.56
2:B:26:ASP:OD1	2:B:26:ASP:O	2.23	0.56
2:B:102:ASN:CB	2:B:408:TYR:CE1	2.88	0.56
2:B:180:THR:C	2:B:398:MET:CE	2.73	0.56
2:B:183:GLU:OE2	2:B:394:GLN:CG	2.53	0.56
2:B:209:LEU:HD13	2:B:227:LEU:CG	2.15	0.56
2:B:212:ILE:CD1	2:B:302:MET:HB2	2.36	0.56
2:B:262:PHE:HB2	2:B:266:HIS:HE1	1.71	0.56
1:A:10:GLY:O	1:A:13:GLY:CA	2.53	0.56
1:A:13:GLY:HA2	1:A:16:ILE:HG21	1.87	0.56
1:A:25:CYS:O	1:A:26:LEU:HD23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:HG13	1:A:325:PRO:HD2	1.87	0.56
2:B:141:LEU:C	2:B:186:ASN:HD21	2.13	0.56
2:B:284:ARG:HD3	2:B:290:GLU:OE1	2.04	0.56
2:B:359:PRO:HB2	2:B:372:LYS:O	2.05	0.56
1:A:192:HIS:CG	1:A:193:THR:N	2.73	0.56
1:A:292:THR:O	1:A:295:CYS:HB2	2.05	0.56
1:A:335:ILE:CG2	1:A:341:ILE:HG13	2.35	0.56
2:B:6:HIS:ND1	2:B:21:TRP:CZ2	2.74	0.56
2:B:223:THR:OG1	2:B:226:ASP:CB	2.54	0.56
2:B:230:LEU:O	2:B:233:ALA:HB3	2.04	0.56
2:B:239:THR:HB	2:B:243:ARG:NH1	2.20	0.56
2:B:250:ALA:HB2	2:B:352:LYS:HZ1	1.70	0.56
1:A:28:HIS:ND1	1:A:29:GLY:N	2.54	0.56
1:A:154:MET:CE	1:A:166:LYS:CD	2.80	0.56
1:A:224:TYR:CE1	3:A:500:GTP:C4	2.94	0.56
1:A:335:ILE:HG22	1:A:341:ILE:HG13	1.88	0.56
2:B:53:TYR:HE1	2:B:87:PHE:HE1	1.46	0.56
2:B:78:VAL:HA	2:B:82:PRO:HG2	1.86	0.56
2:B:151:THR:C	2:B:192:HIS:HD2	2.12	0.56
2:B:288:VAL:C	2:B:290:GLU:N	2.57	0.56
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.86	0.56
1:A:66:VAL:HG21	1:A:125:LEU:HD12	1.87	0.56
2:B:44:LEU:O	2:B:47:GLU:CB	2.54	0.56
2:B:241:CYS:C	2:B:242:LEU:HG	2.31	0.56
2:B:311:ARG:O	2:B:381:SER:CB	2.52	0.56
1:A:2:ARG:HB3	1:A:243:ARG:NH1	2.21	0.56
1:A:141:PHE:HB2	1:A:172:TYR:HA	1.87	0.56
1:A:292:THR:CG2	1:A:319:TYR:OH	2.42	0.56
2:B:40:SER:O	2:B:41:ASP:CB	2.54	0.56
2:B:75:MET:HE2	2:B:79:ARG:CG	2.35	0.56
1:A:33:ASP:OD1	1:A:33:ASP:O	2.23	0.56
1:A:363:VAL:HG12	1:A:364:PRO:CG	2.35	0.56
2:B:191:VAL:HG23	2:B:421:ALA:CB	2.36	0.56
2:B:295:MET:HE3	2:B:375:ALA:CA	2.09	0.56
1:A:14:VAL:HG21	1:A:69:ASP:OD1	2.06	0.55
1:A:97:GLU:CB	1:A:110:ILE:HD13	2.35	0.55
1:A:187:SER:O	1:A:191:THR:HG23	2.07	0.55
1:A:288:VAL:HG22	1:A:373:ARG:HG2	1.88	0.55
1:A:314:ALA:HB3	1:A:380:ASN:ND2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:CA	1:A:75:ILE:HG22	2.33	0.55
1:A:108:TYR:HA	1:A:112:LYS:HE2	1.87	0.55
1:A:288:VAL:O	1:A:291:ILE:CB	2.54	0.55
2:B:7:ILE:CB	2:B:137:LEU:HD21	2.28	0.55
2:B:40:SER:C	2:B:41:ASP:OD1	2.49	0.55
2:B:147:SER:HB3	2:B:189:LEU:HD11	0.56	0.55
2:B:154:ILE:HG23	2:B:198:THR:HG22	1.87	0.55
1:A:22:GLU:O	1:A:25:CYS:HB2	2.07	0.55
1:A:137:VAL:CB	1:A:168:GLU:HG2	2.37	0.55
1:A:217:LEU:CB	1:A:368:LEU:HD11	2.35	0.55
1:A:405:VAL:HG11	1:A:405:VAL:HG21	1.87	0.55
2:B:302:MET:O	2:B:302:MET:CG	2.47	0.55
1:A:157:LEU:HB2	1:A:166:LYS:NZ	2.21	0.55
1:A:306:ASP:CG	1:A:308:ARG:HD2	2.32	0.55
2:B:49:ILE:HA	2:B:61:TYR:CE2	2.41	0.55
2:B:231:VAL:O	2:B:232:SER:C	2.46	0.55
1:A:14:VAL:HG21	1:A:74:VAL:CG1	2.36	0.55
1:A:28:HIS:CD2	1:A:33:ASP:HB3	2.41	0.55
1:A:35:GLN:O	1:A:36:MET:CG	2.54	0.55
1:A:69:ASP:HB3	1:A:71:GLU:O	2.07	0.55
1:A:427:ALA:O	1:A:431:ASP:N	2.19	0.55
2:B:206:ASN:O	2:B:210:TYR:HD2	1.86	0.55
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.55
2:B:287:THR:CA	2:B:290:GLU:HB3	2.36	0.55
2:B:311:ARG:CD	2:B:341:SER:O	2.54	0.55
1:A:45:GLY:O	1:A:46:ASP:OD2	2.22	0.55
2:B:181:VAL:C	2:B:398:MET:HE1	2.31	0.55
1:A:14:VAL:HG21	1:A:74:VAL:HG13	1.88	0.55
2:B:14:ASN:HD21	2:B:69:ASP:HA	1.72	0.55
2:B:103:TRP:CD1	2:B:147:SER:C	2.85	0.55
2:B:174:SER:O	2:B:176:LYS:N	2.39	0.55
2:B:394:GLN:O	2:B:398:MET:CB	2.54	0.55
1:A:313:MET:N	1:A:380:ASN:O	2.40	0.55
2:B:142:GLY:HA2	2:B:185:TYR:CE1	2.37	0.55
2:B:181:VAL:O	2:B:399:PHE:CZ	2.57	0.55
1:A:5:ILE:HD13	1:A:135:PHE:CE1	2.42	0.55
1:A:40:LYS:C	1:A:42:ILE:H	2.08	0.55
2:B:87:PHE:CD1	2:B:88:ARG:C	2.76	0.55
2:B:238:VAL:HG13	2:B:255:LEU:HD13	1.88	0.55
2:B:273:ALA:HB1	2:B:294:GLN:CD	2.32	0.55
1:A:157:LEU:O	1:A:161:TYR:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HD11	1:A:318:LEU:HD11	1.87	0.54
1:A:267:PHE:CD2	1:A:388:TRP:HZ2	2.25	0.54
2:B:170:SER:O	2:B:204:ILE:HB	2.06	0.54
2:B:273:ALA:CB	2:B:294:GLN:CD	2.80	0.54
2:B:316:ALA:O	2:B:378:ILE:N	2.38	0.54
2:B:344:VAL:O	2:B:344:VAL:HG12	2.07	0.54
1:A:105:ARG:HG3	1:A:411:GLU:CD	2.32	0.54
1:A:108:TYR:CZ	1:A:417:GLU:CD	2.85	0.54
1:A:141:PHE:O	1:A:182:VAL:CG1	2.48	0.54
2:B:8:GLN:O	2:B:68:VAL:N	2.41	0.54
2:B:12:CYS:O	2:B:16:ILE:HG13	1.98	0.54
2:B:202:TYR:OH	2:B:238:VAL:HG11	2.08	0.54
1:A:26:LEU:O	1:A:27:GLU:HB2	2.06	0.54
1:A:33:ASP:O	1:A:33:ASP:CG	2.49	0.54
1:A:41:THR:O	1:A:42:ILE:CB	2.43	0.54
1:A:219:ILE:HG21	1:A:219:ILE:HD13	1.87	0.54
2:B:106:GLY:HA2	2:B:111:GLY:H	1.72	0.54
2:B:136:GLN:NE2	2:B:243:ARG:HH12	2.05	0.54
2:B:242:LEU:HB3	2:B:250:ALA:O	2.08	0.54
2:B:313:LEU:N	2:B:381:SER:HA	2.22	0.54
2:B:434:GLN:C	2:B:435:TYR:HD1	2.14	0.54
1:A:9:VAL:HG11	1:A:150:THR:HG23	1.78	0.54
1:A:9:VAL:CB	1:A:138:PHE:O	2.55	0.54
1:A:166:LYS:CD	1:A:197:HIS:HD2	2.20	0.54
1:A:191:THR:HG21	1:A:421:ALA:HA	1.88	0.54
1:A:220:GLU:CB	1:A:220:GLU:CD	2.74	0.54
1:A:256:GLN:O	1:A:260:VAL:CB	2.55	0.54
1:A:344:VAL:HB	1:A:347:CYS:HG	1.68	0.54
2:B:56:ALA:HB1	2:B:62:VAL:H	1.71	0.54
2:B:126:SER:HA	2:B:132:LEU:HD11	1.88	0.54
2:B:175:PRO:HD2	2:B:207:GLU:HG2	1.88	0.54
2:B:195:VAL:O	2:B:195:VAL:HG12	2.08	0.54
2:B:286:LEU:HD12	2:B:372:LYS:CB	2.29	0.54
2:B:295:MET:HE1	2:B:375:ALA:CA	2.29	0.54
1:A:184:PRO:CG	1:A:395:PHE:CG	2.60	0.54
1:A:207:GLU:HG3	1:A:207:GLU:O	2.08	0.54
2:B:6:HIS:HD2	2:B:64:ARG:O	1.90	0.54
1:A:107:HIS:HD2	1:A:151:SER:OG	1.89	0.54
1:A:146:GLY:HA2	1:A:150:THR:CG2	2.37	0.54
1:A:185:TYR:HD2	1:A:408:TYR:HH	0.55	0.54
1:A:220:GLU:CG	1:A:220:GLU:N	2.70	0.54

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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	0.54
2:B:201:THR:OG1	2:B:267:PHE:CD1	2.58	0.54
2:B:244:PHE:CG	2:B:245:PRO:HD3	2.40	0.54
2:B:359:PRO:O	2:B:360:PRO:C	2.49	0.54
1:A:11:GLN:OE1	1:A:74:VAL:HB	2.07	0.54
1:A:20:CYS:C	1:A:24:TYR:CD2	2.80	0.54
1:A:100:ALA:CB	1:A:105:ARG:HB3	2.31	0.54
1:A:166:LYS:HD2	1:A:197:HIS:HD2	1.73	0.54
1:A:208:ALA:HB2	1:A:303:VAL:CA	2.36	0.54
1:A:259:LEU:O	1:A:380:ASN:ND2	2.41	0.54
2:B:197:ASN:CG	2:B:197:ASN:O	2.50	0.54
1:A:274:PRO:C	1:A:275:VAL:HG23	2.33	0.54
2:B:41:ASP:O	2:B:42:LEU:CB	2.56	0.54
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.30	0.54
2:B:48:ARG:HH12	2:B:60:LYS:H	1.54	0.54
2:B:129:CYS:O	2:B:130:ASP:OD1	2.24	0.54
2:B:213:CYS:HA	2:B:217:LEU:CD1	2.06	0.54
1:A:103:TYR:O	1:A:148:GLY:HA3	2.08	0.54
1:A:114:ILE:O	1:A:114:ILE:HG22	2.07	0.54
1:A:148:GLY:O	1:A:152:LEU:N	2.40	0.54
1:A:85:GLN:O	1:A:86:LEU:C	2.39	0.53
1:A:200:CYS:SG	1:A:256:GLN:HA	2.48	0.53
2:B:92:PHE:CE2	2:B:114:LEU:CD1	2.89	0.53
2:B:234:THR:HB	2:B:302:MET:HE1	1.89	0.53
2:B:286:LEU:HD13	2:B:373:MET:H	1.70	0.53
2:B:296:PHE:CE1	2:B:335:VAL:CG1	2.82	0.53
2:B:321:GLY:HA2	2:B:359:PRO:HB3	1.90	0.53
1:A:169:PHE:HZ	1:A:235:VAL:HG22	1.61	0.53
1:A:289:ALA:HB1	1:A:331:ALA:HB1	1.89	0.53
2:B:49:ILE:O	2:B:50:ASN:ND2	2.40	0.53
2:B:118:VAL:O	2:B:122:VAL:HG23	2.07	0.53
2:B:172:VAL:HG21	2:B:205:ASP:OD1	2.09	0.53
2:B:319:PHE:HZ	2:B:332:MET:SD	2.31	0.53
1:A:3:GLU:CA	1:A:31:GLN:CG	2.86	0.53
1:A:171:ILE:H	1:A:203:MET:HE1	1.64	0.53
1:A:212:ILE:HD13	1:A:230:LEU:CD2	2.15	0.53
1:A:219:ILE:O	1:A:222:PRO:HD3	2.09	0.53
1:A:291:ILE:HD13	1:A:373:ARG:C	2.33	0.53
2:B:135:PHE:CG	2:B:166:MET:SD	3.02	0.53
2:B:309:HIS:HB3	2:B:386:GLU:OE2	2.07	0.53
2:B:319:PHE:CZ	2:B:328:VAL:HG12	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:HB3	1:A:203:MET:HE2	1.89	0.53
2:B:23:VAL:O	2:B:26:ASP:HB3	2.08	0.53
2:B:94:PHE:HZ	2:B:110:GLU:O	1.92	0.53
2:B:190:SER:OG	2:B:191:VAL:N	2.41	0.53
2:B:192:HIS:HA	2:B:196:GLU:OE2	2.08	0.53
2:B:301:MET:HE1	2:B:377:PHE:CE1	2.42	0.53
1:A:167:LEU:HD11	1:A:252:LEU:HD22	1.90	0.53
2:B:141:LEU:HD12	2:B:173:PRO:CD	2.37	0.53
2:B:293:GLN:O	2:B:297:ASP:OD1	2.27	0.53
1:A:174:ALA:CB	1:A:390:ARG:NH2	2.52	0.53
1:A:407:TRP:CD2	2:B:257:VAL:CG2	2.88	0.53
1:A:81:GLY:O	1:A:83:TYR:N	2.41	0.53
1:A:237:SER:HA	1:A:320:ARG:HH11	1.73	0.53
1:A:287:SER:HG	1:A:290:GLU:HB2	1.72	0.53
1:A:416:GLY:O	1:A:417:GLU:CB	2.55	0.53
2:B:27:GLU:OE1	2:B:36:TYR:HA	2.09	0.53
2:B:107:HIS:CD2	2:B:151:THR:OG1	2.62	0.53
2:B:158:ARG:HG3	2:B:197:ASN:ND2	2.22	0.53
2:B:339:ASN:HB3	2:B:342:TYR:HB2	1.90	0.53
1:A:21:TRP:N	1:A:21:TRP:CD1	2.76	0.53
1:A:191:THR:HG22	1:A:421:ALA:HA	1.91	0.53
1:A:219:ILE:CG2	1:A:219:ILE:CD1	2.86	0.53
1:A:301:GLN:NE2	1:A:305:CYS:HB2	2.24	0.53
2:B:57:ALA:O	2:B:64:ARG:N	2.42	0.53
2:B:98:GLY:C	2:B:99:ALA:O	2.52	0.53
2:B:135:PHE:CD2	2:B:157:ILE:HG21	2.44	0.53
2:B:192:HIS:CG	2:B:196:GLU:HG3	2.44	0.53
2:B:208:ALA:HB2	2:B:303:ALA:O	2.05	0.53
1:A:126:ALA:C	1:A:132:LEU:HD11	2.32	0.53
1:A:205:ASP:HB2	1:A:303:VAL:CA	2.32	0.53
1:A:282:TYR:CD2	1:A:285:GLN:CA	2.81	0.53
1:A:313:MET:CG	1:A:380:ASN:O	2.57	0.53
1:A:400:ALA:O	1:A:401:LYS:C	2.52	0.53
2:B:32:PRO:HB2	2:B:59:ASN:HD22	0.60	0.53
2:B:42:LEU:O	2:B:43:GLN:CB	2.56	0.53
2:B:244:PHE:O	2:B:245:PRO:C	2.51	0.53
2:B:346:TRP:HE3	2:B:347:ILE:HG13	0.87	0.53
1:A:204:VAL:CG1	1:A:209:ILE:CG1	2.86	0.53
2:B:8:GLN:O	2:B:68:VAL:HB	2.08	0.53
2:B:22:GLU:HA	2:B:83:PHE:HE2	1.73	0.53
2:B:339:ASN:HA	2:B:342:TYR:HD1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TYR:O	1:A:25:CYS:C	2.47	0.52
1:A:53:PHE:HA	1:A:88:HIS:ND1	2.16	0.52
1:A:119:LEU:CA	1:A:122:ILE:HG22	2.38	0.52
1:A:224:TYR:HB2	2:B:325:MET:HB2	1.91	0.52
1:A:233:GLN:O	1:A:234:ILE:C	2.49	0.52
1:A:386:GLU:O	1:A:389:ALA:HB3	2.09	0.52
1:A:179:THR:CG2	1:A:180:ALA:N	2.67	0.52
2:B:139:HIS:C	2:B:139:HIS:ND1	2.67	0.52
2:B:312:TYR:O	2:B:344:VAL:HG21	2.00	0.52
2:B:319:PHE:CZ	2:B:332:MET:SD	3.03	0.52
2:B:342:TYR:O	2:B:343:PHE:CG	2.62	0.52
2:B:360:PRO:HG2	2:B:374:SER:HB3	1.90	0.52
2:B:431:GLU:HA	2:B:434:GLN:CG	2.39	0.52
1:A:83:TYR:O	1:A:84:ARG:HB2	2.09	0.52
1:A:142:GLY:HA2	1:A:185:TYR:CE1	2.43	0.52
1:A:209:ILE:HD12	1:A:227:LEU:HD21	1.90	0.52
1:A:219:ILE:CG2	1:A:219:ILE:HD13	2.39	0.52
1:A:362:VAL:CG1	1:A:363:VAL:N	2.73	0.52
2:B:212:ILE:HD11	2:B:302:MET:HA	1.91	0.52
2:B:339:ASN:HA	2:B:342:TYR:CD1	2.43	0.52
1:A:101:ASN:ND2	3:A:500:GTP:O2G	2.42	0.52
1:A:426:ALA:C	1:A:428:LEU:H	2.14	0.52
2:B:6:HIS:CE1	2:B:21:TRP:CZ2	2.97	0.52
2:B:105:LYS:CE	2:B:411:GLU:CG	2.86	0.52
2:B:399:PHE:CZ	2:B:408:TYR:CZ	2.96	0.52
1:A:13:GLY:O	1:A:16:ILE:CG2	2.56	0.52
1:A:228:ASN:ND2	3:A:500:GTP:C6	2.72	0.52
2:B:212:ILE:HD11	2:B:302:MET:CA	2.40	0.52
2:B:268:PHE:HD1	2:B:380:ASN:CG	2.13	0.52
1:A:5:ILE:CD1	1:A:135:PHE:CZ	2.93	0.52
1:A:311:LYS:O	1:A:312:TYR:C	2.51	0.52
2:B:343:PHE:CG	2:B:350:ASN:ND2	2.78	0.52
2:B:68:VAL:HG13	2:B:149:MET:HE1	1.92	0.52
1:A:205:ASP:HB2	1:A:208:ALA:HB3	1.91	0.52
1:A:282:TYR:O	1:A:284:GLU:C	2.53	0.52
2:B:7:ILE:HG13	2:B:66:ILE:CG2	2.36	0.52
2:B:31:ASP:H	2:B:32:PRO:CD	2.20	0.52
2:B:33:THR:CG2	2:B:34:GLY:N	2.73	0.52
2:B:49:ILE:CA	2:B:61:TYR:CE2	2.93	0.52
2:B:295:MET:HE2	2:B:375:ALA:C	2.34	0.52
2:B:371:LEU:N	5:B:501:TXL:H183	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ASN:C	2:B:428:LEU:H	2.17	0.52
1:A:7:ILE:HG22	1:A:8:HIS:O	2.10	0.52
1:A:223:THR:O	2:B:326:LYS:HE3	2.10	0.52
1:A:272:TYR:CE1	1:A:274:PRO:C	2.70	0.52
1:A:361:THR:C	1:A:362:VAL:CG2	2.82	0.52
2:B:33:THR:HG22	2:B:34:GLY:H	1.73	0.52
2:B:208:ALA:CB	2:B:303:ALA:C	2.81	0.52
2:B:233:ALA:CB	2:B:272:PHE:CD2	2.79	0.52
2:B:259:MET:CE	2:B:268:PHE:CD1	2.93	0.52
2:B:259:MET:HE3	2:B:268:PHE:CD1	2.44	0.52
2:B:295:MET:HE1	2:B:375:ALA:HA	1.92	0.52
2:B:319:PHE:CD1	2:B:319:PHE:N	2.78	0.52
2:B:384:ILE:HG23	2:B:388:PHE:CE2	2.45	0.52
1:A:63:PRO:HB2	1:A:65:ALA:HB2	1.92	0.52
1:A:78:VAL:O	1:A:78:VAL:HG12	2.10	0.52
1:A:83:TYR:C	1:A:84:ARG:CG	2.73	0.52
1:A:209:ILE:O	1:A:213:CYS:SG	2.63	0.52
1:A:224:TYR:HE1	3:A:500:GTP:C2	2.27	0.52
2:B:6:HIS:ND1	2:B:21:TRP:HZ2	2.07	0.52
2:B:28:HIS:CD2	2:B:240:THR:HA	2.45	0.52
2:B:64:ARG:NH2	2:B:125:GLU:C	2.67	0.52
2:B:181:VAL:HA	2:B:398:MET:HE1	1.86	0.52
2:B:181:VAL:C	2:B:399:PHE:CE2	2.85	0.52
1:A:142:GLY:O	1:A:185:TYR:CE1	2.63	0.51
1:A:289:ALA:C	1:A:291:ILE:N	2.69	0.51
2:B:135:PHE:CD2	2:B:157:ILE:HD13	2.45	0.51
2:B:140:SER:OG	2:B:143:GLY:HA3	2.10	0.51
2:B:229:HIS:ND1	5:B:501:TXL:H432	2.25	0.51
2:B:335:VAL:C	2:B:339:ASN:ND2	2.59	0.51
2:B:360:PRO:HD3	2:B:374:SER:HB3	1.91	0.51
1:A:30:ILE:O	1:A:32:PRO:HG3	1.95	0.51
2:B:295:MET:HE2	2:B:376:THR:N	2.25	0.51
2:B:315:VAL:HG13	2:B:377:PHE:CE2	2.45	0.51
2:B:339:ASN:O	2:B:340:SER:O	2.29	0.51
1:A:181:VAL:HG13	1:A:399:TYR:OH	2.11	0.51
1:A:190:THR:O	1:A:191:THR:C	2.52	0.51
1:A:224:TYR:HB2	2:B:325:MET:CG	2.41	0.51
1:A:382:THR:O	1:A:385:ALA:N	2.43	0.51
2:B:9:ALA:O	2:B:13:GLY:HA3	2.10	0.51
2:B:389:LYS:O	2:B:393:GLU:HG2	2.09	0.51
1:A:241:SER:HB2	1:A:356:ASN:CG	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:HD13	2:B:30:ILE:CA	2.35	0.51
2:B:184:PRO:CG	2:B:399:PHE:CB	2.69	0.51
2:B:369:ARG:O	5:B:501:TXL:C22	2.59	0.51
5:B:501:TXL:H192	5:B:501:TXL:C5	2.39	0.51
1:A:41:THR:O	1:A:41:THR:CG2	2.59	0.51
1:A:152:LEU:HD11	1:A:156:ARG:HE	1.75	0.51
1:A:183:GLU:OE1	1:A:183:GLU:HA	2.10	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
2:B:35:SER:HB3	2:B:60:LYS:CE	2.40	0.51
2:B:378:ILE:HG22	2:B:379:GLY:N	2.24	0.51
1:A:6:SER:HB3	1:A:30:ILE:HD12	1.92	0.51
1:A:66:VAL:HG21	1:A:125:LEU:CD1	2.40	0.51
1:A:253:THR:O	1:A:253:THR:CG2	2.57	0.51
1:A:396:ASP:O	1:A:401:LYS:CB	2.34	0.51
1:A:405:VAL:HG23	1:A:409:VAL:HG23	1.89	0.51
2:B:433:GLN:C	2:B:435:TYR:N	2.67	0.51
1:A:105:ARG:NH2	2:B:253:ARG:NH2	2.59	0.51
1:A:150:THR:O	1:A:154:MET:HG2	2.11	0.51
1:A:340:THR:O	1:A:341:ILE:HD13	2.11	0.51
2:B:64:ARG:HH22	2:B:132:LEU:HD11	1.76	0.51
2:B:94:PHE:CE2	2:B:114:LEU:HB2	2.46	0.51
2:B:103:TRP:HE1	2:B:148:GLY:HA2	1.72	0.51
2:B:114:LEU:O	2:B:117:SER:N	2.44	0.51
1:A:155:GLU:CG	1:A:196:GLU:HG3	2.34	0.51
2:B:7:ILE:HG21	2:B:137:LEU:HD22	1.91	0.51
2:B:385:GLN:HG3	2:B:389:LYS:CE	2.04	0.51
2:B:404:PHE:CD2	2:B:404:PHE:O	2.64	0.51
1:A:267:PHE:CD1	1:A:388:TRP:CZ2	2.98	0.51
2:B:39:ASP:O	2:B:40:SER:HB3	2.08	0.51
2:B:184:PRO:CB	2:B:399:PHE:CE2	2.69	0.51
2:B:287:THR:C	2:B:290:GLU:HB3	2.36	0.51
2:B:398:MET:CE	2:B:399:PHE:CE2	2.93	0.51
1:A:158:SER:HB2	1:A:196:GLU:O	2.11	0.51
2:B:75:MET:HE3	2:B:75:MET:CA	2.28	0.51
2:B:154:ILE:CG2	2:B:198:THR:HG22	2.37	0.51
2:B:312:TYR:CG	2:B:381:SER:HB3	2.46	0.51
5:B:501:TXL:H173	5:B:501:TXL:C13	2.37	0.51
5:B:501:TXL:C17	5:B:501:TXL:C13	2.89	0.51
1:A:25:CYS:O	1:A:25:CYS:SG	2.69	0.50
1:A:68:VAL:CG1	1:A:149:PHE:HZ	2.07	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:396:ASP:OD2	1:A:422:ARG:CZ	2.59	0.50
1:A:205:ASP:O	1:A:209:ILE:HG13	2.11	0.50
1:A:221:ARG:N	1:A:222:PRO:CD	2.65	0.50
1:A:340:THR:O	1:A:341:ILE:CG1	2.59	0.50
2:B:259:MET:HG3	2:B:378:ILE:HG21	1.92	0.50
2:B:280:SER:O	2:B:281:GLN:C	2.55	0.50
1:A:178:SER:O	1:A:179:THR:HB	2.10	0.50
2:B:250:ALA:CB	2:B:352:LYS:HZ3	2.23	0.50
2:B:287:THR:CG2	2:B:290:GLU:N	2.68	0.50
1:A:241:SER:HB2	1:A:356:ASN:CB	2.42	0.50
1:A:269:LEU:O	1:A:377:MET:O	2.29	0.50
1:A:306:ASP:OD1	1:A:308:ARG:CD	2.55	0.50
1:A:341:ILE:O	1:A:342:GLN:C	2.52	0.50
2:B:184:PRO:CA	2:B:395:PHE:HD1	2.22	0.50
2:B:226:ASP:OD1	2:B:226:ASP:O	2.30	0.50
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.39	0.50
2:B:308:ARG:CD	2:B:342:TYR:CZ	2.93	0.50
1:A:119:LEU:HA	1:A:122:ILE:HG22	1.93	0.50
1:A:267:PHE:CZ	1:A:388:TRP:CZ2	2.99	0.50
2:B:47:GLU:OE2	2:B:85:GLN:OE1	2.30	0.50
2:B:183:GLU:CD	2:B:394:GLN:HG3	2.34	0.50
2:B:229:HIS:HD1	5:B:501:TXL:H432	1.75	0.50
2:B:384:ILE:HG22	2:B:388:PHE:CE2	2.45	0.50
2:B:29:GLY:O	2:B:58:GLY:O	2.30	0.50
2:B:30:ILE:HG21	2:B:136:GLN:NE2	2.23	0.50
2:B:63:PRO:CG	2:B:86:ILE:O	2.60	0.50
2:B:217:LEU:HD23	2:B:275:LEU:O	2.10	0.50
2:B:230:LEU:HD21	2:B:302:MET:HB2	1.94	0.50
1:A:88:HIS:NE2	1:A:89:PRO:HD2	2.26	0.50
1:A:230:LEU:CD2	1:A:302:MET:HE1	2.41	0.50
1:A:301:GLN:HE21	1:A:305:CYS:HB2	1.76	0.50
2:B:22:GLU:CD	2:B:83:PHE:CD1	2.88	0.50
2:B:33:THR:CA	2:B:59:ASN:ND2	2.72	0.50
2:B:34:GLY:HA2	2:B:37:HIS:NE2	2.26	0.50
2:B:70:LEU:HA	2:B:94:PHE:HB2	1.94	0.50
2:B:101:ASN:O	2:B:102:ASN:ND2	2.43	0.50
1:A:116:ASP:C	1:A:118:VAL:N	2.68	0.50
2:B:250:ALA:CB	2:B:352:LYS:HZ1	2.25	0.50
2:B:332:MET:O	2:B:336:GLN:HG3	2.11	0.50
5:B:501:TXL:O11	5:B:501:TXL:H332	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HG2	1:A:133:GLN:NE2	2.23	0.50
1:A:132:LEU:O	1:A:133:GLN:C	2.54	0.50
1:A:155:GLU:HA	1:A:196:GLU:HB3	1.94	0.50
1:A:209:ILE:HD13	1:A:231:ILE:HG12	1.94	0.50
1:A:252:LEU:CA	1:A:255:PHE:HD2	2.07	0.50
2:B:104:ALA:C	2:B:108:TYR:HD2	2.20	0.50
2:B:259:MET:HB3	2:B:268:PHE:CD1	2.30	0.50
2:B:270:PRO:HB3	2:B:378:ILE:HD13	1.94	0.50
2:B:342:TYR:C	2:B:343:PHE:CG	2.90	0.50
2:B:414:ASP:C	2:B:416:MET:N	2.68	0.50
2:B:416:MET:N	2:B:416:MET:SD	2.85	0.50
1:A:66:VAL:HG22	1:A:125:LEU:HD13	1.92	0.49
1:A:170:SER:OG	1:A:203:MET:CG	1.65	0.49
1:A:205:ASP:HB2	1:A:208:ALA:CB	2.42	0.49
1:A:390:ARG:O	1:A:394:LYS:HG3	2.12	0.49
2:B:12:CYS:SG	4:B:500:GDP:C1'	3.00	0.49
2:B:135:PHE:CB	2:B:166:MET:HE3	2.13	0.49
2:B:151:THR:CB	2:B:192:HIS:NE2	2.28	0.49
2:B:312:TYR:C	2:B:381:SER:HA	2.36	0.49
2:B:389:LYS:HG2	2:B:429:VAL:HG21	1.93	0.49
1:A:166:LYS:CE	1:A:197:HIS:CD2	2.63	0.49
1:A:222:PRO:O	2:B:326:LYS:CB	2.56	0.49
2:B:101:ASN:C	2:B:102:ASN:CG	2.78	0.49
2:B:135:PHE:CE2	2:B:157:ILE:HD13	2.47	0.49
1:A:101:ASN:ND2	3:A:500:GTP:PG	2.85	0.49
1:A:141:PHE:CB	1:A:173:PRO:HD3	2.41	0.49
1:A:179:THR:CG2	1:A:181:VAL:CA	2.88	0.49
1:A:261:PRO:HB2	1:A:346:TRP:HH2	1.77	0.49
2:B:8:GLN:HE22	2:B:21:TRP:CD1	2.27	0.49
2:B:23:VAL:HG22	5:B:501:TXL:C33	2.30	0.49
1:A:70:LEU:HD12	1:A:145:THR:CA	2.40	0.49
1:A:212:ILE:HD12	1:A:230:LEU:HD21	1.75	0.49
2:B:35:SER:H	2:B:60:LYS:NZ	2.09	0.49
2:B:213:CYS:HB3	2:B:219:LEU:HD13	1.93	0.49
2:B:274:PRO:C	2:B:276:THR:CG2	2.85	0.49
2:B:288:VAL:HB	2:B:289:PRO:CD	2.42	0.49
1:A:11:GLN:HG2	3:A:500:GTP:O2A	2.12	0.49
1:A:14:VAL:HB	1:A:74:VAL:CG1	2.43	0.49
1:A:209:ILE:HG12	1:A:302:MET:CE	2.42	0.49
1:A:217:LEU:C	1:A:218:ASP:OD1	2.55	0.49
1:A:369:ALA:O	1:A:370:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:CYS:CB	2:B:219:LEU:HD11	2.30	0.49
2:B:13:GLY:CA	2:B:138:THR:CB	2.85	0.49
2:B:44:LEU:CD1	2:B:63:PRO:HG3	2.42	0.49
2:B:62:VAL:CG1	2:B:63:PRO:N	2.76	0.49
2:B:121:VAL:O	2:B:125:GLU:HG3	2.12	0.49
2:B:183:GLU:OE1	2:B:183:GLU:HA	2.13	0.49
2:B:191:VAL:CG2	2:B:421:ALA:CB	2.90	0.49
2:B:400:ARG:NH1	2:B:422:GLU:OE1	2.37	0.49
1:A:108:TYR:OH	1:A:417:GLU:CG	2.59	0.49
1:A:152:LEU:CD1	1:A:156:ARG:NE	2.75	0.49
1:A:220:GLU:HG3	1:A:220:GLU:N	2.28	0.49
1:A:277:SER:CB	1:A:279:GLU:H	2.23	0.49
1:A:306:ASP:OD1	1:A:308:ARG:N	2.46	0.49
2:B:14:ASN:OD1	2:B:69:ASP:OD1	2.29	0.49
2:B:57:ALA:CA	2:B:64:ARG:HB3	2.35	0.49
2:B:79:ARG:HB2	2:B:86:ILE:HD11	1.95	0.49
1:A:186:ASN:O	1:A:190:THR:N	2.44	0.49
1:A:264:ARG:O	1:A:266:HIS:ND1	2.45	0.49
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.77	0.49
2:B:4:ILE:HG21	2:B:30:ILE:HG21	1.93	0.49
2:B:194:LEU:CD2	2:B:265:LEU:HB3	2.38	0.49
2:B:206:ASN:O	2:B:210:TYR:HE2	1.85	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	1.92	0.49
1:A:99:ALA:HB3	2:B:251:ASP:OD2	2.13	0.49
1:A:134:GLY:HA3	1:A:252:LEU:CD1	2.43	0.49
1:A:142:GLY:O	1:A:185:TYR:CZ	2.66	0.49
2:B:102:ASN:CB	2:B:105:LYS:CD	2.79	0.49
2:B:246:GLY:N	2:B:357:ASP:OD2	2.45	0.49
1:A:3:GLU:HB3	1:A:64:ARG:NH1	2.28	0.49
1:A:14:VAL:HB	1:A:74:VAL:HG11	1.94	0.49
1:A:78:VAL:HG13	1:A:87:PHE:CE1	2.42	0.49
1:A:103:TYR:CZ	1:A:151:SER:OG	2.59	0.49
1:A:104:ALA:O	1:A:108:TYR:HD2	1.96	0.49
1:A:176:GLN:NE2	2:B:333:LEU:CB	2.74	0.49
1:A:197:HIS:C	1:A:198:SER:OG	2.56	0.49
1:A:335:ILE:C	1:A:337:THR:N	2.71	0.49
2:B:15:GLN:C	2:B:17:GLY:N	2.70	0.49
2:B:52:TYR:N	2:B:52:TYR:CD1	2.81	0.49
2:B:108:TYR:OH	2:B:417:GLU:HG3	2.13	0.49
2:B:346:TRP:C	2:B:347:ILE:HG13	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:N	1:A:166:LYS:CE	2.76	0.48
1:A:276:ILE:CD1	1:A:371:VAL:CG2	2.87	0.48
1:A:312:TYR:CE1	1:A:341:ILE:HD12	2.47	0.48
2:B:61:TYR:O	2:B:61:TYR:CD1	2.66	0.48
2:B:192:HIS:CE1	2:B:193:GLN:HG2	2.48	0.48
1:A:34:GLY:O	1:A:35:GLN:HG3	2.13	0.48
1:A:326:LYS:O	1:A:326:LYS:HG2	2.12	0.48
2:B:3:GLU:CD	2:B:64:ARG:NH1	2.71	0.48
2:B:44:LEU:CD1	2:B:86:ILE:O	2.49	0.48
2:B:324:SER:CB	2:B:327:GLU:H	2.25	0.48
2:B:394:GLN:OE1	2:B:394:GLN:HA	2.12	0.48
1:A:103:TYR:HA	1:A:147:SER:HG	1.75	0.48
1:A:220:GLU:CG	1:A:220:GLU:H	2.20	0.48
2:B:25:SER:O	2:B:27:GLU:CG	2.55	0.48
2:B:70:LEU:C	2:B:71:GLU:HG3	2.38	0.48
2:B:102:ASN:CB	2:B:105:LYS:HG3	2.43	0.48
2:B:308:ARG:HD3	2:B:342:TYR:HE2	1.66	0.48
2:B:385:GLN:O	2:B:389:LYS:CG	2.62	0.48
1:A:206:ASN:HD22	1:A:206:ASN:HA	1.46	0.48
1:A:224:TYR:HD1	3:A:500:GTP:C2	2.31	0.48
1:A:292:THR:N	1:A:375:VAL:HG21	2.28	0.48
1:A:397:LEU:CA	1:A:401:LYS:HB2	2.37	0.48
2:B:102:ASN:CA	2:B:408:TYR:CE1	2.91	0.48
1:A:16:ILE:HG23	1:A:138:PHE:CD1	2.48	0.48
1:A:40:LYS:C	1:A:42:ILE:N	2.65	0.48
1:A:180:ALA:CB	1:A:398:MET:CE	2.91	0.48
1:A:200:CYS:SG	1:A:260:VAL:CG2	3.00	0.48
1:A:359:PRO:HB2	1:A:360:PRO:HD2	1.94	0.48
1:A:9:VAL:HG11	1:A:146:GLY:HA2	1.95	0.48
1:A:42:ILE:HD13	1:A:61:HIS:O	2.13	0.48
1:A:73:THR:HB	2:B:249:ASN:ND2	2.27	0.48
1:A:291:ILE:O	1:A:375:VAL:HG21	2.13	0.48
3:A:500:GTP:O1A	2:B:248:LEU:CD1	2.51	0.48
2:B:35:SER:HA	2:B:60:LYS:CE	2.30	0.48
2:B:239:THR:O	2:B:243:ARG:CG	2.51	0.48
2:B:386:GLU:O	2:B:387:LEU:C	2.57	0.48
1:A:172:TYR:CD1	1:A:173:PRO:O	2.64	0.48
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.13	0.48
1:A:217:LEU:CD2	1:A:368:LEU:CD1	2.70	0.48
1:A:256:GLN:O	1:A:260:VAL:HB	2.13	0.48
2:B:50:ASN:HD22	2:B:61:TYR:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:LEU:HA	2:B:117:SER:OG	2.14	0.48
2:B:114:LEU:C	2:B:116:ASP:N	2.71	0.48
2:B:118:VAL:O	2:B:118:VAL:CG1	2.62	0.48
2:B:213:CYS:SG	2:B:227:LEU:HD11	2.52	0.48
2:B:311:ARG:O	2:B:381:SER:CA	2.62	0.48
1:A:15:GLN:O	1:A:18:ASN:HB2	2.13	0.48
1:A:137:VAL:HB	1:A:168:GLU:CG	2.40	0.48
1:A:175:PRO:HD3	1:A:390:ARG:CZ	2.44	0.48
1:A:224:TYR:C	1:A:226:ASN:H	2.21	0.48
1:A:276:ILE:HB	1:A:369:ALA:HB2	1.95	0.48
2:B:2:ARG:NH2	2:B:243:ARG:O	2.46	0.48
2:B:23:VAL:O	2:B:23:VAL:HG12	2.14	0.48
2:B:102:ASN:CA	2:B:408:TYR:HE1	2.18	0.48
1:A:122:ILE:HG23	1:A:123:ARG:N	2.29	0.48
1:A:242:LEU:HD13	1:A:250:VAL:HB	1.94	0.48
1:A:420:GLU:OE1	1:A:420:GLU:HA	2.13	0.48
2:B:56:ALA:C	2:B:62:VAL:HB	2.38	0.48
2:B:188:THR:CG2	2:B:417:GLU:O	2.59	0.48
2:B:209:LEU:HB3	2:B:227:LEU:HD21	1.96	0.48
2:B:241:CYS:O	2:B:242:LEU:HG	2.14	0.48
2:B:394:GLN:O	2:B:398:MET:HB2	2.14	0.48
1:A:73:THR:CB	2:B:249:ASN:HD21	2.27	0.48
1:A:175:PRO:HG3	1:A:304:LYS:NZ	2.29	0.48
1:A:275:VAL:O	1:A:275:VAL:CG1	2.62	0.48
1:A:312:TYR:C	1:A:313:MET:HG2	2.37	0.48
1:A:362:VAL:C	1:A:363:VAL:HG23	2.38	0.48
2:B:109:THR:CG2	2:B:411:GLU:O	2.62	0.48
2:B:238:VAL:HG13	2:B:255:LEU:HD11	1.94	0.48
2:B:311:ARG:H	2:B:382:THR:HB	1.79	0.48
1:A:20:CYS:C	1:A:24:TYR:HD2	2.17	0.47
1:A:108:TYR:OH	1:A:417:GLU:CD	2.56	0.47
1:A:209:ILE:CD1	1:A:231:ILE:CG1	2.90	0.47
2:B:62:VAL:HG12	2:B:63:PRO:O	2.14	0.47
2:B:87:PHE:CD1	2:B:88:ARG:N	2.82	0.47
2:B:119:LEU:HD21	2:B:156:LYS:HD3	1.96	0.47
2:B:143:GLY:O	2:B:185:TYR:OH	2.31	0.47
2:B:328:VAL:HG12	2:B:353:THR:HG21	1.96	0.47
2:B:435:TYR:O	2:B:436:GLN:OE1	2.29	0.47
1:A:3:GLU:OE1	1:A:132:LEU:CD2	2.62	0.47
1:A:9:VAL:HG13	1:A:150:THR:HG22	1.95	0.47
1:A:346:TRP:N	1:A:346:TRP:CD1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PHE:CZ	2:B:257:VAL:O	2.61	0.47
2:B:3:GLU:HA	2:B:31:ASP:HB2	1.86	0.47
2:B:141:LEU:HB3	2:B:186:ASN:ND2	1.87	0.47
2:B:433:GLN:O	2:B:435:TYR:N	2.46	0.47
1:A:250:VAL:CB	1:A:254:GLU:HG2	2.43	0.47
2:B:3:GLU:O	2:B:4:ILE:HG13	2.11	0.47
2:B:103:TRP:HZ3	2:B:413:MET:HE2	1.56	0.47
2:B:292:THR:O	2:B:293:GLN:C	2.54	0.47
1:A:196:GLU:HB3	1:A:197:HIS:CE1	2.50	0.47
1:A:287:SER:O	1:A:291:ILE:HG13	2.13	0.47
1:A:296:PHE:O	1:A:298:PRO:N	2.47	0.47
2:B:347:ILE:N	2:B:348:PRO:HD3	2.27	0.47
1:A:3:GLU:OE1	1:A:132:LEU:HD23	2.14	0.47
1:A:6:SER:O	1:A:66:VAL:N	2.47	0.47
1:A:115:ILE:CB	1:A:152:LEU:HD21	2.43	0.47
1:A:272:TYR:HD1	1:A:275:VAL:CG2	2.28	0.47
1:A:387:ALA:O	1:A:390:ARG:HB2	2.15	0.47
1:A:389:ALA:O	1:A:393:HIS:ND1	2.47	0.47
2:B:23:VAL:HG21	2:B:232:SER:HB2	1.95	0.47
2:B:57:ALA:C	2:B:64:ARG:N	2.69	0.47
2:B:135:PHE:HD2	2:B:166:MET:HE1	1.69	0.47
2:B:201:THR:CG2	2:B:265:LEU:CG	2.87	0.47
2:B:272:PHE:O	2:B:275:LEU:HD21	2.13	0.47
2:B:416:MET:O	2:B:417:GLU:CB	2.55	0.47
1:A:31:GLN:CD	1:A:243:ARG:NE	2.70	0.47
1:A:121:ARG:O	1:A:125:LEU:CG	2.44	0.47
1:A:181:VAL:O	1:A:184:PRO:C	2.58	0.47
1:A:7:ILE:HG21	1:A:153:LEU:CD2	2.43	0.47
1:A:35:GLN:O	1:A:36:MET:HG2	2.13	0.47
1:A:105:ARG:HH12	2:B:253:ARG:NH2	2.11	0.47
1:A:259:LEU:CB	1:A:380:ASN:HD21	2.27	0.47
1:A:262:TYR:CB	1:A:263:PRO:HD3	2.25	0.47
2:B:191:VAL:HG23	2:B:421:ALA:HA	1.87	0.47
1:A:23:LEU:CD2	1:A:233:GLN:HA	2.45	0.47
1:A:261:PRO:HB2	1:A:346:TRP:CH2	2.50	0.47
1:A:429:GLU:O	1:A:433:GLU:CG	2.51	0.47
2:B:275:LEU:CB	2:B:294:GLN:HE22	2.28	0.47
2:B:313:LEU:CD1	2:B:435:TYR:HD2	2.27	0.47
1:A:20:CYS:SG	1:A:138:PHE:CZ	3.06	0.47
1:A:98:ASP:CG	2:B:253:ARG:HH12	2.21	0.47
1:A:103:TYR:HD2	1:A:189:LEU:HG	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ILE:HB	1:A:216:ASN:HD22	1.79	0.47
2:B:112:ALA:HA	2:B:115:VAL:HB	1.96	0.47
2:B:248:LEU:HD23	2:B:353:THR:O	2.15	0.47
1:A:31:GLN:NE2	1:A:243:ARG:HB3	2.30	0.47
1:A:224:TYR:C	1:A:226:ASN:N	2.71	0.47
1:A:229:ARG:O	1:A:233:GLN:CG	2.52	0.47
1:A:271:THR:OG1	1:A:377:MET:N	2.48	0.47
2:B:170:SER:OG	2:B:203:CYS:CA	2.61	0.47
2:B:194:LEU:HD23	2:B:267:PHE:HZ	1.72	0.47
2:B:261:PRO:HG3	2:B:314:THR:HG23	1.97	0.47
1:A:103:TYR:CD2	1:A:188:ILE:HG22	2.50	0.46
1:A:103:TYR:N	1:A:185:TYR:CE2	2.82	0.46
1:A:224:TYR:CB	2:B:325:MET:HB2	2.45	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:430:LYS:O	1:A:434:GLU:HG3	2.15	0.46
2:B:94:PHE:CZ	2:B:110:GLU:O	2.68	0.46
2:B:190:SER:O	2:B:192:HIS:C	2.56	0.46
2:B:294:GLN:HG2	2:B:294:GLN:O	2.14	0.46
2:B:313:LEU:HA	2:B:344:VAL:CG2	2.30	0.46
1:A:20:CYS:SG	1:A:138:PHE:CE1	3.07	0.46
1:A:23:LEU:HD22	1:A:233:GLN:HA	1.96	0.46
1:A:48:SER:O	1:A:49:PHE:HB2	2.14	0.46
1:A:105:ARG:CZ	2:B:253:ARG:NH2	2.79	0.46
1:A:197:HIS:O	1:A:198:SER:OG	2.34	0.46
1:A:334:THR:HA	1:A:337:THR:HG21	1.98	0.46
1:A:349:THR:O	1:A:351:PHE:N	2.48	0.46
2:B:27:GLU:CB	2:B:36:TYR:HB3	2.44	0.46
2:B:211:ASP:O	2:B:215:ARG:HB2	2.14	0.46
1:A:10:GLY:O	1:A:11:GLN:C	2.58	0.46
1:A:228:ASN:O	1:A:232:GLY:N	2.39	0.46
2:B:50:ASN:HB2	2:B:61:TYR:CB	2.45	0.46
2:B:68:VAL:HG13	2:B:149:MET:CE	2.42	0.46
2:B:74:THR:O	2:B:75:MET:O	2.33	0.46
2:B:147:SER:HG	2:B:189:LEU:CD1	2.27	0.46
2:B:270:PRO:HA	2:B:377:PHE:O	2.14	0.46
2:B:273:ALA:HB1	2:B:294:GLN:HB3	1.97	0.46
1:A:3:GLU:CB	1:A:64:ARG:NH1	2.78	0.46
1:A:293:ASN:O	1:A:297:GLU:HG3	2.16	0.46
1:A:307:PRO:C	1:A:309:HIS:N	2.68	0.46
2:B:44:LEU:C	2:B:47:GLU:CG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:ARG:HH22	2:B:132:LEU:HD21	1.79	0.46
2:B:75:MET:CE	2:B:79:ARG:CB	2.90	0.46
2:B:151:THR:HG21	2:B:189:LEU:HA	1.96	0.46
2:B:212:ILE:C	2:B:214:PHE:H	2.23	0.46
1:A:87:PHE:HZ	1:A:92:LEU:HD21	1.80	0.46
1:A:109:THR:HG21	1:A:411:GLU:CB	2.44	0.46
1:A:153:LEU:O	1:A:153:LEU:HG	2.14	0.46
1:A:157:LEU:HB2	1:A:166:LYS:HE2	1.98	0.46
1:A:209:ILE:CD1	1:A:231:ILE:HG12	2.45	0.46
1:A:292:THR:CG2	1:A:319:TYR:CE2	2.98	0.46
1:A:344:VAL:HG12	1:A:345:ASP:H	1.81	0.46
2:B:205:ASP:CG	2:B:304:ALA:N	2.72	0.46
2:B:263:PRO:O	2:B:264:ARG:C	2.57	0.46
1:A:3:GLU:HG3	1:A:131:GLY:O	2.16	0.46
1:A:170:SER:OG	1:A:202:PHE:O	2.34	0.46
1:A:217:LEU:O	1:A:218:ASP:OD1	2.33	0.46
1:A:223:THR:OG1	1:A:225:THR:OG1	2.10	0.46
1:A:340:THR:O	1:A:341:ILE:CD1	2.63	0.46
2:B:102:ASN:CB	2:B:105:LYS:HE3	2.46	0.46
1:A:105:ARG:NH1	2:B:253:ARG:NE	2.62	0.46
1:A:187:SER:OG	1:A:188:ILE:N	2.49	0.46
1:A:312:TYR:HE1	1:A:341:ILE:HD12	1.81	0.46
2:B:33:THR:CG2	2:B:34:GLY:H	2.28	0.46
2:B:194:LEU:CA	2:B:265:LEU:HB2	2.38	0.46
2:B:212:ILE:HD12	2:B:302:MET:HB2	1.98	0.46
2:B:338:LYS:C	2:B:339:ASN:CG	2.83	0.46
1:A:14:VAL:CB	1:A:74:VAL:CG1	2.94	0.46
1:A:107:HIS:ND1	1:A:108:TYR:CD2	2.80	0.46
1:A:155:GLU:HG2	1:A:196:GLU:CB	2.46	0.46
1:A:289:ALA:CB	1:A:331:ALA:HB2	2.44	0.46
1:A:328:VAL:O	1:A:332:ILE:CG1	2.63	0.46
2:B:44:LEU:HG	2:B:85:GLN:CG	2.46	0.46
2:B:48:ARG:NH1	2:B:60:LYS:HG3	2.30	0.46
2:B:141:LEU:CD1	2:B:173:PRO:CD	2.91	0.46
2:B:143:GLY:C	2:B:185:TYR:OH	2.59	0.46
1:A:3:GLU:HB2	1:A:64:ARG:NH2	2.30	0.46
1:A:172:TYR:CE2	1:A:388:TRP:HZ3	2.28	0.46
1:A:312:TYR:CD1	1:A:341:ILE:HG23	2.51	0.46
2:B:68:VAL:HA	2:B:92:PHE:HB2	1.98	0.46
2:B:273:ALA:CB	2:B:294:GLN:HB3	2.46	0.46
2:B:346:TRP:O	2:B:347:ILE:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:HG11	1:A:352:LYS:NZ	2.26	0.46
1:A:275:VAL:O	1:A:368:LEU:CD1	2.64	0.46
2:B:35:SER:CB	2:B:60:LYS:HE3	2.44	0.46
2:B:56:ALA:HB1	2:B:62:VAL:N	2.31	0.46
2:B:179:ASP:O	2:B:180:THR:HG23	2.15	0.46
2:B:249:ASN:O	2:B:249:ASN:OD1	2.34	0.46
2:B:435:TYR:O	2:B:436:GLN:CB	2.56	0.46
1:A:146:GLY:C	1:A:189:LEU:HD13	2.41	0.45
1:A:267:PHE:CD1	1:A:388:TRP:HZ2	2.34	0.45
1:A:306:ASP:OD2	1:A:308:ARG:HB2	2.16	0.45
1:A:343:PHE:HE2	1:A:351:PHE:CZ	1.85	0.45
1:A:363:VAL:HG12	1:A:364:PRO:HG3	1.99	0.45
1:A:384:ILE:O	1:A:386:GLU:N	2.49	0.45
1:A:101:ASN:CA	3:A:500:GTP:O2G	2.61	0.45
1:A:141:PHE:CE1	1:A:170:SER:HB2	2.51	0.45
1:A:174:ALA:HB3	1:A:175:PRO:CD	2.10	0.45
1:A:175:PRO:HD2	1:A:207:GLU:HG2	1.98	0.45
2:B:14:ASN:HB3	2:B:74:THR:CB	2.43	0.45
2:B:241:CYS:O	2:B:242:LEU:CG	2.64	0.45
1:A:8:HIS:HB2	1:A:67:PHE:HA	1.98	0.45
2:B:143:GLY:H	2:B:147:SER:HG	1.56	0.45
2:B:196:GLU:HA	2:B:196:GLU:OE1	2.15	0.45
2:B:318:VAL:HG22	2:B:354:ALA:HB3	1.98	0.45
2:B:384:ILE:HG22	2:B:388:PHE:HE2	1.77	0.45
1:A:35:GLN:C	1:A:36:MET:CG	2.89	0.45
1:A:123:ARG:O	1:A:127:ASP:OD1	2.34	0.45
1:A:238:ILE:CG2	1:A:255:PHE:CZ	2.99	0.45
1:A:277:SER:HB3	1:A:280:LYS:CE	2.36	0.45
1:A:297:GLU:O	1:A:298:PRO:C	2.52	0.45
2:B:102:ASN:HB2	2:B:105:LYS:HG3	1.98	0.45
2:B:140:SER:O	2:B:147:SER:OG	2.25	0.45
2:B:184:PRO:CA	2:B:395:PHE:CD1	2.98	0.45
1:A:103:TYR:CD2	1:A:148:GLY:N	2.85	0.45
1:A:278:ALA:N	1:A:368:LEU:HD22	2.32	0.45
2:B:174:SER:CB	2:B:175:PRO:CD	2.89	0.45
2:B:295:MET:CE	2:B:375:ALA:HA	2.40	0.45
2:B:312:TYR:N	2:B:381:SER:CB	2.80	0.45
2:B:427:ASP:O	2:B:431:GLU:HG3	2.16	0.45
1:A:31:GLN:OE1	1:A:243:ARG:HD3	2.01	0.45
1:A:309:HIS:CB	1:A:386:GLU:OE2	2.65	0.45
1:A:183:GLU:HB3	1:A:394:LYS:HB2	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:C	1:A:342:GLN:HG3	2.42	0.45
2:B:56:ALA:CB	2:B:62:VAL:N	2.80	0.45
2:B:405:LEU:C	2:B:409:THR:HG1	2.11	0.45
2:B:411:GLU:OE1	2:B:411:GLU:HA	2.17	0.45
1:A:180:ALA:CB	1:A:398:MET:HE3	2.26	0.45
1:A:409:VAL:O	1:A:412:GLY:O	2.35	0.45
2:B:66:ILE:HG23	2:B:66:ILE:O	2.16	0.45
2:B:143:GLY:CA	2:B:185:TYR:CE1	2.87	0.45
2:B:210:TYR:O	2:B:211:ASP:C	2.59	0.45
2:B:217:LEU:CD2	2:B:275:LEU:O	2.65	0.45
1:A:82:THR:C	1:A:84:ARG:N	2.73	0.45
1:A:383:ALA:O	1:A:385:ALA:CA	2.60	0.45
2:B:35:SER:CB	2:B:60:LYS:CE	2.94	0.45
2:B:146:GLY:O	2:B:150:GLY:N	2.48	0.45
2:B:194:LEU:HD21	2:B:267:PHE:HE2	1.65	0.45
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.51	0.45
1:A:267:PHE:CE2	1:A:388:TRP:HZ2	2.35	0.45
2:B:94:PHE:CD2	2:B:114:LEU:CD2	3.00	0.45
2:B:250:ALA:HB1	2:B:352:LYS:NZ	2.32	0.45
2:B:313:LEU:HD22	2:B:346:TRP:CH2	2.51	0.45
2:B:319:PHE:O	2:B:355:VAL:HG13	2.16	0.45
2:B:370:GLY:C	5:B:501:TXL:C18	2.72	0.45
1:A:35:GLN:N	1:A:60:LYS:HD3	2.31	0.44
1:A:169:PHE:CZ	1:A:235:VAL:CG2	2.78	0.44
1:A:267:PHE:HA	1:A:268:PRO:HD2	1.57	0.44
1:A:307:PRO:O	1:A:308:ARG:C	2.61	0.44
2:B:102:ASN:CG	2:B:105:LYS:HE3	2.41	0.44
2:B:166:MET:HG2	2:B:197:ASN:O	2.16	0.44
2:B:313:LEU:H	2:B:381:SER:HA	1.81	0.44
1:A:9:VAL:HG13	1:A:150:THR:CG2	2.42	0.44
1:A:26:LEU:HD11	1:A:361:THR:HG23	1.83	0.44
1:A:30:ILE:C	1:A:32:PRO:CG	2.55	0.44
1:A:291:ILE:HD11	1:A:373:ARG:HB2	1.95	0.44
2:B:44:LEU:HD21	2:B:85:GLN:HB2	1.07	0.44
2:B:71:GLU:HG2	2:B:99:ALA:H	1.65	0.44
2:B:75:MET:SD	2:B:93:VAL:HG21	2.57	0.44
2:B:230:LEU:HD21	2:B:302:MET:HG3	1.99	0.44
2:B:426:ASN:C	2:B:426:ASN:HD22	2.25	0.44
1:A:16:ILE:O	1:A:19:ALA:HB3	2.16	0.44
1:A:81:GLY:C	1:A:83:TYR:N	2.68	0.44
1:A:182:VAL:O	1:A:183:GLU:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HD2	1:A:398:MET:HB3	1.99	0.44
1:A:305:CYS:O	1:A:307:PRO:CD	2.56	0.44
1:A:345:ASP:OD2	1:A:439:SER:HA	2.17	0.44
2:B:344:VAL:HB	2:B:347:ILE:HD12	1.99	0.44
2:B:431:GLU:O	2:B:434:GLN:HB2	2.18	0.44
1:A:107:HIS:ND1	1:A:107:HIS:C	2.74	0.44
1:A:122:ILE:HD11	1:A:157:LEU:HD22	1.97	0.44
1:A:152:LEU:HD11	1:A:156:ARG:HH21	1.78	0.44
1:A:152:LEU:O	1:A:156:ARG:HG3	2.17	0.44
1:A:183:GLU:HG3	2:B:348:PRO:HB2	1.98	0.44
2:B:102:ASN:CG	2:B:408:TYR:HD1	2.18	0.44
1:A:34:GLY:O	1:A:35:GLN:CB	2.64	0.44
1:A:97:GLU:OE2	1:A:114:ILE:HD11	2.16	0.44
2:B:151:THR:HG21	2:B:192:HIS:CG	2.36	0.44
2:B:157:ILE:O	2:B:161:TYR:HB2	2.18	0.44
2:B:254:LYS:C	2:B:258:ASN:OD1	2.59	0.44
2:B:265:LEU:HD23	2:B:267:PHE:HZ	1.67	0.44
1:A:137:VAL:CG2	1:A:168:GLU:HG2	2.48	0.44
1:A:297:GLU:C	1:A:299:ALA:H	2.25	0.44
2:B:66:ILE:HG21	2:B:66:ILE:HD13	1.78	0.44
2:B:340:SER:OG	2:B:341:SER:N	2.38	0.44
1:A:206:ASN:OD1	3:A:500:GTP:N2	2.50	0.44
1:A:432:TYR:O	1:A:435:VAL:HB	2.17	0.44
2:B:129:CYS:C	2:B:130:ASP:OD1	2.61	0.44
2:B:166:MET:HG3	2:B:197:ASN:O	2.18	0.44
2:B:234:THR:HG23	2:B:270:PRO:HB2	2.00	0.44
2:B:289:PRO:CD	2:B:290:GLU:H	2.29	0.44
1:A:181:VAL:O	1:A:185:TYR:HB2	2.18	0.44
1:A:328:VAL:O	1:A:332:ILE:HB	2.17	0.44
1:A:437:VAL:O	1:A:437:VAL:CG1	2.64	0.44
2:B:29:GLY:O	2:B:58:GLY:HA3	2.18	0.44
2:B:243:ARG:CZ	2:B:252:LEU:HD21	2.45	0.44
2:B:333:LEU:HG	2:B:337:ASN:HD21	1.82	0.44
1:A:170:SER:OG	1:A:203:MET:CA	2.66	0.44
1:A:179:THR:HG22	1:A:180:ALA:C	2.28	0.44
2:B:6:HIS:CE1	2:B:30:ILE:CG1	3.00	0.44
2:B:64:ARG:HH12	2:B:132:LEU:HD21	1.83	0.44
2:B:94:PHE:CE2	2:B:114:LEU:CB	3.01	0.44
2:B:103:TRP:CD1	2:B:148:GLY:N	2.83	0.44
2:B:133:GLN:NE2	2:B:253:ARG:HB2	2.33	0.44
2:B:259:MET:SD	2:B:378:ILE:CG2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HB3	1:A:187:SER:OG	2.18	0.43
1:A:229:ARG:HH11	1:A:229:ARG:HD2	1.40	0.43
1:A:230:LEU:HG	1:A:302:MET:CE	2.36	0.43
1:A:362:VAL:HG13	1:A:367:ASP:CB	2.48	0.43
2:B:22:GLU:HB3	2:B:83:PHE:CE1	2.46	0.43
2:B:49:ILE:HA	2:B:61:TYR:HE2	1.82	0.43
2:B:194:LEU:HD21	2:B:267:PHE:CZ	2.48	0.43
2:B:236:SER:O	2:B:240:THR:HB	2.18	0.43
2:B:275:LEU:CD1	2:B:300:ASN:ND2	2.67	0.43
2:B:417:GLU:OE1	2:B:417:GLU:HA	2.17	0.43
1:A:38:SER:C	1:A:39:ASP:CG	2.85	0.43
1:A:71:GLU:HG2	1:A:99:ALA:HB2	1.01	0.43
1:A:76:ASP:O	1:A:76:ASP:OD1	2.37	0.43
1:A:241:SER:OG	1:A:242:LEU:N	2.51	0.43
1:A:306:ASP:CG	1:A:308:ARG:CD	2.90	0.43
1:A:306:ASP:C	1:A:308:ARG:N	2.72	0.43
2:B:183:GLU:OE1	2:B:394:GLN:HB2	2.14	0.43
1:A:3:GLU:OE2	1:A:129:CYS:CB	2.59	0.43
1:A:12:ALA:HB1	1:A:171:ILE:HD12	2.00	0.43
1:A:35:GLN:C	1:A:36:MET:HG3	2.42	0.43
1:A:222:PRO:CG	2:B:326:LYS:HD3	2.38	0.43
1:A:273:ALA:HB2	1:A:294:ALA:HB3	1.98	0.43
2:B:6:HIS:CD2	2:B:21:TRP:CZ2	3.03	0.43
2:B:115:VAL:HG11	2:B:152:LEU:HB3	2.00	0.43
2:B:265:LEU:HD21	2:B:267:PHE:CE1	2.52	0.43
2:B:320:ARG:NH2	5:B:501:TXL:C27	2.78	0.43
2:B:385:GLN:OE1	2:B:433:GLN:HB2	2.17	0.43
1:A:31:GLN:NE2	1:A:243:ARG:NE	2.59	0.43
1:A:38:SER:HB3	1:A:45:GLY:HA3	2.00	0.43
1:A:115:ILE:HD11	1:A:156:ARG:CD	2.47	0.43
1:A:157:LEU:HB2	1:A:166:LYS:CE	2.49	0.43
1:A:259:LEU:CA	1:A:380:ASN:HD21	2.31	0.43
1:A:414:GLU:O	1:A:415:GLU:HB2	2.19	0.43
2:B:102:ASN:O	2:B:105:LYS:HB2	2.19	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CE1	2.53	0.43
2:B:321:GLY:HA3	2:B:373:MET:CG	2.15	0.43
1:A:5:ILE:CB	1:A:135:PHE:CE1	3.01	0.43
1:A:7:ILE:HB	1:A:136:SER:O	2.18	0.43
1:A:26:LEU:O	1:A:27:GLU:CB	2.66	0.43
1:A:252:LEU:HD23	1:A:255:PHE:HE2	1.78	0.43
1:A:404:PHE:O	1:A:404:PHE:CG	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.19	0.43
2:B:94:PHE:CE1	2:B:97:SER:HB3	2.52	0.43
2:B:296:PHE:CE2	2:B:335:VAL:CG1	2.98	0.43
2:B:318:VAL:O	2:B:376:THR:N	2.26	0.43
2:B:389:LYS:HG2	2:B:429:VAL:HG11	1.75	0.43
2:B:425:MET:O	2:B:428:LEU:CB	2.63	0.43
1:A:14:VAL:CG2	1:A:74:VAL:CG1	2.96	0.43
1:A:109:THR:HG21	1:A:411:GLU:CD	2.42	0.43
1:A:115:ILE:HD12	1:A:152:LEU:HD23	1.87	0.43
1:A:147:SER:OG	1:A:148:GLY:N	2.50	0.43
1:A:211:ASP:OD1	1:A:214:ARG:NH1	2.51	0.43
1:A:312:TYR:HD1	1:A:341:ILE:O	2.01	0.43
2:B:6:HIS:HE1	2:B:30:ILE:HD12	0.60	0.43
2:B:280:SER:O	2:B:283:TYR:HD1	2.02	0.43
2:B:292:THR:HG22	2:B:332:MET:SD	2.58	0.43
1:A:97:GLU:HG3	1:A:110:ILE:HG23	1.92	0.43
1:A:119:LEU:HA	1:A:122:ILE:CG2	2.48	0.43
1:A:137:VAL:HB	1:A:168:GLU:CB	2.49	0.43
1:A:266:HIS:HD2	1:A:432:TYR:CZ	2.37	0.43
2:B:183:GLU:HB3	2:B:184:PRO:HD3	1.81	0.43
1:A:79:ARG:O	1:A:79:ARG:HG3	2.18	0.43
2:B:4:ILE:HG21	2:B:30:ILE:HG22	1.99	0.43
2:B:21:TRP:CE3	2:B:24:ILE:HD12	2.53	0.43
2:B:24:ILE:CA	2:B:26:ASP:H	2.25	0.43
2:B:186:ASN:HA	2:B:189:LEU:HD12	2.01	0.43
2:B:344:VAL:H	2:B:350:ASN:HD21	1.67	0.43
1:A:58:ALA:C	1:A:60:LYS:N	2.75	0.43
1:A:64:ARG:CZ	1:A:132:LEU:CD2	2.86	0.43
1:A:192:HIS:O	1:A:196:GLU:CB	2.67	0.43
1:A:204:VAL:HG13	1:A:209:ILE:CD1	2.30	0.43
1:A:303:VAL:CG1	1:A:304:LYS:N	2.80	0.43
1:A:340:THR:C	1:A:341:ILE:HD13	2.44	0.43
1:A:397:LEU:HA	1:A:401:LYS:HD2	2.00	0.43
1:A:409:VAL:O	1:A:412:GLY:N	2.40	0.43
1:A:437:VAL:HG12	1:A:438:ASP:OD1	2.19	0.43
2:B:224:TYR:O	2:B:225:GLY:C	2.54	0.43
1:A:141:PHE:HB3	1:A:186:ASN:CG	2.43	0.43
1:A:181:VAL:HG12	1:A:185:TYR:HB2	2.01	0.43
1:A:287:SER:O	1:A:288:VAL:C	2.57	0.43
1:A:298:PRO:O	1:A:301:GLN:HB2	2.18	0.43
2:B:199:ASP:OD2	2:B:256:ALA:HB1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ILE:O	2:B:216:THR:OG1	2.35	0.43
2:B:258:ASN:O	2:B:314:THR:HG21	2.19	0.43
1:A:77:GLU:CA	1:A:80:THR:CB	2.84	0.42
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.86	0.42
1:A:277:SER:HA	1:A:368:LEU:CD2	2.38	0.42
1:A:341:ILE:H	1:A:342:GLN:HG3	1.84	0.42
2:B:27:GLU:HB2	2:B:36:TYR:CB	2.49	0.42
2:B:157:ILE:HG21	2:B:166:MET:CE	2.49	0.42
2:B:320:ARG:HH21	5:B:501:TXL:H27	1.76	0.42
2:B:324:SER:O	2:B:328:VAL:HG23	2.19	0.42
2:B:339:ASN:CA	2:B:342:TYR:HD1	2.32	0.42
2:B:384:ILE:HG21	2:B:388:PHE:HE2	1.79	0.42
2:B:398:MET:SD	2:B:399:PHE:CD2	3.12	0.42
1:A:31:GLN:NE2	1:A:243:ARG:CB	2.57	0.42
1:A:154:MET:HB2	1:A:192:HIS:HE1	1.75	0.42
1:A:264:ARG:O	1:A:265:GLY:C	2.62	0.42
2:B:7:ILE:HG21	2:B:137:LEU:CD2	2.49	0.42
2:B:89:PRO:C	2:B:90:ASP:CG	2.84	0.42
2:B:296:PHE:CD1	2:B:335:VAL:CG1	3.02	0.42
2:B:319:PHE:CE1	2:B:353:THR:HG21	2.44	0.42
2:B:385:GLN:NE2	2:B:433:GLN:HB2	2.34	0.42
2:B:405:LEU:O	2:B:409:THR:CB	2.67	0.42
1:A:101:ASN:O	1:A:102:ASN:CB	2.51	0.42
1:A:184:PRO:HG2	1:A:399:TYR:CD2	2.51	0.42
1:A:194:THR:CG2	1:A:195:LEU:N	2.59	0.42
2:B:48:ARG:O	2:B:61:TYR:CE2	2.72	0.42
2:B:48:ARG:CZ	2:B:60:LYS:HA	2.46	0.42
2:B:152:LEU:O	2:B:155:SER:OG	2.34	0.42
2:B:243:ARG:HH21	2:B:252:LEU:CG	2.31	0.42
2:B:301:MET:HG3	2:B:307:PRO:HG3	2.00	0.42
2:B:313:LEU:HD22	2:B:346:TRP:CZ2	2.55	0.42
2:B:336:GLN:HE21	2:B:351:VAL:CB	2.29	0.42
1:A:252:LEU:HD23	1:A:255:PHE:CD2	2.54	0.42
2:B:27:GLU:OE2	2:B:40:SER:O	2.37	0.42
2:B:111:GLY:O	2:B:115:VAL:CA	2.66	0.42
2:B:114:LEU:O	2:B:118:VAL:HG23	2.20	0.42
2:B:191:VAL:HG23	2:B:421:ALA:HB1	2.00	0.42
2:B:216:THR:HG21	2:B:275:LEU:HD13	2.00	0.42
2:B:311:ARG:C	2:B:381:SER:CB	2.88	0.42
1:A:30:ILE:HB	1:A:64:ARG:HB3	1.90	0.42
1:A:185:TYR:CD1	1:A:185:TYR:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:HB1	1:A:294:ALA:HB1	1.98	0.42
1:A:312:TYR:HA	1:A:381:THR:CB	2.48	0.42
2:B:3:GLU:CA	2:B:31:ASP:CG	2.87	0.42
2:B:115:VAL:HG12	2:B:156:LYS:HZ2	1.84	0.42
2:B:176:LYS:CD	2:B:207:GLU:OE2	2.67	0.42
2:B:398:MET:CG	2:B:399:PHE:N	2.62	0.42
1:A:5:ILE:HB	1:A:135:PHE:CE1	2.55	0.42
1:A:289:ALA:C	1:A:291:ILE:H	2.25	0.42
2:B:223:THR:HG1	2:B:226:ASP:HB2	1.84	0.42
2:B:377:PHE:CD1	2:B:377:PHE:C	2.97	0.42
1:A:344:VAL:HG12	1:A:345:ASP:N	2.34	0.42
1:A:382:THR:O	1:A:383:ALA:C	2.61	0.42
1:A:395:PHE:C	1:A:397:LEU:N	2.76	0.42
2:B:172:VAL:CG2	2:B:205:ASP:OD1	2.67	0.42
1:A:5:ILE:HG13	1:A:64:ARG:NH2	2.31	0.42
1:A:306:ASP:CG	1:A:308:ARG:CB	2.73	0.42
2:B:34:GLY:O	2:B:36:TYR:HD2	2.01	0.42
2:B:142:GLY:N	2:B:186:ASN:CG	2.61	0.42
2:B:237:GLY:C	2:B:241:CYS:HB2	2.28	0.42
2:B:242:LEU:HD13	2:B:250:ALA:O	2.20	0.42
2:B:273:ALA:CB	2:B:294:GLN:OE1	2.60	0.42
2:B:301:MET:CE	2:B:377:PHE:CE1	3.03	0.42
2:B:339:ASN:C	2:B:342:TYR:HD1	2.28	0.42
2:B:391:ILE:C	2:B:394:GLN:HB2	2.45	0.42
2:B:393:GLU:OE1	2:B:393:GLU:HA	2.20	0.42
1:A:276:ILE:HG22	1:A:277:SER:N	2.35	0.42
1:A:296:PHE:HD2	1:A:312:TYR:OH	2.03	0.42
1:A:362:VAL:O	1:A:363:VAL:HG23	2.19	0.42
1:A:397:LEU:CA	1:A:401:LYS:CB	2.84	0.42
2:B:34:GLY:C	2:B:35:SER:HG	2.14	0.42
2:B:96:GLN:OE1	2:B:96:GLN:HA	2.19	0.42
2:B:101:ASN:HD22	2:B:101:ASN:HA	1.47	0.42
2:B:196:GLU:O	2:B:197:ASN:HB3	2.19	0.42
2:B:385:GLN:NE2	2:B:433:GLN:CD	2.62	0.42
1:A:57:GLY:CA	1:A:61:HIS:NE2	2.78	0.42
2:B:62:VAL:HG12	2:B:63:PRO:C	2.45	0.42
2:B:70:LEU:O	2:B:70:LEU:HG	2.20	0.42
2:B:236:SER:O	2:B:241:CYS:N	2.50	0.42
2:B:259:MET:HE2	2:B:379:GLY:H	1.79	0.42
2:B:431:GLU:CA	2:B:434:GLN:HG3	2.50	0.42
1:A:67:PHE:CB	1:A:92:LEU:CD2	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:N	1:A:189:LEU:HD13	2.33	0.41
1:A:173:PRO:HG3	1:A:186:ASN:ND2	2.35	0.41
1:A:179:THR:HG21	1:A:181:VAL:CA	2.46	0.41
2:B:133:GLN:HE21	2:B:253:ARG:NH1	2.04	0.41
2:B:213:CYS:CB	2:B:219:LEU:CD1	2.86	0.41
2:B:262:PHE:CB	2:B:263:PRO:CD	2.78	0.41
2:B:286:LEU:HD13	2:B:372:LYS:C	2.45	0.41
1:A:282:TYR:CD2	1:A:284:GLU:O	2.74	0.41
2:B:35:SER:HB3	2:B:60:LYS:HE3	2.02	0.41
2:B:172:VAL:HG12	2:B:173:PRO:O	2.20	0.41
1:A:31:GLN:NE2	1:A:239:THR:HG23	2.35	0.41
1:A:73:THR:CG2	2:B:249:ASN:HD21	2.24	0.41
1:A:109:THR:HG1	1:A:110:ILE:H	1.68	0.41
1:A:170:SER:OG	1:A:203:MET:CB	2.42	0.41
2:B:151:THR:O	2:B:192:HIS:HD2	2.02	0.41
2:B:184:PRO:CB	2:B:395:PHE:CD1	3.00	0.41
1:A:102:ASN:HA	1:A:408:TYR:CE1	2.56	0.41
1:A:122:ILE:HD13	1:A:157:LEU:HD22	1.94	0.41
1:A:143:GLY:C	1:A:185:TYR:OH	2.63	0.41
1:A:303:VAL:HG12	1:A:304:LYS:H	1.84	0.41
2:B:92:PHE:N	2:B:92:PHE:CD1	2.87	0.41
2:B:154:ILE:CD1	2:B:192:HIS:CE1	2.82	0.41
2:B:435:TYR:CB	2:B:436:GLN:HG3	2.51	0.41
1:A:101:ASN:HD22	3:A:500:GTP:PG	2.42	0.41
1:A:114:ILE:HD13	1:A:114:ILE:HG21	1.84	0.41
1:A:224:TYR:HH	3:A:500:GTP:C2'	2.04	0.41
2:B:241:CYS:C	2:B:243:ARG:H	2.28	0.41
2:B:260:VAL:HG12	2:B:262:PHE:H	1.85	0.41
2:B:346:TRP:CZ2	2:B:435:TYR:CD2	3.05	0.41
1:A:64:ARG:NH2	1:A:132:LEU:CB	2.83	0.41
1:A:104:ALA:C	1:A:108:TYR:HD2	2.28	0.41
1:A:407:TRP:CE2	2:B:256:ALA:O	2.74	0.41
2:B:4:ILE:CG2	2:B:30:ILE:HB	2.50	0.41
2:B:231:VAL:C	2:B:233:ALA:N	2.74	0.41
2:B:253:ARG:HH11	2:B:253:ARG:CB	2.29	0.41
2:B:370:GLY:O	5:B:501:TXL:C18	2.37	0.41
5:B:501:TXL:C21	5:B:501:TXL:C18	2.91	0.41
1:A:9:VAL:HG12	1:A:146:GLY:HA2	2.02	0.41
1:A:70:LEU:CB	1:A:145:THR:HG22	2.36	0.41
1:A:75:ILE:HG23	1:A:76:ASP:N	2.36	0.41
1:A:382:THR:O	1:A:385:ALA:HB2	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLU:HG2	2:B:48:ARG:HH21	1.85	0.41
2:B:47:GLU:CD	2:B:85:GLN:OE1	2.64	0.41
1:A:2:ARG:C	1:A:31:GLN:HG3	2.35	0.41
1:A:224:TYR:CB	2:B:325:MET:CB	2.98	0.41
1:A:277:SER:OG	1:A:279:GLU:C	2.56	0.41
1:A:416:GLY:O	1:A:417:GLU:HB2	2.19	0.41
2:B:14:ASN:ND2	2:B:69:ASP:HA	2.35	0.41
2:B:69:ASP:OD2	2:B:74:THR:HG22	2.15	0.41
2:B:243:ARG:CZ	2:B:252:LEU:HD11	2.48	0.41
2:B:433:GLN:CD	2:B:437:ASP:OD2	2.64	0.41
1:A:107:HIS:HD1	1:A:108:TYR:N	2.18	0.41
1:A:116:ASP:OD1	1:A:156:ARG:NH1	2.54	0.41
1:A:242:LEU:HD22	1:A:250:VAL:HB	2.03	0.41
1:A:311:LYS:CG	1:A:342:GLN:O	2.69	0.41
2:B:150:GLY:O	2:B:154:ILE:CG1	2.45	0.41
2:B:174:SER:HB2	2:B:207:GLU:CG	2.51	0.41
1:A:316:CYS:C	1:A:317:LEU:HD23	2.46	0.41
2:B:48:ARG:HD2	2:B:60:LYS:CA	2.38	0.41
2:B:74:THR:O	2:B:75:MET:C	2.63	0.41
2:B:86:ILE:HB	2:B:87:PHE:H	1.29	0.41
2:B:236:SER:OG	5:B:501:TXL:H27	2.21	0.41
2:B:259:MET:HG3	2:B:378:ILE:CG2	2.50	0.41
1:A:130:THR:O	1:A:131:GLY:O	2.38	0.40
1:A:398:MET:SD	2:B:348:PRO:O	2.79	0.40
1:A:404:PHE:HE2	2:B:257:VAL:HG13	1.86	0.40
2:B:95:GLY:C	2:B:96:GLN:HG2	2.46	0.40
2:B:165:ILE:HD13	2:B:199:ASP:CG	2.46	0.40
2:B:183:GLU:HG3	2:B:398:MET:SD	2.59	0.40
2:B:194:LEU:HD11	2:B:428:LEU:HD22	2.03	0.40
2:B:259:MET:C	2:B:261:PRO:HD3	2.46	0.40
2:B:405:LEU:CG	2:B:405:LEU:O	2.52	0.40
1:A:4:CYS:H	1:A:30:ILE:HG22	1.86	0.40
1:A:115:ILE:HD13	1:A:115:ILE:HG21	1.83	0.40
1:A:217:LEU:HD22	1:A:368:LEU:CG	2.51	0.40
1:A:313:MET:HB2	1:A:380:ASN:HB2	2.03	0.40
2:B:50:ASN:N	2:B:61:TYR:CG	2.83	0.40
2:B:165:ILE:HD12	2:B:256:ALA:CB	2.51	0.40
1:A:147:SER:N	1:A:189:LEU:CD1	2.80	0.40
1:A:191:THR:OG1	1:A:192:HIS:N	2.54	0.40
1:A:271:THR:CB	1:A:377:MET:HB3	2.50	0.40
1:A:311:LYS:O	1:A:382:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:SER:O	2:B:179:ASP:CB	2.64	0.40
2:B:388:PHE:O	2:B:391:ILE:N	2.54	0.40
1:A:76:ASP:O	1:A:80:THR:HA	2.17	0.40
1:A:150:THR:O	1:A:192:HIS:NE2	2.54	0.40
1:A:312:TYR:CG	1:A:381:THR:CG2	2.90	0.40
1:A:416:GLY:C	1:A:418:PHE:H	2.06	0.40
2:B:40:SER:O	2:B:41:ASP:HB2	2.21	0.40
2:B:201:THR:HG21	2:B:267:PHE:CE1	2.56	0.40
2:B:238:VAL:CG1	2:B:255:LEU:CD1	2.98	0.40
2:B:274:PRO:HB2	2:B:371:LEU:CD2	2.51	0.40
2:B:424:ASN:ND2	2:B:424:ASN:C	2.77	0.40
1:A:14:VAL:CG1	1:A:74:VAL:HG13	2.52	0.40
1:A:103:TYR:CZ	1:A:148:GLY:HA2	2.56	0.40
1:A:116:ASP:O	1:A:119:LEU:HB2	2.22	0.40
1:A:154:MET:HB2	1:A:192:HIS:HE2	1.82	0.40
1:A:157:LEU:CB	1:A:166:LYS:HE2	2.50	0.40
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.92	0.40
2:B:282:GLN:HA	2:B:282:GLN:OE1	2.21	0.40
2:B:315:VAL:HB	2:B:351:VAL:HG22	2.04	0.40

All (35) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:CG	1:A:420:GLU:CD[2_444]	0.73	1.47
1:A:1:MET:CE	2:B:72:PRO:CG[1_655]	1.00	1.20
1:A:283:HIS:CG	1:A:420:GLU:OE1[2_444]	1.01	1.19
1:A:283:HIS:ND1	1:A:420:GLU:CD[2_444]	1.11	1.09
1:A:283:HIS:CD2	1:A:420:GLU:CA[2_444]	1.18	1.02
1:A:283:HIS:CD2	1:A:420:GLU:CB[2_444]	1.19	1.01
1:A:283:HIS:NE2	1:A:420:GLU:CB[2_444]	1.42	0.78
1:A:283:HIS:CB	1:A:420:GLU:CD[2_444]	1.42	0.78
1:A:283:HIS:CG	1:A:420:GLU:CG[2_444]	1.42	0.78
1:A:440:VAL:C	2:B:402:LYS:CE[1_655]	1.45	0.75
1:A:283:HIS:ND1	1:A:420:GLU:OE1[2_444]	1.46	0.74
1:A:283:HIS:CB	1:A:420:GLU:OE2[2_444]	1.59	0.61
1:A:1:MET:CB	2:B:96:GLN:NE2[1_655]	1.61	0.59
1:A:326:LYS:NZ	2:B:214:PHE:CZ[1_655]	1.67	0.53
1:A:1:MET:CE	2:B:72:PRO:CB[1_655]	1.68	0.52
1:A:283:HIS:CD2	1:A:420:GLU:OE1[2_444]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:ND1	1:A:420:GLU:CG[2_444]	1.75	0.45
1:A:349:THR:CB	2:B:177:VAL:CG1[1_655]	1.78	0.42
1:A:283:HIS:CD2	1:A:420:GLU:CG[2_444]	1.82	0.38
1:A:440:VAL:C	2:B:402:LYS:NZ[1_655]	1.82	0.38
1:A:1:MET:CA	2:B:96:GLN:NE2[1_655]	1.83	0.37
1:A:254:GLU:OE1	2:B:101:ASN:OD1[1_655]	1.87	0.33
1:A:283:HIS:CB	1:A:420:GLU:OE1[2_444]	1.90	0.30
1:A:283:HIS:CG	1:A:420:GLU:OE2[2_444]	1.90	0.30
1:A:283:HIS:ND1	1:A:420:GLU:OE2[2_444]	1.91	0.29
1:A:283:HIS:CG	1:A:420:GLU:CB[2_444]	1.98	0.22
1:A:283:HIS:CD2	1:A:420:GLU:CD[2_444]	2.01	0.19
1:A:440:VAL:O	2:B:402:LYS:CE[1_655]	2.02	0.18
2:B:284:ARG:NE	2:B:420:GLU:OE2[2_344]	2.05	0.15
1:A:2:ARG:NH2	2:B:71:GLU:OE1[1_655]	2.06	0.14
1:A:326:LYS:NZ	2:B:214:PHE:CE1[1_655]	2.06	0.14
1:A:133:GLN:NE2	2:B:96:GLN:O[1_655]	2.11	0.09
1:A:254:GLU:OE2	2:B:101:ASN:OD1[1_655]	2.13	0.07
1:A:283:HIS:NE2	1:A:420:GLU:CA[2_444]	2.17	0.03
1:A:283:HIS:CE1	1:A:420:GLU:CB[2_444]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	438/440 (100%)	323 (74%)	62 (14%)	53 (12%)	0	4
2	B	425/427 (100%)	297 (70%)	49 (12%)	79 (19%)	0	1
All	All	863/867 (100%)	620 (72%)	111 (13%)	132 (15%)	0	2

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLN

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Mol	Chain	Res	Type
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	GLY
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
2	B	42	LEU

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Mol	Chain	Res	Type
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
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
2	B	32	PRO
2	B	50	ASN

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Mol	Chain	Res	Type
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
1	A	65	ALA
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	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
2	B	389	LYS
2	B	403	ALA
2	B	277	SER

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Mol	Chain	Res	Type
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	369/369 (100%)	353 (96%)	16 (4%)	26	50
2	B	368/368 (100%)	354 (96%)	14 (4%)	29	53
All	All	737/737 (100%)	707 (96%)	30 (4%)	28	52

All (30) 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
1	A	422	ARG
1	A	425	MET
2	B	30	ILE
2	B	101	ASN

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	61	HIS
1	A	85	GLN
1	A	88	HIS
1	A	102	ASN
1	A	107	HIS
1	A	176	GLN
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
1	A	406	HIS
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

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Mol	Chain	Res	Type
2	B	133	GLN
2	B	136	GLN
2	B	193	GLN
2	B	197	ASN
2	B	247	GLN
2	B	249	ASN
2	B	294	GLN
2	B	336	GLN
2	B	337	ASN
2	B	349	ASN
2	B	350	ASN
2	B	426	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	TXL	B	501	-	63,63,63	4.48	48 (76%)	100,100,100	3.47	55 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDP	B	500	-	29,30,30	1.32	3 (10%)	45,47,47	0.96	2 (4%)
3	GTP	A	500	-	33,34,34	1.93	6 (18%)	50,54,54	1.45	5 (10%)

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

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

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	TXL	O3-C4	-10.05	1.26	1.46
5	B	501	TXL	C41-C36	9.35	1.53	1.39
5	B	501	TXL	C37-C36	-8.74	1.26	1.39
5	B	501	TXL	C8-C3	-8.13	1.38	1.57
5	B	501	TXL	O6-C9	-8.05	1.08	1.21
5	B	501	TXL	C25-C24	-7.66	1.27	1.39
5	B	501	TXL	C13-C12	-7.19	1.37	1.51
5	B	501	TXL	C14-C13	7.16	1.66	1.52
3	A	500	GTP	PB-O3A	-7.04	1.51	1.59
5	B	501	TXL	O5-C7	-6.86	1.32	1.43
5	B	501	TXL	C16-C15	-6.79	1.40	1.53
5	B	501	TXL	C6-C7	6.01	1.63	1.53
5	B	501	TXL	C43-C42	-5.87	1.30	1.49
5	B	501	TXL	C12-C11	-5.87	1.26	1.34
5	B	501	TXL	C10-C11	-5.38	1.34	1.50
5	B	501	TXL	O8-C13	-5.36	1.36	1.45
5	B	501	TXL	C14-C1	-5.28	1.43	1.54
5	B	501	TXL	O4-C5	5.28	1.56	1.46
5	B	501	TXL	C20-C4	5.24	1.67	1.53
5	B	501	TXL	C17-C15	4.63	1.62	1.53
5	B	501	TXL	C40-C39	-4.57	1.28	1.38
5	B	501	TXL	C28-C27	-4.47	1.28	1.38
5	B	501	TXL	C4-C3	4.42	1.64	1.54
5	B	501	TXL	C40-C41	4.30	1.46	1.38
5	B	501	TXL	C8-C9	4.26	1.67	1.55
5	B	501	TXL	C24-C23	-4.15	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	TXL	O12-C30	-4.12	1.26	1.34
5	B	501	TXL	O11-C30	4.08	1.29	1.21
3	A	500	GTP	PA-O3A	-4.04	1.55	1.59
5	B	501	TXL	O10-C22	3.92	1.49	1.42
5	B	501	TXL	C30-N1	3.89	1.44	1.34
5	B	501	TXL	C22-C21	-3.55	1.43	1.52
5	B	501	TXL	O12-C31	3.50	1.54	1.48
5	B	501	TXL	C36-C35	-3.28	1.42	1.50
5	B	501	TXL	C23-N1	-3.25	1.39	1.46
3	A	500	GTP	O2'-C2'	-3.10	1.35	1.43
5	B	501	TXL	O2-C35	3.07	1.41	1.34
3	A	500	GTP	O4'-C1'	-3.00	1.35	1.42
5	B	501	TXL	C34-C31	-2.98	1.43	1.51
5	B	501	TXL	O4-C20	-2.89	1.38	1.45
5	B	501	TXL	O8-C21	2.82	1.40	1.34
5	B	501	TXL	C39-C38	-2.78	1.32	1.38
5	B	501	TXL	C28-C29	-2.77	1.34	1.38
5	B	501	TXL	O13-C35	-2.64	1.15	1.22
5	B	501	TXL	C6-C5	-2.54	1.47	1.52
4	B	500	GDP	PB-O2B	-2.53	1.45	1.54
5	B	501	TXL	C4-C5	-2.52	1.50	1.55
5	B	501	TXL	C10-C9	2.51	1.60	1.53
4	B	500	GDP	PB-O1B	-2.47	1.42	1.50
5	B	501	TXL	O3-C42	2.44	1.40	1.35
5	B	501	TXL	O1-C1	-2.36	1.40	1.43
5	B	501	TXL	C32-C31	-2.35	1.45	1.51
3	A	500	GTP	C3'-C4'	-2.34	1.47	1.53
5	B	501	TXL	C26-C25	-2.27	1.35	1.38
4	B	500	GDP	PA-O3A	-2.16	1.57	1.59
3	A	500	GTP	C5'-C4'	-2.16	1.45	1.51
5	B	501	TXL	C1-C2	2.03	1.64	1.57

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	TXL	C39-C38-C37	11.06	133.89	120.24
5	B	501	TXL	C15-C1-C2	10.89	123.89	111.93
5	B	501	TXL	C38-C37-C36	-9.75	110.78	120.36
5	B	501	TXL	O7-C10-C9	7.21	121.53	109.51
5	B	501	TXL	C39-C40-C41	-6.27	112.51	120.24
5	B	501	TXL	C8-C9-C10	6.23	131.96	122.69
3	A	500	GTP	O2B-PB-O3B	5.97	123.40	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	TXL	C13-C12-C11	-5.86	108.07	117.73
5	B	501	TXL	O11-C30-N1	5.77	134.31	124.86
5	B	501	TXL	C11-C10-C9	-5.65	107.54	114.05
5	B	501	TXL	O2-C2-C1	5.41	115.97	104.74
5	B	501	TXL	C6-C5-C4	-5.29	112.44	119.63
5	B	501	TXL	C17-C15-C1	5.25	122.22	111.13
5	B	501	TXL	O4-C5-C6	4.85	122.11	113.17
5	B	501	TXL	C18-C12-C11	4.70	130.93	125.32
5	B	501	TXL	C16-C15-C1	-4.63	101.36	111.13
5	B	501	TXL	O12-C30-N1	-4.51	102.64	110.03
5	B	501	TXL	C33-C31-C32	4.51	122.39	111.13
5	B	501	TXL	O10-C22-C23	4.46	122.24	109.69
5	B	501	TXL	C10-C11-C12	-4.43	113.96	120.65
5	B	501	TXL	C14-C1-C15	-4.28	103.75	111.48
3	A	500	GTP	O3B-PB-O1B	-4.22	98.00	110.70
5	B	501	TXL	C2-O2-C35	4.14	125.37	117.80
5	B	501	TXL	O12-C31-C32	-4.06	91.17	107.21
5	B	501	TXL	O6-C9-C10	-3.96	112.85	117.37
5	B	501	TXL	O3-C42-O14	3.89	130.39	123.61
5	B	501	TXL	C31-O12-C30	-3.87	115.10	120.97
5	B	501	TXL	C19-C8-C9	3.85	116.53	106.56
5	B	501	TXL	C20-C4-C3	3.81	126.21	120.32
5	B	501	TXL	O7-C10-C11	-3.73	105.45	111.48
5	B	501	TXL	O2-C35-C36	3.72	117.88	111.90
5	B	501	TXL	C24-C23-N1	3.63	119.06	112.07
5	B	501	TXL	C15-C11-C12	3.52	124.33	119.60
5	B	501	TXL	C13-O8-C21	-3.23	110.78	116.58
3	A	500	GTP	O3G-PG-O3B	3.12	115.11	104.64
5	B	501	TXL	C24-C23-C22	-3.05	103.87	111.46
5	B	501	TXL	O5-C7-C6	3.01	115.25	109.12
5	B	501	TXL	C1-C2-C3	-2.97	113.75	118.19
5	B	501	TXL	C34-C31-C33	-2.91	103.87	111.13
5	B	501	TXL	C20-C4-C5	-2.84	82.45	85.38
5	B	501	TXL	C37-C36-C35	-2.75	114.33	120.40
5	B	501	TXL	C18-C12-C13	2.70	120.92	116.11
5	B	501	TXL	O3-C42-C43	-2.67	106.15	110.67
5	B	501	TXL	C23-N1-C30	-2.65	116.20	121.69
5	B	501	TXL	O8-C13-C12	-2.55	103.78	109.85
5	B	501	TXL	O4-C5-C4	2.55	93.37	90.58
5	B	501	TXL	O8-C21-O9	2.51	128.48	123.95
5	B	501	TXL	O12-C31-C34	2.50	117.08	107.21
5	B	501	TXL	C19-C8-C3	-2.49	105.67	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	TXL	C41-C36-C35	2.48	125.86	120.40
5	B	501	TXL	C14-C1-C2	-2.38	107.45	111.67
4	B	500	GDP	C1'-N9-C8	2.38	133.48	126.73
5	B	501	TXL	C27-C26-C25	2.36	123.16	120.24
3	A	500	GTP	O3A-PB-O1B	-2.36	103.61	110.70
5	B	501	TXL	O10-C22-C21	-2.34	103.74	110.33
5	B	501	TXL	C3-C4-C5	2.32	123.68	119.49
5	B	501	TXL	O1-C1-C2	-2.28	100.61	105.54
4	B	500	GDP	O2B-PB-O1B	2.26	119.63	110.83
5	B	501	TXL	O3-C4-C5	-2.24	107.09	112.26
3	A	500	GTP	O2G-PG-O3B	2.16	111.87	104.64
5	B	501	TXL	O2-C2-C3	-2.11	104.35	108.17
5	B	501	TXL	O6-C9-C8	-2.03	114.74	119.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

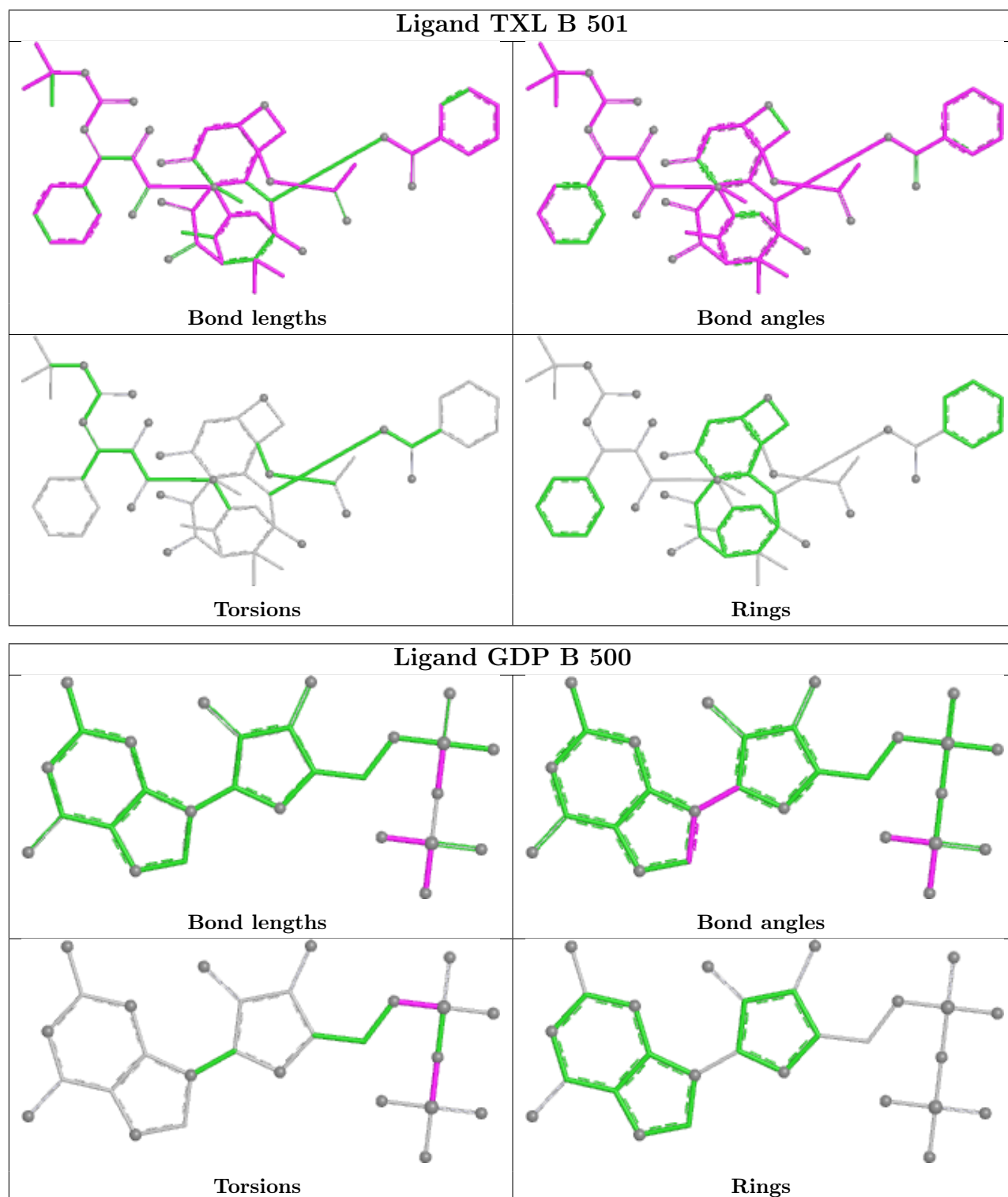
There are no ring outliers.

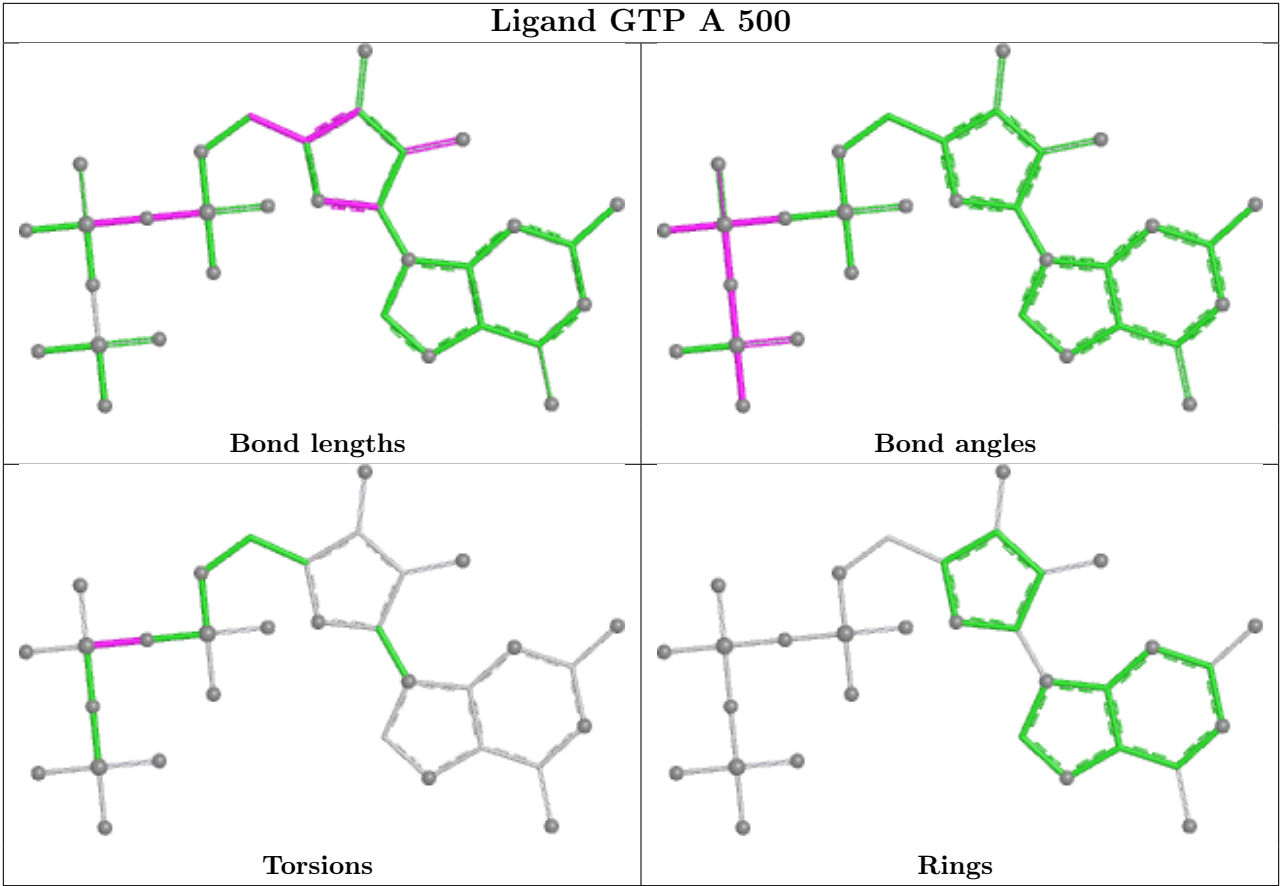
3 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	TXL	60	0
4	B	500	GDP	17	0
3	A	500	GTP	30	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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
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	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	B	244:PHE	C	245:PRO	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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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