Full wwPDB EM Validation Report ⓘ

Dec 13, 2022 – 12:01 AM EST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

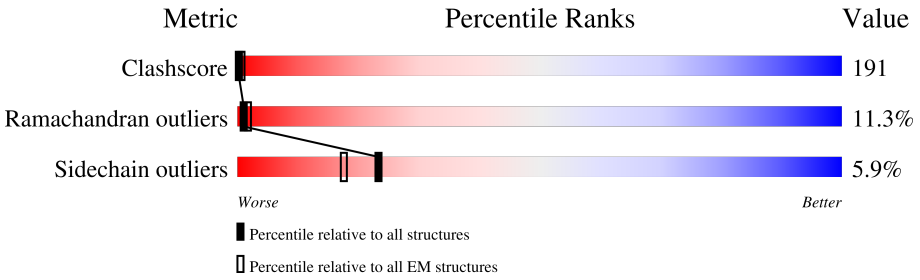
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	451	7% 51% 26% 14% .
2	B	445	5% 47% 28% 16% .
3	K	394	64% 16% . 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	A	500	-	-	X	-
5	GDP	B	501	-	-	X	-
6	TXL	B	502	-	-	X	-

2 Entry composition (i)

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

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TUBULIN ALPHA CHAIN.

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

- Molecule 2 is a protein called TUBULIN BETA CHAIN.

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

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

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

There are 42 discrepancies between the modelled and reference sequences:

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

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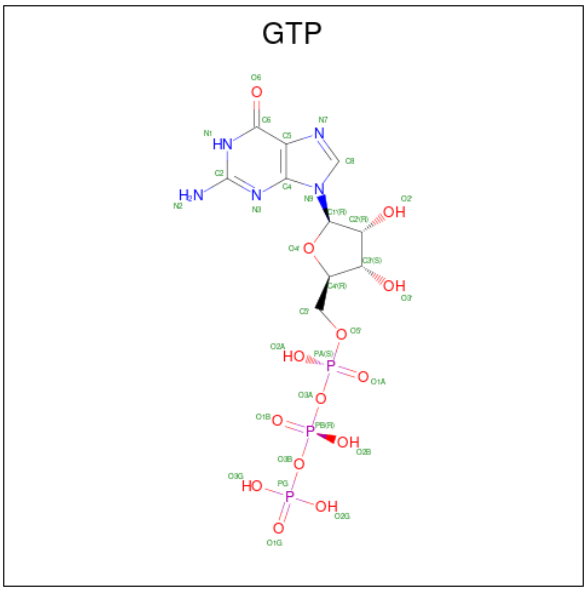
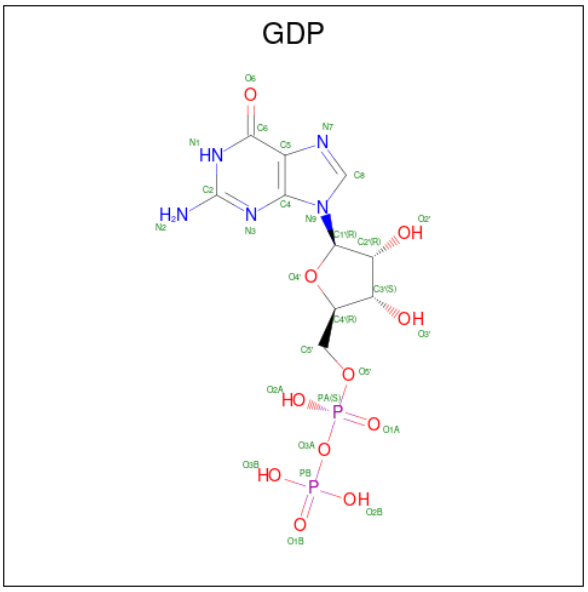
Chain	Residue	Modelled	Actual	Comment	Reference
K	0	ASN	-	see remark 999	UNP P33173
K	1	MET	-	see remark 999	UNP P33173
K	2	PRO	-	see remark 999	UNP P33173
K	202	ALA	PRO	engineered mutation	UNP P33173
K	356	ASN	-	SEE REMARK 999	UNP P33173
K	357	THR	-	SEE REMARK 999	UNP P33173
K	358	VAL	-	SEE REMARK 999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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



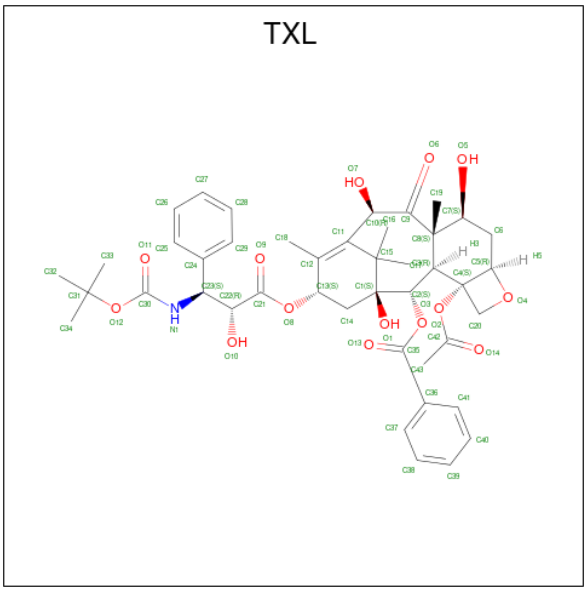
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 6 is TAXOTERE (three-letter code: TXL) (formula: $C_{43}H_{53}NO_{14}$).

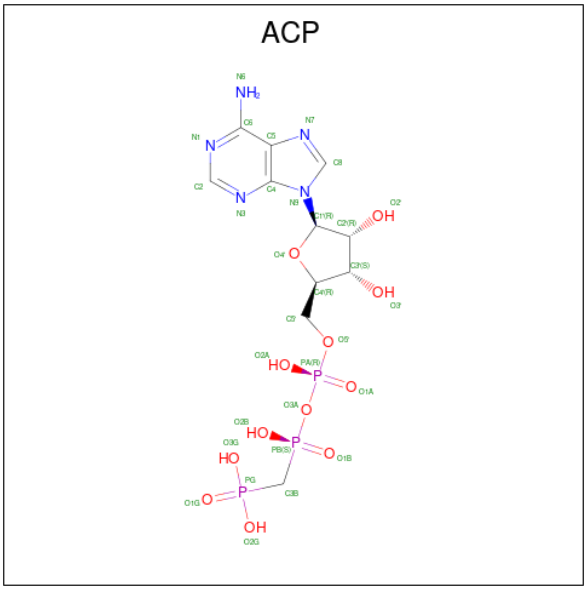


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			58	43	1	14	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



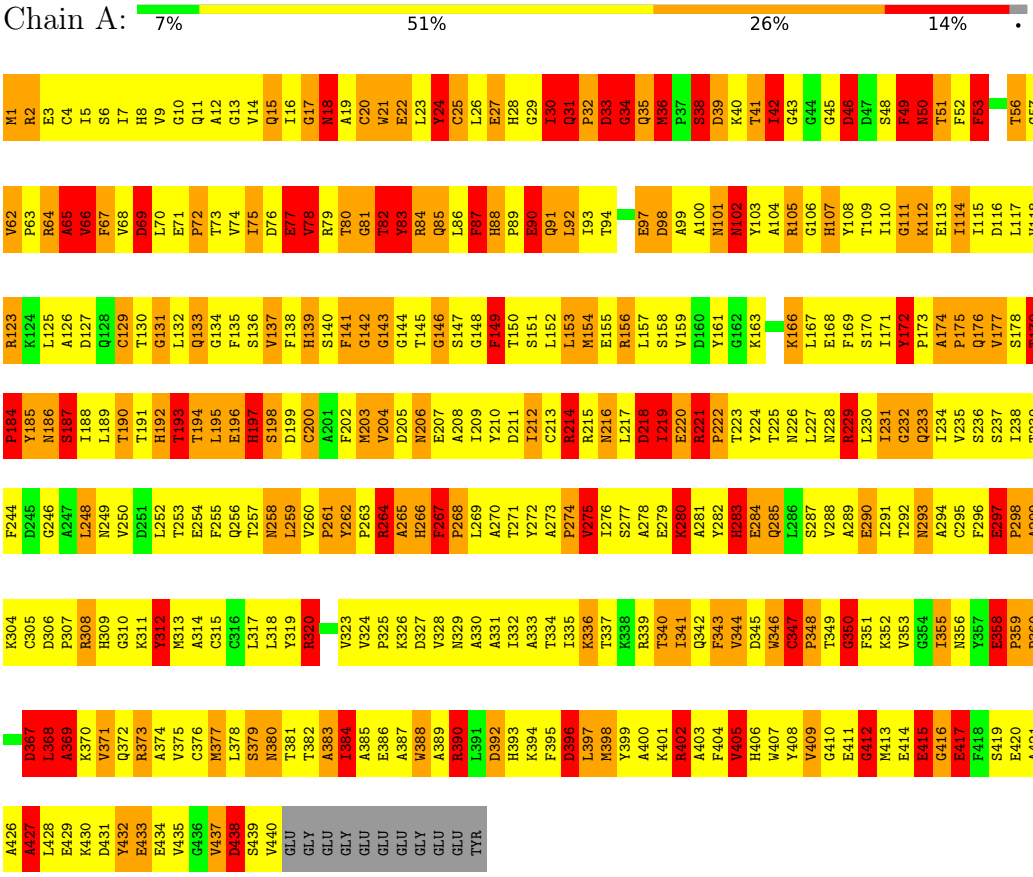
Mol	Chain	Residues	Atoms					AltConf
8	K	1	Total	C	N	O	P	0
			31	11	5	12	3	

3 Residue-property plots (i)

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

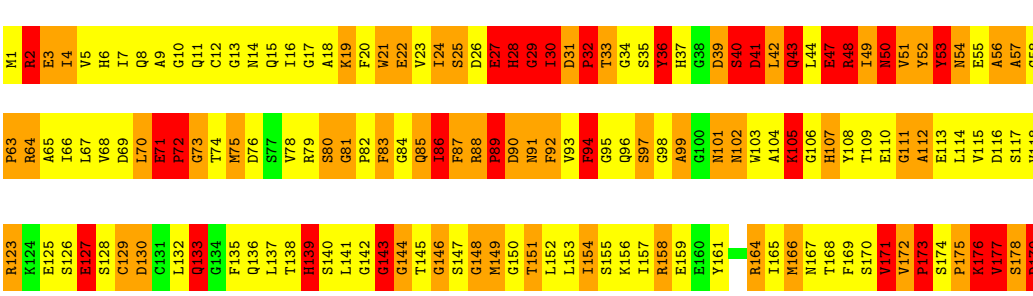
• Molecule 1: TUBULIN ALPHA CHAIN

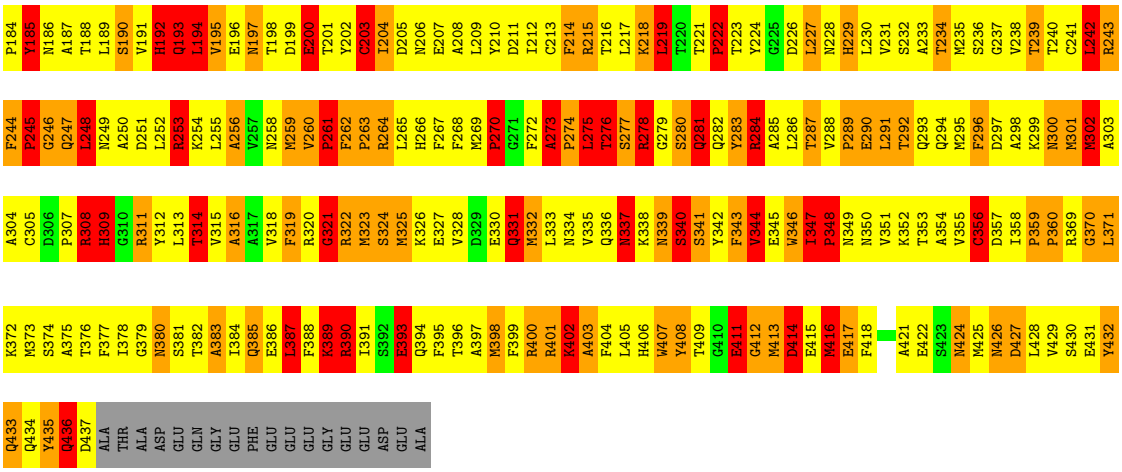
Chain A:



• Molecule 2: TUBULIN BETA CHAIN

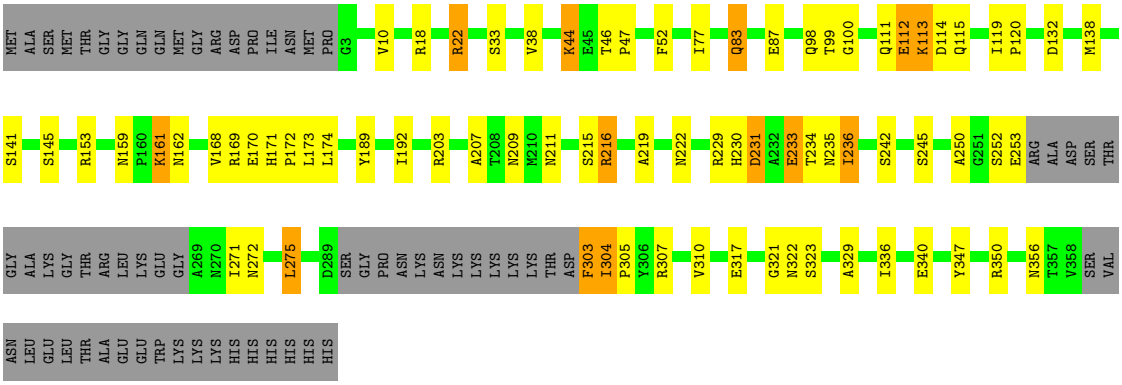
Chain B:





• Molecule 3: KINESIN-LIKE PROTEIN KIF1A

Chain K:



4 Data and refinement statistics (i)

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

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	2.34	109/3508 (3.1%)	2.76	211/4762 (4.4%)
2	B	2.47	110/3434 (3.2%)	3.07	266/4652 (5.7%)
3	K	0.47	0/2708	0.73	2/3655 (0.1%)
All	All	2.05	219/9650 (2.3%)	2.51	479/13069 (3.7%)

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

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

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	278	ARG	CA-CB	34.91	2.30	1.53
2	B	105	LYS	C-N	-29.41	0.80	1.33
2	B	73	GLY	C-N	-28.02	0.69	1.34
1	A	38	SER	C-N	-27.48	0.70	1.34
1	A	347	CYS	C-N	-23.39	0.89	1.34
1	A	218	ASP	C-N	-21.39	0.84	1.34
2	B	321	GLY	C-N	-19.80	0.88	1.34
1	A	219	ILE	CB-CG2	19.43	2.13	1.52
1	A	358	GLU	C-N	-19.17	0.97	1.34
2	B	200	GLU	C-N	-19.09	0.90	1.34
2	B	182	VAL	C-N	-19.09	0.90	1.34
1	A	53	PHE	C-N	-18.99	0.90	1.34
2	B	197	ASN	C-N	-18.84	0.90	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	340	SER	C-N	-18.04	0.92	1.34
2	B	309	HIS	C-N	-17.96	1.00	1.33
1	A	219	ILE	CB-CG1	-17.60	1.04	1.54
1	A	416	GLY	C-N	-16.99	0.94	1.34
1	A	193	THR	C-N	-16.81	0.95	1.34
1	A	350	GLY	C-N	-16.78	0.95	1.34
1	A	415	GLU	C-N	-16.60	1.03	1.33
2	B	247	GLN	C-N	-16.25	0.96	1.34
2	B	417	GLU	C-N	-15.51	0.98	1.34
2	B	346	TRP	C-N	-15.06	0.99	1.34
2	B	71	GLU	C-N	-14.75	1.06	1.34
1	A	31	GLN	C-N	-14.63	1.06	1.34
1	A	409	VAL	C-N	14.56	1.59	1.33
1	A	34	GLY	N-CA	-14.48	1.24	1.46
2	B	270	PRO	C-N	13.99	1.58	1.33
2	B	203	CYS	C-N	-13.92	1.02	1.34
1	A	220	GLU	CB-CG	13.85	1.78	1.52
2	B	275	LEU	C-N	-13.74	1.02	1.34
1	A	221	ARG	C-N	-13.61	1.08	1.34
1	A	371	VAL	C-N	-13.57	1.02	1.34
1	A	69	ASP	C-N	-13.44	1.03	1.34
1	A	405	VAL	C-N	-13.43	1.03	1.34
2	B	387	LEU	C-N	12.85	1.63	1.34
2	B	380	ASN	C-N	-12.72	1.04	1.34
2	B	400	ARG	C-N	-12.39	1.05	1.34
2	B	127	GLU	C-N	-12.23	1.05	1.34
1	A	33	ASP	C-N	-11.71	1.11	1.33
2	B	331	GLN	C-N	-11.60	1.07	1.34
2	B	22	GLU	C-N	-11.53	1.07	1.34
1	A	32	PRO	N-CD	-11.51	1.31	1.47
1	A	190	THR	C-N	-11.41	1.07	1.34
2	B	273	ALA	C-N	-11.35	1.12	1.34
1	A	405	VAL	CB-CG2	11.12	1.76	1.52
1	A	221	ARG	CB-CG	-11.12	1.22	1.52
1	A	216	ASN	C-N	-10.85	1.09	1.34
1	A	402	ARG	C-N	-10.84	1.09	1.34
2	B	344	VAL	C-N	-10.54	1.09	1.34
1	A	21	TRP	C-O	10.22	1.42	1.23
2	B	60	LYS	C-N	-10.19	1.10	1.34
2	B	179	ASP	C-N	-10.16	1.10	1.34
2	B	371	LEU	C-N	-10.11	1.10	1.34
2	B	334	ASN	C-N	-9.97	1.11	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	287	THR	C-N	9.95	1.56	1.34
1	A	87	PHE	C-N	-9.89	1.11	1.34
1	A	43	GLY	C-N	9.82	1.50	1.33
2	B	414	ASP	C-N	-9.79	1.11	1.34
2	B	64	ARG	C-N	-9.74	1.11	1.34
1	A	280	LYS	C-N	-9.40	1.12	1.34
1	A	405	VAL	CB-CG1	-9.24	1.33	1.52
2	B	292	THR	C-N	-9.08	1.13	1.34
2	B	193	GLN	C-O	9.03	1.40	1.23
2	B	71	GLU	C-O	-8.98	1.06	1.23
2	B	54	ASN	N-CA	-8.98	1.28	1.46
1	A	187	SER	C-N	8.97	1.54	1.34
1	A	90	GLU	C-N	-8.92	1.13	1.34
2	B	143	GLY	CA-C	-8.82	1.37	1.51
1	A	222	PRO	N-CD	8.60	1.59	1.47
2	B	146	GLY	C-N	8.49	1.53	1.34
2	B	436	GLN	C-N	-8.46	1.14	1.34
2	B	151	THR	C-N	-8.43	1.14	1.34
1	A	231	ILE	C-O	8.38	1.39	1.23
1	A	379	SER	C-N	-8.20	1.15	1.34
1	A	438	ASP	C-O	8.16	1.38	1.23
2	B	173	PRO	C-N	-8.07	1.15	1.34
1	A	229	ARG	NE-CZ	-8.05	1.22	1.33
2	B	244	PHE	C-N	-8.04	1.19	1.34
2	B	154	ILE	C-N	-8.04	1.15	1.34
1	A	24	TYR	C-N	-8.02	1.15	1.34
2	B	337	ASN	C-N	-7.97	1.15	1.34
2	B	347	ILE	C-N	-7.82	1.19	1.34
1	A	233	GLN	C-N	-7.79	1.16	1.34
2	B	89	PRO	C-N	-7.71	1.16	1.34
2	B	70	LEU	C-N	-7.69	1.16	1.34
1	A	43	GLY	C-O	-7.68	1.11	1.23
2	B	291	LEU	N-CA	-7.62	1.31	1.46
1	A	229	ARG	CA-CB	-7.57	1.37	1.53
2	B	171	VAL	C-N	-7.56	1.16	1.34
1	A	204	VAL	C-N	-7.55	1.16	1.34
2	B	72	PRO	C-N	-7.55	1.19	1.33
2	B	243	ARG	C-N	-7.53	1.16	1.34
2	B	278	ARG	CD-NE	-7.52	1.33	1.46
1	A	274	PRO	C-N	-7.49	1.16	1.34
1	A	367	ASP	C-N	-7.41	1.17	1.34
1	A	346	TRP	C-N	-7.37	1.17	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	218	LYS	C-N	7.35	1.50	1.34
2	B	299	LYS	C-N	-7.29	1.17	1.34
2	B	245	PRO	N-CD	-7.23	1.37	1.47
1	A	222	PRO	CB-CG	7.23	1.86	1.50
2	B	53	TYR	C-N	-7.22	1.17	1.34
1	A	259	LEU	C-N	-7.15	1.17	1.34
2	B	192	HIS	C-O	7.01	1.36	1.23
1	A	2	ARG	N-CA	6.97	1.60	1.46
1	A	184	PRO	CA-CB	-6.96	1.39	1.53
1	A	433	GLU	C-N	-6.75	1.18	1.34
2	B	130	ASP	C-N	-6.74	1.18	1.34
2	B	190	SER	C-N	6.72	1.49	1.34
1	A	34	GLY	C-N	-6.69	1.18	1.34
1	A	80	THR	C-N	-6.65	1.21	1.33
2	B	143	GLY	C-N	-6.64	1.21	1.33
1	A	176	GLN	C-N	6.55	1.49	1.34
1	A	140	SER	C-N	-6.51	1.19	1.34
1	A	172	TYR	CB-CG	6.50	1.61	1.51
1	A	137	VAL	C-N	-6.49	1.19	1.34
2	B	193	GLN	C-N	-6.47	1.19	1.34
1	A	183	GLU	C-N	-6.45	1.22	1.34
1	A	36	MET	C-N	-6.42	1.22	1.34
1	A	146	GLY	C-N	-6.39	1.19	1.34
2	B	348	PRO	C-N	-6.38	1.19	1.34
2	B	244	PHE	N-CA	-6.34	1.33	1.46
1	A	43	GLY	CA-C	6.31	1.61	1.51
2	B	111	GLY	C-N	-6.29	1.19	1.34
2	B	234	THR	C-N	-6.29	1.19	1.34
1	A	22	GLU	C-O	6.28	1.35	1.23
2	B	194	LEU	C-N	-6.26	1.19	1.34
1	A	111	GLY	C-N	-6.26	1.19	1.34
1	A	149	PHE	C-N	-6.25	1.19	1.34
1	A	383	ALA	C-N	-6.24	1.19	1.34
2	B	259	MET	C-N	-6.24	1.19	1.34
2	B	178	SER	C-N	-6.20	1.19	1.34
2	B	1	MET	CA-C	-6.17	1.36	1.52
2	B	412	GLY	C-N	6.15	1.48	1.34
1	A	384	ILE	C-O	-6.15	1.11	1.23
1	A	377	MET	C-N	-6.14	1.20	1.34
2	B	149	MET	C-N	-6.14	1.22	1.33
1	A	1	MET	CA-C	-6.14	1.36	1.52
2	B	393	GLU	C-O	-6.11	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	349	ASN	N-CA	-6.09	1.34	1.46
1	A	27	GLU	C-N	6.08	1.48	1.34
1	A	91	GLN	C-N	6.08	1.48	1.34
1	A	437	VAL	C-N	-6.06	1.20	1.34
1	A	363	VAL	C-N	6.05	1.45	1.34
1	A	283	HIS	C-N	-6.03	1.20	1.34
2	B	407	TRP	CA-CB	-6.00	1.40	1.53
2	B	52	TYR	C-N	-6.00	1.20	1.34
1	A	380	ASN	C-N	-5.97	1.20	1.34
1	A	181	VAL	C-N	5.97	1.47	1.34
2	B	40	SER	N-CA	-5.93	1.34	1.46
1	A	388	TRP	NE1-CE2	-5.92	1.29	1.37
1	A	17	GLY	C-N	5.90	1.47	1.34
2	B	167	ASN	C-N	5.89	1.47	1.34
2	B	107	HIS	C-O	5.83	1.34	1.23
2	B	139	HIS	C-N	5.82	1.47	1.34
2	B	346	TRP	N-CA	-5.82	1.34	1.46
1	A	183	GLU	C-O	-5.78	1.12	1.23
1	A	78	VAL	C-N	-5.77	1.20	1.34
2	B	133	GLN	C-N	-5.76	1.22	1.33
1	A	107	HIS	C-O	5.75	1.34	1.23
2	B	76	ASP	C-O	5.74	1.34	1.23
2	B	168	THR	C-N	5.71	1.47	1.34
1	A	141	PHE	N-CA	-5.71	1.34	1.46
1	A	46	ASP	C-N	5.70	1.47	1.34
1	A	232	GLY	CA-C	-5.70	1.42	1.51
1	A	196	GLU	C-N	-5.68	1.21	1.34
1	A	285	GLN	C-N	-5.68	1.21	1.34
2	B	86	ILE	C-N	5.67	1.47	1.34
1	A	1	MET	C-N	5.65	1.47	1.34
1	A	166	LYS	C-N	-5.62	1.21	1.34
1	A	258	ASN	C-N	-5.61	1.21	1.34
1	A	72	PRO	N-CD	-5.60	1.40	1.47
2	B	51	VAL	C-N	-5.59	1.21	1.34
2	B	92	PHE	C-N	-5.58	1.21	1.34
2	B	356	CYS	C-N	-5.57	1.21	1.34
2	B	52	TYR	N-CA	-5.57	1.35	1.46
2	B	222	PRO	CA-C	-5.54	1.41	1.52
1	A	200	CYS	C-N	-5.52	1.21	1.34
2	B	242	LEU	C-N	-5.51	1.21	1.34
1	A	163	LYS	C-N	-5.51	1.21	1.34
2	B	298	ALA	C-N	5.49	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	ARG	CA-C	-5.48	1.38	1.52
1	A	77	GLU	C-N	5.46	1.46	1.34
2	B	21	TRP	NE1-CE2	-5.45	1.30	1.37
1	A	360	PRO	N-CD	-5.45	1.40	1.47
2	B	383	ALA	C-N	-5.43	1.21	1.34
2	B	2	ARG	C-N	-5.43	1.21	1.34
2	B	53	TYR	CG-CD2	-5.43	1.32	1.39
2	B	296	PHE	C-N	-5.41	1.21	1.34
1	A	20	CYS	C-N	5.41	1.46	1.34
1	A	114	ILE	C-N	-5.38	1.21	1.34
2	B	221	THR	N-CA	5.38	1.57	1.46
2	B	248	LEU	C-N	-5.37	1.21	1.34
2	B	27	GLU	C-N	-5.37	1.21	1.34
1	A	184	PRO	CA-C	-5.35	1.42	1.52
2	B	28	HIS	C-O	-5.34	1.13	1.23
1	A	355	ILE	C-N	-5.34	1.21	1.34
1	A	266	HIS	N-CA	-5.29	1.35	1.46
1	A	229	ARG	CD-NE	-5.28	1.37	1.46
2	B	278	ARG	NE-CZ	-5.27	1.26	1.33
1	A	21	TRP	NE1-CE2	-5.27	1.30	1.37
1	A	339	ARG	CA-C	-5.22	1.39	1.52
1	A	407	TRP	CA-CB	-5.21	1.42	1.53
2	B	261	PRO	CA-C	-5.20	1.42	1.52
2	B	3	GLU	N-CA	-5.19	1.35	1.46
1	A	33	ASP	CA-C	-5.18	1.39	1.52
2	B	435	TYR	CB-CG	-5.17	1.44	1.51
2	B	164	ARG	C-N	5.15	1.45	1.34
2	B	276	THR	C-O	5.13	1.33	1.23
1	A	406	HIS	C-N	-5.13	1.22	1.34
1	A	102	ASN	C-N	-5.13	1.22	1.34
1	A	66	VAL	N-CA	5.10	1.56	1.46
1	A	88	HIS	C-N	-5.09	1.24	1.34
1	A	41	THR	C-N	-5.08	1.22	1.34
2	B	290	GLU	C-O	-5.08	1.13	1.23
2	B	53	TYR	N-CA	-5.06	1.36	1.46
2	B	261	PRO	N-CD	-5.03	1.40	1.47
1	A	24	TYR	C-O	5.01	1.32	1.23
2	B	222	PRO	C-N	-5.01	1.22	1.34

All (479) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	368	LEU	O-C-N	-54.19	35.99	122.70
1	A	363	VAL	C-N-CD	-48.68	13.50	120.60
2	B	273	ALA	C-N-CD	-46.49	18.32	120.60
2	B	105	LYS	O-C-N	-44.51	47.53	123.20
2	B	88	ARG	C-N-CD	-44.07	23.64	120.60
1	A	283	HIS	O-C-N	-34.62	67.31	122.70
1	A	369	ALA	O-C-N	-32.93	70.02	122.70
2	B	73	GLY	O-C-N	-28.93	76.42	122.70
1	A	402	ARG	O-C-N	-27.80	78.22	122.70
2	B	275	LEU	O-C-N	-27.11	79.33	122.70
1	A	1	MET	O-C-N	26.19	164.61	122.70
1	A	358	GLU	C-N-CD	-26.03	63.33	120.60
2	B	143	GLY	O-C-N	-25.65	79.60	123.20
2	B	105	LYS	CA-C-N	25.11	166.41	116.20
2	B	321	GLY	O-C-N	-24.37	83.71	122.70
2	B	179	ASP	O-C-N	-22.45	86.78	122.70
2	B	194	LEU	O-C-N	-21.89	87.67	122.70
1	A	53	PHE	O-C-N	-21.58	88.17	122.70
2	B	85	GLN	O-C-N	21.53	157.15	122.70
2	B	278	ARG	N-CA-CB	21.31	148.96	110.60
2	B	344	VAL	O-C-N	-21.13	88.90	122.70
2	B	73	GLY	CA-C-N	21.08	163.57	117.20
2	B	1	MET	O-C-N	21.00	156.29	122.70
1	A	24	TYR	O-C-N	-20.69	89.59	122.70
2	B	86	ILE	O-C-N	19.94	154.60	122.70
2	B	321	GLY	C-N-CA	19.68	170.90	121.70
2	B	348	PRO	O-C-N	19.56	154.00	122.70
2	B	60	LYS	C-N-CA	18.97	169.13	121.70
2	B	52	TYR	O-C-N	18.60	152.46	122.70
1	A	367	ASP	O-C-N	-18.36	93.33	122.70
1	A	218	ASP	O-C-N	-18.25	93.49	122.70
2	B	402	LYS	C-N-CA	18.24	167.29	121.70
1	A	405	VAL	CA-CB-CG1	18.20	138.20	110.90
2	B	275	LEU	CA-C-N	18.06	156.94	117.20
2	B	411	GLU	C-N-CA	17.57	159.19	122.30
1	A	267	PHE	C-N-CD	-17.45	82.22	120.60
2	B	247	GLN	O-C-N	-17.26	95.09	122.70
2	B	203	CYS	C-N-CA	17.09	164.42	121.70
2	B	194	LEU	C-N-CA	16.91	163.97	121.70
1	A	34	GLY	O-C-N	-16.90	95.66	122.70
2	B	60	LYS	O-C-N	-16.80	95.81	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	127	GLU	O-C-N	-16.75	95.91	122.70
2	B	21	TRP	O-C-N	-16.69	96.00	122.70
1	A	1	MET	CB-CA-C	16.63	143.66	110.40
1	A	1	MET	CA-C-N	-16.28	81.38	117.20
1	A	402	ARG	CA-C-N	16.17	152.77	117.20
1	A	172	TYR	CB-CG-CD1	15.94	130.56	121.00
2	B	179	ASP	C-N-CA	15.80	161.19	121.70
1	A	87	PHE	O-C-N	-15.72	97.55	122.70
2	B	53	TYR	O-C-N	15.72	147.85	122.70
2	B	321	GLY	CA-C-N	15.32	150.90	117.20
2	B	1	MET	CB-CA-C	15.11	140.62	110.40
2	B	194	LEU	CA-C-N	14.98	150.16	117.20
2	B	30	ILE	CB-CA-C	14.96	141.52	111.60
2	B	1	MET	N-CA-C	-14.80	71.05	111.00
2	B	1	MET	CA-C-N	-14.77	84.71	117.20
2	B	343	PHE	O-C-N	14.75	146.30	122.70
2	B	331	GLN	O-C-N	-14.71	99.16	122.70
2	B	86	ILE	CA-C-N	-14.50	85.30	117.20
2	B	247	GLN	CA-C-N	14.42	148.92	117.20
2	B	253	ARG	CD-NE-CZ	14.37	143.72	123.60
1	A	405	VAL	C-N-CA	14.36	157.61	121.70
2	B	344	VAL	C-N-CA	14.10	156.94	121.70
1	A	50	ASN	O-C-N	-14.08	100.17	122.70
1	A	218	ASP	CA-C-N	13.53	146.96	117.20
2	B	85	GLN	CA-C-N	-13.49	87.53	117.20
1	A	283	HIS	C-N-CA	13.46	155.34	121.70
1	A	347	CYS	C-N-CD	-13.35	91.23	120.60
2	B	400	ARG	O-C-N	-13.29	101.44	122.70
2	B	402	LYS	O-C-N	-13.25	101.49	122.70
1	A	38	SER	C-N-CA	13.23	154.78	121.70
1	A	266	HIS	O-C-N	13.16	143.75	122.70
2	B	370	GLY	O-C-N	-13.12	101.71	122.70
1	A	367	ASP	CA-C-N	13.10	146.02	117.20
1	A	1	MET	N-CA-C	-12.99	75.91	111.00
1	A	21	TRP	CA-CB-CG	-12.95	89.09	113.70
2	B	73	GLY	C-N-CA	12.88	153.91	121.70
2	B	411	GLU	O-C-N	-12.88	101.31	123.20
1	A	38	SER	O-C-N	-12.84	102.16	122.70
2	B	182	VAL	C-N-CA	12.69	153.42	121.70
2	B	247	GLN	C-N-CA	12.55	153.08	121.70
2	B	359	PRO	O-C-N	12.55	144.94	121.10
1	A	347	CYS	O-C-N	-12.44	97.47	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	344	VAL	CA-C-N	12.36	144.38	117.20
2	B	348	PRO	CA-C-N	-12.34	90.06	117.20
1	A	183	GLU	O-C-N	-12.29	97.75	121.10
1	A	38	SER	CA-C-N	12.12	143.87	117.20
2	B	89	PRO	O-C-N	-12.04	103.44	122.70
1	A	184	PRO	O-C-N	12.01	141.92	122.70
2	B	203	CYS	O-C-N	-11.99	103.51	122.70
1	A	32	PRO	CA-N-CD	11.98	128.47	111.70
1	A	219	ILE	CA-CB-CG2	-11.97	86.97	110.90
1	A	30	ILE	C-N-CA	11.91	151.46	121.70
1	A	41	THR	O-C-N	11.84	141.65	122.70
2	B	105	LYS	C-N-CA	11.83	147.13	122.30
2	B	52	TYR	CA-C-N	-11.79	91.27	117.20
2	B	179	ASP	CA-C-N	11.76	143.07	117.20
1	A	24	TYR	CA-C-N	11.74	143.04	117.20
2	B	53	TYR	CB-CG-CD2	-11.69	113.99	121.00
1	A	218	ASP	C-N-CA	11.60	150.69	121.70
1	A	280	LYS	O-C-N	-11.56	104.20	122.70
2	B	143	GLY	CA-C-N	11.51	139.23	116.20
1	A	87	PHE	C-N-CA	11.47	150.38	121.70
2	B	53	TYR	CA-C-N	-11.41	92.09	117.20
2	B	30	ILE	O-C-N	-11.37	104.51	122.70
1	A	415	GLU	O-C-N	-11.34	103.93	123.20
1	A	53	PHE	CA-C-N	11.27	142.00	117.20
1	A	179	THR	O-C-N	-11.23	104.73	122.70
2	B	53	TYR	CB-CG-CD1	11.19	127.71	121.00
1	A	1	MET	C-N-CA	11.13	149.53	121.70
2	B	224	TYR	O-C-N	-11.11	104.32	123.20
2	B	400	ARG	C-N-CA	11.10	149.45	121.70
1	A	415	GLU	C-N-CA	11.03	145.47	122.30
1	A	396	ASP	O-C-N	-11.03	105.06	122.70
2	B	347	ILE	C-N-CD	-10.96	96.49	120.60
2	B	47	GLU	C-N-CA	10.96	149.09	121.70
2	B	284	ARG	NE-CZ-NH2	10.82	125.71	120.30
2	B	269	MET	C-N-CD	-10.81	96.81	120.60
2	B	203	CYS	CA-C-N	10.74	140.83	117.20
2	B	192	HIS	O-C-N	-10.65	105.66	122.70
1	A	69	ASP	O-C-N	-10.62	105.71	122.70
1	A	34	GLY	CA-C-N	10.60	140.51	117.20
1	A	415	GLU	CA-C-N	10.53	137.26	116.20
2	B	171	VAL	O-C-N	-10.41	106.05	122.70
2	B	343	PHE	CA-C-N	-10.35	94.44	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	ARG	O-C-N	-10.24	101.64	121.10
1	A	280	LYS	C-N-CA	10.22	147.26	121.70
2	B	264	ARG	NE-CZ-NH2	10.22	125.41	120.30
2	B	127	GLU	CA-C-N	10.20	139.64	117.20
1	A	87	PHE	CA-C-N	10.15	139.54	117.20
2	B	107	HIS	O-C-N	-10.14	106.47	122.70
1	A	107	HIS	O-C-N	-10.12	106.50	122.70
1	A	49	PHE	C-N-CA	10.01	146.72	121.70
1	A	405	VAL	O-C-N	-10.00	106.70	122.70
2	B	289	PRO	O-C-N	10.00	138.69	122.70
1	A	172	TYR	CA-CB-CG	9.96	132.32	113.40
1	A	266	HIS	CA-C-N	-9.95	95.32	117.20
2	B	21	TRP	CA-C-N	9.92	139.01	117.20
1	A	229	ARG	NE-CZ-NH2	9.89	125.25	120.30
2	B	182	VAL	O-C-N	-9.88	106.89	122.70
2	B	311	ARG	NE-CZ-NH2	9.84	125.22	120.30
2	B	29	GLY	O-C-N	9.70	138.23	122.70
2	B	158	ARG	NE-CZ-NH2	9.67	125.13	120.30
2	B	219	LEU	O-C-N	-9.65	107.26	122.70
1	A	121	ARG	NE-CZ-NH2	9.61	125.10	120.30
2	B	435	TYR	CB-CG-CD1	-9.60	115.24	121.00
1	A	90	GLU	O-C-N	-9.60	107.35	122.70
1	A	193	THR	O-C-N	-9.60	107.35	122.70
1	A	61	HIS	CB-CA-C	9.58	129.56	110.40
2	B	49	ILE	O-C-N	-9.54	107.43	122.70
2	B	356	CYS	O-C-N	-9.52	107.47	122.70
2	B	85	GLN	C-N-CA	9.52	145.49	121.70
2	B	52	TYR	C-N-CA	9.49	145.43	121.70
1	A	2	ARG	NE-CZ-NH2	9.48	125.04	120.30
2	B	127	GLU	C-N-CA	9.38	145.16	121.70
2	B	275	LEU	C-N-CA	9.36	145.11	121.70
1	A	416	GLY	C-N-CA	9.34	145.06	121.70
2	B	193	GLN	O-C-N	-9.34	107.75	122.70
2	B	414	ASP	C-N-CA	9.34	145.05	121.70
1	A	229	ARG	NE-CZ-NH1	-9.32	115.64	120.30
2	B	322	ARG	NE-CZ-NH2	9.32	124.96	120.30
2	B	370	GLY	CA-C-N	9.27	137.60	117.20
1	A	320	ARG	NE-CZ-NH2	9.23	124.92	120.30
2	B	185	TYR	CA-CB-CG	9.18	130.84	113.40
1	A	65	ALA	CB-CA-C	-9.17	96.35	110.10
2	B	48	ARG	NE-CZ-NH2	9.12	124.86	120.30
1	A	409	VAL	O-C-N	9.08	138.64	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	TYR	CB-CG-CD2	-9.06	115.57	121.00
1	A	367	ASP	C-N-CA	8.98	144.15	121.70
2	B	49	ILE	C-N-CA	8.96	144.11	121.70
2	B	200	GLU	O-C-N	-8.95	108.38	122.70
1	A	21	TRP	O-C-N	-8.94	108.39	122.70
1	A	347	CYS	CA-C-N	8.86	141.92	117.10
2	B	278	ARG	CB-CA-C	-8.84	92.73	110.40
1	A	219	ILE	CG1-CB-CG2	-8.76	92.12	111.40
2	B	94	PHE	CB-CG-CD1	-8.72	114.69	120.80
1	A	139	HIS	CA-CB-CG	8.69	128.37	113.60
1	A	32	PRO	N-CA-CB	-8.66	92.91	103.30
1	A	183	GLU	CA-C-N	8.65	141.31	117.10
1	A	31	GLN	C-N-CD	-8.63	101.62	120.60
1	A	222	PRO	N-CA-CB	8.61	113.63	103.30
1	A	42	ILE	CA-C-N	8.60	133.40	116.20
1	A	56	THR	C-N-CA	-8.58	104.27	122.30
2	B	414	ASP	O-C-N	-8.58	108.97	122.70
2	B	29	GLY	C-N-CA	8.50	142.96	121.70
1	A	412	GLY	O-C-N	-8.49	109.11	122.70
1	A	24	TYR	C-N-CA	8.48	142.89	121.70
2	B	400	ARG	CA-C-N	8.46	135.81	117.20
2	B	436	GLN	C-N-CA	8.45	142.82	121.70
2	B	47	GLU	O-C-N	-8.41	109.24	122.70
2	B	24	ILE	O-C-N	-8.41	109.25	122.70
2	B	229	HIS	O-C-N	-8.39	109.27	122.70
1	A	190	THR	O-C-N	-8.34	109.35	122.70
1	A	297	GLU	O-C-N	8.30	136.88	121.10
2	B	92	PHE	CA-CB-CG	-8.29	94.01	113.90
2	B	200	GLU	C-N-CA	8.27	142.38	121.70
2	B	177	VAL	CA-C-O	8.27	137.47	120.10
2	B	53	TYR	N-CA-CB	8.25	125.45	110.60
2	B	400	ARG	NE-CZ-NH2	8.25	124.42	120.30
2	B	309	HIS	O-C-N	-8.18	109.30	123.20
2	B	411	GLU	CA-C-N	8.13	132.46	116.20
1	A	369	ALA	C-N-CA	8.10	141.95	121.70
2	B	406	HIS	CA-CB-CG	-8.10	99.84	113.60
1	A	184	PRO	CA-C-N	-8.08	99.42	117.20
2	B	402	LYS	CA-C-N	8.08	134.97	117.20
1	A	422	ARG	NE-CZ-NH2	8.07	124.34	120.30
2	B	215	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	A	221	ARG	CA-C-N	8.05	139.63	117.10
1	A	43	GLY	CA-C-N	-7.96	100.27	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	89	PRO	C-N-CA	7.96	141.59	121.70
1	A	65	ALA	N-CA-C	7.95	132.46	111.00
1	A	113	GLU	O-C-N	-7.93	110.00	122.70
2	B	370	GLY	C-N-CA	7.92	141.51	121.70
1	A	190	THR	CA-C-N	7.91	134.60	117.20
1	A	215	ARG	NE-CZ-NH2	7.91	124.25	120.30
2	B	245	PRO	CA-N-CD	7.91	122.77	111.70
2	B	164	ARG	NE-CZ-NH2	7.90	124.25	120.30
2	B	289	PRO	CA-C-N	-7.88	99.86	117.20
2	B	59	ASN	C-N-CA	7.87	141.38	121.70
2	B	299	LYS	O-C-N	7.87	135.29	122.70
2	B	302	MET	CG-SD-CE	7.84	112.74	100.20
2	B	171	VAL	CA-C-N	7.76	134.28	117.20
1	A	221	ARG	C-N-CD	-7.73	103.59	120.60
2	B	21	TRP	C-N-CA	-7.71	102.42	121.70
2	B	359	PRO	CA-C-N	-7.71	95.52	117.10
1	A	33	ASP	C-N-CA	-7.71	106.12	122.30
2	B	182	VAL	CA-C-N	7.68	134.10	117.20
1	A	298	PRO	O-C-N	-7.66	110.45	122.70
2	B	412	GLY	O-C-N	-7.66	110.45	122.70
1	A	340	THR	O-C-N	7.64	134.93	122.70
2	B	356	CYS	CA-C-N	7.64	134.02	117.20
1	A	67	PHE	CA-CB-CG	-7.64	95.57	113.90
2	B	50	ASN	CA-C-N	-7.62	100.43	117.20
1	A	15	GLN	O-C-N	7.59	134.85	122.70
1	A	405	VAL	CA-C-N	7.59	133.90	117.20
2	B	407	TRP	CA-CB-CG	-7.55	99.35	113.70
1	A	31	GLN	N-CA-C	7.52	131.30	111.00
2	B	185	TYR	CB-CG-CD1	7.51	125.51	121.00
2	B	64	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	373	ARG	CD-NE-CZ	7.49	134.08	123.60
1	A	392	ASP	CA-C-O	-7.48	104.39	120.10
1	A	18	ASN	O-C-N	7.48	134.66	122.70
2	B	151	THR	O-C-N	-7.45	110.79	122.70
2	B	253	ARG	NE-CZ-NH2	7.43	124.02	120.30
2	B	346	TRP	CA-C-N	-7.42	100.87	117.20
1	A	417	GLU	O-C-N	7.40	134.55	122.70
1	A	339	ARG	O-C-N	7.39	134.52	122.70
2	B	2	ARG	O-C-N	7.35	134.46	122.70
2	B	308	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	A	34	GLY	C-N-CA	7.30	139.96	121.70
1	A	377	MET	CG-SD-CE	7.30	111.89	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	29	GLY	CA-C-N	-7.30	101.14	117.20
1	A	264	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	B	143	GLY	C-N-CA	7.26	137.55	122.30
1	A	416	GLY	O-C-N	-7.22	111.14	122.70
2	B	19	LYS	CD-CE-NZ	7.20	128.26	111.70
2	B	200	GLU	CA-C-N	7.20	133.03	117.20
1	A	50	ASN	CA-C-N	7.19	133.01	117.20
1	A	32	PRO	N-CD-CG	-7.15	92.47	103.20
2	B	290	GLU	O-C-N	7.15	134.14	122.70
2	B	264	ARG	NH1-CZ-NH2	-7.15	111.53	119.40
1	A	302	MET	CG-SD-CE	7.14	111.62	100.20
2	B	387	LEU	C-N-CA	-7.08	104.00	121.70
2	B	24	ILE	C-N-CA	-7.05	104.06	121.70
1	A	340	THR	CA-C-N	-7.01	101.78	117.20
2	B	331	GLN	CA-C-N	6.99	132.59	117.20
1	A	197	HIS	CA-C-N	-6.92	101.97	117.20
1	A	2	ARG	CB-CA-C	-6.92	96.56	110.40
2	B	89	PRO	CA-C-N	6.91	132.40	117.20
2	B	276	THR	C-N-CA	6.91	138.97	121.70
1	A	61	HIS	CA-CB-CG	6.90	125.33	113.60
2	B	149	MET	CG-SD-CE	6.90	111.24	100.20
2	B	412	GLY	C-N-CA	6.88	138.91	121.70
2	B	269	MET	CG-SD-CE	6.87	111.19	100.20
1	A	17	GLY	O-C-N	6.86	133.68	122.70
1	A	203	MET	O-C-N	6.86	133.68	122.70
2	B	32	PRO	O-C-N	6.86	133.67	122.70
2	B	349	ASN	CB-CA-C	6.84	124.09	110.40
2	B	340	SER	C-N-CA	-6.84	104.60	121.70
2	B	30	ILE	CA-C-N	6.83	132.24	117.20
1	A	355	ILE	CA-C-O	-6.82	105.79	120.10
1	A	368	LEU	C-N-CA	6.79	138.67	121.70
2	B	346	TRP	CD1-CG-CD2	6.79	111.73	106.30
2	B	193	GLN	C-N-CA	6.78	138.65	121.70
1	A	72	PRO	O-C-N	6.76	133.52	122.70
2	B	151	THR	CA-C-N	6.75	132.06	117.20
1	A	409	VAL	CA-C-N	-6.72	102.77	116.20
2	B	436	GLN	O-C-N	-6.70	111.98	122.70
2	B	398	MET	CG-SD-CE	6.67	110.87	100.20
2	B	1	MET	C-N-CA	6.67	138.37	121.70
1	A	290	GLU	O-C-N	6.65	133.35	122.70
1	A	85	GLN	O-C-N	-6.65	112.06	122.70
2	B	281	GLN	O-C-N	-6.65	112.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	91	ASN	CA-CB-CG	6.64	128.01	113.40
1	A	425	MET	CG-SD-CE	6.64	110.82	100.20
2	B	224	TYR	CA-C-N	6.63	129.46	116.20
1	A	384	ILE	CA-C-N	-6.61	102.66	117.20
1	A	203	MET	CG-SD-CE	6.60	110.75	100.20
2	B	113	GLU	CA-C-O	6.59	133.94	120.10
1	A	78	VAL	O-C-N	-6.58	112.16	122.70
2	B	166	MET	CG-SD-CE	6.58	110.73	100.20
2	B	348	PRO	C-N-CA	6.58	138.15	121.70
1	A	113	GLU	CA-C-O	6.58	133.91	120.10
1	A	197	HIS	O-C-N	6.57	133.21	122.70
1	A	369	ALA	CA-C-N	-6.57	102.75	117.20
1	A	221	ARG	C-N-CA	6.55	149.53	122.00
2	B	219	LEU	CB-CA-C	-6.55	97.75	110.20
2	B	263	PRO	N-CA-C	6.55	129.12	112.10
2	B	243	ARG	NE-CZ-NH2	6.53	123.57	120.30
2	B	413	MET	CG-SD-CE	6.52	110.64	100.20
1	A	49	PHE	O-C-N	-6.52	112.27	122.70
1	A	83	TYR	CA-CB-CG	-6.51	101.03	113.40
1	A	140	SER	O-C-N	6.48	133.07	122.70
1	A	275	VAL	O-C-N	6.48	133.07	122.70
1	A	398	MET	CG-SD-CE	6.47	110.55	100.20
1	A	396	ASP	CA-C-N	6.47	131.43	117.20
1	A	297	GLU	CA-C-N	-6.45	99.04	117.10
2	B	60	LYS	CA-C-N	6.44	131.38	117.20
2	B	36	TYR	O-C-N	-6.42	112.42	122.70
2	B	290	GLU	CA-C-N	-6.41	103.10	117.20
1	A	111	GLY	CA-C-O	-6.40	109.07	120.60
2	B	111	GLY	CA-C-O	-6.39	109.10	120.60
2	B	332	MET	CG-SD-CE	6.38	110.41	100.20
1	A	407	TRP	CA-CB-CG	-6.38	101.58	113.70
1	A	262	TYR	CB-CG-CD2	6.37	124.82	121.00
1	A	402	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	A	290	GLU	CA-C-N	-6.32	103.30	117.20
1	A	312	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	A	371	VAL	O-C-N	6.30	132.78	122.70
1	A	214	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	280	LYS	CA-C-N	6.26	130.97	117.20
1	A	105	ARG	CD-NE-CZ	6.25	132.35	123.60
2	B	346	TRP	N-CA-CB	6.25	121.85	110.60
1	A	187	SER	CA-C-N	-6.25	103.46	117.20
2	B	243	ARG	O-C-N	6.22	132.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	ARG	NE-CZ-NH2	6.21	123.41	120.30
2	B	59	ASN	O-C-N	-6.21	112.77	122.70
1	A	111	GLY	CA-C-N	6.21	130.85	117.20
2	B	111	GLY	CA-C-N	6.20	130.85	117.20
1	A	412	GLY	C-N-CA	6.18	137.16	121.70
1	A	390	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	43	GLY	O-C-N	6.13	133.62	123.20
2	B	177	VAL	O-C-N	-6.13	112.90	122.70
2	B	390	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	A	274	PRO	O-C-N	-6.10	112.94	122.70
2	B	323	MET	CG-SD-CE	6.10	109.96	100.20
2	B	390	ARG	NE-CZ-NH1	6.09	123.34	120.30
2	B	154	ILE	C-N-CA	6.08	136.91	121.70
1	A	172	TYR	CB-CA-C	6.07	122.55	110.40
2	B	314	THR	N-CA-CB	6.04	121.77	110.30
2	B	52	TYR	CB-CG-CD2	-6.03	117.38	121.00
2	B	331	GLN	C-N-CA	5.99	136.68	121.70
2	B	433	GLN	CA-C-N	-5.99	104.03	117.20
2	B	234	THR	CA-C-N	5.97	130.34	117.20
2	B	308	ARG	NH1-CZ-NH2	-5.97	112.83	119.40
1	A	42	ILE	C-N-CA	5.96	134.82	122.30
2	B	433	GLN	O-C-N	5.96	132.24	122.70
1	A	41	THR	CA-C-N	-5.95	104.11	117.20
2	B	301	MET	CG-SD-CE	5.94	109.71	100.20
2	B	407	TRP	CD1-CG-CD2	5.94	111.05	106.30
2	B	324	SER	O-C-N	5.94	132.20	122.70
2	B	412	GLY	CA-C-N	5.93	130.26	117.20
1	A	1	MET	CG-SD-CE	5.91	109.65	100.20
1	A	82	THR	O-C-N	5.90	132.14	122.70
1	A	82	THR	C-N-CA	5.89	136.43	121.70
2	B	185	TYR	CB-CG-CD2	-5.89	117.47	121.00
2	B	123	ARG	NE-CZ-NH2	5.86	123.23	120.30
2	B	416	MET	CG-SD-CE	5.85	109.56	100.20
2	B	244	PHE	CB-CA-C	5.84	122.09	110.40
2	B	171	VAL	C-N-CA	5.84	136.30	121.70
2	B	72	PRO	CA-C-N	5.84	127.88	116.20
1	A	90	GLU	CA-C-N	5.84	130.04	117.20
2	B	308	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	B	278	ARG	NE-CZ-NH1	5.81	123.21	120.30
2	B	36	TYR	CA-C-N	5.80	129.96	117.20
2	B	259	MET	CG-SD-CE	5.79	109.46	100.20
2	B	283	TYR	C-N-CA	5.78	136.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	324	SER	CA-C-N	-5.78	104.50	117.20
2	B	167	ASN	C-N-CA	-5.77	107.28	121.70
1	A	182	VAL	CA-C-N	5.75	129.85	117.20
1	A	50	ASN	C-N-CA	5.74	136.05	121.70
2	B	219	LEU	C-N-CA	-5.70	107.45	121.70
1	A	297	GLU	C-N-CD	5.70	140.36	128.40
2	B	2	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	B	414	ASP	CA-C-N	5.68	129.69	117.20
2	B	417	GLU	C-N-CA	5.65	135.82	121.70
2	B	284	ARG	NH1-CZ-NH2	-5.64	113.20	119.40
3	K	153	ARG	NE-CZ-NH1	-5.63	117.48	120.30
2	B	219	LEU	CA-C-N	5.63	129.58	117.20
2	B	43	GLN	O-C-N	5.62	131.70	122.70
2	B	113	GLU	O-C-N	-5.62	113.71	122.70
2	B	325	MET	CG-SD-CE	5.61	109.18	100.20
1	A	92	LEU	C-N-CA	5.61	135.73	121.70
1	A	274	PRO	CA-C-N	5.61	129.54	117.20
2	B	28	HIS	CA-C-N	-5.61	104.99	116.20
1	A	379	SER	CA-C-N	-5.60	104.88	117.20
2	B	50	ASN	CA-C-O	5.60	131.86	120.10
1	A	413	MET	CG-SD-CE	5.59	109.14	100.20
2	B	192	HIS	CA-C-N	5.58	129.47	117.20
1	A	343	PHE	O-C-N	5.58	131.62	122.70
1	A	154	MET	CG-SD-CE	5.57	109.11	100.20
2	B	390	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
1	A	90	GLU	C-N-CA	5.56	135.59	121.70
1	A	339	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	A	139	HIS	N-CA-CB	-5.55	100.61	110.60
2	B	349	ASN	N-CA-C	-5.55	96.02	111.00
2	B	389	LYS	CB-CA-C	5.54	121.48	110.40
2	B	346	TRP	O-C-N	5.51	131.51	122.70
2	B	178	SER	CA-C-O	-5.51	108.53	120.10
2	B	299	LYS	C-N-CA	-5.50	107.94	121.70
2	B	154	ILE	O-C-N	-5.50	113.90	122.70
2	B	264	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	71	GLU	O-C-N	-5.48	110.69	121.10
2	B	245	PRO	N-CA-CB	-5.48	96.58	102.60
1	A	221	ARG	CA-CB-CG	5.44	125.37	113.40
1	A	297	GLU	C-N-CA	-5.44	99.15	122.00
1	A	262	TYR	CA-CB-CG	5.43	123.72	113.40
1	A	222	PRO	CA-CB-CG	-5.41	93.71	104.00
2	B	86	ILE	C-N-CA	5.41	135.23	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	253	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
1	A	65	ALA	O-C-N	-5.38	114.10	122.70
2	B	32	PRO	CA-C-N	-5.37	105.38	117.20
1	A	84	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	62	VAL	O-C-N	5.36	131.29	121.10
2	B	72	PRO	O-C-N	-5.36	114.09	123.20
2	B	4	ILE	O-C-N	5.36	131.27	122.70
1	A	379	SER	O-C-N	5.35	131.26	122.70
2	B	49	ILE	CA-C-N	5.34	128.94	117.20
1	A	336	LYS	O-C-N	5.33	131.23	122.70
1	A	360	PRO	C-N-CA	-5.31	108.42	121.70
1	A	390	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	141	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	186	ASN	C-N-CA	5.29	134.93	121.70
1	A	17	GLY	CA-C-N	-5.29	105.57	117.20
1	A	97	GLU	O-C-N	5.28	131.15	122.70
2	B	173	PRO	O-C-N	-5.26	114.28	122.70
2	B	193	GLN	CA-C-N	5.26	128.77	117.20
1	A	390	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
1	A	407	TRP	CD1-CG-CD2	5.25	110.50	106.30
2	B	256	ALA	CA-C-N	5.25	128.74	117.20
1	A	36	MET	C-N-CD	-5.25	109.06	120.60
2	B	41	ASP	O-C-N	5.25	131.09	122.70
2	B	185	TYR	N-CA-CB	-5.24	101.17	110.60
1	A	42	ILE	CA-C-O	-5.23	109.11	120.10
2	B	176	LYS	O-C-N	-5.23	114.34	122.70
2	B	278	ARG	CA-CB-CG	5.22	124.88	113.40
1	A	195	LEU	CA-C-O	-5.21	109.17	120.10
2	B	2	ARG	CA-C-N	-5.20	105.77	117.20
2	B	48	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	A	221	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	433	GLN	C-N-CA	-5.18	108.76	121.70
1	A	123	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	A	69	ASP	CA-C-N	5.17	128.57	117.20
1	A	405	VAL	N-CA-CB	-5.17	100.14	111.50
2	B	435	TYR	CD1-CG-CD2	5.16	123.58	117.90
1	A	299	ALA	CA-C-N	5.16	128.55	117.20
2	B	264	ARG	CB-CA-C	5.16	120.71	110.40
1	A	298	PRO	CA-C-N	5.14	128.51	117.20
1	A	412	GLY	CA-C-N	5.14	128.51	117.20
2	B	322	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	A	31	GLN	O-C-N	5.14	130.86	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	60	LYS	CA-C-O	5.13	130.88	120.10
3	K	113	LYS	N-CA-C	5.13	124.85	111.00
2	B	408	TYR	CB-CG-CD2	-5.12	117.93	121.00
2	B	214	PHE	CB-CG-CD2	-5.11	117.22	120.80
2	B	289	PRO	C-N-CA	-5.10	108.95	121.70
1	A	17	GLY	C-N-CA	-5.09	108.97	121.70
1	A	427	ALA	O-C-N	5.08	130.83	122.70
2	B	346	TRP	CE2-CD2-CG	-5.08	103.24	107.30
2	B	172	VAL	C-N-CD	-5.07	109.45	120.60
1	A	438	ASP	CA-C-N	5.06	128.34	117.20
2	B	1	MET	CG-SD-CE	5.06	108.29	100.20
2	B	246	GLY	N-CA-C	5.06	125.74	113.10
1	A	203	MET	CA-C-N	-5.05	106.10	117.20
1	A	308	ARG	NE-CZ-NH2	5.05	122.82	120.30
2	B	53	TYR	C-N-CA	5.05	134.32	121.70
2	B	337	ASN	O-C-N	-5.04	114.63	122.70
2	B	139	HIS	N-CA-CB	-5.03	101.55	110.60
2	B	260	VAL	C-N-CD	-5.01	109.57	120.60

There are no chirality outliers.

All (116) planarity outliers are listed below:

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

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

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

5.2 Too-close contacts (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	3252	1687	0
2	B	3359	0	3171	1861	0
3	K	2667	0	2614	154	0
4	A	32	0	11	21	0
5	B	28	0	12	17	0
6	B	58	0	51	57	0
7	K	1	0	0	0	0
8	K	31	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9606	0	9125	3576	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 191.

All (3576) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:LEU:HD22	2:B:418:PHE:CZ	1.17	1.68
2:B:151:THR:CB	2:B:192:HIS:CD2	1.75	1.68
2:B:229:HIS:CE1	6:B:502:TXL:H343	1.28	1.67
1:A:115:ILE:HD12	1:A:152:LEU:CG	1.26	1.64
2:B:184:PRO:HG2	2:B:399:PHE:CE2	1.12	1.63
2:B:147:SER:HB3	2:B:189:LEU:CD1	1.19	1.63
2:B:287:THR:HB	2:B:290:GLU:CB	1.26	1.63
1:A:217:LEU:HD13	1:A:368:LEU:CD1	1.25	1.63
1:A:405:VAL:CG2	1:A:405:VAL:CB	1.76	1.63
2:B:346:TRP:CE3	2:B:347:ILE:HG13	1.25	1.63
1:A:53:PHE:N	1:A:88:HIS:CE1	1.68	1.62
2:B:405:LEU:CD1	2:B:408:TYR:CB	1.75	1.61
2:B:158:ARG:CB	2:B:197:ASN:CB	1.76	1.60
1:A:326:LYS:NZ	2:B:214:PHE:CZ	1.67	1.59
1:A:115:ILE:CD1	1:A:152:LEU:HG	1.15	1.59
1:A:220:GLU:CB	1:A:220:GLU:CG	1.78	1.58
1:A:212:ILE:HD11	1:A:230:LEU:CD2	1.25	1.57
2:B:181:VAL:CG1	2:B:399:PHE:HZ	1.17	1.57
2:B:158:ARG:HB2	2:B:197:ASN:CB	1.14	1.57
1:A:296:PHE:CE1	1:A:335:ILE:HD13	1.38	1.57
2:B:346:TRP:CZ3	2:B:347:ILE:HD11	1.34	1.57
1:A:204:VAL:CG1	1:A:209:ILE:HD11	1.17	1.57
2:B:6:HIS:CE1	2:B:30:ILE:HD12	1.39	1.57
2:B:158:ARG:CD	2:B:197:ASN:HB2	1.30	1.56
2:B:151:THR:HG22	2:B:192:HIS:CE1	1.39	1.56
2:B:158:ARG:CG	2:B:197:ASN:HB2	1.13	1.56
1:A:31:GLN:HE22	1:A:243:ARG:CG	1.15	1.55
1:A:424:ASP:CG	3:K:307:ARG:HH12	1.03	1.55
2:B:70:LEU:HD12	2:B:94:PHE:CD2	1.40	1.54
1:A:103:TYR:CE2	1:A:189:LEU:HD23	1.41	1.54
1:A:349:THR:CB	2:B:177:VAL:CG1	1.78	1.53
1:A:70:LEU:HD12	1:A:145:THR:CG2	1.07	1.53
1:A:100:ALA:CB	1:A:105:ARG:HD3	1.38	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CD2	1:A:189:LEU:HD23	1.44	1.53
2:B:295:MET:CE	2:B:375:ALA:HB1	1.08	1.53
2:B:399:PHE:CE1	2:B:408:TYR:HE2	1.22	1.53
2:B:151:THR:CA	2:B:192:HIS:CD2	1.89	1.51
2:B:181:VAL:HG13	2:B:399:PHE:CZ	1.40	1.51
2:B:158:ARG:CA	2:B:197:ASN:HD22	0.89	1.50
2:B:169:PHE:CE1	2:B:235:MET:HG2	1.45	1.50
1:A:62:VAL:CG1	1:A:63:PRO:HD2	1.39	1.50
2:B:184:PRO:CG	2:B:399:PHE:CG	1.92	1.50
2:B:346:TRP:CE3	2:B:347:ILE:CG1	1.90	1.50
1:A:210:TYR:CE2	1:A:227:LEU:HD22	1.45	1.49
1:A:64:ARG:HH22	1:A:132:LEU:CD2	1.22	1.49
1:A:264:ARG:NH2	3:K:307:ARG:HD2	1.24	1.49
2:B:405:LEU:CD2	2:B:418:PHE:CZ	1.91	1.49
2:B:405:LEU:HD13	2:B:408:TYR:CD2	1.48	1.49
1:A:107:HIS:HB2	1:A:148:GLY:CA	1.42	1.48
2:B:192:HIS:CA	2:B:196:GLU:HG3	1.42	1.48
2:B:259:MET:HB3	2:B:268:PHE:CE1	1.47	1.48
1:A:272:TYR:CE1	1:A:274:PRO:O	1.64	1.47
1:A:349:THR:HB	2:B:177:VAL:CG1	1.00	1.47
2:B:399:PHE:HE1	2:B:408:TYR:CE2	1.30	1.47
2:B:295:MET:CE	2:B:375:ALA:CB	1.93	1.47
1:A:70:LEU:CD1	1:A:145:THR:HG22	0.98	1.46
1:A:349:THR:CB	2:B:177:VAL:HG11	1.34	1.46
1:A:31:GLN:CD	1:A:243:ARG:HD2	1.08	1.46
2:B:405:LEU:CD2	2:B:418:PHE:CE2	2.00	1.46
2:B:405:LEU:HD11	2:B:408:TYR:CB	1.34	1.45
1:A:212:ILE:CD1	1:A:230:LEU:HD21	1.45	1.45
2:B:399:PHE:CE1	2:B:408:TYR:CE2	2.03	1.45
1:A:158:SER:CB	1:A:197:HIS:CB	1.84	1.44
2:B:405:LEU:CD1	2:B:408:TYR:HB2	0.96	1.44
1:A:103:TYR:CD2	1:A:147:SER:HB2	1.50	1.44
2:B:151:THR:HB	2:B:192:HIS:CD2	1.39	1.44
1:A:397:LEU:CD2	1:A:401:LYS:HD2	1.47	1.44
1:A:107:HIS:CB	1:A:148:GLY:HA3	1.47	1.44
2:B:239:THR:O	2:B:243:ARG:CD	1.65	1.44
2:B:19:LYS:CB	2:B:228:ASN:HB3	1.45	1.43
2:B:286:LEU:CD1	2:B:372:LYS:HB2	1.47	1.43
2:B:107:HIS:C	2:B:152:LEU:HD11	1.35	1.43
2:B:135:PHE:HB3	2:B:166:MET:CE	1.47	1.43
2:B:158:ARG:HD2	2:B:197:ASN:CA	1.44	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:CD1	2:B:94:PHE:CD2	1.99	1.43
2:B:172:VAL:CG1	2:B:173:PRO:HD2	1.46	1.42
2:B:19:LYS:HG3	2:B:228:ASN:CB	1.46	1.42
1:A:264:ARG:HH21	3:K:307:ARG:CB	1.31	1.42
2:B:87:PHE:CE1	2:B:89:PRO:HG2	1.52	1.42
2:B:151:THR:HA	2:B:192:HIS:CD2	1.49	1.42
1:A:53:PHE:CA	1:A:88:HIS:CE1	2.01	1.41
1:A:222:PRO:CB	1:A:222:PRO:CG	1.86	1.41
2:B:151:THR:HG22	2:B:192:HIS:ND1	1.24	1.41
1:A:64:ARG:NH2	1:A:132:LEU:HD22	1.31	1.41
1:A:424:ASP:CB	3:K:307:ARG:HH12	1.34	1.40
2:B:147:SER:CB	2:B:189:LEU:HD11	0.95	1.40
1:A:250:VAL:HG13	1:A:254:GLU:CB	1.48	1.40
1:A:172:TYR:OH	1:A:387:ALA:CB	1.64	1.40
2:B:184:PRO:CB	2:B:399:PHE:CD2	2.05	1.40
1:A:68:VAL:HG11	1:A:149:PHE:CZ	1.57	1.39
1:A:277:SER:OG	1:A:280:LYS:CG	1.68	1.39
2:B:19:LYS:CG	2:B:228:ASN:HB3	1.50	1.39
2:B:57:ALA:HA	2:B:64:ARG:CB	1.52	1.39
1:A:204:VAL:CG2	1:A:231:ILE:HG23	1.50	1.39
2:B:7:ILE:HB	2:B:137:LEU:CD2	1.51	1.39
2:B:87:PHE:CD1	2:B:88:ARG:O	1.76	1.38
1:A:250:VAL:HG13	1:A:254:GLU:CG	1.54	1.38
2:B:175:PRO:O	2:B:176:LYS:CE	1.70	1.38
1:A:176:GLN:O	1:A:177:VAL:CG2	1.69	1.37
1:A:288:VAL:CG2	1:A:373:ARG:HD3	1.52	1.37
2:B:103:TRP:CD1	2:B:189:LEU:HD23	1.57	1.37
2:B:184:PRO:CD	2:B:399:PHE:CD2	2.07	1.37
2:B:158:ARG:HA	2:B:197:ASN:ND2	1.04	1.36
2:B:184:PRO:HG2	2:B:399:PHE:CG	1.55	1.36
1:A:264:ARG:NH2	3:K:307:ARG:HB3	1.40	1.36
2:B:158:ARG:CB	2:B:197:ASN:HB2	1.44	1.36
2:B:147:SER:CB	2:B:189:LEU:CD1	1.79	1.36
1:A:179:THR:HG22	1:A:181:VAL:N	1.42	1.35
2:B:20:PHE:CE2	2:B:235:MET:HB3	1.50	1.35
2:B:97:SER:HB2	2:B:110:GLU:OE1	1.19	1.35
2:B:24:ILE:O	2:B:26:ASP:N	1.60	1.35
2:B:32:PRO:CB	2:B:59:ASN:HD22	1.25	1.35
2:B:435:TYR:O	2:B:436:GLN:CG	1.72	1.35
1:A:182:VAL:HG13	1:A:186:ASN:ND2	1.40	1.35
1:A:217:LEU:CD1	1:A:368:LEU:HD11	1.55	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TRP:CE3	2:B:413:MET:HE1	1.61	1.34
1:A:272:TYR:CZ	1:A:274:PRO:HG2	1.62	1.34
2:B:175:PRO:O	2:B:176:LYS:CD	1.74	1.34
2:B:192:HIS:HA	2:B:196:GLU:CG	1.55	1.34
1:A:212:ILE:CD1	1:A:230:LEU:CD2	2.02	1.34
2:B:96:GLN:O	2:B:98:GLY:N	1.59	1.34
2:B:103:TRP:CZ3	2:B:413:MET:HE2	1.62	1.34
2:B:201:THR:CG2	2:B:265:LEU:HD21	1.57	1.34
2:B:151:THR:HA	2:B:192:HIS:NE2	1.04	1.33
2:B:305:CYS:SG	2:B:384:ILE:HD13	1.67	1.33
1:A:2:ARG:NH2	2:B:71:GLU:HB3	1.42	1.33
1:A:53:PHE:N	1:A:88:HIS:NE2	1.75	1.33
1:A:158:SER:CB	1:A:197:HIS:HB3	1.49	1.33
2:B:19:LYS:CG	2:B:228:ASN:CB	2.02	1.33
2:B:294:GLN:CG	2:B:300:ASN:OD1	1.77	1.33
2:B:405:LEU:HD22	2:B:418:PHE:CE2	1.56	1.33
1:A:31:GLN:N	1:A:32:PRO:CD	1.76	1.32
1:A:31:GLN:NE2	1:A:243:ARG:CD	1.92	1.32
1:A:306:ASP:OD1	1:A:308:ARG:CG	1.76	1.32
2:B:346:TRP:CZ3	2:B:347:ILE:CD1	2.10	1.32
2:B:22:GLU:HG2	2:B:83:PHE:CD2	1.63	1.32
1:A:277:SER:CB	1:A:280:LYS:HG2	1.59	1.32
2:B:75:MET:CE	2:B:79:ARG:HD2	1.60	1.32
1:A:179:THR:CG2	1:A:181:VAL:H	1.42	1.32
1:A:369:ALA:CB	1:A:371:VAL:HG23	1.56	1.32
1:A:424:ASP:CG	3:K:307:ARG:NH1	1.81	1.32
2:B:259:MET:HE1	2:B:379:GLY:CA	1.57	1.32
2:B:158:ARG:CG	2:B:197:ASN:CB	1.95	1.32
1:A:184:PRO:HG3	1:A:395:PHE:CB	1.57	1.31
2:B:107:HIS:O	2:B:152:LEU:HD11	1.28	1.31
2:B:181:VAL:CG1	2:B:399:PHE:CZ	2.03	1.31
2:B:244:PHE:CD2	2:B:245:PRO:HD2	1.65	1.31
2:B:335:VAL:O	2:B:339:ASN:ND2	1.60	1.31
2:B:158:ARG:HD2	2:B:197:ASN:CB	1.59	1.31
2:B:175:PRO:O	2:B:176:LYS:HE2	1.22	1.31
1:A:30:ILE:O	1:A:32:PRO:CG	1.78	1.31
1:A:108:TYR:O	1:A:112:LYS:CD	1.76	1.31
2:B:311:ARG:HG2	2:B:341:SER:O	1.21	1.30
1:A:250:VAL:CG2	1:A:352:LYS:HE2	1.60	1.30
1:A:31:GLN:CD	1:A:243:ARG:CD	1.99	1.30
1:A:250:VAL:CG1	1:A:254:GLU:HB3	1.61	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:HIS:O	2:B:196:GLU:CB	1.80	1.30
1:A:103:TYR:CD2	1:A:189:LEU:CD2	2.13	1.29
1:A:291:ILE:HG22	1:A:375:VAL:CG2	1.62	1.29
2:B:201:THR:HG21	2:B:265:LEU:CD2	1.60	1.29
2:B:12:CYS:O	2:B:16:ILE:HG12	1.25	1.29
1:A:266:HIS:CD2	1:A:432:TYR:HE1	1.50	1.29
1:A:423:GLU:OE2	3:K:172:PRO:HA	1.23	1.29
2:B:189:LEU:O	2:B:193:GLN:HG3	1.31	1.29
2:B:435:TYR:O	2:B:436:GLN:HG3	1.20	1.29
1:A:38:SER:O	1:A:39:ASP:N	1.58	1.29
2:B:107:HIS:CA	2:B:152:LEU:HD11	1.63	1.29
2:B:4:ILE:HD12	2:B:30:ILE:C	1.53	1.29
2:B:229:HIS:CG	6:B:502:TXL:H38	1.67	1.29
2:B:268:PHE:CE1	2:B:380:ASN:ND2	1.99	1.29
2:B:107:HIS:CD2	2:B:152:LEU:HG	1.66	1.28
2:B:114:LEU:HD12	2:B:117:SER:OG	1.24	1.28
2:B:180:THR:O	2:B:398:MET:CE	1.78	1.28
1:A:2:ARG:CG	1:A:133:GLN:OE1	1.82	1.28
2:B:151:THR:CG2	2:B:192:HIS:CG	2.16	1.28
1:A:184:PRO:CG	1:A:395:PHE:CD2	2.17	1.28
2:B:192:HIS:O	2:B:196:GLU:HB2	1.17	1.28
2:B:319:PHE:CE1	2:B:353:THR:HG23	1.67	1.28
1:A:31:GLN:N	1:A:32:PRO:HD3	1.05	1.27
1:A:433:GLU:O	1:A:437:VAL:HG23	1.32	1.27
1:A:306:ASP:OD1	1:A:308:ARG:HG3	1.17	1.27
2:B:151:THR:HG22	2:B:192:HIS:CG	1.67	1.27
2:B:151:THR:CA	2:B:192:HIS:NE2	1.82	1.27
2:B:312:TYR:HA	2:B:381:SER:CB	1.63	1.27
2:B:142:GLY:C	2:B:185:TYR:CE1	2.07	1.27
2:B:183:GLU:HB2	2:B:184:PRO:CD	1.59	1.27
2:B:295:MET:HE1	2:B:375:ALA:CB	1.51	1.27
2:B:237:GLY:HA2	2:B:241:CYS:SG	1.74	1.27
1:A:31:GLN:NE2	1:A:243:ARG:CG	1.93	1.27
1:A:53:PHE:HA	1:A:88:HIS:CE1	1.64	1.27
2:B:145:THR:O	2:B:149:MET:HB3	1.19	1.27
1:A:101:ASN:O	1:A:102:ASN:CG	1.72	1.26
2:B:405:LEU:CD1	2:B:408:TYR:CD2	2.06	1.26
2:B:75:MET:HE1	2:B:79:ARG:CD	1.64	1.26
2:B:182:VAL:HG13	2:B:186:ASN:ND2	1.48	1.26
1:A:38:SER:C	1:A:39:ASP:CA	2.04	1.26
1:A:383:ALA:O	1:A:385:ALA:N	1.69	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:CE1	2:B:88:ARG:O	1.87	1.26
2:B:94:PHE:HD1	2:B:94:PHE:O	1.16	1.26
1:A:204:VAL:CG1	1:A:209:ILE:CD1	2.13	1.26
1:A:219:ILE:CB	1:A:219:ILE:CG2	2.13	1.26
1:A:204:VAL:HG21	1:A:231:ILE:CG2	1.47	1.26
2:B:193:GLN:O	2:B:265:LEU:CD2	1.82	1.26
1:A:424:ASP:OD1	3:K:307:ARG:NH2	1.70	1.25
2:B:3:GLU:OE1	2:B:130:ASP:CB	1.84	1.25
2:B:183:GLU:CB	2:B:184:PRO:HD3	1.63	1.25
2:B:312:TYR:O	2:B:344:VAL:CG2	1.84	1.25
1:A:172:TYR:OH	1:A:387:ALA:HB3	1.11	1.25
2:B:12:CYS:O	2:B:16:ILE:CG1	1.82	1.25
1:A:288:VAL:HG22	1:A:373:ARG:CD	1.65	1.25
2:B:57:ALA:CA	2:B:64:ARG:HB2	1.64	1.25
2:B:92:PHE:CD2	2:B:114:LEU:HD11	1.70	1.25
2:B:103:TRP:HD1	2:B:189:LEU:CD2	1.49	1.25
2:B:287:THR:O	2:B:291:LEU:CG	1.81	1.25
1:A:264:ARG:HH22	3:K:307:ARG:CD	1.48	1.25
2:B:405:LEU:CD1	2:B:408:TYR:CG	2.20	1.25
1:A:424:ASP:HA	3:K:307:ARG:CZ	1.65	1.24
2:B:103:TRP:CD1	2:B:189:LEU:CD2	2.18	1.24
1:A:97:GLU:CB	1:A:110:ILE:HG21	1.65	1.24
1:A:206:ASN:ND2	1:A:227:LEU:CD2	2.00	1.24
1:A:257:THR:HG22	2:B:407:TRP:CE3	1.71	1.24
1:A:108:TYR:CA	1:A:112:LYS:HE3	1.67	1.24
2:B:44:LEU:HD23	2:B:85:GLN:CG	1.35	1.24
2:B:103:TRP:CE3	2:B:413:MET:CE	2.21	1.24
1:A:77:GLU:HA	1:A:80:THR:OG1	1.09	1.24
1:A:108:TYR:O	1:A:112:LYS:CE	1.85	1.24
2:B:4:ILE:HD13	2:B:30:ILE:CG2	1.68	1.24
2:B:35:SER:O	2:B:37:HIS:N	1.71	1.24
2:B:319:PHE:HE1	2:B:353:THR:CG2	1.50	1.24
1:A:30:ILE:CG2	1:A:64:ARG:HG2	1.68	1.23
1:A:31:GLN:OE1	1:A:243:ARG:CD	1.85	1.23
1:A:259:LEU:O	1:A:261:PRO:HD3	1.38	1.23
1:A:276:ILE:O	1:A:368:LEU:HB3	1.31	1.23
1:A:326:LYS:NZ	2:B:214:PHE:CE1	2.06	1.23
2:B:382:THR:CG2	2:B:436:GLN:OE1	1.78	1.23
1:A:9:VAL:HG11	1:A:150:THR:CG2	1.67	1.23
1:A:185:TYR:HD2	1:A:408:TYR:OH	0.92	1.23
1:A:291:ILE:CG2	1:A:375:VAL:HG23	1.65	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:THR:CG2	2:B:289:PRO:HD2	1.67	1.23
1:A:360:PRO:CG	1:A:371:VAL:O	1.86	1.23
2:B:107:HIS:HA	2:B:152:LEU:CD1	1.67	1.23
2:B:111:GLY:O	2:B:115:VAL:HG23	1.32	1.23
2:B:244:PHE:CE2	2:B:358:ILE:HD12	1.73	1.23
2:B:20:PHE:CE2	2:B:235:MET:CB	2.01	1.23
1:A:77:GLU:CA	1:A:80:THR:OG1	1.86	1.23
2:B:143:GLY:N	2:B:185:TYR:CE1	2.05	1.23
1:A:30:ILE:O	1:A:32:PRO:HG2	1.27	1.22
1:A:206:ASN:ND2	1:A:227:LEU:HD21	1.51	1.22
2:B:87:PHE:HE1	2:B:89:PRO:CG	1.51	1.22
2:B:102:ASN:HD22	2:B:105:LYS:CE	1.49	1.22
2:B:75:MET:CE	2:B:79:ARG:CD	2.17	1.22
1:A:20:CYS:O	1:A:24:TYR:CD2	1.91	1.22
1:A:312:TYR:O	1:A:344:VAL:CG2	1.87	1.22
2:B:229:HIS:CD2	6:B:502:TXL:H38	1.54	1.22
2:B:287:THR:CB	2:B:290:GLU:HB2	1.67	1.22
1:A:26:LEU:HD11	1:A:361:THR:CG2	1.69	1.22
1:A:48:SER:O	1:A:56:THR:CG2	1.87	1.22
1:A:78:VAL:CG1	1:A:87:PHE:HE1	1.53	1.22
1:A:424:ASP:CB	3:K:307:ARG:NH1	2.00	1.22
1:A:3:GLU:HA	1:A:31:GLN:CB	1.70	1.22
1:A:272:TYR:HE1	1:A:274:PRO:O	0.94	1.22
2:B:6:HIS:HE1	2:B:30:ILE:CD1	1.53	1.22
2:B:69:ASP:OD2	2:B:74:THR:HB	1.32	1.22
1:A:93:ILE:CD1	1:A:118:VAL:HG22	1.70	1.21
1:A:210:TYR:CE2	1:A:227:LEU:CD2	2.21	1.21
2:B:36:TYR:CE2	2:B:244:PHE:CE1	1.94	1.21
1:A:4:CYS:HB2	1:A:30:ILE:CG2	1.68	1.21
1:A:108:TYR:C	1:A:112:LYS:HE3	1.59	1.21
1:A:220:GLU:C	1:A:222:PRO:HD3	1.61	1.21
1:A:423:GLU:OE1	3:K:170:GLU:HG3	1.30	1.21
2:B:97:SER:CB	2:B:110:GLU:OE1	1.89	1.21
2:B:175:PRO:O	2:B:176:LYS:CG	1.88	1.21
1:A:242:LEU:HD12	1:A:255:PHE:CZ	1.73	1.21
2:B:184:PRO:CD	2:B:399:PHE:HD2	1.49	1.21
2:B:237:GLY:O	2:B:241:CYS:HB2	1.33	1.21
1:A:416:GLY:HA3	3:K:169:ARG:NH2	1.54	1.21
2:B:319:PHE:CE1	2:B:328:VAL:CG1	2.24	1.21
1:A:217:LEU:HD13	1:A:368:LEU:HD13	1.21	1.20
2:B:143:GLY:N	2:B:185:TYR:HE1	1.35	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:TYR:HA	2:B:381:SER:CA	1.71	1.20
1:A:107:HIS:HB2	1:A:148:GLY:C	1.59	1.20
1:A:217:LEU:CD1	1:A:368:LEU:CD1	2.14	1.20
1:A:272:TYR:CE1	1:A:274:PRO:HG2	1.75	1.20
2:B:229:HIS:CE1	6:B:502:TXL:C34	2.23	1.20
2:B:435:TYR:C	2:B:436:GLN:HG3	1.17	1.20
1:A:28:HIS:CE1	1:A:29:GLY:O	1.93	1.20
1:A:184:PRO:HG3	1:A:395:PHE:CD2	1.74	1.20
2:B:192:HIS:CA	2:B:196:GLU:CG	2.12	1.20
1:A:396:ASP:O	1:A:401:LYS:HB2	1.40	1.20
2:B:87:PHE:CE1	2:B:89:PRO:CG	2.23	1.20
2:B:175:PRO:HD3	2:B:390:ARG:NH2	1.57	1.20
2:B:20:PHE:HE2	2:B:235:MET:CB	1.24	1.19
1:A:176:GLN:O	1:A:177:VAL:HG23	1.03	1.19
1:A:220:GLU:O	1:A:222:PRO:CD	1.89	1.19
1:A:344:VAL:HB	1:A:347:CYS:SG	1.80	1.19
2:B:107:HIS:O	2:B:152:LEU:CD1	1.89	1.19
2:B:169:PHE:CE1	2:B:235:MET:CG	2.25	1.19
1:A:16:ILE:HD13	1:A:138:PHE:CD1	1.75	1.19
2:B:135:PHE:CB	2:B:166:MET:CE	2.20	1.19
2:B:295:MET:HE3	2:B:375:ALA:CB	1.65	1.19
1:A:30:ILE:C	1:A:32:PRO:CD	2.11	1.19
1:A:174:ALA:CB	1:A:175:PRO:CD	2.20	1.19
2:B:321:GLY:HA3	2:B:373:MET:HG3	1.22	1.19
1:A:343:PHE:CE2	1:A:351:PHE:CZ	2.30	1.19
2:B:151:THR:CG2	2:B:192:HIS:CE1	2.26	1.19
1:A:115:ILE:CD1	1:A:152:LEU:CG	1.92	1.18
1:A:332:ILE:CD1	1:A:353:VAL:HG21	1.70	1.18
1:A:2:ARG:HG2	1:A:133:GLN:OE1	1.06	1.18
2:B:259:MET:CE	2:B:379:GLY:HA2	1.72	1.18
2:B:346:TRP:HE3	2:B:347:ILE:CG1	1.34	1.18
1:A:4:CYS:SG	1:A:252:LEU:HD11	1.83	1.18
2:B:44:LEU:O	2:B:47:GLU:HG3	1.01	1.18
2:B:250:ALA:HA	2:B:254:LYS:HD2	1.25	1.18
1:A:184:PRO:CB	1:A:395:PHE:HD2	1.55	1.18
1:A:312:TYR:HA	1:A:381:THR:HG22	1.26	1.18
2:B:32:PRO:CB	2:B:59:ASN:ND2	1.79	1.18
1:A:31:GLN:OE1	1:A:243:ARG:HD2	1.03	1.17
1:A:103:TYR:CD1	1:A:188:ILE:CG2	2.26	1.17
1:A:115:ILE:HD13	1:A:156:ARG:CZ	1.74	1.17
1:A:3:GLU:O	1:A:132:LEU:O	1.59	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:O	1:A:56:THR:HG21	1.02	1.17
2:B:33:THR:N	2:B:59:ASN:HD22	1.42	1.17
2:B:370:GLY:O	6:B:502:TXL:H183	1.43	1.17
1:A:264:ARG:NH2	3:K:307:ARG:CD	2.04	1.17
1:A:437:VAL:O	1:A:438:ASP:OD1	1.62	1.17
2:B:180:THR:O	2:B:398:MET:HE3	1.41	1.17
1:A:108:TYR:O	1:A:112:LYS:HE3	1.40	1.17
2:B:41:ASP:O	2:B:42:LEU:HG	1.45	1.17
2:B:175:PRO:C	2:B:176:LYS:HG2	1.54	1.17
1:A:62:VAL:CG1	1:A:63:PRO:CD	2.22	1.16
1:A:2:ARG:HH21	2:B:71:GLU:CB	1.57	1.16
1:A:105:ARG:HH21	1:A:110:ILE:HD11	1.03	1.16
1:A:220:GLU:O	1:A:222:PRO:HD2	1.45	1.16
2:B:7:ILE:HA	2:B:66:ILE:CG2	1.75	1.16
2:B:294:GLN:HG2	2:B:300:ASN:OD1	1.01	1.16
1:A:31:GLN:NE2	1:A:243:ARG:HD2	1.51	1.16
2:B:174:SER:CB	2:B:207:GLU:HB3	1.73	1.16
2:B:183:GLU:CD	2:B:394:GLN:HB3	1.66	1.16
2:B:435:TYR:C	2:B:436:GLN:CG	2.06	1.16
2:B:44:LEU:O	2:B:47:GLU:CG	1.91	1.16
1:A:100:ALA:CB	1:A:105:ARG:CD	2.23	1.16
1:A:115:ILE:HD12	1:A:152:LEU:CD2	1.75	1.16
1:A:137:VAL:HG21	1:A:154:MET:SD	1.85	1.16
1:A:312:TYR:HE2	1:A:377:MET:HE1	1.10	1.16
2:B:135:PHE:CB	2:B:166:MET:HE3	1.73	1.15
2:B:191:VAL:CG2	2:B:421:ALA:HA	1.75	1.15
2:B:183:GLU:HB2	2:B:398:MET:SD	1.85	1.15
2:B:287:THR:HB	2:B:290:GLU:HB3	1.21	1.15
2:B:287:THR:HG22	2:B:289:PRO:HD2	1.20	1.15
2:B:151:THR:CG2	2:B:192:HIS:CD2	2.27	1.15
2:B:209:LEU:HD13	2:B:227:LEU:HG	1.21	1.15
2:B:260:VAL:HG22	2:B:266:HIS:HB2	1.21	1.15
2:B:405:LEU:HD12	2:B:408:TYR:CB	1.56	1.15
2:B:22:GLU:HB3	2:B:83:PHE:CE2	1.81	1.15
2:B:22:GLU:HB3	2:B:83:PHE:CZ	1.82	1.15
2:B:50:ASN:N	2:B:61:TYR:CD2	2.15	1.15
2:B:158:ARG:CB	2:B:197:ASN:HD22	1.60	1.15
2:B:234:THR:OG1	2:B:302:MET:SD	2.05	1.15
2:B:234:THR:OG1	2:B:302:MET:CE	1.95	1.15
2:B:241:CYS:SG	2:B:320:ARG:NH1	2.20	1.15
1:A:217:LEU:HD11	1:A:368:LEU:HD21	1.15	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:HD22	2:B:186:ASN:HB3	1.21	1.14
2:B:172:VAL:CG1	2:B:173:PRO:CD	2.25	1.14
2:B:242:LEU:HD13	2:B:250:ALA:HB3	1.28	1.14
3:K:159:ASN:ND2	3:K:161:LYS:HG3	1.62	1.14
2:B:104:ALA:HA	2:B:108:TYR:CD2	1.83	1.14
2:B:105:LYS:HE2	2:B:411:GLU:OE2	1.48	1.14
2:B:151:THR:HB	2:B:192:HIS:CG	1.81	1.14
2:B:313:LEU:CD2	2:B:344:VAL:HG11	1.75	1.14
1:A:174:ALA:HB1	1:A:175:PRO:CD	1.75	1.14
1:A:155:GLU:HG3	1:A:192:HIS:CD2	1.82	1.14
1:A:184:PRO:HG3	1:A:395:PHE:CG	1.81	1.14
2:B:277:SER:HB2	2:B:280:SER:HB2	1.30	1.14
1:A:296:PHE:CE1	1:A:335:ILE:CD1	2.31	1.13
2:B:151:THR:CB	2:B:192:HIS:CG	2.31	1.13
2:B:296:PHE:CZ	2:B:335:VAL:HG11	1.83	1.13
1:A:397:LEU:HD23	1:A:401:LYS:HD2	1.19	1.13
2:B:22:GLU:CG	2:B:83:PHE:CD2	2.30	1.13
2:B:313:LEU:HD23	2:B:344:VAL:CG2	1.79	1.13
2:B:7:ILE:CG1	2:B:66:ILE:HG21	1.77	1.13
2:B:56:ALA:HB3	2:B:62:VAL:CB	1.78	1.13
2:B:244:PHE:HE2	2:B:358:ILE:CD1	1.60	1.13
2:B:405:LEU:CD1	2:B:408:TYR:HD2	1.53	1.13
1:A:59:GLY:O	1:A:62:VAL:O	1.63	1.13
1:A:217:LEU:CG	1:A:368:LEU:HD11	1.78	1.13
2:B:154:ILE:HG21	2:B:198:THR:CG2	1.79	1.13
2:B:154:ILE:CG2	2:B:198:THR:HG23	1.78	1.13
2:B:184:PRO:CG	2:B:399:PHE:CE2	1.90	1.13
2:B:193:GLN:O	2:B:265:LEU:HD22	0.96	1.13
1:A:206:ASN:HD22	1:A:227:LEU:HD21	0.97	1.13
1:A:62:VAL:HG13	1:A:63:PRO:CD	1.77	1.12
2:B:103:TRP:CZ3	2:B:413:MET:CE	2.28	1.12
1:A:57:GLY:HA3	1:A:61:HIS:CE1	1.83	1.12
1:A:266:HIS:CD2	1:A:432:TYR:CE1	2.38	1.12
1:A:312:TYR:CE2	1:A:377:MET:CE	2.32	1.12
2:B:36:TYR:CE2	2:B:244:PHE:HE1	1.46	1.12
2:B:107:HIS:CE1	2:B:152:LEU:HD21	1.84	1.12
2:B:320:ARG:HG2	2:B:374:SER:OG	1.47	1.12
2:B:385:GLN:CG	2:B:389:LYS:HE3	1.79	1.12
1:A:31:GLN:NE2	1:A:243:ARG:HG3	1.56	1.12
1:A:62:VAL:HG12	1:A:63:PRO:HD2	1.24	1.12
1:A:182:VAL:CG1	1:A:186:ASN:ND2	2.12	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASN:HD22	2:B:105:LYS:NZ	1.45	1.12
1:A:38:SER:CA	1:A:39:ASP:N	2.11	1.12
1:A:97:GLU:CB	1:A:110:ILE:CG2	2.27	1.12
1:A:103:TYR:HD2	1:A:147:SER:CB	1.59	1.12
2:B:192:HIS:O	2:B:196:GLU:CG	1.98	1.12
2:B:286:LEU:HD11	2:B:372:LYS:HB2	1.13	1.12
2:B:287:THR:HG22	2:B:289:PRO:CD	1.79	1.12
2:B:390:ARG:O	2:B:394:GLN:HG2	1.46	1.12
2:B:154:ILE:HG21	2:B:198:THR:HG23	1.21	1.11
2:B:319:PHE:CD1	2:B:328:VAL:HG11	1.85	1.11
1:A:10:GLY:O	1:A:13:GLY:N	1.83	1.11
1:A:30:ILE:HG21	1:A:64:ARG:HG2	1.15	1.11
1:A:328:VAL:HG13	1:A:332:ILE:HD11	1.31	1.11
2:B:107:HIS:CA	2:B:152:LEU:CD1	2.25	1.11
2:B:107:HIS:NE2	2:B:152:LEU:HD23	1.64	1.11
1:A:179:THR:HG21	1:A:181:VAL:HB	1.13	1.11
1:A:184:PRO:CG	1:A:395:PHE:HD2	1.56	1.11
2:B:181:VAL:HG12	2:B:399:PHE:HZ	1.05	1.11
1:A:48:SER:OG	1:A:56:THR:HB	1.51	1.11
1:A:107:HIS:CB	1:A:148:GLY:CA	2.17	1.11
2:B:48:ARG:HH11	2:B:60:LYS:CA	1.62	1.11
2:B:201:THR:CG2	2:B:265:LEU:HD11	1.79	1.11
1:A:30:ILE:HB	1:A:64:ARG:HB2	1.24	1.11
1:A:397:LEU:HD22	1:A:401:LYS:HD2	1.27	1.11
2:B:107:HIS:CD2	2:B:152:LEU:CD2	2.34	1.11
2:B:176:LYS:HE3	2:B:207:GLU:OE2	1.49	1.11
2:B:385:GLN:HG3	2:B:389:LYS:HE3	1.21	1.11
2:B:97:SER:HB2	2:B:110:GLU:CD	1.71	1.10
2:B:111:GLY:C	2:B:115:VAL:HG23	1.69	1.10
2:B:287:THR:CB	2:B:290:GLU:CB	2.23	1.10
1:A:97:GLU:HB3	1:A:110:ILE:CG2	1.81	1.10
1:A:177:VAL:HG12	1:A:178:SER:H	1.04	1.10
1:A:191:THR:HG21	1:A:421:ALA:CB	1.81	1.10
1:A:204:VAL:HG11	1:A:209:ILE:HD11	1.10	1.10
2:B:80:SER:C	2:B:82:PRO:HD2	1.70	1.10
2:B:158:ARG:CB	2:B:197:ASN:ND2	2.10	1.10
1:A:2:ARG:O	1:A:31:GLN:HG3	1.51	1.10
1:A:266:HIS:NE2	1:A:432:TYR:HE1	1.48	1.10
2:B:107:HIS:CD2	2:B:152:LEU:CG	2.32	1.10
2:B:158:ARG:CB	2:B:197:ASN:CG	2.19	1.10
1:A:210:TYR:CZ	1:A:227:LEU:HD22	1.87	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:THR:O	2:B:398:MET:HE1	1.51	1.10
1:A:169:PHE:CZ	1:A:235:VAL:HG22	1.85	1.10
1:A:3:GLU:CA	1:A:31:GLN:HB2	1.82	1.09
1:A:105:ARG:NH2	1:A:110:ILE:HD11	1.67	1.09
1:A:176:GLN:C	1:A:177:VAL:HG23	1.71	1.09
2:B:4:ILE:CD1	2:B:30:ILE:HA	1.83	1.09
2:B:66:ILE:HG13	2:B:121:VAL:CG1	1.82	1.09
2:B:312:TYR:HA	2:B:381:SER:HB3	1.30	1.09
1:A:277:SER:OG	1:A:280:LYS:HG2	0.93	1.09
2:B:158:ARG:CD	2:B:197:ASN:CB	2.09	1.09
2:B:242:LEU:N	2:B:356:CYS:SG	2.25	1.09
1:A:22:GLU:HG2	1:A:85:GLN:HE22	0.94	1.09
1:A:70:LEU:CG	1:A:145:THR:HG22	1.81	1.09
1:A:158:SER:HB3	1:A:197:HIS:CB	1.35	1.09
1:A:174:ALA:HB1	1:A:175:PRO:HD3	1.27	1.09
1:A:174:ALA:HB1	1:A:390:ARG:HH22	1.03	1.09
2:B:44:LEU:CD2	2:B:85:GLN:HG3	1.78	1.09
2:B:278:ARG:CA	2:B:278:ARG:CB	2.30	1.09
2:B:312:TYR:O	2:B:344:VAL:HG23	1.47	1.09
1:A:100:ALA:HB1	1:A:105:ARG:HD3	1.13	1.09
1:A:183:GLU:HB3	1:A:394:LYS:HB3	1.24	1.09
2:B:3:GLU:HA	2:B:31:ASP:CB	1.83	1.09
2:B:414:ASP:OD2	3:K:253:GLU:OE2	1.67	1.09
2:B:56:ALA:HB3	2:B:62:VAL:HB	1.35	1.09
2:B:94:PHE:O	2:B:94:PHE:CD1	2.05	1.09
2:B:158:ARG:HB2	2:B:197:ASN:CG	1.72	1.09
3:K:18[B]:ARG:HH21	3:K:336:ILE:HD12	1.15	1.09
1:A:108:TYR:CE2	1:A:417:GLU:OE2	2.06	1.08
1:A:349:THR:CB	2:B:177:VAL:HG12	1.58	1.08
2:B:7:ILE:CA	2:B:66:ILE:HG23	1.75	1.08
2:B:44:LEU:HD23	2:B:85:GLN:HG3	1.12	1.08
2:B:175:PRO:CD	2:B:390:ARG:HH21	1.66	1.08
1:A:100:ALA:HB2	1:A:105:ARG:HD3	1.18	1.08
1:A:184:PRO:HG3	1:A:395:PHE:HB2	1.33	1.08
1:A:217:LEU:HG	1:A:218:ASP:H	0.96	1.08
2:B:7:ILE:HG12	2:B:66:ILE:HD13	1.09	1.08
2:B:103:TRP:HZ3	2:B:108:TYR:OH	1.33	1.08
2:B:150:GLY:O	2:B:154:ILE:HG13	1.52	1.08
3:K:252:SER:O	3:K:253:GLU:HG2	1.53	1.08
1:A:103:TYR:CD1	1:A:188:ILE:HG21	1.86	1.08
1:A:332:ILE:HD13	1:A:353:VAL:HG21	1.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ALA:HB1	2:B:272:PHE:CD2	1.87	1.08
1:A:204:VAL:HG12	1:A:209:ILE:HD11	1.09	1.08
1:A:262:TYR:HB3	1:A:263:PRO:CD	1.84	1.08
1:A:296:PHE:HE1	1:A:335:ILE:CD1	1.67	1.08
2:B:33:THR:H	2:B:59:ASN:ND2	1.47	1.08
2:B:56:ALA:HB3	2:B:62:VAL:CG2	1.81	1.08
2:B:80:SER:O	2:B:82:PRO:HD2	1.52	1.08
2:B:147:SER:OG	2:B:189:LEU:HD11	1.50	1.08
2:B:243:ARG:HH21	2:B:252:LEU:HD21	1.17	1.08
2:B:382:THR:HG21	2:B:436:GLN:OE1	1.51	1.08
1:A:237:SER:O	1:A:241:SER:OG	1.69	1.08
1:A:423:GLU:OE1	3:K:170:GLU:CG	2.01	1.08
2:B:24:ILE:O	2:B:25:SER:C	1.80	1.08
2:B:405:LEU:HD21	2:B:418:PHE:CE2	1.82	1.08
1:A:26:LEU:HD11	1:A:361:THR:HG21	1.23	1.07
1:A:250:VAL:HG13	1:A:254:GLU:HB3	1.08	1.07
2:B:36:TYR:CD2	2:B:244:PHE:HE1	1.43	1.07
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.10	1.07
1:A:24:TYR:O	1:A:26:LEU:N	1.87	1.07
1:A:100:ALA:HB2	1:A:105:ARG:CD	1.80	1.07
1:A:171:ILE:N	1:A:203:MET:HE1	1.55	1.07
1:A:250:VAL:HG21	1:A:352:LYS:HE2	1.13	1.07
2:B:313:LEU:CD2	2:B:344:VAL:CG1	2.31	1.07
2:B:313:LEU:HD22	2:B:344:VAL:HG11	1.13	1.07
2:B:346:TRP:O	2:B:347:ILE:HB	1.50	1.07
1:A:184:PRO:CG	1:A:395:PHE:HA	1.84	1.07
1:A:292:THR:HG22	1:A:319:TYR:OH	1.53	1.07
2:B:33:THR:O	2:B:59:ASN:ND2	1.87	1.07
2:B:305:CYS:SG	2:B:384:ILE:CD1	2.41	1.07
1:A:360:PRO:HG3	1:A:371:VAL:O	0.91	1.07
2:B:3:GLU:OE1	2:B:130:ASP:HB2	0.91	1.07
2:B:158:ARG:HD2	2:B:197:ASN:N	1.70	1.07
2:B:259:MET:CB	2:B:268:PHE:CE1	2.38	1.07
1:A:103:TYR:CD2	1:A:147:SER:CB	2.36	1.07
1:A:192:HIS:ND1	1:A:193:THR:N	2.03	1.06
2:B:24:ILE:C	2:B:26:ASP:N	2.01	1.06
2:B:48:ARG:HB2	2:B:61:TYR:HA	1.34	1.06
2:B:103:TRP:NE1	2:B:189:LEU:HD23	1.70	1.06
2:B:192:HIS:C	2:B:196:GLU:HG3	1.73	1.06
2:B:319:PHE:CE1	2:B:328:VAL:HG11	1.87	1.06
2:B:3:GLU:HB3	2:B:132:LEU:HD23	1.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:CD	2:B:228:ASN:HB2	1.84	1.06
2:B:35:SER:N	2:B:60:LYS:HE3	1.71	1.06
2:B:154:ILE:HD12	2:B:192:HIS:CE1	1.90	1.06
2:B:244:PHE:CG	2:B:245:PRO:HD2	1.89	1.06
2:B:397:ALA:HA	2:B:401:ARG:HD3	1.33	1.06
2:B:405:LEU:HD12	2:B:408:TYR:CG	1.88	1.06
2:B:102:ASN:HB2	2:B:105:LYS:HD2	1.33	1.06
1:A:78:VAL:HG11	1:A:87:PHE:HE1	1.19	1.06
1:A:103:TYR:CD1	1:A:188:ILE:HG22	1.89	1.06
2:B:102:ASN:HD22	2:B:105:LYS:HE3	1.17	1.06
2:B:141:LEU:CD1	2:B:172:VAL:HA	1.86	1.06
2:B:174:SER:OG	2:B:207:GLU:CB	2.02	1.06
1:A:103:TYR:OH	1:A:151:SER:CB	2.04	1.06
1:A:277:SER:OG	1:A:280:LYS:N	1.87	1.06
1:A:420:GLU:CD	3:K:170:GLU:O	1.93	1.06
2:B:53:TYR:CD1	2:B:87:PHE:CZ	2.44	1.06
2:B:107:HIS:NE2	2:B:152:LEU:CD2	2.18	1.06
2:B:192:HIS:C	2:B:196:GLU:CG	2.24	1.06
1:A:93:ILE:HD13	1:A:118:VAL:HG22	1.11	1.05
1:A:97:GLU:HB2	1:A:110:ILE:HG21	1.38	1.05
3:K:233:GLU:HG3	3:K:234:THR:H	0.90	1.05
1:A:32:PRO:O	1:A:34:GLY:N	1.89	1.05
1:A:70:LEU:HD12	1:A:145:THR:CB	1.86	1.05
2:B:7:ILE:CB	2:B:137:LEU:CD2	2.34	1.05
2:B:22:GLU:CB	2:B:83:PHE:CE2	2.39	1.05
2:B:265:LEU:HD23	2:B:267:PHE:CZ	1.92	1.05
2:B:311:ARG:CG	2:B:341:SER:O	2.04	1.05
2:B:313:LEU:N	2:B:380:ASN:O	1.86	1.05
2:B:435:TYR:O	2:B:436:GLN:CD	1.95	1.05
1:A:59:GLY:C	1:A:62:VAL:O	1.95	1.05
1:A:312:TYR:CE2	1:A:377:MET:HE1	1.89	1.05
2:B:107:HIS:HA	2:B:152:LEU:HD12	1.35	1.05
1:A:174:ALA:CB	1:A:175:PRO:HD2	1.86	1.05
2:B:41:ASP:C	2:B:42:LEU:HG	1.76	1.05
2:B:48:ARG:HH11	2:B:60:LYS:HA	1.17	1.05
2:B:141:LEU:HD12	2:B:172:VAL:CA	1.86	1.05
2:B:259:MET:CE	2:B:379:GLY:CA	2.29	1.05
1:A:205:ASP:OD1	1:A:303:VAL:CG2	1.98	1.05
1:A:217:LEU:HD11	1:A:368:LEU:CD2	1.86	1.05
2:B:32:PRO:HB2	2:B:59:ASN:ND2	1.00	1.05
2:B:103:TRP:HD1	2:B:189:LEU:HD21	1.17	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:LYS:O	2:B:330:GLU:HG3	1.56	1.05
1:A:31:GLN:HE22	1:A:243:ARG:HG3	0.94	1.04
1:A:256:GLN:HB3	2:B:407:TRP:CH2	1.91	1.04
1:A:312:TYR:CD2	1:A:381:THR:CG2	2.40	1.04
1:A:45:GLY:O	1:A:46:ASP:CB	1.98	1.04
1:A:183:GLU:HB3	1:A:394:LYS:CB	1.87	1.04
2:B:102:ASN:OD1	2:B:408:TYR:CE1	2.09	1.04
2:B:44:LEU:HD21	2:B:86:ILE:N	1.67	1.04
2:B:70:LEU:CD1	2:B:94:PHE:HD2	1.47	1.04
2:B:244:PHE:CD2	2:B:245:PRO:CD	2.39	1.04
1:A:30:ILE:HB	1:A:64:ARG:CB	1.87	1.04
1:A:121:ARG:O	1:A:125:LEU:HG	1.56	1.04
1:A:306:ASP:OD1	1:A:308:ARG:CB	2.05	1.04
2:B:3:GLU:C	2:B:4:ILE:HG13	1.77	1.04
2:B:4:ILE:CD1	2:B:30:ILE:HG22	1.88	1.04
2:B:19:LYS:HD2	2:B:228:ASN:HB2	1.39	1.04
2:B:56:ALA:O	2:B:59:ASN:O	1.73	1.04
2:B:172:VAL:HG13	2:B:173:PRO:HD2	1.05	1.04
2:B:308:ARG:HD3	2:B:342:TYR:CE2	1.92	1.04
1:A:126:ALA:O	1:A:132:LEU:HD11	1.57	1.04
2:B:69:ASP:OD2	2:B:74:THR:CB	2.06	1.04
2:B:70:LEU:HD23	2:B:145:THR:HG22	1.04	1.04
2:B:147:SER:HB3	2:B:189:LEU:CG	1.77	1.04
2:B:147:SER:CA	2:B:189:LEU:CD1	2.36	1.04
1:A:62:VAL:HG13	1:A:63:PRO:HD2	1.07	1.03
1:A:155:GLU:CG	1:A:192:HIS:CD2	2.41	1.03
2:B:66:ILE:HG13	2:B:121:VAL:HG11	1.04	1.03
2:B:92:PHE:HD2	2:B:114:LEU:HD11	1.04	1.03
2:B:172:VAL:HG12	2:B:173:PRO:CD	1.88	1.03
2:B:275:LEU:HG	2:B:294:GLN:NE2	1.73	1.03
1:A:45:GLY:O	1:A:46:ASP:CG	1.96	1.03
1:A:179:THR:HG21	1:A:181:VAL:CB	1.87	1.03
2:B:44:LEU:C	2:B:47:GLU:HG3	1.79	1.03
2:B:194:LEU:HA	2:B:265:LEU:CB	1.88	1.03
1:A:193:THR:O	1:A:194:THR:O	1.77	1.03
1:A:217:LEU:CD2	1:A:368:LEU:HD11	1.88	1.03
1:A:266:HIS:NE2	1:A:432:TYR:CE1	2.26	1.03
1:A:424:ASP:OD1	3:K:307:ARG:CZ	2.05	1.03
2:B:49:ILE:C	2:B:61:TYR:CD2	2.32	1.03
3:K:233:GLU:HG3	3:K:234:THR:N	1.73	1.03
2:B:69:ASP:CG	2:B:74:THR:HB	1.77	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:VAL:O	2:B:82:PRO:HG2	1.59	1.02
2:B:135:PHE:CD2	2:B:166:MET:HE1	1.94	1.02
2:B:275:LEU:HG	2:B:294:GLN:HE22	1.21	1.02
2:B:287:THR:O	2:B:291:LEU:HG	0.85	1.02
1:A:16:ILE:HD13	1:A:138:PHE:HD1	0.88	1.02
2:B:4:ILE:HD12	2:B:30:ILE:O	1.57	1.02
2:B:6:HIS:CE1	2:B:30:ILE:CD1	2.32	1.02
2:B:145:THR:O	2:B:149:MET:CB	2.05	1.02
1:A:191:THR:O	1:A:194:THR:HB	1.56	1.02
2:B:7:ILE:HG12	2:B:66:ILE:HG21	1.34	1.02
2:B:80:SER:O	2:B:82:PRO:CD	2.07	1.02
1:A:206:ASN:O	1:A:210:TYR:HD2	1.41	1.02
1:A:328:VAL:HG13	1:A:332:ILE:CD1	1.90	1.02
2:B:23:VAL:HG22	6:B:502:TXL:H333	1.41	1.02
2:B:268:PHE:CD1	2:B:380:ASN:ND2	2.28	1.02
1:A:4:CYS:HB2	1:A:30:ILE:HG23	1.03	1.02
2:B:107:HIS:CE1	2:B:152:LEU:CD2	2.42	1.02
1:A:70:LEU:CG	1:A:145:THR:CG2	2.36	1.01
2:B:49:ILE:C	2:B:61:TYR:HD2	1.63	1.01
1:A:36:MET:SD	1:A:61:HIS:N	2.33	1.01
1:A:252:LEU:HA	1:A:255:PHE:HD2	1.18	1.01
2:B:19:LYS:HB2	2:B:228:ASN:HB3	1.42	1.01
2:B:151:THR:CG2	2:B:192:HIS:ND1	2.14	1.01
2:B:175:PRO:O	2:B:176:LYS:HG2	1.49	1.01
2:B:190:SER:O	2:B:193:GLN:N	1.92	1.01
2:B:201:THR:HG23	2:B:265:LEU:CD1	1.91	1.01
1:A:115:ILE:HD11	1:A:152:LEU:HG	1.40	1.01
2:B:384:ILE:O	2:B:386:GLU:N	1.93	1.01
1:A:405:VAL:HG22	1:A:409:VAL:HG23	1.39	1.01
2:B:286:LEU:CD1	2:B:372:LYS:CB	2.39	1.01
2:B:370:GLY:C	6:B:502:TXL:H183	1.81	1.01
1:A:108:TYR:O	1:A:112:LYS:HD2	1.61	1.00
1:A:296:PHE:CZ	1:A:335:ILE:HG21	1.95	1.00
2:B:200:GLU:OE2	2:B:256:ALA:HA	1.56	1.00
2:B:260:VAL:CG1	2:B:262:PHE:O	2.08	1.00
2:B:385:GLN:CG	2:B:389:LYS:CE	2.37	1.00
1:A:103:TYR:HD2	1:A:189:LEU:CD2	1.59	1.00
1:A:343:PHE:HE2	1:A:351:PHE:HZ	1.08	1.00
2:B:242:LEU:HD22	2:B:250:ALA:H	1.23	1.00
2:B:396:THR:OG1	2:B:422:GLU:OE2	1.79	1.00
2:B:422:GLU:O	2:B:426:ASN:HB2	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.42	1.00
1:A:324:VAL:HB	1:A:327:ASP:CG	1.82	1.00
2:B:343:PHE:HB3	2:B:350:ASN:HD22	1.26	1.00
2:B:103:TRP:NE1	2:B:148:GLY:HA2	1.75	1.00
1:A:103:TYR:CE1	1:A:188:ILE:HG22	1.96	1.00
1:A:143:GLY:O	1:A:146:GLY:N	1.95	1.00
1:A:217:LEU:HG	1:A:218:ASP:N	1.76	1.00
1:A:431:ASP:HA	3:K:303:PHE:CD1	1.96	1.00
2:B:296:PHE:CE1	2:B:335:VAL:HG11	1.96	1.00
2:B:313:LEU:HA	2:B:344:VAL:HG21	1.43	1.00
2:B:194:LEU:HA	2:B:265:LEU:HB3	1.44	1.00
2:B:320:ARG:HG2	2:B:374:SER:HG	1.25	1.00
2:B:405:LEU:HD12	2:B:408:TYR:HB2	1.03	1.00
1:A:88:HIS:CG	1:A:89:PRO:HD2	1.95	1.00
1:A:174:ALA:CB	1:A:390:ARG:HH22	1.75	1.00
1:A:185:TYR:CD2	1:A:408:TYR:OH	1.85	1.00
1:A:219:ILE:CG2	1:A:219:ILE:CG1	2.40	1.00
1:A:433:GLU:O	1:A:437:VAL:CG2	2.10	1.00
2:B:243:ARG:NH2	2:B:252:LEU:HD11	1.77	1.00
1:A:312:TYR:O	1:A:344:VAL:HG23	1.58	0.99
1:A:397:LEU:CD2	1:A:401:LYS:CD	2.40	0.99
1:A:424:ASP:HA	3:K:307:ARG:NH2	1.77	0.99
2:B:24:ILE:C	2:B:26:ASP:H	1.55	0.99
2:B:111:GLY:O	2:B:115:VAL:N	1.95	0.99
2:B:181:VAL:HG22	2:B:404:PHE:CE2	1.97	0.99
2:B:275:LEU:HD11	2:B:300:ASN:ND2	1.78	0.99
2:B:284:ARG:HD2	2:B:290:GLU:OE1	1.62	0.99
1:A:45:GLY:O	1:A:46:ASP:HB2	1.60	0.99
1:A:145:THR:O	1:A:149:PHE:HB3	1.62	0.99
2:B:192:HIS:CB	2:B:196:GLU:HG3	1.90	0.99
1:A:256:GLN:O	1:A:260:VAL:HG23	1.61	0.99
2:B:191:VAL:HG21	2:B:421:ALA:HA	1.42	0.99
2:B:312:TYR:HA	2:B:381:SER:HA	1.43	0.99
1:A:184:PRO:CD	1:A:395:PHE:HA	1.91	0.99
1:A:276:ILE:HD12	1:A:371:VAL:HG22	1.41	0.99
1:A:397:LEU:HD22	1:A:401:LYS:CD	1.93	0.99
1:A:31:GLN:HE22	1:A:243:ARG:CD	1.67	0.99
2:B:44:LEU:HD11	2:B:86:ILE:O	1.63	0.99
1:A:204:VAL:HG23	1:A:231:ILE:HG23	1.41	0.99
1:A:104:ALA:HA	1:A:108:TYR:CD2	1.97	0.99
1:A:174:ALA:HB3	1:A:175:PRO:HD2	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:O	1:A:378:LEU:HA	1.61	0.99
1:A:78:VAL:CG1	1:A:87:PHE:CE1	2.46	0.99
1:A:205:ASP:CB	1:A:303:VAL:HA	1.92	0.99
1:A:343:PHE:CZ	1:A:351:PHE:CZ	2.50	0.99
1:A:416:GLY:CA	3:K:169:ARG:NH2	2.25	0.99
2:B:70:LEU:HD11	2:B:94:PHE:CD2	1.92	0.99
2:B:384:ILE:C	2:B:386:GLU:H	1.52	0.99
1:A:242:LEU:HB3	1:A:250:VAL:O	1.63	0.99
1:A:270:ALA:O	1:A:302:MET:HG2	1.63	0.99
1:A:312:TYR:O	1:A:344:VAL:HG22	1.62	0.99
2:B:295:MET:HE1	2:B:375:ALA:HB1	1.03	0.99
1:A:22:GLU:HG2	1:A:85:GLN:NE2	1.78	0.98
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.58	0.98
2:B:199:ASP:OD2	2:B:256:ALA:HB2	1.62	0.98
2:B:405:LEU:HD22	2:B:418:PHE:CE1	1.98	0.98
2:B:70:LEU:HD23	2:B:145:THR:CG2	1.93	0.98
2:B:155:SER:O	2:B:159:GLU:HG3	1.63	0.98
2:B:343:PHE:HD1	2:B:350:ASN:ND2	1.62	0.98
1:A:42:ILE:O	1:A:42:ILE:HG22	1.60	0.98
1:A:72:PRO:O	1:A:76:ASP:N	1.96	0.98
1:A:97:GLU:HB3	1:A:110:ILE:HG21	1.36	0.98
2:B:154:ILE:CG2	2:B:198:THR:CG2	2.40	0.98
1:A:103:TYR:CE2	1:A:189:LEU:HA	1.98	0.98
2:B:102:ASN:HB2	2:B:105:LYS:CD	1.92	0.98
2:B:173:PRO:CG	2:B:391:ILE:HD11	1.92	0.98
2:B:275:LEU:CD1	2:B:294:GLN:HE21	1.75	0.98
2:B:79:ARG:O	2:B:80:SER:CB	2.10	0.98
1:A:51:THR:HG22	1:A:52:PHE:N	1.74	0.98
1:A:68:VAL:CG1	1:A:149:PHE:CZ	2.47	0.98
1:A:76:ASP:O	1:A:80:THR:N	1.97	0.98
2:B:174:SER:OG	2:B:207:GLU:HB2	1.63	0.98
1:A:30:ILE:O	1:A:32:PRO:CD	2.08	0.98
2:B:36:TYR:CD2	2:B:244:PHE:CE1	2.22	0.98
2:B:173:PRO:HG3	2:B:391:ILE:HD11	1.45	0.98
2:B:286:LEU:HD11	2:B:371:LEU:O	1.62	0.98
2:B:384:ILE:C	2:B:386:GLU:N	2.11	0.98
2:B:182:VAL:HG13	2:B:186:ASN:HD22	1.29	0.97
1:A:101:ASN:O	1:A:102:ASN:ND2	1.97	0.97
1:A:206:ASN:ND2	1:A:227:LEU:HD23	1.79	0.97
2:B:414:ASP:HB2	3:K:253:GLU:CD	1.83	0.97
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:HB2	2:B:65:ALA:HA	1.46	0.97
2:B:102:ASN:ND2	2:B:105:LYS:NZ	2.12	0.97
2:B:103:TRP:CD1	2:B:148:GLY:CA	2.48	0.97
2:B:201:THR:HG23	2:B:265:LEU:HD11	0.97	0.97
1:A:194:THR:HG22	1:A:195:LEU:HG	1.44	0.97
1:A:419:SER:HB2	3:K:172:PRO:HB3	1.46	0.97
1:A:429:GLU:O	1:A:433:GLU:HG3	1.63	0.97
2:B:181:VAL:HG13	2:B:399:PHE:CE1	1.97	0.97
1:A:51:THR:HG22	1:A:52:PHE:H	1.26	0.97
1:A:115:ILE:HG21	1:A:152:LEU:HD21	1.45	0.97
1:A:241:SER:HB2	1:A:356:ASN:ND2	1.78	0.97
1:A:250:VAL:HG13	1:A:254:GLU:HG2	1.44	0.97
2:B:142:GLY:CA	2:B:182:VAL:HG22	1.94	0.97
2:B:262:PHE:HB3	2:B:263:PRO:HD2	1.43	0.97
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.06	0.97
1:A:217:LEU:CD1	1:A:368:LEU:HD21	1.95	0.97
1:A:9:VAL:CG1	1:A:150:THR:CG2	2.42	0.97
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.29	0.97
1:A:177:VAL:CG1	1:A:178:SER:H	1.78	0.97
1:A:241:SER:HB2	1:A:356:ASN:HD22	1.27	0.97
1:A:310:GLY:O	1:A:342:GLN:OE1	1.82	0.97
1:A:115:ILE:HD13	1:A:156:ARG:NE	1.80	0.97
1:A:217:LEU:HD13	1:A:368:LEU:HD11	1.02	0.97
1:A:313:MET:CE	1:A:346:TRP:CH2	2.47	0.97
1:A:107:HIS:HB2	1:A:148:GLY:HA3	1.01	0.97
2:B:111:GLY:O	2:B:115:VAL:CG2	2.12	0.97
2:B:7:ILE:HB	2:B:137:LEU:HD23	1.01	0.96
2:B:33:THR:N	2:B:59:ASN:ND2	2.04	0.96
2:B:103:TRP:HE3	2:B:413:MET:HE1	1.27	0.96
2:B:158:ARG:CA	2:B:197:ASN:ND2	1.74	0.96
3:K:233:GLU:CG	3:K:234:THR:H	1.76	0.96
1:A:424:ASP:CA	3:K:307:ARG:CZ	2.43	0.96
2:B:19:LYS:CG	2:B:228:ASN:HB2	1.86	0.96
2:B:206:ASN:O	2:B:210:TYR:CE2	2.18	0.96
2:B:206:ASN:O	2:B:210:TYR:CD2	2.18	0.96
2:B:70:LEU:HD11	2:B:94:PHE:CE2	2.00	0.96
2:B:229:HIS:CD2	6:B:502:TXL:H37	1.98	0.96
1:A:108:TYR:HA	1:A:112:LYS:HE3	1.47	0.96
2:B:7:ILE:CB	2:B:137:LEU:HD23	1.95	0.96
1:A:78:VAL:HG11	1:A:87:PHE:CE1	2.00	0.96
1:A:177:VAL:HG12	1:A:178:SER:N	1.79	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:HG2	2:B:4:ILE:H	1.27	0.96
2:B:39:ASP:O	2:B:40:SER:OG	1.82	0.96
2:B:405:LEU:HD11	2:B:408:TYR:HB3	1.44	0.96
1:A:2:ARG:NH2	2:B:71:GLU:CB	2.22	0.96
1:A:204:VAL:HG12	1:A:209:ILE:CD1	1.87	0.96
1:A:422:ARG:O	1:A:426:ALA:HB2	1.63	0.96
2:B:22:GLU:CD	2:B:83:PHE:CG	2.39	0.96
2:B:229:HIS:HE1	6:B:502:TXL:H343	1.30	0.96
2:B:229:HIS:HD2	6:B:502:TXL:C38	1.47	0.96
2:B:287:THR:CG2	2:B:289:PRO:CD	2.38	0.96
1:A:31:GLN:N	1:A:32:PRO:HD2	1.81	0.96
2:B:260:VAL:HG13	2:B:266:HIS:ND1	1.78	0.96
2:B:346:TRP:CE3	2:B:347:ILE:CD1	2.43	0.96
1:A:2:ARG:HG2	1:A:133:GLN:CD	1.85	0.96
1:A:119:LEU:HD11	1:A:156:ARG:HD3	1.48	0.96
1:A:191:THR:O	1:A:194:THR:CB	2.14	0.96
2:B:107:HIS:C	2:B:152:LEU:CD1	2.27	0.96
2:B:208:ALA:CB	2:B:303:ALA:O	2.13	0.96
1:A:68:VAL:HG11	1:A:149:PHE:HZ	1.30	0.95
1:A:333:ALA:O	1:A:337:THR:HG23	1.66	0.95
2:B:275:LEU:HD12	2:B:294:GLN:HE21	1.29	0.95
1:A:372:GLN:O	1:A:373:ARG:HG3	1.65	0.95
2:B:53:TYR:HE1	2:B:89:PRO:HG3	1.29	0.95
2:B:346:TRP:O	2:B:347:ILE:CB	2.09	0.95
1:A:68:VAL:HG11	1:A:149:PHE:CE1	2.01	0.95
1:A:205:ASP:OD1	1:A:303:VAL:HG22	1.18	0.95
1:A:250:VAL:CG2	1:A:352:LYS:CE	2.43	0.95
1:A:309:HIS:CG	1:A:386:GLU:OE2	2.19	0.95
2:B:181:VAL:O	2:B:399:PHE:CE2	2.19	0.95
1:A:212:ILE:HD13	1:A:230:LEU:HD21	1.49	0.95
1:A:424:ASP:CA	3:K:307:ARG:NH2	2.30	0.95
1:A:426:ALA:O	1:A:429:GLU:N	2.00	0.95
2:B:243:ARG:HH21	2:B:252:LEU:CD2	1.78	0.95
2:B:346:TRP:CZ3	2:B:347:ILE:CG1	2.45	0.95
1:A:2:ARG:HH21	2:B:71:GLU:HB3	0.79	0.95
1:A:171:ILE:N	1:A:203:MET:CE	2.24	0.95
1:A:141:PHE:O	1:A:182:VAL:HG13	1.66	0.95
2:B:101:ASN:O	2:B:102:ASN:CG	2.05	0.95
1:A:184:PRO:CB	1:A:395:PHE:CD2	2.45	0.95
1:A:313:MET:HE3	1:A:346:TRP:CH2	2.01	0.95
2:B:4:ILE:CD1	2:B:30:ILE:O	2.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ARG:O	2:B:80:SER:HB3	1.66	0.95
2:B:151:THR:HG22	2:B:192:HIS:CD2	1.96	0.95
2:B:343:PHE:HD1	2:B:350:ASN:CG	1.67	0.95
2:B:426:ASN:O	2:B:429:VAL:N	2.00	0.95
1:A:16:ILE:CD1	1:A:138:PHE:HD1	1.78	0.95
1:A:229:ARG:O	1:A:233:GLN:HG3	1.66	0.95
2:B:3:GLU:HA	2:B:31:ASP:HB3	1.47	0.95
2:B:151:THR:HB	2:B:192:HIS:HD2	1.31	0.95
2:B:147:SER:HA	2:B:189:LEU:HD13	1.47	0.95
2:B:274:PRO:O	2:B:276:THR:HG23	1.67	0.95
2:B:287:THR:HG21	2:B:289:PRO:HG2	1.49	0.95
1:A:158:SER:HB2	1:A:197:HIS:CB	1.67	0.95
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.49	0.95
1:A:314:ALA:HB3	1:A:380:ASN:HD22	1.31	0.95
2:B:259:MET:HB3	2:B:268:PHE:CZ	2.02	0.95
1:A:141:PHE:O	1:A:186:ASN:ND2	1.58	0.94
2:B:398:MET:O	2:B:401:ARG:HB3	1.66	0.94
2:B:174:SER:OG	2:B:207:GLU:HB3	1.65	0.94
1:A:59:GLY:CA	1:A:62:VAL:O	2.15	0.94
2:B:184:PRO:CD	2:B:399:PHE:CE2	2.37	0.94
1:A:20:CYS:O	1:A:24:TYR:HD2	1.46	0.94
1:A:252:LEU:HA	1:A:255:PHE:CD2	2.02	0.94
1:A:294:ALA:O	1:A:300:ASN:ND2	1.99	0.94
1:A:257:THR:CG2	2:B:407:TRP:CE3	2.50	0.94
1:A:405:VAL:CG2	1:A:405:VAL:CG1	2.44	0.94
2:B:19:LYS:HG3	2:B:228:ASN:HB2	1.43	0.94
2:B:241:CYS:SG	2:B:320:ARG:HD3	2.08	0.94
2:B:287:THR:HG22	2:B:290:GLU:H	1.29	0.94
2:B:382:THR:HG23	2:B:436:GLN:OE1	1.64	0.94
1:A:3:GLU:HA	1:A:31:GLN:HB2	0.94	0.94
2:B:56:ALA:HB1	2:B:60:LYS:O	1.68	0.94
2:B:433:GLN:HG2	2:B:437:ASP:OD2	1.65	0.94
1:A:103:TYR:CE2	1:A:189:LEU:CD2	2.38	0.94
1:A:212:ILE:HD11	1:A:230:LEU:HD22	0.96	0.94
1:A:217:LEU:HD22	1:A:368:LEU:HD11	1.47	0.94
2:B:182:VAL:CG1	2:B:186:ASN:ND2	2.30	0.94
1:A:65:ALA:CB	1:A:91:GLN:OE1	2.16	0.94
2:B:126:SER:HA	2:B:132:LEU:HD12	1.50	0.94
2:B:295:MET:CE	2:B:375:ALA:CA	2.45	0.94
2:B:319:PHE:HE1	2:B:353:THR:HG23	0.77	0.94
2:B:158:ARG:CD	2:B:197:ASN:CA	2.39	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PHE:CE2	1:A:351:PHE:HZ	1.81	0.93
1:A:397:LEU:HA	1:A:401:LYS:CB	1.96	0.93
2:B:97:SER:O	2:B:110:GLU:OE2	1.84	0.93
2:B:279:GLY:C	2:B:281:GLN:H	1.62	0.93
1:A:36:MET:SD	1:A:61:HIS:CA	2.56	0.93
1:A:119:LEU:O	1:A:122:ILE:HG22	1.65	0.93
1:A:369:ALA:HB2	1:A:371:VAL:HG23	1.46	0.93
1:A:64:ARG:NH2	1:A:132:LEU:CD2	2.05	0.93
2:B:48:ARG:NH1	2:B:60:LYS:HA	1.83	0.93
2:B:71:GLU:O	2:B:73:GLY:N	2.01	0.93
1:A:181:VAL:O	1:A:184:PRO:O	1.87	0.93
1:A:272:TYR:CD1	1:A:274:PRO:O	2.22	0.93
1:A:312:TYR:CA	1:A:381:THR:HG22	1.99	0.93
2:B:151:THR:HG22	2:B:192:HIS:NE2	1.83	0.93
2:B:184:PRO:CD	2:B:398:MET:SD	2.57	0.93
2:B:274:PRO:HB3	2:B:371:LEU:HD21	1.50	0.93
2:B:343:PHE:CD1	2:B:350:ASN:ND2	2.37	0.93
2:B:414:ASP:CB	3:K:253:GLU:CD	2.37	0.93
3:K:159:ASN:HD22	3:K:161:LYS:HG3	1.26	0.93
1:A:217:LEU:CD1	1:A:368:LEU:CD2	2.46	0.93
1:A:250:VAL:HG22	1:A:352:LYS:HE2	1.49	0.93
2:B:48:ARG:NH1	2:B:60:LYS:CA	2.31	0.93
2:B:343:PHE:HB3	2:B:350:ASN:ND2	1.83	0.93
1:A:258:ASN:OD1	1:A:352:LYS:HD2	1.69	0.93
1:A:420:GLU:OE1	3:K:170:GLU:O	1.87	0.93
2:B:75:MET:HE2	2:B:79:ARG:CD	1.99	0.93
2:B:142:GLY:HA2	2:B:185:TYR:CD1	2.03	0.93
1:A:15:GLN:HA	1:A:18:ASN:ND2	1.83	0.93
1:A:204:VAL:CG2	1:A:231:ILE:CG2	2.24	0.93
2:B:142:GLY:HA2	2:B:182:VAL:HG22	1.49	0.93
2:B:154:ILE:HD12	2:B:192:HIS:NE2	1.83	0.93
1:A:250:VAL:CG1	1:A:254:GLU:CG	2.46	0.93
1:A:405:VAL:CG2	1:A:409:VAL:HG23	1.98	0.93
2:B:101:ASN:O	2:B:102:ASN:CB	2.17	0.93
3:K:252:SER:HA	3:K:275:LEU:HD11	1.50	0.93
1:A:108:TYR:O	1:A:112:LYS:CG	2.17	0.92
1:A:256:GLN:O	1:A:260:VAL:CG2	2.16	0.92
1:A:369:ALA:HB3	1:A:371:VAL:HG23	1.50	0.92
1:A:83:TYR:CD2	1:A:83:TYR:O	2.22	0.92
1:A:155:GLU:HG2	1:A:196:GLU:HG3	1.51	0.92
1:A:423:GLU:OE2	3:K:172:PRO:CA	2.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:CA	2:B:66:ILE:CG2	2.38	0.92
2:B:106:GLY:O	2:B:111:GLY:HA3	1.70	0.92
2:B:275:LEU:CG	2:B:294:GLN:NE2	2.32	0.92
1:A:31:GLN:HE22	1:A:243:ARG:CB	1.81	0.92
1:A:59:GLY:HA2	1:A:62:VAL:O	1.70	0.92
1:A:106:GLY:O	1:A:111:GLY:HA3	1.70	0.92
1:A:53:PHE:CA	1:A:88:HIS:NE2	2.20	0.92
1:A:107:HIS:CD2	1:A:148:GLY:O	2.23	0.92
2:B:107:HIS:ND1	2:B:152:LEU:HD21	1.85	0.92
2:B:386:GLU:O	2:B:388:PHE:N	2.01	0.92
1:A:238:ILE:HG23	1:A:255:PHE:CE1	2.05	0.92
1:A:250:VAL:HG22	1:A:254:GLU:HG2	1.50	0.92
1:A:288:VAL:HG22	1:A:373:ARG:HD3	0.93	0.92
3:K:216:ARG:HH11	3:K:216:ARG:HG3	1.33	0.92
1:A:277:SER:H	1:A:280:LYS:CG	1.82	0.92
1:A:349:THR:CG2	2:B:177:VAL:CG1	2.46	0.92
1:A:428:LEU:O	1:A:432:TYR:HB2	1.70	0.92
1:A:107:HIS:CB	1:A:148:GLY:C	2.36	0.92
1:A:158:SER:HB3	1:A:197:HIS:HB2	1.51	0.92
1:A:184:PRO:CG	1:A:395:PHE:CA	2.47	0.92
1:A:184:PRO:CG	1:A:395:PHE:CB	2.45	0.92
2:B:33:THR:H	2:B:59:ASN:HD22	0.93	0.92
1:A:107:HIS:HD2	1:A:148:GLY:O	1.51	0.91
2:B:49:ILE:CA	2:B:61:TYR:HD2	1.82	0.91
2:B:70:LEU:CD2	2:B:145:THR:HG22	1.98	0.91
2:B:104:ALA:HA	2:B:108:TYR:HD2	1.20	0.91
2:B:181:VAL:O	2:B:399:PHE:HE2	1.50	0.91
2:B:158:ARG:HD2	2:B:197:ASN:HA	1.52	0.91
2:B:241:CYS:O	2:B:242:LEU:HB2	1.69	0.91
1:A:332:ILE:HD13	1:A:353:VAL:CG2	1.99	0.91
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.05	0.91
2:B:126:SER:HA	2:B:132:LEU:CD1	2.01	0.91
2:B:19:LYS:CB	2:B:228:ASN:CB	2.40	0.91
2:B:70:LEU:CD1	2:B:94:PHE:CE2	2.52	0.91
1:A:26:LEU:CD1	1:A:361:THR:OG1	2.19	0.91
1:A:103:TYR:HE2	1:A:189:LEU:HA	1.32	0.91
1:A:103:TYR:CG	1:A:188:ILE:CG2	2.54	0.91
1:A:277:SER:H	1:A:280:LYS:HG3	1.34	0.91
1:A:420:GLU:CD	3:K:170:GLU:H	1.73	0.91
2:B:78:VAL:C	2:B:82:PRO:HG2	1.91	0.91
1:A:349:THR:CG2	2:B:177:VAL:HG12	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:CD2	2:B:86:ILE:H	1.61	0.91
2:B:319:PHE:CZ	2:B:328:VAL:CG1	2.54	0.91
2:B:24:ILE:O	2:B:27:GLU:N	2.04	0.91
2:B:184:PRO:CB	2:B:399:PHE:CG	2.41	0.91
2:B:102:ASN:ND2	2:B:105:LYS:CE	2.33	0.91
2:B:260:VAL:HG12	2:B:262:PHE:O	1.69	0.91
1:A:9:VAL:HG11	1:A:150:THR:HG21	1.53	0.91
1:A:100:ALA:HB1	1:A:105:ARG:CD	1.91	0.91
1:A:115:ILE:HD13	1:A:152:LEU:CG	2.01	0.91
1:A:250:VAL:HG22	1:A:352:LYS:CE	2.00	0.91
2:B:75:MET:CE	2:B:79:ARG:HD3	1.99	0.90
2:B:229:HIS:NE2	6:B:502:TXL:H343	1.82	0.90
2:B:229:HIS:CB	6:B:502:TXL:H38	2.01	0.90
2:B:312:TYR:CA	2:B:381:SER:HB3	2.01	0.90
1:A:420:GLU:OE2	3:K:170:GLU:O	1.89	0.90
2:B:11:GLN:HB3	5:B:501:GDP:PA	2.11	0.90
2:B:14:ASN:HB3	2:B:74:THR:CG2	2.01	0.90
2:B:56:ALA:HB3	2:B:62:VAL:HG23	1.54	0.90
2:B:158:ARG:CG	2:B:197:ASN:CG	2.38	0.90
2:B:268:PHE:HE1	2:B:380:ASN:ND2	1.65	0.90
1:A:72:PRO:O	1:A:75:ILE:CG2	2.19	0.90
1:A:328:VAL:CG1	1:A:353:VAL:HG11	2.00	0.90
2:B:66:ILE:CG1	2:B:121:VAL:HG11	1.99	0.90
1:A:254:GLU:OE1	2:B:101:ASN:OD1	1.87	0.90
1:A:305:CYS:O	1:A:307:PRO:HD3	1.71	0.90
2:B:200:GLU:HB3	2:B:268:PHE:HE2	1.37	0.90
2:B:405:LEU:CD2	2:B:418:PHE:HZ	1.84	0.90
2:B:44:LEU:CG	2:B:85:GLN:HG3	2.02	0.90
2:B:158:ARG:HA	2:B:197:ASN:HD21	1.35	0.90
2:B:183:GLU:HB2	2:B:184:PRO:HD3	0.90	0.90
2:B:229:HIS:CG	6:B:502:TXL:C38	2.41	0.90
1:A:257:THR:HG22	2:B:407:TRP:HE3	1.36	0.90
2:B:185:TYR:O	2:B:189:LEU:HG	1.72	0.90
2:B:243:ARG:NH2	2:B:252:LEU:HD21	1.86	0.90
1:A:184:PRO:HB3	1:A:395:PHE:HD2	1.33	0.90
2:B:39:ASP:O	2:B:40:SER:CB	2.16	0.90
2:B:259:MET:CB	2:B:268:PHE:CZ	2.55	0.90
2:B:275:LEU:CD1	2:B:294:GLN:NE2	2.35	0.90
1:A:67:PHE:HB2	1:A:92:LEU:HD23	1.53	0.90
1:A:312:TYR:CD2	1:A:381:THR:HG21	2.06	0.90
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:LEU:CD1	2:B:418:PHE:HZ	1.85	0.90
1:A:5:ILE:HG21	1:A:135:PHE:HE1	1.35	0.90
1:A:107:HIS:CG	1:A:148:GLY:CA	2.54	0.90
1:A:328:VAL:HG12	1:A:332:ILE:HD12	1.53	0.90
2:B:4:ILE:HD13	2:B:30:ILE:HG22	0.93	0.90
2:B:86:ILE:HD12	2:B:91:ASN:HD21	1.33	0.90
1:A:3:GLU:O	1:A:132:LEU:C	2.08	0.90
1:A:204:VAL:HG11	1:A:209:ILE:CD1	1.92	0.90
1:A:206:ASN:O	1:A:210:TYR:CD2	2.25	0.90
2:B:151:THR:CG2	2:B:192:HIS:NE2	2.35	0.90
1:A:405:VAL:HG22	1:A:409:VAL:CG2	2.01	0.89
2:B:102:ASN:ND2	2:B:105:LYS:HE3	1.85	0.89
2:B:192:HIS:HA	2:B:196:GLU:HG2	1.53	0.89
2:B:94:PHE:CD1	2:B:97:SER:HB3	2.06	0.89
2:B:189:LEU:O	2:B:193:GLN:CG	2.19	0.89
2:B:312:TYR:CA	2:B:381:SER:CB	2.49	0.89
1:A:93:ILE:HD13	1:A:118:VAL:CG2	2.01	0.89
1:A:155:GLU:O	1:A:159:VAL:HG23	1.72	0.89
1:A:276:ILE:O	1:A:368:LEU:CB	2.21	0.89
1:A:420:GLU:OE1	3:K:170:GLU:N	2.05	0.89
2:B:172:VAL:HG11	2:B:387:LEU:HD11	1.54	0.89
2:B:184:PRO:HD2	2:B:399:PHE:CE2	2.06	0.89
2:B:278:ARG:O	2:B:281:GLN:HB3	1.71	0.89
1:A:431:ASP:HA	3:K:303:PHE:CE1	2.07	0.89
2:B:239:THR:O	2:B:243:ARG:HD2	0.72	0.89
1:A:30:ILE:C	1:A:32:PRO:HD3	1.81	0.89
1:A:100:ALA:HB1	1:A:105:ARG:HB3	1.55	0.89
1:A:194:THR:HG22	1:A:195:LEU:H	1.38	0.89
2:B:25:SER:O	2:B:27:GLU:HG3	1.73	0.89
2:B:295:MET:HE3	2:B:375:ALA:HB1	0.91	0.89
2:B:311:ARG:O	2:B:382:THR:N	2.05	0.89
1:A:64:ARG:HH22	1:A:132:LEU:HD22	0.76	0.89
1:A:72:PRO:HA	1:A:75:ILE:CG2	2.02	0.89
1:A:103:TYR:H	1:A:408:TYR:HE1	0.96	0.89
1:A:183:GLU:OE2	1:A:394:LYS:NZ	1.77	0.89
1:A:250:VAL:HG13	1:A:352:LYS:NZ	1.86	0.89
2:B:80:SER:O	2:B:82:PRO:N	2.05	0.89
1:A:291:ILE:CD1	1:A:373:ARG:HB3	2.03	0.89
1:A:326:LYS:NZ	2:B:214:PHE:CE2	2.40	0.89
1:A:4:CYS:CB	1:A:30:ILE:HG23	1.99	0.89
1:A:276:ILE:HG21	1:A:282:TYR:CD1	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:HE21	2:B:21:TRP:HE1	1.21	0.89
2:B:173:PRO:HG3	2:B:391:ILE:CD1	2.03	0.89
2:B:405:LEU:HD13	2:B:408:TYR:HD2	0.74	0.89
1:A:328:VAL:CG1	1:A:332:ILE:CD1	2.50	0.89
1:A:191:THR:CG2	1:A:421:ALA:HB1	2.03	0.89
2:B:7:ILE:HD12	2:B:137:LEU:HD21	1.55	0.89
2:B:19:LYS:HG3	2:B:228:ASN:CG	1.93	0.89
2:B:183:GLU:OE1	2:B:394:GLN:CB	2.21	0.89
1:A:2:ARG:NH2	2:B:71:GLU:OE1	2.06	0.88
1:A:88:HIS:ND1	1:A:89:PRO:HD2	1.88	0.88
1:A:239:THR:HG23	1:A:243:ARG:HG3	1.54	0.88
2:B:20:PHE:CE2	2:B:235:MET:HB2	2.06	0.88
2:B:200:GLU:OE2	2:B:256:ALA:CA	2.15	0.88
2:B:346:TRP:HE3	2:B:347:ILE:HG12	1.33	0.88
3:K:252:SER:HA	3:K:275:LEU:CD1	2.02	0.88
1:A:382:THR:O	1:A:385:ALA:HB3	1.71	0.88
2:B:33:THR:C	2:B:59:ASN:HD21	1.76	0.88
2:B:346:TRP:CE3	2:B:347:ILE:HG12	2.06	0.88
1:A:231:ILE:HD13	1:A:302:MET:CE	2.03	0.88
2:B:87:PHE:HD1	2:B:88:ARG:O	1.47	0.88
2:B:183:GLU:CD	2:B:394:GLN:CB	2.41	0.88
2:B:435:TYR:N	2:B:435:TYR:HD1	1.66	0.88
1:A:41:THR:O	1:A:42:ILE:HB	1.73	0.88
1:A:328:VAL:CG1	1:A:332:ILE:HD12	2.03	0.88
2:B:11:GLN:CB	5:B:501:GDP:O2A	2.20	0.88
2:B:42:LEU:O	2:B:43:GLN:HG3	1.74	0.88
3:K:234:THR:HB	3:K:236:ILE:HD11	1.55	0.88
1:A:166:LYS:O	1:A:199:ASP:HB2	1.72	0.88
2:B:169:PHE:CE1	2:B:235:MET:SD	2.67	0.88
2:B:313:LEU:HD23	2:B:344:VAL:HG21	1.52	0.88
1:A:277:SER:HB3	1:A:280:LYS:HE2	1.56	0.88
2:B:20:PHE:HE2	2:B:235:MET:HB3	0.80	0.88
2:B:53:TYR:CE1	2:B:87:PHE:CZ	2.62	0.88
2:B:151:THR:CA	2:B:192:HIS:HD2	1.82	0.88
2:B:313:LEU:HD22	2:B:344:VAL:CG1	1.98	0.88
1:A:133:GLN:O	1:A:252:LEU:HD12	1.73	0.88
1:A:382:THR:O	1:A:385:ALA:CB	2.22	0.88
2:B:385:GLN:NE2	2:B:433:GLN:OE1	2.07	0.88
2:B:98:GLY:O	2:B:99:ALA:O	1.91	0.88
2:B:284:ARG:CD	2:B:290:GLU:OE1	2.22	0.88
1:A:76:ASP:O	1:A:80:THR:OG1	1.91	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:CB	1:A:394:LYS:HB3	2.04	0.87
2:B:4:ILE:HD12	2:B:30:ILE:CA	2.03	0.87
2:B:142:GLY:HA3	2:B:182:VAL:CG2	2.04	0.87
2:B:154:ILE:HD13	2:B:198:THR:HG21	1.56	0.87
2:B:49:ILE:CA	2:B:61:TYR:CD2	2.57	0.87
2:B:104:ALA:CA	2:B:108:TYR:HD2	1.85	0.87
2:B:114:LEU:CD1	2:B:117:SER:OG	2.19	0.87
1:A:220:GLU:O	1:A:222:PRO:HD3	1.60	0.87
1:A:258:ASN:CG	1:A:352:LYS:HD2	1.93	0.87
2:B:302:MET:O	2:B:302:MET:HG2	1.72	0.87
6:B:502:TXL:H173	6:B:502:TXL:H13	1.57	0.87
1:A:277:SER:HA	1:A:368:LEU:HD22	1.56	0.87
1:A:311:LYS:HB3	1:A:342:GLN:O	1.74	0.87
1:A:53:PHE:N	1:A:88:HIS:HE1	1.41	0.87
1:A:191:THR:CG2	1:A:421:ALA:CB	2.53	0.87
1:A:425:MET:O	1:A:428:LEU:HB3	1.73	0.87
2:B:275:LEU:CG	2:B:294:GLN:HE22	1.85	0.87
1:A:23:LEU:CD2	1:A:236:SER:HB3	2.04	0.87
2:B:48:ARG:HD2	2:B:60:LYS:HA	1.55	0.87
2:B:184:PRO:HD3	2:B:398:MET:SD	2.14	0.87
2:B:433:GLN:HG2	2:B:437:ASP:CG	1.95	0.87
1:A:59:GLY:O	1:A:62:VAL:C	2.12	0.87
1:A:424:ASP:CA	3:K:307:ARG:NH1	2.37	0.87
2:B:274:PRO:CB	2:B:371:LEU:HD21	2.04	0.87
1:A:115:ILE:O	1:A:119:LEU:HG	1.75	0.87
1:A:196:GLU:O	1:A:197:HIS:ND1	2.08	0.87
1:A:383:ALA:O	1:A:384:ILE:C	2.07	0.87
2:B:6:HIS:CD2	2:B:21:TRP:HH2	1.92	0.87
1:A:208:ALA:O	1:A:212:ILE:HG23	1.75	0.86
2:B:22:GLU:OE2	2:B:83:PHE:HB2	1.74	0.86
2:B:320:ARG:CG	2:B:374:SER:OG	2.23	0.86
1:A:209:ILE:CD1	1:A:227:LEU:HD11	1.93	0.86
2:B:53:TYR:CE1	2:B:87:PHE:CE1	2.62	0.86
2:B:151:THR:CA	2:B:192:HIS:HE2	1.68	0.86
2:B:172:VAL:HG12	2:B:173:PRO:N	1.89	0.86
2:B:244:PHE:HE2	2:B:358:ILE:HD12	1.06	0.86
2:B:312:TYR:CA	2:B:381:SER:HA	2.06	0.86
1:A:313:MET:HB2	1:A:380:ASN:O	1.75	0.86
2:B:158:ARG:HG3	2:B:197:ASN:CG	1.94	0.86
2:B:384:ILE:CG2	2:B:388:PHE:HE2	1.88	0.86
1:A:9:VAL:HG11	1:A:150:THR:HG22	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:HE2	1:A:189:LEU:HD23	1.29	0.86
2:B:279:GLY:O	2:B:281:GLN:N	2.08	0.86
1:A:158:SER:HB2	1:A:197:HIS:HB3	0.87	0.86
2:B:118:VAL:HG11	2:B:153:LEU:HD22	1.54	0.86
2:B:276:THR:OG1	6:B:502:TXL:H62	1.74	0.86
1:A:303:VAL:CG1	1:A:305:CYS:SG	2.64	0.86
2:B:339:ASN:O	2:B:342:TYR:N	2.09	0.86
1:A:65:ALA:HB1	1:A:91:GLN:OE1	1.73	0.86
1:A:224:TYR:HE1	4:A:500:GTP:N3	1.73	0.86
1:A:231:ILE:HD13	1:A:302:MET:HE1	1.57	0.86
2:B:29:GLY:O	2:B:58:GLY:C	2.14	0.86
2:B:87:PHE:CD1	2:B:89:PRO:HG2	2.03	0.86
2:B:405:LEU:HD12	2:B:408:TYR:CD2	2.00	0.86
3:K:317:GLU:OE1	3:K:322:ASN:HB3	1.74	0.86
1:A:184:PRO:HG3	1:A:395:PHE:CA	2.06	0.86
1:A:250:VAL:CG1	1:A:254:GLU:CB	2.34	0.86
1:A:424:ASP:OD1	3:K:307:ARG:NH1	2.06	0.86
2:B:385:GLN:HE22	2:B:433:GLN:CD	1.79	0.86
1:A:108:TYR:HA	1:A:112:LYS:CE	2.05	0.86
1:A:109:THR:HG21	1:A:411:GLU:OE1	1.75	0.86
2:B:144:GLY:N	2:B:185:TYR:CE1	2.44	0.86
2:B:435:TYR:N	2:B:435:TYR:CD1	2.31	0.86
1:A:424:ASP:N	3:K:307:ARG:HH22	1.74	0.86
2:B:7:ILE:HA	2:B:66:ILE:HG23	0.89	0.86
2:B:107:HIS:CG	2:B:152:LEU:HD21	2.11	0.86
2:B:194:LEU:CD2	2:B:267:PHE:CE2	2.58	0.86
2:B:327:GLU:O	2:B:331:GLN:HG2	1.75	0.86
1:A:272:TYR:CE1	1:A:274:PRO:CG	2.59	0.85
2:B:184:PRO:CG	2:B:399:PHE:CD2	0.91	0.85
2:B:241:CYS:HG	2:B:320:ARG:NH1	1.70	0.85
2:B:430:SER:O	2:B:434:GLN:HG3	1.76	0.85
2:B:127:GLU:O	2:B:129:CYS:N	2.09	0.85
2:B:147:SER:CA	2:B:189:LEU:HD13	2.04	0.85
2:B:313:LEU:HD23	2:B:344:VAL:HG22	1.58	0.85
2:B:53:TYR:CD1	2:B:87:PHE:CE1	2.63	0.85
2:B:178:SER:HB3	5:B:501:GDP:O3'	1.74	0.85
1:A:306:ASP:OD2	1:A:308:ARG:HD2	1.76	0.85
2:B:13:GLY:CA	2:B:138:THR:OG1	2.24	0.85
2:B:254:LYS:O	2:B:258:ASN:OD1	1.94	0.85
1:A:23:LEU:HD23	1:A:236:SER:HB3	1.57	0.85
1:A:250:VAL:HG12	1:A:254:GLU:HB3	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:HD12	1:A:371:VAL:CG2	2.06	0.85
2:B:44:LEU:HD21	2:B:86:ILE:H	1.00	0.85
2:B:102:ASN:HA	2:B:408:TYR:HE1	1.42	0.85
1:A:83:TYR:O	1:A:84:ARG:HG3	1.76	0.85
1:A:88:HIS:CE1	1:A:89:PRO:HD2	2.12	0.85
1:A:103:TYR:HA	1:A:147:SER:OG	1.77	0.85
1:A:174:ALA:HB1	1:A:390:ARG:NH2	1.81	0.85
2:B:7:ILE:HG13	2:B:66:ILE:HG21	1.58	0.85
1:A:154:MET:HB2	1:A:192:HIS:CE1	2.11	0.85
1:A:383:ALA:C	1:A:385:ALA:N	2.23	0.85
2:B:287:THR:HB	2:B:290:GLU:HB2	0.86	0.85
2:B:405:LEU:HD21	2:B:418:PHE:HE2	1.41	0.85
1:A:184:PRO:HB2	1:A:399:TYR:CD2	2.12	0.85
1:A:282:TYR:CD2	1:A:285:GLN:HA	2.11	0.85
2:B:41:ASP:O	2:B:42:LEU:CG	2.25	0.85
2:B:57:ALA:CA	2:B:64:ARG:CB	2.38	0.85
2:B:229:HIS:NE2	6:B:502:TXL:C37	2.40	0.85
1:A:193:THR:O	1:A:197:HIS:O	1.94	0.84
1:A:204:VAL:HG13	1:A:302:MET:HE2	1.58	0.84
1:A:276:ILE:HD13	1:A:282:TYR:CD1	2.11	0.84
1:A:64:ARG:HH22	1:A:132:LEU:HD23	1.41	0.84
1:A:175:PRO:HD3	1:A:390:ARG:NH2	1.91	0.84
2:B:244:PHE:CG	2:B:245:PRO:CD	2.56	0.84
2:B:405:LEU:O	2:B:405:LEU:HG	1.75	0.84
2:B:174:SER:HB2	2:B:207:GLU:HB3	1.59	0.84
2:B:181:VAL:HA	2:B:398:MET:CE	2.06	0.84
1:A:107:HIS:CG	1:A:148:GLY:HA3	2.13	0.84
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.10	0.84
2:B:75:MET:HA	2:B:75:MET:HE3	1.58	0.84
2:B:158:ARG:CB	2:B:197:ASN:HB3	1.70	0.84
2:B:226:ASP:OD2	6:B:502:TXL:H40	1.77	0.84
2:B:233:ALA:HB1	2:B:272:PHE:CG	2.12	0.84
1:A:271:THR:OG1	1:A:377:MET:HB3	1.76	0.84
1:A:273:ALA:HB1	1:A:294:ALA:HB3	1.60	0.84
2:B:49:ILE:N	2:B:61:TYR:HD2	1.75	0.84
2:B:385:GLN:HG2	2:B:389:LYS:HD2	1.58	0.84
2:B:158:ARG:HB2	2:B:197:ASN:HB3	0.85	0.84
2:B:199:ASP:OD2	2:B:256:ALA:CB	2.26	0.84
2:B:428:LEU:O	2:B:432:TYR:HB2	1.77	0.84
2:B:182:VAL:HG13	2:B:186:ASN:HD21	1.41	0.84
2:B:184:PRO:HG3	2:B:399:PHE:CB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:THR:C	2:B:243:ARG:HD2	1.95	0.84
1:A:16:ILE:CD1	1:A:138:PHE:CD1	2.59	0.84
1:A:349:THR:OG1	2:B:177:VAL:HG12	1.77	0.84
2:B:135:PHE:CG	2:B:166:MET:HE1	2.11	0.84
2:B:275:LEU:HD12	2:B:294:GLN:NE2	1.92	0.84
1:A:1:MET:O	1:A:130:THR:O	1.94	0.83
2:B:158:ARG:HG3	2:B:197:ASN:CB	2.08	0.83
2:B:201:THR:OG1	2:B:267:PHE:HA	1.78	0.83
2:B:289:PRO:O	2:B:293:GLN:HB2	1.78	0.83
1:A:104:ALA:HA	1:A:108:TYR:HD2	1.39	0.83
1:A:176:GLN:O	1:A:177:VAL:HG22	1.77	0.83
2:B:23:VAL:CG2	6:B:502:TXL:H333	2.09	0.83
2:B:166:MET:HB2	2:B:198:THR:HA	1.61	0.83
2:B:172:VAL:HG12	2:B:173:PRO:HD2	1.43	0.83
1:A:217:LEU:HD22	1:A:368:LEU:CD1	2.08	0.83
2:B:68:VAL:HG11	2:B:149:MET:HE2	1.60	0.83
2:B:169:PHE:HE1	2:B:235:MET:HG2	0.82	0.83
2:B:226:ASP:OD1	6:B:502:TXL:C39	2.25	0.83
2:B:244:PHE:CB	2:B:245:PRO:HD2	2.05	0.83
2:B:388:PHE:C	2:B:390:ARG:H	1.80	0.83
1:A:70:LEU:CD1	1:A:145:THR:CG2	1.89	0.83
1:A:133:GLN:NE2	2:B:96:GLN:O	2.11	0.83
1:A:292:THR:HG22	1:A:319:TYR:CZ	2.12	0.83
2:B:183:GLU:CB	2:B:398:MET:SD	2.65	0.83
2:B:401:ARG:HG3	2:B:402:LYS:H	1.41	0.83
1:A:115:ILE:CD1	1:A:152:LEU:CD2	2.45	0.83
2:B:433:GLN:HG2	2:B:437:ASP:OD1	1.78	0.83
1:A:33:ASP:OD2	1:A:244:PHE:HD2	1.62	0.83
1:A:277:SER:OG	1:A:280:LYS:CB	2.25	0.83
1:A:288:VAL:HG22	1:A:373:ARG:CG	2.08	0.83
2:B:14:ASN:HB3	2:B:74:THR:HG21	1.59	0.83
1:A:77:GLU:HA	1:A:80:THR:CB	2.08	0.83
2:B:11:GLN:HB3	5:B:501:GDP:O2A	1.79	0.83
2:B:222:PRO:O	2:B:223:THR:HG23	1.79	0.83
1:A:51:THR:CG2	1:A:52:PHE:H	1.92	0.83
1:A:273:ALA:HB1	1:A:294:ALA:CB	2.07	0.83
2:B:339:ASN:O	2:B:342:TYR:HB2	1.79	0.83
1:A:30:ILE:C	1:A:32:PRO:HD2	1.98	0.82
1:A:72:PRO:C	1:A:75:ILE:HG22	1.99	0.82
1:A:97:GLU:HB3	1:A:110:ILE:HG23	1.61	0.82
1:A:424:ASP:N	3:K:307:ARG:NH2	2.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:N	2:B:60:LYS:CE	2.42	0.82
2:B:174:SER:CB	2:B:207:GLU:CB	2.52	0.82
2:B:174:SER:HB2	2:B:175:PRO:HD2	1.59	0.82
2:B:288:VAL:N	2:B:289:PRO:HD2	1.92	0.82
1:A:202:PHE:CE1	1:A:378:LEU:HD13	2.14	0.82
2:B:19:LYS:HB3	2:B:228:ASN:HB3	1.60	0.82
2:B:68:VAL:CG1	2:B:149:MET:CE	2.58	0.82
2:B:105:LYS:HG2	2:B:411:GLU:CG	2.09	0.82
1:A:312:TYR:CE2	1:A:377:MET:HE3	2.12	0.82
2:B:48:ARG:NH1	2:B:60:LYS:CG	2.42	0.82
2:B:143:GLY:N	2:B:147:SER:OG	2.12	0.82
2:B:313:LEU:HD23	2:B:344:VAL:CG1	2.08	0.82
1:A:2:ARG:CB	1:A:133:GLN:OE1	2.27	0.82
1:A:18:ASN:O	1:A:22:GLU:HG3	1.78	0.82
2:B:14:ASN:CB	2:B:74:THR:OG1	2.27	0.82
1:A:194:THR:HG22	1:A:195:LEU:N	1.95	0.82
1:A:219:ILE:CG2	1:A:219:ILE:CA	2.57	0.82
1:A:264:ARG:O	1:A:266:HIS:CE1	2.32	0.82
2:B:53:TYR:CD1	2:B:87:PHE:HZ	1.96	0.82
2:B:229:HIS:CG	6:B:502:TXL:C37	2.62	0.82
2:B:414:ASP:CB	3:K:253:GLU:OE2	2.28	0.82
1:A:13:GLY:O	1:A:16:ILE:HG22	1.80	0.82
1:A:264:ARG:NH2	3:K:307:ARG:CG	2.41	0.82
1:A:184:PRO:CD	1:A:395:PHE:CA	2.58	0.82
1:A:313:MET:HA	1:A:344:VAL:HG21	1.60	0.82
2:B:22:GLU:OE2	2:B:83:PHE:CB	2.27	0.82
2:B:175:PRO:HD3	2:B:390:ARG:HH21	0.74	0.82
2:B:194:LEU:HA	2:B:265:LEU:HB2	1.60	0.82
2:B:194:LEU:HD23	2:B:265:LEU:HB3	1.62	0.82
1:A:81:GLY:O	1:A:82:THR:C	2.18	0.82
1:A:424:ASP:HB3	3:K:307:ARG:NH1	1.90	0.82
2:B:169:PHE:CZ	2:B:235:MET:SD	2.73	0.82
2:B:311:ARG:O	2:B:381:SER:HB2	1.80	0.82
1:A:291:ILE:HG22	1:A:375:VAL:HG23	0.84	0.82
1:A:332:ILE:CD1	1:A:353:VAL:CG2	2.54	0.82
2:B:87:PHE:HE1	2:B:89:PRO:HG2	0.84	0.82
2:B:169:PHE:HE1	2:B:235:MET:CG	1.76	0.82
2:B:241:CYS:O	2:B:242:LEU:CB	2.27	0.82
1:A:70:LEU:HB2	1:A:145:THR:HG21	1.62	0.81
1:A:107:HIS:HB3	1:A:148:GLY:HA3	1.60	0.81
1:A:264:ARG:NH2	3:K:307:ARG:CB	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ILE:HD13	2:B:199:ASP:OD2	1.79	0.81
3:K:234:THR:HB	3:K:236:ILE:CD1	2.10	0.81
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.62	0.81
1:A:76:ASP:O	1:A:80:THR:CA	2.27	0.81
1:A:108:TYR:O	1:A:112:LYS:HG3	1.80	0.81
1:A:250:VAL:CG1	1:A:352:LYS:NZ	2.43	0.81
1:A:256:GLN:HB3	2:B:407:TRP:HH2	1.45	0.81
1:A:320:ARG:HG2	1:A:374:ALA:HB3	1.60	0.81
1:A:383:ALA:C	1:A:385:ALA:H	1.84	0.81
2:B:6:HIS:CD2	2:B:21:TRP:CH2	2.68	0.81
2:B:30:ILE:CG2	2:B:243:ARG:NH1	2.44	0.81
2:B:35:SER:HA	2:B:60:LYS:HE2	1.62	0.81
2:B:119:LEU:O	2:B:123:ARG:HG3	1.80	0.81
2:B:135:PHE:CG	2:B:166:MET:CE	2.63	0.81
2:B:184:PRO:HB3	2:B:395:PHE:CE1	2.16	0.81
1:A:20:CYS:O	1:A:24:TYR:CE2	2.33	0.81
1:A:106:GLY:O	1:A:111:GLY:CA	2.29	0.81
2:B:106:GLY:O	2:B:111:GLY:CA	2.29	0.81
2:B:135:PHE:HB3	2:B:166:MET:HE3	0.83	0.81
2:B:287:THR:CG2	2:B:290:GLU:H	1.92	0.81
1:A:30:ILE:CG2	1:A:64:ARG:CG	2.55	0.81
1:A:64:ARG:CZ	1:A:132:LEU:HD22	2.10	0.81
1:A:312:TYR:HA	1:A:381:THR:CG2	2.09	0.81
2:B:13:GLY:HA2	2:B:138:THR:CB	2.10	0.81
1:A:154:MET:CE	1:A:166:LYS:HD3	2.11	0.81
1:A:193:THR:O	1:A:194:THR:C	2.05	0.81
1:A:397:LEU:HA	1:A:401:LYS:HB2	1.57	0.81
2:B:102:ASN:HB3	2:B:408:TYR:HD1	1.46	0.81
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.11	0.81
2:B:287:THR:HG22	2:B:288:VAL:N	1.95	0.81
1:A:101:ASN:HA	4:A:500:GTP:O2G	1.81	0.81
2:B:141:LEU:HD22	2:B:186:ASN:CB	2.09	0.81
1:A:416:GLY:CA	3:K:169:ARG:HH22	1.94	0.81
2:B:405:LEU:CG	2:B:408:TYR:HB2	2.07	0.81
2:B:226:ASP:CG	6:B:502:TXL:H39	2.00	0.81
2:B:287:THR:CB	2:B:290:GLU:HB3	1.99	0.81
1:A:9:VAL:CG1	1:A:150:THR:HG22	2.08	0.80
2:B:4:ILE:CD1	2:B:30:ILE:CA	2.58	0.80
1:A:343:PHE:HZ	1:A:351:PHE:CE2	1.99	0.80
2:B:4:ILE:HD12	2:B:30:ILE:HA	1.48	0.80
2:B:22:GLU:HG2	2:B:83:PHE:HD2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ARG:NH1	2:B:60:LYS:HG2	1.95	0.80
2:B:142:GLY:CA	2:B:185:TYR:CE1	2.64	0.80
1:A:301:GLN:NE2	1:A:305:CYS:O	2.12	0.80
2:B:6:HIS:NE2	2:B:21:TRP:HH2	1.77	0.80
2:B:190:SER:O	2:B:192:HIS:N	2.14	0.80
2:B:250:ALA:CA	2:B:254:LYS:HD2	2.09	0.80
1:A:88:HIS:CG	1:A:89:PRO:CD	2.63	0.80
1:A:144:GLY:HA2	1:A:185:TYR:OH	1.81	0.80
1:A:276:ILE:HG21	1:A:282:TYR:HD1	1.44	0.80
1:A:361:THR:HG22	1:A:362:VAL:N	1.96	0.80
2:B:14:ASN:CG	2:B:69:ASP:OD1	2.20	0.80
2:B:80:SER:C	2:B:82:PRO:CD	2.48	0.80
2:B:226:ASP:CG	6:B:502:TXL:C39	2.49	0.80
2:B:286:LEU:HD12	2:B:372:LYS:HB2	1.61	0.80
1:A:116:ASP:O	1:A:119:LEU:N	2.15	0.80
1:A:221:ARG:N	1:A:222:PRO:HD3	1.97	0.80
2:B:385:GLN:HG2	2:B:389:LYS:CE	2.09	0.80
2:B:64:ARG:NH2	2:B:125:GLU:O	2.13	0.80
1:A:76:ASP:C	1:A:80:THR:HG1	1.84	0.80
2:B:12:CYS:O	2:B:16:ILE:CB	2.29	0.80
2:B:56:ALA:CB	2:B:62:VAL:HB	2.11	0.80
1:A:80:THR:O	1:A:81:GLY:C	2.19	0.80
2:B:10:GLY:O	2:B:14:ASN:ND2	2.14	0.80
2:B:13:GLY:HA2	2:B:138:THR:HB	1.62	0.80
2:B:385:GLN:HG2	2:B:389:LYS:CD	2.11	0.80
1:A:103:TYR:CG	1:A:188:ILE:HG22	2.16	0.80
1:A:209:ILE:HG12	1:A:302:MET:HE3	1.64	0.80
2:B:95:GLY:O	2:B:96:GLN:HB2	1.81	0.80
2:B:286:LEU:HD13	2:B:373:MET:N	1.96	0.80
1:A:212:ILE:CD1	1:A:230:LEU:HD22	1.89	0.80
2:B:96:GLN:C	2:B:98:GLY:N	2.31	0.80
2:B:175:PRO:HB2	2:B:176:LYS:HE2	1.64	0.80
2:B:208:ALA:HB1	2:B:303:ALA:O	1.82	0.80
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.58	0.80
2:B:385:GLN:HG3	2:B:389:LYS:CE	2.04	0.80
1:A:179:THR:CG2	1:A:181:VAL:HB	2.04	0.79
1:A:256:GLN:HB3	2:B:407:TRP:CZ3	2.16	0.79
2:B:142:GLY:CA	2:B:185:TYR:CD1	2.65	0.79
2:B:194:LEU:CD2	2:B:267:PHE:HE2	1.93	0.79
1:A:15:GLN:O	1:A:18:ASN:N	2.14	0.79
1:A:396:ASP:OD2	1:A:422:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLY:C	3:K:169:ARG:HH22	1.84	0.79
2:B:35:SER:CA	2:B:60:LYS:CE	2.60	0.79
2:B:105:LYS:CE	2:B:411:GLU:OE2	2.27	0.79
1:A:6:SER:HA	1:A:136:SER:OG	1.81	0.79
1:A:108:TYR:CA	1:A:112:LYS:CE	2.54	0.79
1:A:271:THR:OG1	1:A:377:MET:CB	2.30	0.79
1:A:424:ASP:HA	3:K:307:ARG:NH1	1.96	0.79
2:B:178:SER:CB	5:B:501:GDP:HO3'	1.94	0.79
2:B:265:LEU:HD23	2:B:267:PHE:CE1	2.17	0.79
1:A:179:THR:CG2	1:A:181:VAL:CB	2.58	0.79
1:A:431:ASP:HB3	3:K:303:PHE:HE1	1.47	0.79
2:B:30:ILE:HG21	2:B:136:GLN:HE22	1.47	0.79
2:B:176:LYS:CE	2:B:207:GLU:OE2	2.29	0.79
1:A:5:ILE:HG21	1:A:135:PHE:CE1	2.18	0.79
1:A:133:GLN:NE2	2:B:98:GLY:HA2	1.96	0.79
1:A:343:PHE:CZ	1:A:351:PHE:CE2	2.69	0.79
1:A:369:ALA:CB	1:A:371:VAL:CG2	2.51	0.79
1:A:420:GLU:OE2	3:K:170:GLU:C	2.20	0.79
1:A:119:LEU:O	1:A:122:ILE:CG2	2.30	0.79
1:A:272:TYR:CZ	1:A:274:PRO:CG	2.56	0.79
1:A:420:GLU:HG3	3:K:169:ARG:HE	1.44	0.79
2:B:49:ILE:N	2:B:61:TYR:CD2	2.51	0.79
1:A:206:ASN:HD21	1:A:227:LEU:HD23	1.42	0.79
2:B:75:MET:HE2	2:B:79:ARG:HD3	1.63	0.79
2:B:243:ARG:HH21	2:B:252:LEU:HD11	1.47	0.79
2:B:405:LEU:HD13	2:B:418:PHE:HZ	1.47	0.79
1:A:196:GLU:O	1:A:197:HIS:CB	2.30	0.79
2:B:7:ILE:CG1	2:B:66:ILE:CG2	2.58	0.79
2:B:7:ILE:HG12	2:B:66:ILE:CD1	2.04	0.79
2:B:287:THR:CG2	2:B:289:PRO:HG2	2.12	0.79
1:A:258:ASN:OD1	1:A:352:LYS:CD	2.29	0.79
1:A:309:HIS:CD2	1:A:386:GLU:OE2	2.36	0.79
2:B:184:PRO:HG3	2:B:399:PHE:CD2	1.33	0.79
1:A:220:GLU:C	1:A:222:PRO:CD	2.37	0.79
1:A:306:ASP:OD1	1:A:308:ARG:HB2	1.79	0.79
2:B:218:LYS:O	2:B:219:LEU:O	2.00	0.79
2:B:259:MET:HE1	2:B:379:GLY:HA2	0.80	0.79
2:B:323:MET:HG2	2:B:324:SER:N	1.98	0.79
2:B:340:SER:HG	2:B:341:SER:N	1.79	0.79
1:A:17:GLY:O	1:A:21:TRP:N	2.11	0.78
1:A:172:TYR:CE2	1:A:388:TRP:CZ3	2.70	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ASP:OD2	2:B:74:THR:CG2	2.31	0.78
2:B:213:CYS:HB3	2:B:219:LEU:HD11	1.64	0.78
2:B:343:PHE:CD1	2:B:350:ASN:CG	2.55	0.78
1:A:109:THR:CG2	1:A:411:GLU:HB3	2.12	0.78
1:A:155:GLU:OE2	1:A:192:HIS:HD2	1.65	0.78
2:B:48:ARG:NH1	2:B:60:LYS:N	2.32	0.78
1:A:115:ILE:CG2	1:A:152:LEU:HD21	2.12	0.78
2:B:66:ILE:HB	2:B:125:GLU:OE2	1.84	0.78
2:B:244:PHE:CD2	2:B:358:ILE:HD12	2.18	0.78
2:B:300:ASN:ND2	2:B:300:ASN:O	2.16	0.78
2:B:401:ARG:HG3	2:B:402:LYS:N	1.99	0.78
1:A:179:THR:HG22	1:A:180:ALA:N	1.95	0.78
1:A:179:THR:HG22	1:A:181:VAL:H	0.63	0.78
2:B:44:LEU:CD2	2:B:85:GLN:CG	2.15	0.78
2:B:53:TYR:CE1	2:B:89:PRO:HG3	2.17	0.78
1:A:191:THR:HG21	1:A:421:ALA:HB2	1.63	0.78
1:A:409:VAL:HG22	1:A:414:GLU:HG2	1.64	0.78
2:B:142:GLY:C	2:B:185:TYR:CZ	2.56	0.78
2:B:305:CYS:SG	2:B:387:LEU:HB2	2.24	0.78
1:A:3:GLU:HA	1:A:31:GLN:CG	2.11	0.78
1:A:32:PRO:C	1:A:34:GLY:N	2.32	0.78
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.56	0.78
2:B:414:ASP:CG	3:K:253:GLU:OE2	2.22	0.78
1:A:4:CYS:CB	1:A:30:ILE:CG2	2.57	0.78
1:A:303:VAL:HG11	1:A:305:CYS:SG	2.22	0.78
1:A:313:MET:HE1	1:A:346:TRP:CZ2	2.19	0.78
2:B:4:ILE:HD13	2:B:30:ILE:CB	2.13	0.78
2:B:7:ILE:CD1	2:B:137:LEU:HD21	2.14	0.78
2:B:34:GLY:O	2:B:35:SER:OG	2.01	0.78
2:B:194:LEU:HD23	2:B:267:PHE:CZ	2.19	0.78
1:A:65:ALA:O	1:A:66:VAL:HG23	1.83	0.78
1:A:72:PRO:O	1:A:75:ILE:HG22	1.83	0.78
2:B:4:ILE:HG21	2:B:30:ILE:CG2	2.12	0.78
2:B:102:ASN:HA	2:B:408:TYR:CE1	2.18	0.78
2:B:107:HIS:CG	2:B:152:LEU:HG	2.19	0.78
2:B:144:GLY:N	2:B:185:TYR:CZ	2.52	0.78
1:A:93:ILE:HD11	1:A:121:ARG:HD2	1.66	0.78
1:A:440:VAL:HB	2:B:402:LYS:HZ1	1.48	0.78
2:B:8:GLN:NE2	2:B:21:TRP:NE1	2.31	0.78
1:A:153:LEU:O	1:A:157:LEU:HG	1.84	0.78
1:A:344:VAL:CB	1:A:347:CYS:SG	2.69	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:CG1	2:B:66:ILE:HD13	2.05	0.78
2:B:48:ARG:CD	2:B:60:LYS:HA	2.13	0.78
2:B:105:LYS:HE2	2:B:411:GLU:CD	2.03	0.78
2:B:128:SER:O	2:B:129:CYS:HB2	1.84	0.78
2:B:184:PRO:CG	2:B:399:PHE:HD2	0.66	0.78
2:B:273:ALA:HB1	2:B:294:GLN:OE1	1.83	0.78
2:B:286:LEU:CD1	2:B:371:LEU:O	2.32	0.78
1:A:158:SER:OG	1:A:196:GLU:O	2.02	0.77
1:A:277:SER:OG	1:A:280:LYS:CA	2.32	0.77
2:B:184:PRO:HD2	2:B:399:PHE:HE2	1.46	0.77
2:B:275:LEU:HD11	2:B:300:ASN:HD21	1.49	0.77
2:B:319:PHE:CZ	2:B:328:VAL:HG13	2.19	0.77
1:A:152:LEU:HD11	1:A:156:ARG:CZ	2.13	0.77
1:A:155:GLU:OE2	1:A:192:HIS:CD2	2.37	0.77
1:A:296:PHE:HE1	1:A:335:ILE:HD13	0.98	0.77
2:B:107:HIS:CG	2:B:152:LEU:CD2	2.67	0.77
2:B:320:ARG:NH2	6:B:502:TXL:H27	1.98	0.77
2:B:346:TRP:CD2	2:B:347:ILE:HG13	2.14	0.77
2:B:399:PHE:CZ	2:B:408:TYR:OH	2.37	0.77
1:A:155:GLU:HG3	1:A:192:HIS:NE2	1.99	0.77
1:A:206:ASN:HD21	4:A:500:GTP:N2	1.82	0.77
2:B:102:ASN:OD1	2:B:408:TYR:HE1	1.62	0.77
2:B:383:ALA:O	2:B:386:GLU:HG3	1.84	0.77
1:A:70:LEU:CG	1:A:145:THR:HG21	2.14	0.77
1:A:103:TYR:O	1:A:107:HIS:HB3	1.85	0.77
1:A:262:TYR:HB3	1:A:263:PRO:HD3	1.65	0.77
2:B:75:MET:HE1	2:B:79:ARG:HD2	0.82	0.77
2:B:104:ALA:HA	2:B:108:TYR:CE2	2.19	0.77
2:B:229:HIS:CE1	6:B:502:TXL:O11	2.38	0.77
1:A:70:LEU:HB2	1:A:145:THR:CG2	2.14	0.77
1:A:154:MET:HE3	1:A:166:LYS:HD3	1.67	0.77
2:B:107:HIS:HD2	2:B:152:LEU:HG	1.48	0.77
2:B:92:PHE:CE2	2:B:114:LEU:HD11	2.20	0.77
2:B:105:LYS:CG	2:B:411:GLU:HG3	2.14	0.77
2:B:243:ARG:HH21	2:B:252:LEU:CD1	1.98	0.77
2:B:262:PHE:HB3	2:B:263:PRO:CD	2.14	0.77
6:B:502:TXL:H162	6:B:502:TXL:C9	2.15	0.77
1:A:105:ARG:NH2	1:A:110:ILE:CD1	2.46	0.77
1:A:252:LEU:HD23	1:A:255:PHE:CE2	2.19	0.77
1:A:288:VAL:HG23	1:A:373:ARG:HD3	1.62	0.77
2:B:103:TRP:HZ3	2:B:108:TYR:HH	0.89	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HG22	2:B:196:GLU:O	1.85	0.77
2:B:249:ASN:O	2:B:254:LYS:NZ	2.16	0.77
2:B:319:PHE:CD1	2:B:328:VAL:CG1	2.58	0.77
2:B:229:HIS:ND1	6:B:502:TXL:O11	2.18	0.77
2:B:252:LEU:O	2:B:255:LEU:HB2	1.85	0.77
2:B:425:MET:O	2:B:428:LEU:HB3	1.84	0.77
1:A:72:PRO:O	1:A:75:ILE:HG23	1.82	0.77
1:A:105:ARG:HH21	1:A:110:ILE:CD1	1.92	0.77
1:A:192:HIS:O	1:A:196:GLU:HG2	1.85	0.77
1:A:306:ASP:CG	1:A:308:ARG:HB2	2.06	0.77
2:B:107:HIS:O	2:B:152:LEU:HD13	1.82	0.77
1:A:108:TYR:HE2	1:A:417:GLU:OE2	1.63	0.77
1:A:206:ASN:HD21	1:A:227:LEU:CD2	1.87	0.77
2:B:104:ALA:CA	2:B:108:TYR:CD2	2.63	0.77
2:B:147:SER:CB	2:B:189:LEU:HD13	2.08	0.77
2:B:277:SER:CB	2:B:280:SER:HB2	2.12	0.77
1:A:217:LEU:HD13	1:A:368:LEU:CG	2.12	0.76
2:B:86:ILE:HD12	2:B:91:ASN:ND2	1.99	0.76
2:B:222:PRO:O	2:B:223:THR:CG2	2.32	0.76
1:A:3:GLU:OE2	1:A:129:CYS:HB3	1.82	0.76
1:A:97:GLU:CG	1:A:110:ILE:CG2	2.63	0.76
3:K:216:ARG:HH11	3:K:216:ARG:CG	1.98	0.76
1:A:148:GLY:HA2	1:A:151:SER:OG	1.85	0.76
2:B:107:HIS:CG	2:B:152:LEU:CG	2.69	0.76
2:B:213:CYS:HB3	2:B:219:LEU:CD1	2.16	0.76
2:B:346:TRP:HZ3	2:B:347:ILE:HD11	0.95	0.76
1:A:115:ILE:CD1	1:A:152:LEU:CD1	2.63	0.76
1:A:115:ILE:HD13	1:A:152:LEU:CD1	2.16	0.76
1:A:423:GLU:C	3:K:307:ARG:NH2	2.39	0.76
2:B:27:GLU:O	2:B:36:TYR:HB3	1.86	0.76
2:B:295:MET:HE1	2:B:375:ALA:CA	2.12	0.76
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.20	0.76
1:A:273:ALA:CB	1:A:294:ALA:HB3	2.16	0.76
2:B:103:TRP:CZ3	2:B:108:TYR:CZ	2.73	0.76
1:A:420:GLU:OE1	3:K:170:GLU:CA	2.34	0.76
2:B:400:ARG:HD3	2:B:422:GLU:OE1	1.85	0.76
2:B:105:LYS:HG2	2:B:411:GLU:CD	2.06	0.76
2:B:200:GLU:HB3	2:B:268:PHE:CE2	2.21	0.76
2:B:237:GLY:CA	2:B:241:CYS:SG	2.68	0.76
1:A:80:THR:O	1:A:83:TYR:N	2.19	0.76
2:B:12:CYS:SG	5:B:501:GDP:C4	2.79	0.76

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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	0.76
2:B:234:THR:OG1	2:B:302:MET:HE2	1.86	0.76
2:B:308:ARG:HD3	2:B:342:TYR:CZ	2.21	0.76
2:B:399:PHE:HZ	2:B:408:TYR:OH	1.68	0.76
2:B:399:PHE:O	2:B:403:ALA:HA	1.86	0.76
1:A:38:SER:C	1:A:39:ASP:N	0.70	0.76
1:A:173:PRO:HG3	1:A:182:VAL:HG12	1.66	0.76
2:B:181:VAL:HG12	2:B:399:PHE:CZ	1.95	0.76
1:A:62:VAL:HG12	1:A:63:PRO:CD	2.06	0.75
1:A:97:GLU:HG3	1:A:110:ILE:CG2	2.16	0.75
1:A:97:GLU:O	1:A:98:ASP:HB3	1.85	0.75
1:A:183:GLU:HB2	1:A:398:MET:SD	2.26	0.75
1:A:228:ASN:ND2	4:A:500:GTP:HN1	1.84	0.75
2:B:142:GLY:HA3	2:B:182:VAL:HG22	1.65	0.75
2:B:273:ALA:N	2:B:274:PRO:HD2	1.45	0.75
1:A:266:HIS:HD2	1:A:432:TYR:CE1	2.04	0.75
2:B:48:ARG:HH11	2:B:60:LYS:CG	1.97	0.75
2:B:135:PHE:CB	2:B:166:MET:SD	2.74	0.75
2:B:237:GLY:O	2:B:241:CYS:CB	2.26	0.75
2:B:384:ILE:CG2	2:B:388:PHE:CE2	2.69	0.75
1:A:420:GLU:OE1	3:K:170:GLU:HB3	1.87	0.75
2:B:169:PHE:CZ	2:B:235:MET:HG2	2.17	0.75
1:A:383:ALA:O	1:A:386:GLU:N	2.18	0.75
2:B:42:LEU:C	2:B:43:GLN:HG3	2.07	0.75
2:B:68:VAL:CG1	2:B:149:MET:HE1	2.15	0.75
2:B:105:LYS:HG2	2:B:411:GLU:HG3	1.67	0.75
2:B:268:PHE:CD1	2:B:380:ASN:CG	2.59	0.75
2:B:96:GLN:O	2:B:97:SER:C	2.21	0.75
2:B:184:PRO:HA	2:B:395:PHE:HD1	1.52	0.75
1:A:66:VAL:CG2	1:A:125:LEU:CD1	2.64	0.75
1:A:83:TYR:C	1:A:84:ARG:HG3	2.05	0.75
1:A:313:MET:CB	1:A:380:ASN:O	2.34	0.75
2:B:141:LEU:CD1	2:B:173:PRO:HD3	2.16	0.75
2:B:170:SER:OG	2:B:203:CYS:HA	1.86	0.75
2:B:405:LEU:HD11	2:B:408:TYR:HB2	0.78	0.75
1:A:176:GLN:C	1:A:177:VAL:CG2	2.42	0.75
1:A:431:ASP:CA	3:K:303:PHE:CE1	2.70	0.75
2:B:87:PHE:CD1	2:B:89:PRO:HD2	2.20	0.75
2:B:102:ASN:CG	2:B:408:TYR:CE1	2.60	0.75
2:B:192:HIS:CA	2:B:196:GLU:HG2	2.11	0.75
1:A:151:SER:HB2	1:A:192:HIS:CB	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ASP:CB	3:K:303:PHE:HE1	2.00	0.75
2:B:70:LEU:HD12	2:B:94:PHE:HD2	0.68	0.75
2:B:143:GLY:O	5:B:501:GDP:PB	2.40	0.75
2:B:181:VAL:HA	2:B:398:MET:HE2	1.67	0.75
2:B:398:MET:HG2	2:B:399:PHE:N	2.01	0.75
1:A:154:MET:HE3	1:A:166:LYS:CD	2.17	0.75
2:B:53:TYR:HE1	2:B:89:PRO:CG	1.98	0.75
1:A:103:TYR:HD2	1:A:189:LEU:CG	2.00	0.74
1:A:184:PRO:HD3	1:A:395:PHE:N	2.01	0.74
1:A:311:LYS:CB	1:A:342:GLN:O	2.34	0.74
1:A:416:GLY:C	3:K:169:ARG:NH2	2.39	0.74
2:B:6:HIS:NE2	2:B:21:TRP:CH2	2.55	0.74
2:B:75:MET:HE2	2:B:79:ARG:CB	2.17	0.74
2:B:103:TRP:CZ3	2:B:108:TYR:CE2	2.75	0.74
2:B:154:ILE:HD13	2:B:198:THR:CG2	2.17	0.74
2:B:312:TYR:O	2:B:344:VAL:HG22	1.84	0.74
2:B:22:GLU:CG	2:B:83:PHE:CE2	2.70	0.74
2:B:326:LYS:O	2:B:330:GLU:CG	2.35	0.74
2:B:343:PHE:CB	2:B:350:ASN:ND2	2.50	0.74
2:B:405:LEU:HD21	2:B:418:PHE:CZ	2.03	0.74
1:A:42:ILE:O	1:A:42:ILE:CG2	2.30	0.74
1:A:326:LYS:O	1:A:330:ALA:HB3	1.87	0.74
1:A:361:THR:O	1:A:362:VAL:HG23	1.86	0.74
1:A:416:GLY:HA3	3:K:169:ARG:HH21	1.47	0.74
1:A:88:HIS:CD2	1:A:89:PRO:CD	2.70	0.74
1:A:287:SER:OG	1:A:290:GLU:HB2	1.87	0.74
1:A:313:MET:HE1	1:A:346:TRP:CH2	2.22	0.74
1:A:349:THR:OG1	2:B:177:VAL:CG1	2.35	0.74
2:B:135:PHE:HB3	2:B:166:MET:HE1	1.66	0.74
2:B:229:HIS:NE2	6:B:502:TXL:H37	2.01	0.74
1:A:26:LEU:HD11	1:A:361:THR:CB	2.17	0.74
1:A:319:TYR:O	1:A:355:ILE:HA	1.87	0.74
2:B:89:PRO:O	2:B:90:ASP:OD1	2.05	0.74
2:B:287:THR:CG2	2:B:289:PRO:CG	2.65	0.74
2:B:319:PHE:CE1	2:B:328:VAL:HG12	2.18	0.74
2:B:188:THR:HG22	2:B:417:GLU:O	1.87	0.74
2:B:226:ASP:OD1	6:B:502:TXL:H39	1.87	0.74
1:A:103:TYR:OH	1:A:151:SER:HB3	1.87	0.74
1:A:179:THR:CG2	1:A:181:VAL:HG23	2.18	0.74
1:A:219:ILE:CG2	1:A:219:ILE:HG12	2.16	0.74
1:A:224:TYR:CE1	4:A:500:GTP:N3	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:MET:CE	1:A:346:TRP:CZ2	2.70	0.74
2:B:7:ILE:HB	2:B:137:LEU:HD21	1.62	0.74
2:B:56:ALA:CB	2:B:62:VAL:HG23	2.18	0.74
2:B:234:THR:CB	2:B:302:MET:HE2	2.17	0.74
2:B:319:PHE:CE1	2:B:353:THR:CG2	2.42	0.74
1:A:57:GLY:HA3	1:A:61:HIS:NE2	2.01	0.74
1:A:196:GLU:O	1:A:197:HIS:HB3	1.87	0.74
1:A:206:ASN:HD21	4:A:500:GTP:HN22	1.35	0.74
2:B:6:HIS:CG	2:B:21:TRP:HZ2	2.05	0.74
2:B:35:SER:CA	2:B:60:LYS:HE3	2.16	0.74
2:B:75:MET:HE2	2:B:79:ARG:HB3	1.69	0.74
2:B:265:LEU:CD2	2:B:267:PHE:CE1	2.71	0.74
2:B:279:GLY:C	2:B:281:GLN:N	2.35	0.74
2:B:284:ARG:HD2	2:B:290:GLU:CD	2.08	0.74
2:B:296:PHE:CE2	2:B:335:VAL:HG11	2.22	0.74
1:A:137:VAL:HB	1:A:168:GLU:HG2	1.70	0.74
2:B:192:HIS:HA	2:B:196:GLU:CD	2.08	0.74
2:B:213:CYS:SG	2:B:227:LEU:CD1	2.75	0.74
1:A:33:ASP:OD2	1:A:244:PHE:CD2	2.39	0.74
1:A:209:ILE:HG23	1:A:230:LEU:CD2	2.17	0.74
2:B:9:ALA:HA	2:B:68:VAL:O	1.86	0.74
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.18	0.73
1:A:277:SER:CA	1:A:280:LYS:HG2	2.18	0.73
1:A:369:ALA:HB1	1:A:371:VAL:HG23	1.67	0.73
1:A:107:HIS:CD2	1:A:148:GLY:CA	2.71	0.73
2:B:123:ARG:O	2:B:127:GLU:HG3	1.87	0.73
2:B:184:PRO:HG2	2:B:399:PHE:CD2	0.29	0.73
2:B:244:PHE:CE2	2:B:358:ILE:CD1	2.48	0.73
2:B:272:PHE:CD1	2:B:274:PRO:HG2	2.24	0.73
2:B:336:GLN:NE2	2:B:351:VAL:HB	2.03	0.73
2:B:397:ALA:O	2:B:401:ARG:HG2	1.87	0.73
1:A:70:LEU:CB	1:A:145:THR:CG2	2.65	0.73
1:A:172:TYR:CZ	1:A:387:ALA:HB1	2.22	0.73
1:A:206:ASN:ND2	4:A:500:GTP:HN22	1.85	0.73
1:A:431:ASP:O	1:A:435:VAL:HG23	1.88	0.73
2:B:244:PHE:HD2	2:B:245:PRO:HD2	1.45	0.73
1:A:2:ARG:NH2	2:B:99:ALA:CB	2.52	0.73
2:B:8:GLN:NE2	2:B:21:TRP:CD1	2.56	0.73
1:A:65:ALA:HB2	1:A:91:GLN:OE1	1.87	0.73
1:A:153:LEU:O	1:A:157:LEU:CD1	2.37	0.73
1:A:158:SER:H	1:A:166:LYS:NZ	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:HG23	1:A:181:VAL:HG23	1.70	0.73
2:B:265:LEU:O	2:B:267:PHE:CE2	2.41	0.73
2:B:313:LEU:CD2	2:B:344:VAL:HG13	2.17	0.73
1:A:3:GLU:HB3	1:A:64:ARG:CZ	2.18	0.73
1:A:264:ARG:HH21	3:K:307:ARG:HB3	0.57	0.73
1:A:277:SER:CB	1:A:280:LYS:CG	2.51	0.73
1:A:282:TYR:HD2	1:A:285:GLN:HA	1.52	0.73
1:A:282:TYR:HD2	1:A:285:GLN:CA	2.01	0.73
2:B:44:LEU:HD11	2:B:86:ILE:C	2.09	0.73
2:B:53:TYR:CE1	2:B:87:PHE:HZ	2.07	0.73
2:B:181:VAL:CG2	2:B:404:PHE:CE2	2.70	0.73
2:B:265:LEU:CD2	2:B:267:PHE:CZ	2.71	0.73
1:A:100:ALA:HB2	1:A:105:ARG:NE	2.04	0.73
1:A:210:TYR:CD2	1:A:227:LEU:HD22	2.20	0.73
1:A:349:THR:HG21	2:B:177:VAL:HG12	1.71	0.73
2:B:35:SER:H	2:B:60:LYS:HE3	1.53	0.73
2:B:142:GLY:HA3	2:B:182:VAL:HG21	1.71	0.73
2:B:229:HIS:HB2	6:B:502:TXL:H38	1.68	0.73
2:B:239:THR:HA	2:B:243:ARG:CZ	2.19	0.73
1:A:314:ALA:O	1:A:379:SER:HA	1.89	0.73
1:A:420:GLU:CD	3:K:170:GLU:N	2.40	0.73
2:B:21:TRP:HA	2:B:24:ILE:HD12	1.71	0.73
2:B:92:PHE:CE1	2:B:121:VAL:HG21	2.23	0.73
2:B:288:VAL:H	2:B:289:PRO:HD2	1.54	0.73
2:B:383:ALA:O	2:B:386:GLU:CG	2.37	0.73
3:K:159:ASN:HD22	3:K:161:LYS:CG	2.02	0.73
1:A:97:GLU:O	1:A:110:ILE:HD13	1.88	0.73
1:A:250:VAL:CG1	1:A:254:GLU:HG2	2.15	0.73
2:B:286:LEU:HD11	2:B:372:LYS:CB	2.07	0.73
2:B:14:ASN:HB2	2:B:74:THR:OG1	1.89	0.73
2:B:105:LYS:HE2	2:B:411:GLU:CG	2.18	0.73
2:B:259:MET:HB2	2:B:268:PHE:CZ	2.23	0.73
1:A:250:VAL:CG2	1:A:254:GLU:HG2	2.19	0.72
2:B:101:ASN:O	2:B:102:ASN:HB2	1.88	0.72
2:B:194:LEU:HD21	2:B:267:PHE:CE2	2.23	0.72
2:B:280:SER:O	2:B:282:GLN:N	2.21	0.72
1:A:36:MET:SD	1:A:60:LYS:HB2	2.29	0.72
1:A:142:GLY:C	1:A:185:TYR:CE1	2.62	0.72
1:A:234:ILE:HD12	1:A:270:ALA:HB1	1.71	0.72
2:B:184:PRO:HG3	2:B:399:PHE:CG	1.84	0.72
1:A:277:SER:HB2	1:A:279:GLU:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:CD2	1:A:381:THR:HG22	2.23	0.72
1:A:397:LEU:HD22	1:A:401:LYS:CE	2.20	0.72
2:B:19:LYS:CD	2:B:228:ASN:CB	2.53	0.72
2:B:158:ARG:CD	2:B:197:ASN:N	2.51	0.72
2:B:20:PHE:CZ	2:B:235:MET:HB3	2.22	0.72
2:B:242:LEU:HD22	2:B:250:ALA:N	2.01	0.72
2:B:286:LEU:HB3	2:B:373:MET:HB3	1.71	0.72
1:A:144:GLY:N	4:A:500:GTP:O2G	2.19	0.72
2:B:3:GLU:CB	2:B:132:LEU:HD23	2.14	0.72
2:B:133:GLN:NE2	2:B:253:ARG:NH1	2.38	0.72
2:B:178:SER:HB2	5:B:501:GDP:O3'	1.89	0.72
2:B:259:MET:CE	2:B:379:GLY:N	2.51	0.72
1:A:6:SER:HB3	1:A:30:ILE:CD1	2.19	0.72
2:B:53:TYR:CE1	2:B:87:PHE:HE1	2.07	0.72
6:B:502:TXL:H181	6:B:502:TXL:C21	2.19	0.72
1:A:5:ILE:CD1	1:A:135:PHE:CE1	2.73	0.72
1:A:70:LEU:CB	1:A:145:THR:HG21	2.20	0.72
1:A:115:ILE:CD1	1:A:156:ARG:CZ	2.62	0.72
1:A:184:PRO:HD3	1:A:395:PHE:CA	2.19	0.72
1:A:231:ILE:CD1	1:A:302:MET:HE2	2.19	0.72
2:B:6:HIS:CG	2:B:21:TRP:CZ2	2.77	0.72
2:B:226:ASP:OD2	6:B:502:TXL:C40	2.37	0.72
1:A:101:ASN:O	1:A:102:ASN:OD1	2.07	0.72
1:A:291:ILE:C	1:A:375:VAL:HG21	2.10	0.72
2:B:7:ILE:CG2	2:B:137:LEU:HD22	2.19	0.72
2:B:15:GLN:CD	5:B:501:GDP:O6	2.29	0.72
2:B:128:SER:O	2:B:129:CYS:CB	2.37	0.72
1:A:152:LEU:HD11	1:A:156:ARG:NH2	2.05	0.72
1:A:210:TYR:CZ	1:A:227:LEU:CD2	2.60	0.72
1:A:341:ILE:CG2	1:A:343:PHE:CE2	2.72	0.72
1:A:9:VAL:HB	1:A:138:PHE:O	1.88	0.71
2:B:288:VAL:O	2:B:292:THR:N	2.19	0.71
1:A:152:LEU:HD11	1:A:156:ARG:NE	2.04	0.71
1:A:179:THR:CG2	1:A:181:VAL:N	2.21	0.71
1:A:228:ASN:ND2	4:A:500:GTP:O6	2.23	0.71
3:K:18[B]:ARG:NH2	3:K:336:ILE:HD12	1.98	0.71
1:A:104:ALA:HA	1:A:108:TYR:CE2	2.25	0.71
1:A:291:ILE:HD11	1:A:373:ARG:HB3	1.72	0.71
1:A:294:ALA:C	1:A:300:ASN:ND2	2.43	0.71
2:B:143:GLY:CA	2:B:185:TYR:HE1	2.03	0.71
2:B:183:GLU:OE1	2:B:394:GLN:HB3	1.83	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:HIS:C	2:B:196:GLU:HG2	2.09	0.71
2:B:323:MET:HG2	2:B:324:SER:H	1.55	0.71
1:A:184:PRO:CB	1:A:399:TYR:CD2	2.73	0.71
1:A:184:PRO:HG2	1:A:395:PHE:CD2	2.20	0.71
1:A:289:ALA:HB1	1:A:331:ALA:CB	2.20	0.71
1:A:319:TYR:CE2	1:A:375:VAL:HG22	2.26	0.71
1:A:336:LYS:HG2	1:A:336:LYS:O	1.88	0.71
2:B:360:PRO:CD	2:B:374:SER:HB3	2.20	0.71
2:B:397:ALA:CA	2:B:401:ARG:HD3	2.19	0.71
1:A:53:PHE:HA	1:A:88:HIS:NE2	1.92	0.71
1:A:292:THR:HG22	1:A:319:TYR:HH	1.55	0.71
2:B:3:GLU:HG2	2:B:4:ILE:N	2.04	0.71
2:B:204:ILE:O	2:B:204:ILE:HG22	1.90	0.71
1:A:220:GLU:CG	1:A:220:GLU:CA	2.67	0.71
2:B:111:GLY:CA	2:B:115:VAL:HG23	2.20	0.71
2:B:183:GLU:HB2	2:B:184:PRO:HD2	1.70	0.71
1:A:36:MET:SD	1:A:61:HIS:HA	2.30	0.71
1:A:217:LEU:CG	1:A:218:ASP:H	1.86	0.71
1:A:231:ILE:CD1	1:A:302:MET:CE	2.69	0.71
1:A:292:THR:HG22	1:A:319:TYR:CE2	2.25	0.71
2:B:405:LEU:HD13	2:B:418:PHE:CZ	2.25	0.71
2:B:414:ASP:HB2	3:K:253:GLU:OE1	1.89	0.71
2:B:95:GLY:O	2:B:96:GLN:CB	2.39	0.71
2:B:191:VAL:CG2	2:B:421:ALA:CA	2.61	0.71
2:B:242:LEU:HD13	2:B:250:ALA:CB	2.15	0.71
1:A:241:SER:CB	1:A:356:ASN:ND2	2.53	0.71
2:B:213:CYS:SG	2:B:227:LEU:HD12	2.31	0.71
2:B:311:ARG:C	2:B:381:SER:HB2	2.11	0.71
1:A:256:GLN:CB	2:B:407:TRP:CZ3	2.74	0.71
2:B:7:ILE:CG2	2:B:137:LEU:CD2	2.69	0.71
2:B:132:LEU:HB2	2:B:164:ARG:NH1	2.06	0.71
2:B:184:PRO:HB2	2:B:399:PHE:CD2	2.23	0.71
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.71	0.71
2:B:259:MET:SD	2:B:378:ILE:HG22	2.31	0.71
2:B:284:ARG:HB3	2:B:287:THR:OG1	1.90	0.71
1:A:341:ILE:HG21	1:A:343:PHE:CE2	2.26	0.70
1:A:349:THR:CA	2:B:177:VAL:HG11	2.18	0.70
2:B:102:ASN:HB3	2:B:408:TYR:CD1	2.25	0.70
2:B:184:PRO:HG3	2:B:399:PHE:HB2	1.70	0.70
2:B:243:ARG:NH2	2:B:252:LEU:CD1	2.52	0.70
1:A:100:ALA:O	1:A:144:GLY:HA3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HG2	1:A:395:PHE:HA	1.72	0.70
1:A:253:THR:O	1:A:253:THR:HG22	1.90	0.70
1:A:254:GLU:CD	2:B:101:ASN:OD1	2.28	0.70
2:B:254:LYS:O	2:B:258:ASN:CG	2.28	0.70
2:B:416:MET:O	2:B:417:GLU:HB2	1.90	0.70
3:K:168:VAL:HG21	3:K:310:VAL:HG13	1.72	0.70
1:A:4:CYS:SG	1:A:252:LEU:CD1	2.72	0.70
1:A:30:ILE:HD12	1:A:64:ARG:HB3	1.72	0.70
1:A:239:THR:O	1:A:243:ARG:HB2	1.91	0.70
1:A:395:PHE:CE1	1:A:422:ARG:HG3	2.26	0.70
2:B:142:GLY:CA	2:B:182:VAL:CG2	2.65	0.70
2:B:287:THR:CG2	2:B:288:VAL:N	2.55	0.70
2:B:338:LYS:O	2:B:339:ASN:CG	2.29	0.70
1:A:167:LEU:CD1	1:A:252:LEU:HD22	2.21	0.70
2:B:75:MET:CE	2:B:75:MET:HA	2.21	0.70
2:B:147:SER:OG	2:B:189:LEU:CD1	2.21	0.70
2:B:175:PRO:O	2:B:176:LYS:HD3	1.88	0.70
2:B:222:PRO:C	2:B:223:THR:HG23	2.11	0.70
1:A:264:ARG:HH21	3:K:307:ARG:CG	1.97	0.70
2:B:2:ARG:CG	2:B:2:ARG:O	2.36	0.70
2:B:7:ILE:HG12	2:B:66:ILE:CG2	2.16	0.70
2:B:102:ASN:CB	2:B:408:TYR:CD1	2.73	0.70
2:B:183:GLU:CG	2:B:394:GLN:HB3	2.21	0.70
1:A:28:HIS:CG	1:A:29:GLY:H	2.10	0.70
1:A:76:ASP:C	1:A:80:THR:OG1	2.29	0.70
1:A:119:LEU:C	1:A:122:ILE:HG22	2.11	0.70
1:A:242:LEU:HD22	1:A:250:VAL:H	1.56	0.70
2:B:19:LYS:HD2	2:B:228:ASN:CB	2.18	0.70
2:B:35:SER:H	2:B:60:LYS:CE	2.02	0.70
3:K:252:SER:O	3:K:253:GLU:CG	2.37	0.70
1:A:16:ILE:HG21	1:A:138:PHE:CD1	2.26	0.70
1:A:30:ILE:CB	1:A:64:ARG:CB	2.66	0.70
1:A:30:ILE:CB	1:A:64:ARG:HB2	2.15	0.70
2:B:53:TYR:HE1	2:B:87:PHE:CE1	2.08	0.70
2:B:104:ALA:HA	2:B:413:MET:CE	2.22	0.70
1:A:3:GLU:HB2	1:A:132:LEU:HA	1.74	0.70
1:A:273:ALA:N	1:A:274:PRO:HD2	2.07	0.70
1:A:70:LEU:CD1	1:A:145:THR:CB	2.60	0.70
1:A:103:TYR:OH	1:A:151:SER:OG	2.08	0.70
1:A:288:VAL:O	1:A:291:ILE:HG13	1.92	0.70
1:A:312:TYR:CB	1:A:381:THR:HG22	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ALA:HB2	1:A:371:VAL:CG2	2.21	0.70
2:B:44:LEU:HB2	2:B:84:GLY:HA2	1.74	0.70
2:B:133:GLN:HE21	2:B:253:ARG:HH11	1.39	0.70
2:B:35:SER:HB3	2:B:60:LYS:CG	2.22	0.70
2:B:313:LEU:CA	2:B:344:VAL:HG21	2.22	0.70
1:A:66:VAL:HG22	1:A:125:LEU:CD1	2.23	0.69
2:B:169:PHE:CZ	2:B:235:MET:CG	2.75	0.69
2:B:242:LEU:CA	2:B:356:CYS:SG	2.79	0.69
2:B:265:LEU:O	2:B:267:PHE:CD2	2.45	0.69
1:A:122:ILE:CD1	1:A:157:LEU:HD22	2.23	0.69
2:B:48:ARG:HH11	2:B:60:LYS:CB	2.04	0.69
2:B:103:TRP:CD1	2:B:189:LEU:HD21	2.08	0.69
2:B:165:ILE:CD1	2:B:199:ASP:OD2	2.40	0.69
2:B:190:SER:O	2:B:191:VAL:C	2.30	0.69
2:B:386:GLU:C	2:B:388:PHE:N	2.43	0.69
1:A:30:ILE:HG22	1:A:64:ARG:HG2	1.70	0.69
1:A:158:SER:N	1:A:166:LYS:NZ	2.40	0.69
1:A:291:ILE:HD11	1:A:373:ARG:CB	2.22	0.69
2:B:183:GLU:CB	2:B:184:PRO:CD	2.29	0.69
2:B:201:THR:CG2	2:B:265:LEU:CD1	2.59	0.69
2:B:191:VAL:HG21	2:B:421:ALA:CA	2.21	0.69
2:B:253:ARG:HH11	2:B:253:ARG:HB2	1.58	0.69
1:A:17:GLY:O	1:A:21:TRP:HD1	1.76	0.69
2:B:242:LEU:HD23	2:B:356:CYS:SG	2.33	0.69
2:B:259:MET:CE	2:B:378:ILE:HG22	2.22	0.69
1:A:5:ILE:HD12	1:A:135:PHE:CE1	2.28	0.69
1:A:13:GLY:HA2	1:A:16:ILE:HG22	1.75	0.69
1:A:48:SER:OG	1:A:56:THR:CB	2.37	0.69
1:A:108:TYR:OH	1:A:417:GLU:HG3	1.91	0.69
1:A:115:ILE:CD1	1:A:156:ARG:HD2	2.23	0.69
1:A:271:THR:O	1:A:376:CYS:HA	1.92	0.69
2:B:3:GLU:OE2	2:B:64:ARG:NH1	2.25	0.69
2:B:289:PRO:HA	2:B:292:THR:OG1	1.93	0.69
1:A:395:PHE:CD1	1:A:422:ARG:HG3	2.28	0.69
1:A:401:LYS:HG2	1:A:402:ARG:HG3	1.75	0.69
1:A:405:VAL:CG2	1:A:409:VAL:CG2	2.65	0.69
2:B:229:HIS:CE1	6:B:502:TXL:H37	2.27	0.69
1:A:51:THR:CG2	1:A:52:PHE:N	2.45	0.69
1:A:72:PRO:CA	1:A:75:ILE:CG2	2.70	0.69
1:A:115:ILE:HD13	1:A:152:LEU:HD11	1.73	0.69
2:B:2:ARG:O	2:B:2:ARG:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:PRO:HD2	2:B:398:MET:SD	2.32	0.69
2:B:244:PHE:CB	2:B:245:PRO:CD	2.71	0.69
2:B:259:MET:O	2:B:261:PRO:HD3	1.93	0.69
2:B:390:ARG:O	2:B:394:GLN:CG	2.33	0.69
1:A:258:ASN:O	1:A:314:ALA:HB1	1.92	0.69
2:B:405:LEU:O	2:B:409:THR:OG1	2.07	0.69
1:A:344:VAL:HB	1:A:347:CYS:HG	1.55	0.69
2:B:14:ASN:ND2	2:B:69:ASP:OD1	2.25	0.69
2:B:53:TYR:HD1	2:B:87:PHE:CZ	2.05	0.69
2:B:320:ARG:HE	2:B:360:PRO:HG3	1.58	0.69
1:A:158:SER:CB	1:A:196:GLU:O	2.41	0.68
1:A:422:ARG:O	1:A:426:ALA:CB	2.41	0.68
2:B:97:SER:OG	2:B:110:GLU:OE1	2.10	0.68
1:A:103:TYR:CE2	1:A:189:LEU:CA	2.75	0.68
1:A:107:HIS:CD2	1:A:148:GLY:HA2	2.29	0.68
2:B:194:LEU:HD23	2:B:267:PHE:CE2	2.28	0.68
2:B:371:LEU:O	2:B:372:LYS:HB2	1.93	0.68
1:A:17:GLY:O	1:A:21:TRP:CD1	2.46	0.68
2:B:141:LEU:CD2	2:B:186:ASN:HB3	2.12	0.68
2:B:184:PRO:HG3	2:B:399:PHE:HD2	0.76	0.68
1:A:241:SER:CB	1:A:356:ASN:HD22	2.04	0.68
1:A:424:ASP:CG	3:K:307:ARG:CZ	2.53	0.68
2:B:183:GLU:CG	2:B:398:MET:SD	2.82	0.68
2:B:339:ASN:O	2:B:342:TYR:CB	2.40	0.68
2:B:405:LEU:O	2:B:409:THR:N	2.26	0.68
1:A:5:ILE:HD11	1:A:132:LEU:HD13	1.76	0.68
1:A:172:TYR:CZ	1:A:387:ALA:CB	2.74	0.68
1:A:184:PRO:CG	1:A:399:TYR:HD2	2.05	0.68
1:A:200:CYS:SG	1:A:259:LEU:HB2	2.32	0.68
1:A:397:LEU:HD22	1:A:401:LYS:NZ	2.08	0.68
2:B:35:SER:CA	2:B:60:LYS:HE2	2.21	0.68
2:B:194:LEU:CD2	2:B:267:PHE:CZ	2.75	0.68
2:B:369:ARG:O	6:B:502:TXL:C21	2.41	0.68
1:A:58:ALA:HB3	1:A:60:LYS:HG3	1.75	0.68
1:A:202:PHE:HE1	1:A:378:LEU:HD13	1.55	0.68
1:A:257:THR:CG2	2:B:407:TRP:HE3	2.01	0.68
2:B:31:ASP:H	2:B:32:PRO:HD3	1.59	0.68
1:A:1:MET:C	2:B:96:GLN:CD	2.42	0.68
1:A:88:HIS:CG	1:A:89:PRO:N	2.62	0.68
1:A:200:CYS:SG	1:A:260:VAL:HG23	2.33	0.68
1:A:312:TYR:CG	1:A:381:THR:HG22	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HD12	1:A:135:PHE:CZ	2.28	0.68
2:B:328:VAL:O	2:B:332:MET:HG2	1.93	0.68
1:A:16:ILE:CG2	1:A:138:PHE:CD1	2.77	0.68
1:A:145:THR:C	1:A:149:PHE:HB3	2.13	0.68
1:A:155:GLU:HG2	1:A:196:GLU:CG	2.21	0.68
1:A:184:PRO:HB3	1:A:395:PHE:CD2	2.19	0.68
2:B:42:LEU:O	2:B:43:GLN:CG	2.42	0.68
2:B:44:LEU:O	2:B:44:LEU:HG	1.93	0.68
2:B:135:PHE:HB2	2:B:166:MET:SD	2.34	0.68
1:A:66:VAL:CG2	1:A:125:LEU:HD13	2.24	0.68
1:A:97:GLU:HB3	1:A:110:ILE:HD13	1.74	0.67
1:A:102:ASN:C	1:A:185:TYR:HE2	1.98	0.67
2:B:104:ALA:HA	2:B:413:MET:HE3	1.73	0.67
2:B:229:HIS:CG	6:B:502:TXL:H37	2.28	0.67
1:A:315:CYS:SG	1:A:343:PHE:CE1	2.87	0.67
2:B:11:GLN:HB2	5:B:501:GDP:O2A	1.95	0.67
1:A:100:ALA:HB1	1:A:105:ARG:CB	2.22	0.67
1:A:103:TYR:N	1:A:408:TYR:HE1	1.81	0.67
2:B:295:MET:HE1	2:B:375:ALA:HB2	1.68	0.67
1:A:275:VAL:O	1:A:275:VAL:HG12	1.94	0.67
1:A:296:PHE:CE1	1:A:335:ILE:HG21	2.28	0.67
2:B:242:LEU:HD21	2:B:354:ALA:HB1	1.77	0.67
2:B:352:LYS:HG2	2:B:353:THR:N	2.09	0.67
1:A:83:TYR:O	1:A:84:ARG:CG	2.41	0.67
1:A:220:GLU:H	1:A:220:GLU:HG3	1.58	0.67
1:A:317:LEU:HA	1:A:376:CYS:O	1.94	0.67
2:B:22:GLU:HG2	2:B:83:PHE:CE2	2.26	0.67
2:B:102:ASN:ND2	2:B:105:LYS:HZ2	1.93	0.67
2:B:144:GLY:N	2:B:185:TYR:OH	2.27	0.67
2:B:175:PRO:C	2:B:176:LYS:HE2	2.12	0.67
1:A:57:GLY:HA3	1:A:61:HIS:ND1	2.08	0.67
1:A:77:GLU:O	1:A:80:THR:HB	1.95	0.67
1:A:196:GLU:O	1:A:197:HIS:CG	2.48	0.67
2:B:96:GLN:O	2:B:98:GLY:CA	2.42	0.67
2:B:405:LEU:CG	2:B:418:PHE:CZ	2.77	0.67
1:A:30:ILE:HG21	1:A:64:ARG:CG	2.09	0.67
2:B:201:THR:HG21	2:B:265:LEU:CG	2.24	0.67
2:B:244:PHE:O	2:B:245:PRO:O	2.12	0.67
2:B:286:LEU:HD13	2:B:372:LYS:HB2	1.67	0.67
1:A:154:MET:HE1	1:A:166:LYS:HB3	1.76	0.67
1:A:239:THR:O	1:A:243:ARG:CG	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:O	1:A:237:SER:OG	2.11	0.67
1:A:361:THR:O	1:A:362:VAL:CG2	2.41	0.67
1:A:399:TYR:O	1:A:403:ALA:HA	1.94	0.67
2:B:44:LEU:CB	2:B:85:GLN:HG3	2.24	0.67
1:A:311:LYS:O	1:A:312:TYR:O	2.12	0.66
2:B:6:HIS:O	2:B:66:ILE:N	2.23	0.66
2:B:30:ILE:HG23	2:B:243:ARG:NH1	2.08	0.66
1:A:205:ASP:HB2	1:A:302:MET:O	1.96	0.66
2:B:272:PHE:CE1	2:B:274:PRO:HG2	2.30	0.66
2:B:359:PRO:CB	2:B:372:LYS:O	2.43	0.66
2:B:401:ARG:CG	2:B:402:LYS:H	2.03	0.66
1:A:22:GLU:O	1:A:25:CYS:CB	2.44	0.66
1:A:191:THR:HG21	1:A:421:ALA:CA	2.24	0.66
2:B:181:VAL:CG2	2:B:404:PHE:HE2	2.08	0.66
2:B:181:VAL:CA	2:B:398:MET:HE1	2.25	0.66
1:A:48:SER:O	1:A:50:ASN:ND2	2.22	0.66
1:A:103:TYR:N	1:A:408:TYR:CE1	2.61	0.66
1:A:153:LEU:O	1:A:157:LEU:CG	2.42	0.66
1:A:254:GLU:OE2	2:B:101:ASN:OD1	2.13	0.66
1:A:272:TYR:CE2	1:A:274:PRO:HG2	2.26	0.66
1:A:328:VAL:HG13	1:A:353:VAL:HG11	1.77	0.66
2:B:184:PRO:HA	2:B:395:PHE:CD1	2.30	0.66
2:B:234:THR:OG1	2:B:302:MET:HE1	1.93	0.66
2:B:284:ARG:O	2:B:286:LEU:N	2.28	0.66
2:B:431:GLU:HA	2:B:434:GLN:CD	2.15	0.66
1:A:14:VAL:HB	1:A:74:VAL:HG21	1.78	0.66
1:A:41:THR:O	1:A:42:ILE:CB	2.44	0.66
1:A:126:ALA:O	1:A:132:LEU:CD1	2.41	0.66
1:A:312:TYR:HD2	1:A:381:THR:CG2	2.04	0.66
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.76	0.66
2:B:22:GLU:CA	2:B:83:PHE:CE2	2.79	0.66
2:B:30:ILE:CG2	2:B:136:GLN:HE22	2.09	0.66
2:B:103:TRP:CZ3	2:B:108:TYR:OH	2.18	0.66
2:B:158:ARG:HH11	2:B:197:ASN:H	1.41	0.66
2:B:184:PRO:HB3	2:B:395:PHE:CD1	2.30	0.66
2:B:197:ASN:OD1	2:B:197:ASN:O	2.13	0.66
2:B:388:PHE:C	2:B:390:ARG:N	2.49	0.66
1:A:88:HIS:CD2	1:A:89:PRO:N	2.63	0.66
1:A:172:TYR:HD1	1:A:173:PRO:O	1.79	0.66
2:B:229:HIS:NE2	6:B:502:TXL:C34	2.50	0.66
1:A:75:ILE:HD12	1:A:93:ILE:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:CE1	1:A:435:VAL:HG13	2.31	0.66
1:A:262:TYR:CB	1:A:263:PRO:CD	2.57	0.66
2:B:182:VAL:CG1	2:B:186:ASN:HD22	2.01	0.66
2:B:407:TRP:N	2:B:407:TRP:CD1	2.58	0.66
1:A:313:MET:HA	1:A:344:VAL:CG2	2.25	0.66
1:A:405:VAL:CG2	1:A:405:VAL:HG11	2.25	0.66
2:B:158:ARG:HA	2:B:197:ASN:HD22	0.52	0.66
1:A:146:GLY:HA2	1:A:150:THR:HG23	1.76	0.66
1:A:202:PHE:CD1	1:A:378:LEU:HD22	2.30	0.66
1:A:242:LEU:CD1	1:A:255:PHE:CZ	2.67	0.66
2:B:151:THR:HA	2:B:192:HIS:HE2	0.85	0.66
2:B:301:MET:HE2	2:B:377:PHE:CE1	2.31	0.66
1:A:184:PRO:CG	1:A:395:PHE:CG	2.60	0.66
1:A:223:THR:H	1:A:226:ASN:HD22	1.44	0.66
2:B:141:LEU:HD12	2:B:172:VAL:HA	0.91	0.66
2:B:391:ILE:O	2:B:394:GLN:HB2	1.95	0.66
1:A:65:ALA:O	1:A:66:VAL:CG2	2.43	0.65
1:A:223:THR:HG1	1:A:225:THR:HG1	1.33	0.65
1:A:291:ILE:CD1	1:A:373:ARG:CB	2.74	0.65
1:A:348:PRO:O	1:A:349:THR:OG1	2.13	0.65
2:B:8:GLN:HB2	2:B:67:LEU:HD12	1.78	0.65
2:B:44:LEU:CG	2:B:85:GLN:CG	2.67	0.65
2:B:142:GLY:O	2:B:185:TYR:CZ	2.49	0.65
2:B:268:PHE:CD1	2:B:380:ASN:OD1	2.49	0.65
1:A:107:HIS:CD2	1:A:151:SER:OG	2.49	0.65
1:A:109:THR:HG21	1:A:411:GLU:HB3	1.78	0.65
1:A:179:THR:CG2	1:A:181:VAL:CG2	2.74	0.65
2:B:44:LEU:HB3	2:B:85:GLN:HG3	1.76	0.65
2:B:87:PHE:CE1	2:B:89:PRO:HG3	2.28	0.65
2:B:92:PHE:CD2	2:B:114:LEU:CD1	2.64	0.65
2:B:259:MET:HE2	2:B:379:GLY:N	2.10	0.65
1:A:2:ARG:HH21	2:B:71:GLU:CG	2.08	0.65
1:A:239:THR:CG2	1:A:243:ARG:HG3	2.23	0.65
1:A:437:VAL:C	1:A:438:ASP:OD1	2.33	0.65
2:B:153:LEU:O	2:B:157:ILE:HG13	1.95	0.65
2:B:234:THR:HB	2:B:302:MET:HE2	1.77	0.65
1:A:238:ILE:HG23	1:A:255:PHE:CZ	2.32	0.65
1:A:239:THR:O	1:A:243:ARG:CB	2.44	0.65
1:A:288:VAL:O	1:A:291:ILE:CG1	2.44	0.65
2:B:107:HIS:CD2	2:B:152:LEU:HD23	2.19	0.65
1:A:143:GLY:O	1:A:144:GLY:C	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:HIS:O	1:A:198:SER:CB	2.45	0.65
2:B:34:GLY:O	2:B:36:TYR:CD2	2.49	0.65
2:B:103:TRP:CD1	2:B:148:GLY:HA3	2.31	0.65
1:A:2:ARG:HH21	2:B:99:ALA:HB2	1.61	0.65
1:A:311:LYS:C	1:A:312:TYR:O	2.31	0.65
2:B:23:VAL:HG21	2:B:232:SER:CB	2.26	0.65
2:B:53:TYR:CE1	2:B:89:PRO:CG	2.78	0.65
2:B:94:PHE:CD2	2:B:114:LEU:HD22	2.32	0.65
2:B:111:GLY:O	2:B:115:VAL:CB	2.45	0.65
2:B:336:GLN:HE21	2:B:351:VAL:HB	1.60	0.65
2:B:399:PHE:CZ	2:B:408:TYR:CE2	2.80	0.65
1:A:115:ILE:HD11	1:A:156:ARG:HD2	1.79	0.65
1:A:142:GLY:HA2	1:A:185:TYR:CD1	2.32	0.65
1:A:277:SER:CA	1:A:368:LEU:HD22	2.24	0.65
2:B:57:ALA:C	2:B:64:ARG:H	2.00	0.65
2:B:141:LEU:HD12	2:B:173:PRO:HD3	1.77	0.65
1:A:1:MET:O	2:B:96:GLN:NE2	2.27	0.65
1:A:5:ILE:HG13	1:A:64:ARG:HH21	1.60	0.65
1:A:277:SER:N	1:A:280:LYS:HG2	2.11	0.65
2:B:111:GLY:C	2:B:115:VAL:CG2	2.56	0.65
2:B:296:PHE:CE1	2:B:335:VAL:HG21	2.32	0.65
3:K:231:ASP:O	3:K:233:GLU:HG2	1.96	0.65
1:A:77:GLU:N	1:A:80:THR:OG1	2.30	0.65
1:A:80:THR:O	1:A:82:THR:N	2.30	0.65
2:B:12:CYS:SG	5:B:501:GDP:O4'	2.55	0.65
2:B:165:ILE:HD13	2:B:256:ALA:CB	2.26	0.65
2:B:183:GLU:CD	2:B:394:GLN:CG	2.65	0.65
2:B:435:TYR:CA	2:B:436:GLN:HG3	2.18	0.65
1:A:397:LEU:HD23	1:A:401:LYS:CD	2.11	0.65
2:B:68:VAL:HG13	2:B:149:MET:HE1	1.79	0.65
2:B:92:PHE:CE1	2:B:121:VAL:CG2	2.80	0.65
2:B:246:GLY:HA2	2:B:357:ASP:CG	2.18	0.65
1:A:2:ARG:NH2	2:B:99:ALA:HB3	2.11	0.64
1:A:5:ILE:HB	1:A:135:PHE:CD1	2.32	0.64
1:A:83:TYR:O	1:A:84:ARG:CB	2.44	0.64
1:A:219:ILE:CG2	1:A:219:ILE:C	2.65	0.64
2:B:342:TYR:C	2:B:343:PHE:CD2	2.71	0.64
1:A:104:ALA:CA	1:A:108:TYR:HD2	2.08	0.64
1:A:209:ILE:HD13	1:A:227:LEU:CD1	2.24	0.64
2:B:3:GLU:C	2:B:4:ILE:CG1	2.58	0.64
2:B:33:THR:HG22	2:B:34:GLY:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:MET:HB3	2:B:268:PHE:HE1	1.45	0.64
2:B:399:PHE:CE1	2:B:408:TYR:CZ	2.80	0.64
1:A:41:THR:O	1:A:41:THR:HG22	1.97	0.64
1:A:217:LEU:CD1	1:A:277:SER:HA	2.27	0.64
2:B:13:GLY:HA2	2:B:138:THR:OG1	1.95	0.64
2:B:200:GLU:CB	2:B:268:PHE:HE2	2.09	0.64
2:B:397:ALA:C	2:B:401:ARG:HB2	2.17	0.64
1:A:13:GLY:CA	1:A:16:ILE:HG22	2.26	0.64
1:A:22:GLU:O	1:A:25:CYS:HB3	1.97	0.64
1:A:77:GLU:C	1:A:80:THR:H	2.01	0.64
1:A:238:ILE:O	1:A:255:PHE:HZ	1.80	0.64
1:A:250:VAL:HG21	1:A:352:LYS:CE	2.08	0.64
1:A:287:SER:OG	1:A:290:GLU:CB	2.45	0.64
2:B:53:TYR:HD1	2:B:87:PHE:CE1	2.11	0.64
2:B:92:PHE:HE1	2:B:121:VAL:CG2	2.10	0.64
2:B:118:VAL:O	2:B:118:VAL:HG12	1.98	0.64
2:B:422:GLU:O	2:B:426:ASN:CB	2.41	0.64
1:A:57:GLY:CA	1:A:61:HIS:CE1	2.71	0.64
2:B:103:TRP:HE1	2:B:189:LEU:HD23	1.59	0.64
2:B:166:MET:O	2:B:199:ASP:HB3	1.97	0.64
2:B:384:ILE:O	2:B:385:GLN:C	2.33	0.64
2:B:426:ASN:C	2:B:428:LEU:N	2.51	0.64
1:A:97:GLU:CB	1:A:110:ILE:HG23	2.21	0.64
1:A:267:PHE:O	1:A:380:ASN:OD1	2.15	0.64
1:A:296:PHE:CZ	1:A:335:ILE:HD13	2.22	0.64
2:B:5:VAL:HG11	2:B:135:PHE:CE2	2.33	0.64
2:B:183:GLU:OE1	2:B:394:GLN:HG3	1.98	0.64
2:B:183:GLU:OE2	2:B:394:GLN:CD	2.36	0.64
1:A:291:ILE:HD12	1:A:373:ARG:HB3	1.77	0.64
1:A:317:LEU:O	1:A:353:VAL:HA	1.98	0.64
1:A:426:ALA:O	1:A:428:LEU:N	2.31	0.64
2:B:319:PHE:CE2	2:B:328:VAL:HG13	2.32	0.64
1:A:13:GLY:C	1:A:16:ILE:HG22	2.18	0.64
2:B:32:PRO:CA	2:B:59:ASN:HD22	2.05	0.64
2:B:133:GLN:NE2	2:B:253:ARG:HH11	1.94	0.64
1:A:103:TYR:CG	1:A:188:ILE:HG21	2.22	0.64
1:A:282:TYR:O	1:A:284:GLU:N	2.31	0.64
1:A:361:THR:CG2	1:A:362:VAL:N	2.59	0.64
1:A:361:THR:C	1:A:362:VAL:HG23	2.18	0.64
2:B:12:CYS:SG	5:B:501:GDP:N9	2.71	0.64
2:B:57:ALA:O	2:B:62:VAL:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:SER:O	2:B:81:GLY:C	2.35	0.64
2:B:92:PHE:HE1	2:B:121:VAL:HG21	1.62	0.64
2:B:154:ILE:HG23	2:B:198:THR:CG2	2.26	0.64
2:B:272:PHE:CZ	6:B:502:TXL:H28	2.33	0.64
1:A:1:MET:N	2:B:96:GLN:OE1	2.31	0.63
1:A:102:ASN:CA	1:A:185:TYR:HE2	2.11	0.63
1:A:179:THR:HB	1:A:182:VAL:HG23	1.79	0.63
1:A:192:HIS:O	1:A:196:GLU:CG	2.46	0.63
2:B:6:HIS:CE1	2:B:21:TRP:CH2	2.86	0.63
2:B:154:ILE:HD12	2:B:192:HIS:HE2	1.60	0.63
1:A:72:PRO:HA	1:A:75:ILE:HG21	1.80	0.63
1:A:237:SER:HA	1:A:320:ARG:NH1	2.13	0.63
1:A:264:ARG:NH1	1:A:424:ASP:O	2.32	0.63
1:A:303:VAL:HG12	1:A:305:CYS:SG	2.38	0.63
1:A:426:ALA:C	1:A:428:LEU:N	2.51	0.63
2:B:166:MET:CG	2:B:197:ASN:O	2.46	0.63
2:B:201:THR:HG21	2:B:265:LEU:HD21	0.74	0.63
1:A:2:ARG:NH2	2:B:99:ALA:HB2	2.13	0.63
1:A:172:TYR:HE2	1:A:388:TRP:CZ3	2.12	0.63
2:B:47:GLU:HG2	2:B:63:PRO:HD3	1.80	0.63
2:B:69:ASP:CG	2:B:74:THR:CB	2.60	0.63
2:B:101:ASN:O	2:B:105:LYS:HD2	1.97	0.63
2:B:231:VAL:HA	2:B:302:MET:CE	2.28	0.63
2:B:296:PHE:O	2:B:297:ASP:C	2.34	0.63
3:K:159:ASN:ND2	3:K:161:LYS:CG	2.52	0.63
1:A:67:PHE:HB2	1:A:92:LEU:CD2	2.28	0.63
2:B:174:SER:HB2	2:B:175:PRO:CD	2.29	0.63
2:B:386:GLU:C	2:B:388:PHE:H	2.01	0.63
1:A:28:HIS:CG	1:A:29:GLY:N	2.64	0.63
1:A:72:PRO:C	1:A:75:ILE:CG2	2.64	0.63
1:A:103:TYR:CZ	1:A:188:ILE:HG22	2.34	0.63
1:A:282:TYR:CE2	1:A:284:GLU:O	2.51	0.63
1:A:324:VAL:O	1:A:327:ASP:HB2	1.97	0.63
2:B:66:ILE:CG1	2:B:121:VAL:CG1	2.69	0.63
2:B:234:THR:CB	2:B:302:MET:CE	2.75	0.63
2:B:250:ALA:HB2	2:B:352:LYS:NZ	2.13	0.63
2:B:288:VAL:N	2:B:289:PRO:CD	2.59	0.63
2:B:313:LEU:CD2	2:B:344:VAL:HG21	2.28	0.63
2:B:426:ASN:O	2:B:428:LEU:N	2.32	0.63
1:A:132:LEU:O	1:A:134:GLY:N	2.30	0.63
1:A:191:THR:CG2	1:A:421:ALA:HA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:O	1:A:302:MET:CG	2.43	0.63
2:B:405:LEU:CD1	2:B:418:PHE:CZ	2.71	0.63
6:B:502:TXL:H192	6:B:502:TXL:C20	2.29	0.63
1:A:155:GLU:CD	1:A:192:HIS:HD2	1.88	0.63
1:A:304:LYS:HG2	1:A:304:LYS:O	1.98	0.63
1:A:420:GLU:OE1	3:K:170:GLU:C	2.36	0.63
2:B:30:ILE:HG22	2:B:243:ARG:NH1	2.14	0.63
2:B:274:PRO:HB2	2:B:371:LEU:HD11	1.81	0.63
2:B:398:MET:O	2:B:401:ARG:CB	2.45	0.63
2:B:398:MET:HE2	2:B:399:PHE:CE2	2.34	0.63
1:A:97:GLU:HA	1:A:97:GLU:OE1	1.97	0.63
1:A:142:GLY:CA	1:A:185:TYR:CE1	2.82	0.63
1:A:151:SER:HB2	1:A:192:HIS:HB2	1.79	0.63
1:A:184:PRO:CG	1:A:395:PHE:HB2	2.19	0.63
1:A:14:VAL:HA	1:A:67:PHE:CE1	2.34	0.63
1:A:210:TYR:HE2	1:A:227:LEU:CD2	2.02	0.63
1:A:282:TYR:CE2	1:A:285:GLN:HA	2.33	0.63
1:A:296:PHE:O	1:A:297:GLU:C	2.31	0.63
2:B:4:ILE:CD1	2:B:30:ILE:CB	2.77	0.63
2:B:35:SER:HB3	2:B:60:LYS:HG3	1.81	0.63
2:B:70:LEU:O	2:B:71:GLU:CG	2.47	0.63
2:B:101:ASN:ND2	2:B:185:TYR:OH	2.31	0.63
1:A:404:PHE:CD2	1:A:404:PHE:O	2.52	0.62
2:B:11:GLN:HB3	5:B:501:GDP:O1A	1.97	0.62
2:B:133:GLN:O	2:B:133:GLN:HG2	1.99	0.62
1:A:133:GLN:NE2	2:B:98:GLY:CA	2.61	0.62
1:A:154:MET:HB2	1:A:192:HIS:NE2	2.14	0.62
1:A:202:PHE:CE1	1:A:378:LEU:HD22	2.34	0.62
3:K:303:PHE:C	3:K:303:PHE:CD2	2.72	0.62
1:A:115:ILE:CD1	1:A:156:ARG:NE	2.59	0.62
2:B:23:VAL:O	2:B:26:ASP:CB	2.47	0.62
2:B:181:VAL:CA	2:B:398:MET:CE	2.77	0.62
1:A:2:ARG:O	1:A:243:ARG:NH1	2.32	0.62
1:A:57:GLY:HA3	1:A:61:HIS:CD2	2.34	0.62
1:A:224:TYR:CE1	4:A:500:GTP:C2	2.86	0.62
1:A:277:SER:N	1:A:280:LYS:CG	2.58	0.62
1:A:103:TYR:CD2	1:A:189:LEU:CG	2.78	0.62
1:A:257:THR:HG22	2:B:407:TRP:CD2	2.32	0.62
2:B:241:CYS:SG	2:B:320:ARG:CD	2.84	0.62
1:A:224:TYR:CD1	4:A:500:GTP:C2	2.88	0.62
1:A:288:VAL:O	1:A:291:ILE:HB	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:O	1:A:334:THR:OG1	2.13	0.62
2:B:169:PHE:HA	2:B:202:TYR:HB2	1.81	0.62
2:B:424:ASN:O	2:B:424:ASN:ND2	2.32	0.62
2:B:427:ASP:O	2:B:431:GLU:N	2.18	0.62
3:K:171:HIS:CD2	3:K:174:LEU:H	2.17	0.62
1:A:106:GLY:O	1:A:111:GLY:N	2.32	0.62
1:A:108:TYR:CZ	1:A:417:GLU:OE2	2.53	0.62
1:A:122:ILE:CD1	1:A:157:LEU:CD2	2.77	0.62
2:B:18:ALA:O	2:B:22:GLU:HG3	2.00	0.62
2:B:22:GLU:CD	2:B:83:PHE:CD2	2.70	0.62
2:B:106:GLY:O	2:B:111:GLY:N	2.32	0.62
2:B:165:ILE:HD13	2:B:256:ALA:HB1	1.80	0.62
2:B:246:GLY:HA2	2:B:357:ASP:OD2	2.00	0.62
2:B:342:TYR:O	2:B:343:PHE:CD2	2.52	0.62
1:A:107:HIS:CD2	1:A:148:GLY:C	2.72	0.62
2:B:289:PRO:O	2:B:293:GLN:CB	2.48	0.62
1:A:259:LEU:HB3	1:A:380:ASN:HD21	1.64	0.62
2:B:40:SER:O	2:B:41:ASP:CG	2.38	0.62
2:B:141:LEU:HB3	2:B:186:ASN:ND2	1.87	0.62
2:B:209:LEU:HD13	2:B:227:LEU:CG	2.15	0.62
1:A:289:ALA:HB1	1:A:331:ALA:HB2	1.82	0.62
2:B:183:GLU:OE1	2:B:394:GLN:CG	2.48	0.62
1:A:14:VAL:HB	1:A:74:VAL:CG2	2.30	0.61
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.35	0.61
1:A:341:ILE:HG22	1:A:343:PHE:CE2	2.35	0.61
2:B:13:GLY:HA3	2:B:138:THR:OG1	1.97	0.61
2:B:102:ASN:CB	2:B:408:TYR:HD1	2.07	0.61
2:B:216:THR:HG21	2:B:275:LEU:CD1	2.29	0.61
2:B:288:VAL:O	2:B:291:LEU:N	2.33	0.61
2:B:360:PRO:CG	2:B:374:SER:HB3	2.30	0.61
2:B:433:GLN:CG	2:B:437:ASP:OD1	2.48	0.61
1:A:3:GLU:CB	1:A:64:ARG:CZ	2.77	0.61
1:A:361:THR:HG22	1:A:362:VAL:H	1.63	0.61
2:B:238:VAL:HG13	2:B:255:LEU:CD1	2.30	0.61
2:B:241:CYS:SG	2:B:320:ARG:CZ	2.89	0.61
2:B:313:LEU:HD13	2:B:435:TYR:HD2	1.65	0.61
1:A:38:SER:C	1:A:39:ASP:CB	2.68	0.61
1:A:139:HIS:HB3	1:A:169:PHE:O	2.00	0.61
1:A:420:GLU:OE1	3:K:170:GLU:CB	2.47	0.61
2:B:4:ILE:HD11	2:B:30:ILE:O	1.98	0.61
2:B:22:GLU:HA	2:B:83:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASN:HB2	2:B:105:LYS:CG	2.29	0.61
2:B:173:PRO:HG2	2:B:391:ILE:HD11	1.78	0.61
1:A:276:ILE:HD13	1:A:282:TYR:CG	2.35	0.61
1:A:397:LEU:HA	1:A:401:LYS:HB3	1.78	0.61
2:B:78:VAL:CA	2:B:82:PRO:HG2	2.29	0.61
2:B:165:ILE:CD1	2:B:256:ALA:CB	2.79	0.61
2:B:250:ALA:CB	2:B:352:LYS:NZ	2.63	0.61
2:B:433:GLN:O	2:B:434:GLN:C	2.34	0.61
1:A:175:PRO:HD3	1:A:390:ARG:HH22	1.62	0.61
1:A:194:THR:CG2	1:A:195:LEU:HG	2.27	0.61
1:A:242:LEU:HD13	1:A:250:VAL:O	2.00	0.61
1:A:269:LEU:HD21	1:A:384:ILE:HD11	1.83	0.61
1:A:273:ALA:CB	1:A:294:ALA:CB	2.78	0.61
2:B:104:ALA:O	2:B:108:TYR:HB2	2.01	0.61
2:B:246:GLY:CA	2:B:357:ASP:OD2	2.48	0.61
1:A:204:VAL:HG13	1:A:302:MET:CE	2.28	0.61
1:A:313:MET:CE	1:A:346:TRP:HH2	2.12	0.61
2:B:274:PRO:C	2:B:276:THR:HG23	2.21	0.61
1:A:34:GLY:O	1:A:60:LYS:NZ	2.34	0.61
2:B:30:ILE:CG2	2:B:243:ARG:HH12	2.13	0.61
2:B:346:TRP:HZ3	2:B:347:ILE:CD1	1.79	0.61
1:A:9:VAL:CG1	1:A:146:GLY:HA2	2.31	0.61
1:A:209:ILE:CD1	1:A:227:LEU:CD1	2.67	0.61
1:A:277:SER:OG	1:A:280:LYS:CD	2.47	0.61
2:B:12:CYS:O	2:B:16:ILE:HB	1.98	0.61
2:B:31:ASP:N	2:B:32:PRO:CD	2.64	0.61
2:B:250:ALA:CB	2:B:352:LYS:HZ3	2.13	0.61
2:B:287:THR:HG22	2:B:289:PRO:N	2.14	0.61
1:A:83:TYR:O	1:A:83:TYR:CG	2.54	0.61
1:A:115:ILE:HD12	1:A:152:LEU:HG	0.67	0.61
1:A:172:TYR:CE1	1:A:387:ALA:HB1	2.34	0.61
2:B:15:GLN:O	2:B:18:ALA:HB3	2.00	0.61
2:B:295:MET:SD	2:B:375:ALA:HB1	2.36	0.61
2:B:433:GLN:CG	2:B:437:ASP:OD2	2.43	0.61
1:A:158:SER:CB	1:A:197:HIS:HB2	2.14	0.61
1:A:262:TYR:HE1	1:A:435:VAL:HG13	1.65	0.61
1:A:358:GLU:O	1:A:359:PRO:O	2.19	0.61
2:B:30:ILE:HG23	2:B:243:ARG:HH11	1.65	0.61
2:B:398:MET:HG2	2:B:399:PHE:H	1.64	0.61
1:A:97:GLU:O	1:A:110:ILE:CD1	2.48	0.60
1:A:109:THR:HG23	1:A:411:GLU:HB3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:HG3	2:B:228:ASN:ND2	2.16	0.60
2:B:34:GLY:HA2	2:B:37:HIS:CD2	2.36	0.60
2:B:78:VAL:HA	2:B:82:PRO:CG	2.32	0.60
2:B:79:ARG:O	2:B:80:SER:OG	2.19	0.60
2:B:223:THR:OG1	2:B:226:ASP:HB2	2.00	0.60
2:B:398:MET:CG	2:B:399:PHE:H	2.12	0.60
6:B:502:TXL:C9	6:B:502:TXL:C16	2.79	0.60
3:K:252:SER:HA	3:K:275:LEU:HD12	1.83	0.60
1:A:14:VAL:HG11	1:A:74:VAL:HG13	1.84	0.60
1:A:122:ILE:HD13	1:A:157:LEU:CD2	2.31	0.60
2:B:103:TRP:HZ3	2:B:413:MET:HE2	1.21	0.60
2:B:190:SER:C	2:B:192:HIS:N	2.53	0.60
1:A:184:PRO:HG2	1:A:399:TYR:HD2	1.67	0.60
2:B:141:LEU:HD13	2:B:173:PRO:HD3	1.81	0.60
2:B:184:PRO:HB2	2:B:399:PHE:CG	2.33	0.60
2:B:323:MET:CG	2:B:324:SER:H	2.13	0.60
1:A:151:SER:HB2	1:A:155:GLU:OE2	2.01	0.60
1:A:315:CYS:SG	1:A:343:PHE:HE1	2.21	0.60
2:B:4:ILE:HG21	2:B:30:ILE:HB	1.82	0.60
2:B:53:TYR:HE1	2:B:87:PHE:HE1	1.46	0.60
2:B:102:ASN:ND2	2:B:105:LYS:HZ1	1.96	0.60
2:B:339:ASN:O	2:B:342:TYR:CA	2.50	0.60
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.83	0.60
1:A:420:GLU:HG3	3:K:169:ARG:NE	2.16	0.60
2:B:103:TRP:O	2:B:107:HIS:HB3	2.02	0.60
2:B:107:HIS:CE1	2:B:152:LEU:HD23	2.22	0.60
2:B:136:GLN:HE22	2:B:243:ARG:HH12	1.49	0.60
2:B:151:THR:CB	2:B:192:HIS:NE2	2.28	0.60
1:A:5:ILE:CG2	1:A:135:PHE:CE1	2.83	0.60
1:A:264:ARG:O	1:A:265:ALA:O	2.19	0.60
1:A:327:ASP:O	1:A:331:ALA:HB3	2.01	0.60
1:A:396:ASP:O	1:A:401:LYS:CB	2.34	0.60
2:B:49:ILE:O	2:B:50:ASN:CG	2.40	0.60
1:A:193:THR:HG1	1:A:194:THR:N	1.97	0.60
1:A:237:SER:HB2	1:A:376:CYS:SG	2.41	0.60
1:A:362:VAL:HG13	1:A:367:ASP:HB3	1.83	0.60
1:A:420:GLU:CD	3:K:170:GLU:C	2.58	0.60
2:B:139:HIS:NE2	2:B:193:GLN:NE2	2.49	0.60
1:A:237:SER:CB	1:A:376:CYS:SG	2.90	0.60
1:A:427:ALA:O	1:A:431:ASP:N	2.19	0.60
2:B:78:VAL:O	2:B:82:PRO:CG	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:VAL:HG12	2:B:156:LYS:NZ	2.16	0.60
2:B:141:LEU:HG	2:B:171:VAL:O	2.01	0.60
1:A:191:THR:CG2	1:A:421:ALA:CA	2.79	0.60
1:A:217:LEU:CD1	1:A:368:LEU:CG	2.75	0.60
1:A:294:ALA:C	1:A:300:ASN:HD22	2.00	0.60
1:A:434:GLU:HB2	3:K:303:PHE:CG	2.37	0.60
1:A:437:VAL:O	1:A:437:VAL:HG12	2.01	0.60
2:B:22:GLU:OE1	2:B:83:PHE:CD1	2.55	0.60
2:B:151:THR:C	2:B:192:HIS:CD2	2.73	0.60
2:B:198:THR:O	2:B:265:LEU:HD13	2.02	0.60
1:A:2:ARG:HB3	1:A:243:ARG:HH12	1.67	0.60
1:A:45:GLY:C	1:A:46:ASP:CG	2.58	0.60
1:A:100:ALA:HB1	1:A:105:ARG:CG	2.31	0.60
1:A:350:GLY:HA2	2:B:180:THR:HG22	1.84	0.60
2:B:20:PHE:HZ	2:B:239:THR:HG21	1.67	0.60
2:B:320:ARG:HG3	2:B:320:ARG:O	2.00	0.60
3:K:159:ASN:HD21	3:K:161:LYS:HG3	1.64	0.60
1:A:6:SER:OG	1:A:65:ALA:N	2.34	0.59
1:A:8:HIS:HE1	1:A:17:GLY:HA3	1.65	0.59
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.02	0.59
1:A:26:LEU:HD11	1:A:361:THR:OG1	1.94	0.59
1:A:57:GLY:HA3	1:A:61:HIS:CG	2.37	0.59
1:A:153:LEU:O	1:A:157:LEU:HD12	2.01	0.59
1:A:297:GLU:C	1:A:299:ALA:N	2.55	0.59
2:B:41:ASP:C	2:B:42:LEU:CG	2.54	0.59
2:B:219:LEU:CD2	2:B:226:ASP:OD2	2.50	0.59
1:A:219:ILE:HG22	1:A:219:ILE:O	2.02	0.59
1:A:362:VAL:HG12	1:A:363:VAL:N	2.17	0.59
2:B:182:VAL:CG1	2:B:186:ASN:HD21	2.05	0.59
2:B:274:PRO:O	2:B:276:THR:CG2	2.46	0.59
2:B:295:MET:HE3	2:B:375:ALA:C	2.22	0.59
1:A:4:CYS:HB2	1:A:30:ILE:HG21	1.76	0.59
1:A:144:GLY:CA	1:A:185:TYR:OH	2.50	0.59
2:B:158:ARG:CG	2:B:197:ASN:ND2	2.61	0.59
2:B:174:SER:HB2	2:B:207:GLU:CB	2.26	0.59
2:B:226:ASP:CG	6:B:502:TXL:C40	2.70	0.59
1:A:173:PRO:HG3	1:A:182:VAL:CG1	2.32	0.59
1:A:324:VAL:CG1	1:A:325:PRO:HD2	2.33	0.59
2:B:14:ASN:HB3	2:B:74:THR:OG1	2.01	0.59
1:A:74:VAL:O	1:A:77:GLU:HB2	2.03	0.59
1:A:209:ILE:O	1:A:212:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:VAL:HG12	2:B:63:PRO:N	2.18	0.59
2:B:268:PHE:HA	2:B:380:ASN:OD1	2.03	0.59
2:B:383:ALA:O	2:B:386:GLU:CB	2.51	0.59
2:B:431:GLU:HA	2:B:434:GLN:NE2	2.17	0.59
1:A:236:SER:O	1:A:240:ALA:HB3	2.02	0.59
1:A:324:VAL:HB	1:A:327:ASP:OD2	2.03	0.59
2:B:175:PRO:CB	2:B:176:LYS:HE2	2.32	0.59
2:B:178:SER:O	2:B:179:ASP:HB2	2.00	0.59
2:B:216:THR:HG21	2:B:275:LEU:HD12	1.83	0.59
1:A:100:ALA:CB	1:A:105:ARG:CG	2.81	0.59
1:A:117:LEU:O	1:A:121:ARG:HG3	2.02	0.59
1:A:221:ARG:N	1:A:222:PRO:CD	2.65	0.59
1:A:385:ALA:HB2	1:A:432:TYR:HD2	1.68	0.59
1:A:397:LEU:HA	1:A:401:LYS:CD	2.33	0.59
1:A:423:GLU:OE1	3:K:170:GLU:HG2	1.99	0.59
2:B:23:VAL:O	2:B:26:ASP:HB2	2.02	0.59
2:B:346:TRP:HZ2	2:B:435:TYR:CD2	2.21	0.59
3:K:83[A]:GLN:NE2	3:K:87:GLU:OE2	2.36	0.59
1:A:36:MET:SD	1:A:60:LYS:CB	2.90	0.59
1:A:65:ALA:CB	1:A:91:GLN:CD	2.71	0.59
1:A:101:ASN:C	1:A:102:ASN:CG	2.59	0.59
1:A:310:GLY:HA3	1:A:382:THR:OG1	2.03	0.59
2:B:27:GLU:HB2	2:B:36:TYR:HB3	1.84	0.59
2:B:251:ASP:O	2:B:253:ARG:N	2.35	0.59
2:B:274:PRO:CB	2:B:371:LEU:HD11	2.32	0.59
2:B:397:ALA:O	2:B:401:ARG:CG	2.50	0.59
1:A:196:GLU:C	1:A:197:HIS:ND1	2.56	0.59
1:A:282:TYR:O	1:A:284:GLU:CA	2.50	0.59
1:A:78:VAL:HG13	1:A:87:PHE:HE1	1.61	0.59
1:A:143:GLY:O	1:A:145:THR:N	2.36	0.59
1:A:191:THR:O	1:A:194:THR:OG1	2.19	0.59
1:A:202:PHE:HA	1:A:268:PRO:HG2	1.85	0.59
1:A:303:VAL:HG12	1:A:304:LYS:N	2.17	0.59
1:A:335:ILE:C	1:A:337:THR:H	2.06	0.59
2:B:192:HIS:ND1	2:B:192:HIS:C	2.57	0.59
2:B:340:SER:O	2:B:343:PHE:N	2.35	0.59
2:B:383:ALA:O	2:B:386:GLU:HB2	2.03	0.59
1:A:65:ALA:HB1	1:A:91:GLN:CD	2.23	0.58
1:A:291:ILE:O	1:A:294:ALA:HB3	2.03	0.58
1:A:264:ARG:HH22	3:K:307:ARG:HD2	0.55	0.58
1:A:273:ALA:N	1:A:274:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CD2	2:B:64:ARG:O	2.56	0.58
2:B:194:LEU:HD21	2:B:267:PHE:HE2	1.65	0.58
3:K:171:HIS:HD2	3:K:173:LEU:H	1.51	0.58
3:K:303:PHE:CD2	3:K:303:PHE:O	2.56	0.58
1:A:28:HIS:ND1	1:A:29:GLY:O	2.32	0.58
1:A:103:TYR:CE1	1:A:188:ILE:CG2	2.67	0.58
1:A:185:TYR:CE1	1:A:189:LEU:HD11	2.39	0.58
2:B:4:ILE:HD13	2:B:30:ILE:HA	1.66	0.58
2:B:29:GLY:HA2	2:B:30:ILE:HG12	1.85	0.58
2:B:48:ARG:C	2:B:61:TYR:CD2	2.76	0.58
2:B:78:VAL:HA	2:B:82:PRO:HG2	1.86	0.58
2:B:181:VAL:HG22	2:B:404:PHE:CD2	2.39	0.58
2:B:272:PHE:CE2	6:B:502:TXL:H28	2.38	0.58
2:B:325:MET:HE1	2:B:355:VAL:HB	1.86	0.58
2:B:346:TRP:O	2:B:347:ILE:CG1	2.51	0.58
2:B:414:ASP:OD2	3:K:253:GLU:CD	2.40	0.58
3:K:100:GLY:H	8:K:503:ACP:H3B1	1.68	0.58
1:A:76:ASP:O	1:A:80:THR:CB	2.51	0.58
1:A:82:THR:C	1:A:84:ARG:H	2.07	0.58
1:A:171:ILE:H	1:A:203:MET:HE1	1.58	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.03	0.58
2:B:29:GLY:O	2:B:58:GLY:CA	2.52	0.58
2:B:133:GLN:HE21	2:B:253:ARG:HB2	1.68	0.58
2:B:184:PRO:CG	2:B:399:PHE:CB	2.69	0.58
2:B:400:ARG:CD	2:B:422:GLU:OE1	2.51	0.58
1:A:18:ASN:O	1:A:22:GLU:CG	2.51	0.58
1:A:107:HIS:HB2	1:A:149:PHE:N	2.17	0.58
1:A:155:GLU:CD	1:A:192:HIS:CD2	2.68	0.58
3:K:171:HIS:HD2	3:K:174:LEU:H	1.51	0.58
1:A:361:THR:CG2	1:A:362:VAL:H	2.15	0.58
2:B:70:LEU:O	2:B:71:GLU:HG3	2.03	0.58
3:K:234:THR:CB	3:K:236:ILE:HD11	2.31	0.58
1:A:141:PHE:HB3	1:A:173:PRO:HD3	1.84	0.58
1:A:197:HIS:O	1:A:198:SER:HB3	2.03	0.58
1:A:328:VAL:O	1:A:332:ILE:HG13	2.04	0.58
1:A:100:ALA:CB	1:A:105:ARG:HB3	2.31	0.58
1:A:208:ALA:HB2	1:A:303:VAL:HA	1.85	0.58
1:A:312:TYR:CE1	1:A:341:ILE:HG23	2.38	0.58
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.86	0.58
2:B:385:GLN:O	2:B:389:LYS:HG3	2.04	0.58
1:A:9:VAL:HG11	1:A:150:THR:HG23	1.78	0.58

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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	0.58
1:A:97:GLU:CG	1:A:110:ILE:HG23	2.33	0.58
1:A:169:PHE:HZ	1:A:235:VAL:HG22	1.61	0.58
1:A:242:LEU:CB	1:A:250:VAL:O	2.47	0.58
2:B:55:GLU:C	2:B:57:ALA:N	2.56	0.58
2:B:338:LYS:O	2:B:339:ASN:OD1	2.22	0.58
1:A:2:ARG:O	1:A:31:GLN:CG	2.39	0.58
1:A:30:ILE:O	1:A:32:PRO:HG3	1.95	0.58
1:A:45:GLY:O	1:A:46:ASP:OD2	2.22	0.58
1:A:85:GLN:O	1:A:87:PHE:N	2.37	0.58
1:A:275:VAL:O	1:A:368:LEU:HD13	2.04	0.58
1:A:324:VAL:HB	1:A:327:ASP:OD1	2.03	0.58
1:A:346:TRP:CE3	1:A:346:TRP:O	2.56	0.58
2:B:4:ILE:HG21	2:B:30:ILE:CB	2.34	0.58
2:B:22:GLU:CG	2:B:83:PHE:CG	2.80	0.58
2:B:105:LYS:CE	2:B:411:GLU:HG3	2.34	0.58
2:B:142:GLY:HA2	2:B:185:TYR:CG	2.37	0.58
2:B:181:VAL:O	2:B:399:PHE:CZ	2.57	0.58
2:B:302:MET:O	2:B:302:MET:CG	2.47	0.58
1:A:103:TYR:CE2	1:A:147:SER:C	2.76	0.57
1:A:115:ILE:CD1	1:A:156:ARG:CD	2.82	0.57
1:A:175:PRO:HG2	1:A:207:GLU:HG2	1.86	0.57
1:A:192:HIS:ND1	1:A:192:HIS:C	2.57	0.57
2:B:213:CYS:HA	2:B:217:LEU:CD1	2.06	0.57
1:A:26:LEU:CD1	1:A:361:THR:HG21	2.15	0.57
2:B:308:ARG:O	2:B:342:TYR:HE2	1.86	0.57
1:A:182:VAL:HG12	1:A:186:ASN:ND2	2.14	0.57
2:B:311:ARG:O	2:B:381:SER:CB	2.52	0.57
1:A:14:VAL:CG1	1:A:74:VAL:HG22	2.35	0.57
1:A:14:VAL:CG2	1:A:69:ASP:OD1	2.52	0.57
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.30	0.57
2:B:7:ILE:CB	2:B:137:LEU:HD21	2.28	0.57
2:B:57:ALA:HA	2:B:64:ARG:HB2	0.68	0.57
2:B:104:ALA:HB2	2:B:413:MET:SD	2.44	0.57
1:A:8:HIS:CE1	1:A:17:GLY:HA3	2.39	0.57
1:A:23:LEU:CD2	1:A:236:SER:CB	2.81	0.57
1:A:23:LEU:HD21	1:A:236:SER:CB	2.34	0.57
1:A:102:ASN:C	1:A:185:TYR:CE2	2.78	0.57
1:A:206:ASN:CG	4:A:500:GTP:HN22	2.06	0.57
1:A:242:LEU:HD12	1:A:255:PHE:CE2	2.34	0.57
1:A:271:THR:CG2	1:A:377:MET:HB3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:O	1:A:341:ILE:HG12	2.04	0.57
2:B:22:GLU:C	2:B:24:ILE:H	2.06	0.57
2:B:229:HIS:O	2:B:230:LEU:C	2.43	0.57
3:K:18[A]:ARG:HE	3:K:22[A]:ARG:NH2	2.03	0.57
1:A:141:PHE:O	1:A:182:VAL:CG1	2.48	0.57
2:B:295:MET:CE	2:B:375:ALA:C	2.72	0.57
2:B:259:MET:HE2	2:B:379:GLY:CA	2.32	0.57
2:B:319:PHE:CZ	2:B:328:VAL:HG12	2.36	0.57
1:A:13:GLY:HA2	1:A:16:ILE:HG21	1.87	0.57
1:A:103:TYR:OH	1:A:151:SER:HB2	1.98	0.57
1:A:434:GLU:CB	3:K:303:PHE:CG	2.87	0.57
2:B:68:VAL:CG1	2:B:149:MET:HE2	2.24	0.57
2:B:242:LEU:HA	2:B:356:CYS:SG	2.45	0.57
2:B:371:LEU:O	2:B:372:LYS:CB	2.50	0.57
1:A:77:GLU:O	1:A:83:TYR:HB2	2.05	0.57
1:A:191:THR:HG23	1:A:421:ALA:HB1	1.86	0.57
2:B:7:ILE:O	2:B:137:LEU:HA	2.04	0.57
2:B:26:ASP:OD1	2:B:26:ASP:O	2.23	0.57
2:B:89:PRO:O	2:B:90:ASP:CG	2.43	0.57
2:B:123:ARG:O	2:B:126:SER:OG	2.20	0.57
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.87	0.57
1:A:184:PRO:CB	1:A:399:TYR:HD2	2.15	0.57
1:A:217:LEU:CB	1:A:368:LEU:HD11	2.35	0.57
1:A:254:GLU:OE2	1:A:352:LYS:HE3	2.04	0.57
2:B:192:HIS:HA	2:B:196:GLU:HG3	1.24	0.57
2:B:230:LEU:O	2:B:233:ALA:HB3	2.04	0.57
2:B:274:PRO:HB2	2:B:371:LEU:CD1	2.34	0.57
2:B:388:PHE:O	2:B:390:ARG:N	2.38	0.57
1:A:267:PHE:CG	1:A:388:TRP:HZ2	2.23	0.56
1:A:335:ILE:CG2	1:A:341:ILE:HG13	2.35	0.56
2:B:201:THR:OG1	2:B:267:PHE:CD1	2.58	0.56
2:B:371:LEU:N	6:B:502:TXL:H183	2.20	0.56
3:K:18[B]:ARG:HH21	3:K:336:ILE:CD1	2.04	0.56
1:A:48:SER:HG	1:A:56:THR:HB	1.63	0.56
1:A:64:ARG:HH22	1:A:132:LEU:CG	2.09	0.56
1:A:122:ILE:O	1:A:126:ALA:N	2.35	0.56
2:B:3:GLU:CD	2:B:64:ARG:HH12	2.09	0.56
2:B:56:ALA:HB1	2:B:62:VAL:H	1.70	0.56
2:B:92:PHE:HD2	2:B:114:LEU:CD1	1.97	0.56
2:B:158:ARG:NH1	2:B:197:ASN:H	2.03	0.56
3:K:119:ILE:HB	3:K:120:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:13:GLY:CA	2.53	0.56
1:A:33:ASP:O	1:A:33:ASP:OD1	2.23	0.56
1:A:89:PRO:O	1:A:90:GLU:HB2	2.04	0.56
1:A:97:GLU:CB	1:A:110:ILE:HD13	2.35	0.56
1:A:106:GLY:HA2	1:A:111:GLY:H	1.69	0.56
1:A:170:SER:OG	1:A:203:MET:CG	1.65	0.56
1:A:228:ASN:ND2	4:A:500:GTP:N1	2.49	0.56
1:A:239:THR:O	1:A:243:ARG:HG2	2.05	0.56
1:A:242:LEU:HD11	1:A:318:LEU:HD11	1.87	0.56
1:A:292:THR:O	1:A:295:CYS:HB2	2.05	0.56
1:A:327:ASP:O	1:A:331:ALA:CB	2.53	0.56
2:B:21:TRP:HA	2:B:24:ILE:CD1	2.34	0.56
2:B:33:THR:C	2:B:59:ASN:ND2	2.44	0.56
2:B:102:ASN:CB	2:B:408:TYR:CE1	2.88	0.56
2:B:154:ILE:HG23	2:B:198:THR:HG22	1.87	0.56
2:B:239:THR:HB	2:B:243:ARG:NH1	2.20	0.56
2:B:244:PHE:CG	2:B:245:PRO:HD3	2.40	0.56
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.87	0.56
3:K:77[B]:ILE:H	3:K:77[B]:ILE:HD12	1.70	0.56
3:K:207:ALA:HA	3:K:211:ASN:OD1	2.06	0.56
1:A:28:HIS:ND1	1:A:29:GLY:N	2.54	0.56
1:A:30:ILE:C	1:A:32:PRO:CG	2.55	0.56
1:A:326:LYS:NZ	2:B:214:PHE:HZ	1.81	0.56
1:A:14:VAL:HG21	1:A:69:ASP:OD1	2.06	0.56
1:A:325:PRO:CG	2:B:223:THR:HA	2.36	0.56
1:A:341:ILE:HG22	1:A:343:PHE:CD2	2.40	0.56
1:A:405:VAL:HG11	1:A:405:VAL:HG21	1.87	0.56
1:A:431:ASP:HA	3:K:303:PHE:HD1	1.64	0.56
2:B:49:ILE:HA	2:B:61:TYR:CE2	2.41	0.56
2:B:262:PHE:HB2	2:B:266:HIS:HE1	1.71	0.56
1:A:219:ILE:HG21	1:A:219:ILE:HD13	1.87	0.56
1:A:258:ASN:OD1	1:A:352:LYS:CE	2.53	0.56
2:B:274:PRO:CB	2:B:371:LEU:CD2	2.81	0.56
2:B:359:PRO:HB2	2:B:372:LYS:O	2.05	0.56
1:A:9:VAL:CG2	1:A:138:PHE:O	2.54	0.56
1:A:107:HIS:CG	1:A:148:GLY:C	2.77	0.56
1:A:267:PHE:CE1	1:A:388:TRP:CZ2	2.93	0.56
1:A:288:VAL:O	1:A:291:ILE:CB	2.54	0.56
2:B:6:HIS:ND1	2:B:21:TRP:CZ2	2.74	0.56
2:B:55:GLU:C	2:B:57:ALA:H	2.07	0.56
2:B:64:ARG:HH21	2:B:125:GLU:HB3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:252:SER:CA	3:K:275:LEU:HD11	2.31	0.56
1:A:2:ARG:HB3	1:A:243:ARG:NH1	2.21	0.56
1:A:14:VAL:HG21	1:A:74:VAL:HG13	1.88	0.56
1:A:23:LEU:HD21	1:A:236:SER:HB3	1.86	0.56
1:A:192:HIS:CG	1:A:193:THR:N	2.73	0.56
1:A:332:ILE:HD11	1:A:353:VAL:HG21	1.78	0.56
2:B:176:LYS:C	2:B:177:VAL:HG13	2.25	0.56
2:B:183:GLU:OE2	2:B:394:GLN:CG	2.53	0.56
2:B:212:ILE:CD1	2:B:302:MET:HB2	2.35	0.56
2:B:311:ARG:CD	2:B:341:SER:O	2.54	0.56
1:A:62:VAL:HG13	1:A:63:PRO:HD3	1.80	0.56
1:A:228:ASN:HD21	4:A:500:GTP:HN1	1.48	0.56
2:B:170:SER:O	2:B:204:ILE:HB	2.06	0.56
2:B:191:VAL:HG23	2:B:421:ALA:CB	2.36	0.56
1:A:35:GLN:O	1:A:36:MET:CG	2.54	0.55
1:A:107:HIS:HD2	1:A:151:SER:OG	1.88	0.55
1:A:174:ALA:HB3	1:A:175:PRO:CD	2.10	0.55
1:A:187:SER:O	1:A:191:THR:HG23	2.07	0.55
1:A:324:VAL:HG13	1:A:325:PRO:HD2	1.87	0.55
2:B:44:LEU:O	2:B:47:GLU:CB	2.54	0.55
1:A:180:ALA:HB1	1:A:398:MET:CE	2.36	0.55
2:B:87:PHE:HE1	2:B:89:PRO:HG3	1.58	0.55
2:B:158:ARG:HH11	2:B:197:ASN:N	2.03	0.55
2:B:223:THR:OG1	2:B:226:ASP:CB	2.54	0.55
2:B:394:GLN:O	2:B:398:MET:CB	2.54	0.55
1:A:25:CYS:O	1:A:26:LEU:HD23	2.06	0.55
1:A:115:ILE:CD1	1:A:152:LEU:HD21	2.32	0.55
1:A:141:PHE:HB2	1:A:172:TYR:HA	1.87	0.55
1:A:157:LEU:HB2	1:A:166:LYS:NZ	2.21	0.55
1:A:208:ALA:HB2	1:A:303:VAL:CA	2.36	0.55
2:B:50:ASN:N	2:B:61:TYR:CE2	2.71	0.55
1:A:66:VAL:HG21	1:A:125:LEU:HD12	1.87	0.55
1:A:306:ASP:CG	1:A:308:ARG:CG	2.69	0.55
2:B:414:ASP:HB3	3:K:253:GLU:OE2	2.05	0.55
1:A:33:ASP:OD1	1:A:33:ASP:C	2.40	0.55
1:A:217:LEU:CD2	1:A:368:LEU:CD1	2.70	0.55
1:A:292:THR:CG2	1:A:319:TYR:OH	2.42	0.55
2:B:40:SER:O	2:B:41:ASP:CB	2.54	0.55
2:B:147:SER:HB3	2:B:189:LEU:HD11	0.56	0.55
2:B:174:SER:O	2:B:176:LYS:N	2.39	0.55
2:B:385:GLN:CD	2:B:433:GLN:HB2	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG21	1:A:74:VAL:CG1	2.36	0.55
1:A:69:ASP:HB3	1:A:71:GLU:O	2.07	0.55
2:B:175:PRO:HD2	2:B:207:GLU:HG2	1.88	0.55
2:B:191:VAL:HG22	2:B:421:ALA:HA	1.79	0.55
2:B:296:PHE:CD1	2:B:335:VAL:HG11	2.40	0.55
1:A:209:ILE:HD11	1:A:231:ILE:CD1	2.17	0.55
1:A:230:LEU:HG	1:A:302:MET:CE	2.36	0.55
2:B:103:TRP:HE3	2:B:413:MET:CE	1.90	0.55
2:B:294:GLN:CD	2:B:300:ASN:OD1	2.45	0.55
1:A:9:VAL:CG1	1:A:150:THR:HG23	2.31	0.55
1:A:133:GLN:HE22	2:B:98:GLY:HA2	1.69	0.55
1:A:219:ILE:C	1:A:219:ILE:HG22	2.26	0.55
2:B:56:ALA:CB	2:B:62:VAL:CG2	2.69	0.55
2:B:288:VAL:C	2:B:291:LEU:H	2.10	0.55
2:B:296:PHE:CE1	2:B:335:VAL:CG1	2.83	0.55
2:B:313:LEU:N	2:B:381:SER:HA	2.22	0.55
1:A:224:TYR:CE1	4:A:500:GTP:C4	2.94	0.55
1:A:11:GLN:OE1	1:A:74:VAL:HB	2.07	0.55
1:A:26:LEU:O	1:A:27:GLU:HB2	2.06	0.55
1:A:70:LEU:HG	1:A:145:THR:HG21	1.87	0.55
1:A:137:VAL:CB	1:A:168:GLU:HG2	2.37	0.55
1:A:154:MET:HE3	1:A:166:LYS:HD2	1.88	0.55
2:B:265:LEU:HD23	2:B:267:PHE:HZ	1.67	0.55
3:K:159:ASN:C	3:K:161:LYS:H	2.09	0.55
1:A:103:TYR:CZ	1:A:151:SER:OG	2.59	0.54
1:A:289:ALA:HB1	1:A:331:ALA:HB1	1.89	0.54
2:B:22:GLU:CD	2:B:83:PHE:CB	2.72	0.54
2:B:287:THR:CA	2:B:290:GLU:HB3	2.36	0.54
1:A:68:VAL:CG1	1:A:149:PHE:HZ	2.07	0.54
1:A:154:MET:CE	1:A:166:LYS:CD	2.79	0.54
2:B:344:VAL:O	2:B:344:VAL:HG12	2.07	0.54
1:A:28:HIS:CD2	1:A:33:ASP:HB3	2.41	0.54
1:A:166:LYS:CD	1:A:197:HIS:HD2	2.20	0.54
1:A:166:LYS:HD2	1:A:197:HIS:HD2	1.73	0.54
2:B:102:ASN:CA	2:B:408:TYR:HE1	2.18	0.54
1:A:313:MET:N	1:A:380:ASN:O	2.40	0.54
2:B:129:CYS:O	2:B:130:ASP:OD1	2.24	0.54
2:B:136:GLN:NE2	2:B:243:ARG:HH12	2.05	0.54
2:B:280:SER:C	2:B:282:GLN:H	2.07	0.54
2:B:287:THR:CG2	2:B:290:GLU:N	2.68	0.54
2:B:308:ARG:HD3	2:B:342:TYR:HE2	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLY:HA2	1:A:151:SER:HG	1.71	0.54
1:A:179:THR:CG2	1:A:180:ALA:N	2.67	0.54
1:A:440:VAL:N	2:B:402:LYS:NZ	2.55	0.54
2:B:6:HIS:HB2	2:B:65:ALA:CA	2.28	0.54
2:B:14:ASN:HD21	2:B:69:ASP:HA	1.72	0.54
2:B:23:VAL:O	2:B:26:ASP:HB3	2.08	0.54
2:B:49:ILE:O	2:B:50:ASN:ND2	2.40	0.54
2:B:416:MET:O	2:B:417:GLU:CB	2.55	0.54
1:A:5:ILE:HD13	1:A:135:PHE:CE1	2.42	0.54
1:A:53:PHE:HA	1:A:88:HIS:ND1	2.16	0.54
2:B:143:GLY:C	2:B:185:TYR:CE1	2.80	0.54
1:A:108:TYR:HA	1:A:112:LYS:HE2	1.86	0.54
1:A:148:GLY:O	1:A:152:LEU:N	2.40	0.54
1:A:220:GLU:CG	1:A:220:GLU:N	2.70	0.54
1:A:416:GLY:O	1:A:417:GLU:CB	2.55	0.54
2:B:48:ARG:HH11	2:B:60:LYS:HG2	1.60	0.54
2:B:106:GLY:HA2	2:B:111:GLY:H	1.72	0.54
2:B:118:VAL:O	2:B:122:VAL:HG23	2.07	0.54
2:B:284:ARG:HD3	2:B:290:GLU:OE1	2.05	0.54
1:A:146:GLY:HA2	1:A:150:THR:CG2	2.37	0.54
1:A:157:LEU:O	1:A:161:TYR:HB2	2.07	0.54
1:A:259:LEU:O	1:A:380:ASN:ND2	2.41	0.54
1:A:267:PHE:CD2	1:A:388:TRP:HZ2	2.25	0.54
2:B:32:PRO:C	2:B:59:ASN:HD22	2.06	0.54
2:B:105:LYS:CE	2:B:411:GLU:CG	2.86	0.54
2:B:309:HIS:HB3	2:B:386:GLU:OE2	2.07	0.54
1:A:200:CYS:SG	1:A:256:GLN:HA	2.48	0.54
1:A:209:ILE:HD12	1:A:227:LEU:HD21	1.90	0.54
2:B:35:SER:HA	2:B:60:LYS:CE	2.30	0.54
2:B:202:TYR:OH	2:B:238:VAL:HG11	2.08	0.54
2:B:206:ASN:O	2:B:210:TYR:HD2	1.86	0.54
2:B:360:PRO:HG2	2:B:374:SER:HB3	1.90	0.54
2:B:399:PHE:CZ	2:B:408:TYR:CZ	2.96	0.54
2:B:414:ASP:C	2:B:416:MET:H	2.05	0.54
1:A:119:LEU:CA	1:A:122:ILE:HG22	2.38	0.54
1:A:252:LEU:CA	1:A:255:PHE:HD2	2.07	0.54
1:A:431:ASP:CA	3:K:303:PHE:HE1	2.16	0.54
2:B:143:GLY:C	2:B:185:TYR:HE1	2.11	0.54
1:A:81:GLY:O	1:A:83:TYR:N	2.41	0.53
1:A:151:SER:CB	1:A:192:HIS:CB	2.75	0.53
1:A:167:LEU:HD11	1:A:252:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HG22	1:A:341:ILE:HG13	1.88	0.53
2:B:41:ASP:O	2:B:42:LEU:CB	2.56	0.53
2:B:158:ARG:HG3	2:B:197:ASN:ND2	2.22	0.53
2:B:321:GLY:HA2	2:B:359:PRO:HB3	1.90	0.53
1:A:9:VAL:CB	1:A:138:PHE:O	2.54	0.53
1:A:22:GLU:O	1:A:25:CYS:HB2	2.07	0.53
1:A:114:ILE:O	1:A:114:ILE:HG22	2.07	0.53
2:B:135:PHE:CD2	2:B:157:ILE:HG21	2.44	0.53
2:B:238:VAL:HG13	2:B:255:LEU:HD13	1.88	0.53
2:B:339:ASN:HA	2:B:342:TYR:CD1	2.43	0.53
1:A:154:MET:HE1	1:A:166:LYS:HD3	1.90	0.53
1:A:256:GLN:O	1:A:260:VAL:CB	2.55	0.53
1:A:363:VAL:HG12	1:A:364:PRO:CG	2.35	0.53
1:A:386:GLU:O	1:A:389:ALA:HB3	2.09	0.53
2:B:4:ILE:HD13	2:B:30:ILE:CA	2.35	0.53
2:B:31:ASP:H	2:B:32:PRO:CD	2.20	0.53
2:B:195:VAL:O	2:B:195:VAL:HG12	2.08	0.53
2:B:293:GLN:O	2:B:297:ASP:OD1	2.27	0.53
1:A:424:ASP:CA	3:K:307:ARG:HH22	2.08	0.53
2:B:8:GLN:O	2:B:68:VAL:HB	2.08	0.53
2:B:94:PHE:HZ	2:B:110:GLU:O	1.92	0.53
2:B:172:VAL:HG21	2:B:205:ASP:OD1	2.09	0.53
2:B:201:THR:CG2	2:B:265:LEU:CD2	2.43	0.53
1:A:2:ARG:HG2	1:A:133:GLN:NE2	2.23	0.53
1:A:108:TYR:C	1:A:112:LYS:HG3	2.29	0.53
1:A:194:THR:CG2	1:A:195:LEU:H	2.02	0.53
1:A:277:SER:H	1:A:280:LYS:HG2	1.60	0.53
1:A:313:MET:CG	1:A:380:ASN:O	2.57	0.53
2:B:102:ASN:CA	2:B:408:TYR:CE1	2.91	0.53
2:B:141:LEU:HD12	2:B:173:PRO:CD	2.37	0.53
1:A:191:THR:HG21	1:A:421:ALA:HA	1.88	0.53
1:A:219:ILE:CG2	1:A:219:ILE:CD1	2.86	0.53
2:B:7:ILE:HG21	2:B:137:LEU:HD22	1.91	0.53
2:B:42:LEU:O	2:B:43:GLN:CB	2.56	0.53
2:B:339:ASN:HB3	2:B:342:TYR:HB2	1.90	0.53
1:A:34:GLY:C	1:A:35:GLN:HG3	2.29	0.53
2:B:242:LEU:HB3	2:B:250:ALA:O	2.08	0.53
2:B:288:VAL:C	2:B:290:GLU:N	2.57	0.53
3:K:321:GLY:O	3:K:356:ASN:HB3	2.08	0.53
1:A:103:TYR:O	1:A:148:GLY:HA3	2.08	0.53
1:A:180:ALA:HB1	1:A:398:MET:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:HG3	1:A:207:GLU:O	2.08	0.53
1:A:220:GLU:CG	1:A:220:GLU:H	2.20	0.53
2:B:40:SER:C	2:B:41:ASP:CG	2.67	0.53
1:A:142:GLY:HA2	1:A:185:TYR:CE1	2.43	0.53
2:B:92:PHE:CE2	2:B:114:LEU:CD1	2.89	0.53
1:A:191:THR:HG22	1:A:421:ALA:HA	1.91	0.53
2:B:6:HIS:ND1	2:B:21:TRP:HZ2	2.07	0.53
2:B:57:ALA:O	2:B:64:ARG:N	2.42	0.53
2:B:360:PRO:HD3	2:B:374:SER:HB3	1.91	0.53
2:B:6:HIS:CE1	2:B:21:TRP:CZ2	2.97	0.52
2:B:184:PRO:CA	2:B:395:PHE:HD1	2.22	0.52
2:B:342:TYR:O	2:B:343:PHE:CG	2.62	0.52
1:A:40:LYS:C	1:A:42:ILE:H	2.08	0.52
1:A:256:GLN:HB2	2:B:407:TRP:CZ3	2.44	0.52
2:B:6:HIS:HD2	2:B:64:ARG:O	1.90	0.52
2:B:126:SER:HA	2:B:132:LEU:HD11	1.88	0.52
2:B:184:PRO:CB	2:B:399:PHE:CE2	2.69	0.52
1:A:219:ILE:O	1:A:222:PRO:HD3	2.09	0.52
2:B:107:HIS:CD2	2:B:151:THR:OG1	2.62	0.52
2:B:181:VAL:C	2:B:398:MET:HE1	2.29	0.52
2:B:181:VAL:C	2:B:399:PHE:HE2	2.12	0.52
2:B:190:SER:OG	2:B:191:VAL:N	2.42	0.52
2:B:206:ASN:O	2:B:210:TYR:HE2	1.85	0.52
1:A:21:TRP:N	1:A:21:TRP:CD1	2.76	0.52
1:A:63:PRO:HB2	1:A:65:ALA:HB2	1.92	0.52
1:A:288:VAL:CG2	1:A:373:ARG:CD	2.44	0.52
1:A:325:PRO:HG2	2:B:223:THR:HA	1.91	0.52
2:B:64:ARG:HH21	2:B:125:GLU:C	2.13	0.52
2:B:135:PHE:CD2	2:B:157:ILE:HD13	2.45	0.52
2:B:251:ASP:O	2:B:254:LYS:N	2.33	0.52
2:B:286:LEU:HD13	2:B:373:MET:H	1.70	0.52
2:B:339:ASN:HA	2:B:342:TYR:HD1	1.73	0.52
1:A:13:GLY:O	1:A:16:ILE:CG2	2.56	0.52
1:A:101:ASN:ND2	4:A:500:GTP:O2G	2.42	0.52
2:B:22:GLU:HA	2:B:83:PHE:HE2	1.73	0.52
2:B:141:LEU:C	2:B:186:ASN:ND2	2.63	0.52
2:B:192:HIS:HA	2:B:196:GLU:OE2	2.08	0.52
1:A:237:SER:HA	1:A:320:ARG:HH11	1.73	0.52
2:B:9:ALA:O	2:B:13:GLY:HA3	2.10	0.52
2:B:135:PHE:CG	2:B:166:MET:SD	3.02	0.52
3:K:216:ARG:HD2	3:K:216:ARG:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:O	1:A:86:LEU:C	2.39	0.52
1:A:97:GLU:HG3	1:A:110:ILE:HG23	1.92	0.52
1:A:296:PHE:HD2	1:A:312:TYR:HH	1.55	0.52
1:A:301:GLN:NE2	1:A:305:CYS:HB2	2.24	0.52
2:B:268:PHE:HD1	2:B:380:ASN:CG	2.13	0.52
2:B:319:PHE:HZ	2:B:332:MET:SD	2.31	0.52
1:A:83:TYR:O	1:A:84:ARG:HB2	2.09	0.52
2:B:319:PHE:CZ	2:B:332:MET:SD	3.03	0.52
2:B:320:ARG:HH22	6:B:502:TXL:H27	1.70	0.52
2:B:431:GLU:HA	2:B:434:GLN:CG	2.39	0.52
1:A:152:LEU:HD11	1:A:156:ARG:HE	1.75	0.52
1:A:179:THR:CG2	1:A:181:VAL:CA	2.88	0.52
1:A:362:VAL:CG1	1:A:363:VAL:N	2.73	0.52
2:B:151:THR:HG21	2:B:192:HIS:CG	2.36	0.52
2:B:212:ILE:HD11	2:B:302:MET:CA	2.40	0.52
2:B:389:LYS:O	2:B:393:GLU:HG2	2.09	0.52
6:B:502:TXL:H192	6:B:502:TXL:C5	2.39	0.52
2:B:27:GLU:OE1	2:B:36:TYR:HA	2.09	0.52
2:B:154:ILE:CG2	2:B:198:THR:HG22	2.37	0.52
2:B:208:ALA:HB2	2:B:303:ALA:O	2.05	0.52
2:B:212:ILE:HD11	2:B:302:MET:HA	1.91	0.52
1:A:7:ILE:HG22	1:A:8:HIS:O	2.10	0.51
1:A:108:TYR:CB	1:A:112:LYS:HE3	2.35	0.51
2:B:8:GLN:O	2:B:68:VAL:N	2.41	0.51
2:B:33:THR:CA	2:B:59:ASN:ND2	2.72	0.51
2:B:49:ILE:CA	2:B:61:TYR:CE2	2.93	0.51
2:B:57:ALA:CA	2:B:64:ARG:HB3	2.35	0.51
2:B:241:CYS:C	2:B:242:LEU:HG	2.31	0.51
2:B:301:MET:HE1	2:B:377:PHE:CD1	2.44	0.51
2:B:313:LEU:CD2	2:B:344:VAL:CG2	2.71	0.51
1:A:172:TYR:CE2	1:A:388:TRP:HZ3	2.28	0.51
1:A:419:SER:OG	3:K:172:PRO:HD3	2.10	0.51
2:B:259:MET:CE	2:B:268:PHE:CD1	2.93	0.51
2:B:259:MET:HG3	2:B:378:ILE:HG21	1.92	0.51
2:B:343:PHE:CG	2:B:350:ASN:ND2	2.78	0.51
3:K:83[A]:GLN:O	3:K:87:GLU:HG3	2.10	0.51
1:A:25:CYS:O	1:A:25:CYS:SG	2.69	0.51
1:A:205:ASP:HB2	1:A:208:ALA:HB3	1.91	0.51
1:A:306:ASP:OD1	1:A:308:ARG:CD	2.55	0.51
1:A:431:ASP:CB	3:K:303:PHE:CE1	2.86	0.51
2:B:141:LEU:C	2:B:186:ASN:HD21	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:LEU:CA	2:B:265:LEU:HB2	2.38	0.51
2:B:319:PHE:CD1	2:B:319:PHE:N	2.78	0.51
2:B:398:MET:CE	2:B:399:PHE:CE2	2.93	0.51
2:B:400:ARG:NH1	2:B:422:GLU:OE1	2.37	0.51
1:A:70:LEU:HG	1:A:145:THR:CG2	2.32	0.51
1:A:288:VAL:HG22	1:A:373:ARG:HG2	1.88	0.51
1:A:340:THR:O	1:A:341:ILE:HD13	2.11	0.51
2:B:140:SER:OG	2:B:143:GLY:HA3	2.10	0.51
2:B:250:ALA:HA	2:B:254:LYS:CD	2.17	0.51
2:B:320:ARG:HH21	6:B:502:TXL:H27	1.76	0.51
1:A:108:TYR:OH	1:A:417:GLU:CG	2.59	0.51
1:A:178:SER:O	1:A:179:THR:HB	2.10	0.51
1:A:405:VAL:HG23	1:A:409:VAL:HG23	1.90	0.51
2:B:359:PRO:O	2:B:360:PRO:C	2.49	0.51
2:B:378:ILE:HG22	2:B:379:GLY:N	2.24	0.51
3:K:33:SER:HB2	3:K:52:PHE:O	2.10	0.51
1:A:17:GLY:C	1:A:21:TRP:HD1	2.13	0.51
1:A:209:ILE:CG2	1:A:230:LEU:HD23	2.29	0.51
1:A:267:PHE:CD1	1:A:388:TRP:CZ2	2.98	0.51
1:A:396:ASP:OD2	1:A:422:ARG:CZ	2.59	0.51
2:B:35:SER:HB3	2:B:60:LYS:CE	2.40	0.51
2:B:40:SER:C	2:B:41:ASP:OD1	2.49	0.51
2:B:101:ASN:O	2:B:102:ASN:ND2	2.43	0.51
2:B:114:LEU:O	2:B:117:SER:N	2.44	0.51
2:B:192:HIS:CG	2:B:196:GLU:HG3	2.44	0.51
2:B:229:HIS:HD1	6:B:502:TXL:H432	1.75	0.51
2:B:259:MET:HE2	2:B:268:PHE:CD1	2.46	0.51
2:B:315:VAL:HG13	2:B:377:PHE:CE2	2.45	0.51
2:B:404:PHE:CD2	2:B:404:PHE:O	2.64	0.51
1:A:269:LEU:O	1:A:377:MET:O	2.29	0.51
2:B:28:HIS:CD2	2:B:240:THR:HA	2.45	0.51
2:B:259:MET:CE	2:B:379:GLY:C	2.78	0.51
2:B:262:PHE:CB	2:B:263:PRO:CD	2.78	0.51
2:B:339:ASN:O	2:B:340:SER:O	2.29	0.51
2:B:369:ARG:O	6:B:502:TXL:C22	2.59	0.51
1:A:3:GLU:CA	1:A:31:GLN:CG	2.86	0.51
1:A:41:THR:O	1:A:41:THR:CG2	2.59	0.51
1:A:181:VAL:HG13	1:A:399:TYR:OH	2.11	0.51
1:A:212:ILE:HD13	1:A:230:LEU:CD2	2.14	0.51
1:A:219:ILE:CG2	1:A:219:ILE:HD13	2.39	0.51
1:A:426:ALA:C	1:A:428:LEU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:THR:HG22	2:B:34:GLY:H	1.73	0.51
2:B:68:VAL:HG11	2:B:149:MET:CE	2.24	0.51
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.51
1:A:420:GLU:OE2	3:K:170:GLU:N	2.43	0.51
2:B:94:PHE:CE2	2:B:114:LEU:HB2	2.46	0.51
2:B:188:THR:CG2	2:B:417:GLU:O	2.59	0.51
2:B:197:ASN:CG	2:B:197:ASN:O	2.50	0.51
2:B:229:HIS:ND1	6:B:502:TXL:H432	2.25	0.51
2:B:384:ILE:HG22	2:B:388:PHE:CE2	2.45	0.51
1:A:141:PHE:CB	1:A:173:PRO:HD3	2.41	0.50
1:A:186:ASN:O	1:A:190:THR:N	2.44	0.50
1:A:250:VAL:HG11	1:A:352:LYS:NZ	2.26	0.50
2:B:270:PRO:HB3	2:B:378:ILE:HD13	1.93	0.50
2:B:316:ALA:O	2:B:378:ILE:N	2.38	0.50
2:B:318:VAL:O	2:B:376:THR:N	2.26	0.50
2:B:321:GLY:HA3	2:B:373:MET:CG	2.15	0.50
3:K:83[B]:GLN:O	3:K:87:GLU:HG3	2.10	0.50
3:K:171:HIS:CD2	3:K:173:LEU:H	2.28	0.50
1:A:142:GLY:O	1:A:185:TYR:CE1	2.63	0.50
1:A:205:ASP:O	1:A:209:ILE:HG13	2.11	0.50
1:A:230:LEU:HG	1:A:302:MET:HE1	1.92	0.50
2:B:14:ASN:OD1	2:B:69:ASP:OD1	2.29	0.50
2:B:34:GLY:HA2	2:B:37:HIS:NE2	2.26	0.50
2:B:194:LEU:CD2	2:B:265:LEU:HB3	2.38	0.50
2:B:194:LEU:HD23	2:B:267:PHE:HZ	1.72	0.50
2:B:201:THR:CG2	2:B:265:LEU:CG	2.87	0.50
6:B:502:TXL:C17	6:B:502:TXL:C13	2.89	0.50
1:A:105:ARG:HG3	1:A:411:GLU:CD	2.32	0.50
1:A:405:VAL:CG2	1:A:405:VAL:CA	2.77	0.50
2:B:44:LEU:CD1	2:B:63:PRO:HG3	2.42	0.50
2:B:222:PRO:C	2:B:223:THR:CG2	2.72	0.50
2:B:278:ARG:CB	2:B:278:ARG:C	2.79	0.50
2:B:312:TYR:O	2:B:344:VAL:HG21	2.00	0.50
2:B:332:MET:O	2:B:336:GLN:HG3	2.11	0.50
3:K:138:MET:SD	3:K:229:ARG:HB2	2.52	0.50
1:A:78:VAL:HG13	1:A:87:PHE:CE1	2.42	0.50
1:A:103:TYR:HD2	1:A:189:LEU:HG	1.76	0.50
1:A:150:THR:O	1:A:154:MET:HG2	2.11	0.50
1:A:155:GLU:HA	1:A:196:GLU:HB3	1.94	0.50
1:A:277:SER:HB3	1:A:280:LYS:CE	2.36	0.50
1:A:301:GLN:HE21	1:A:305:CYS:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:HG13	2:B:66:ILE:CG2	2.36	0.50
2:B:64:ARG:HH22	2:B:132:LEU:HD11	1.76	0.50
2:B:213:CYS:SG	2:B:227:LEU:HD11	2.52	0.50
2:B:217:LEU:HD23	2:B:275:LEU:O	2.10	0.50
2:B:231:VAL:O	2:B:232:SER:C	2.46	0.50
2:B:389:LYS:HG2	2:B:429:VAL:HG21	1.93	0.50
1:A:88:HIS:NE2	1:A:89:PRO:HD2	2.26	0.50
1:A:253:THR:O	1:A:253:THR:CG2	2.57	0.50
1:A:267:PHE:CZ	1:A:388:TRP:CZ2	2.99	0.50
2:B:35:SER:H	2:B:60:LYS:NZ	2.09	0.50
2:B:259:MET:HE1	2:B:379:GLY:N	2.14	0.50
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.39	0.50
1:A:97:GLU:O	1:A:98:ASP:CB	2.57	0.50
1:A:183:GLU:OE1	1:A:183:GLU:HA	2.10	0.50
1:A:397:LEU:CA	1:A:401:LYS:HB2	2.37	0.50
2:B:19:LYS:HG3	2:B:228:ASN:HB3	1.30	0.50
1:A:196:GLU:C	1:A:197:HIS:CG	2.83	0.50
1:A:242:LEU:HD12	1:A:255:PHE:HZ	1.62	0.50
1:A:274:PRO:C	1:A:275:VAL:HG23	2.32	0.50
1:A:382:THR:O	1:A:385:ALA:N	2.43	0.50
2:B:295:MET:HE3	2:B:375:ALA:CA	2.25	0.50
2:B:312:TYR:CG	2:B:381:SER:HB3	2.46	0.50
6:B:502:TXL:O11	6:B:502:TXL:H332	2.12	0.50
2:B:33:THR:CG2	2:B:34:GLY:N	2.73	0.50
2:B:288:VAL:HB	2:B:289:PRO:CD	2.42	0.50
2:B:295:MET:CE	2:B:375:ALA:HA	2.40	0.50
2:B:416:MET:N	2:B:416:MET:SD	2.85	0.50
1:A:78:VAL:O	1:A:78:VAL:HG12	2.10	0.50
1:A:108:TYR:CZ	1:A:417:GLU:CD	2.85	0.50
1:A:340:THR:O	1:A:341:ILE:CG1	2.59	0.50
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.77	0.50
1:A:423:GLU:HB3	3:K:170:GLU:HG2	1.94	0.50
2:B:3:GLU:HA	2:B:31:ASP:CG	2.19	0.50
2:B:3:GLU:O	2:B:4:ILE:HG13	2.11	0.50
2:B:12:CYS:SG	5:B:501:GDP:C1'	3.00	0.50
2:B:44:LEU:CD1	2:B:86:ILE:O	2.49	0.50
2:B:63:PRO:CG	2:B:86:ILE:O	2.60	0.50
2:B:384:ILE:HG23	2:B:388:PHE:CE2	2.45	0.50
1:A:14:VAL:HB	1:A:74:VAL:HG11	1.94	0.49
1:A:229:ARG:O	1:A:233:GLN:CG	2.52	0.49
1:A:264:ARG:O	1:A:266:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LYS:O	1:A:326:LYS:HG2	2.12	0.49
2:B:62:VAL:CG1	2:B:63:PRO:N	2.75	0.49
2:B:246:GLY:N	2:B:357:ASP:OD2	2.45	0.49
2:B:273:ALA:CB	2:B:294:GLN:CD	2.80	0.49
1:A:134:GLY:HA3	1:A:252:LEU:CD1	2.43	0.49
2:B:233:ALA:CB	2:B:272:PHE:CD2	2.79	0.49
2:B:433:GLN:O	2:B:435:TYR:N	2.46	0.49
1:A:101:ASN:O	1:A:102:ASN:CB	2.51	0.49
1:A:261:PRO:HB2	1:A:346:TRP:HH2	1.77	0.49
1:A:306:ASP:CG	1:A:308:ARG:HD2	2.31	0.49
1:A:6:SER:HB3	1:A:30:ILE:HD12	1.92	0.49
1:A:20:CYS:C	1:A:24:TYR:CD2	2.80	0.49
1:A:241:SER:HB2	1:A:356:ASN:CB	2.42	0.49
1:A:313:MET:HE3	1:A:346:TRP:CZ2	2.39	0.49
2:B:121:VAL:O	2:B:125:GLU:HG3	2.12	0.49
2:B:324:SER:CB	2:B:327:GLU:H	2.25	0.49
1:A:158:SER:HB2	1:A:196:GLU:O	2.11	0.49
1:A:205:ASP:HB2	1:A:208:ALA:CB	2.42	0.49
1:A:209:ILE:O	1:A:213:CYS:SG	2.63	0.49
3:K:317:GLU:CD	3:K:322:ASN:H	2.15	0.49
1:A:119:LEU:HA	1:A:122:ILE:HG22	1.94	0.49
1:A:142:GLY:O	1:A:185:TYR:CZ	2.66	0.49
1:A:194:THR:CG2	1:A:195:LEU:N	2.59	0.49
1:A:359:PRO:HB2	1:A:360:PRO:HD2	1.94	0.49
2:B:29:GLY:O	2:B:58:GLY:O	2.30	0.49
2:B:308:ARG:CD	2:B:342:TYR:CZ	2.93	0.49
2:B:394:GLN:OE1	2:B:394:GLN:HA	2.12	0.49
6:B:502:TXL:H173	6:B:502:TXL:C13	2.37	0.49
1:A:11:GLN:HG2	4:A:500:GTP:O2A	2.13	0.49
1:A:121:ARG:O	1:A:125:LEU:CG	2.44	0.49
1:A:200:CYS:SG	1:A:260:VAL:CG2	3.01	0.49
2:B:108:TYR:OH	2:B:417:GLU:HG3	2.13	0.49
2:B:135:PHE:CE2	2:B:157:ILE:HD13	2.47	0.49
2:B:244:PHE:O	2:B:245:PRO:C	2.51	0.49
1:A:14:VAL:HG12	1:A:74:VAL:HG22	1.95	0.49
1:A:97:GLU:HG3	1:A:110:ILE:HG22	1.93	0.49
1:A:101:ASN:ND2	4:A:500:GTP:PG	2.85	0.49
1:A:231:ILE:HD13	1:A:302:MET:HE2	1.80	0.49
1:A:306:ASP:OD1	1:A:308:ARG:N	2.46	0.49
1:A:314:ALA:HB3	1:A:380:ASN:ND2	2.13	0.49
1:A:369:ALA:O	1:A:370:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:CG	2:B:4:ILE:H	2.09	0.49
2:B:226:ASP:OD1	2:B:226:ASP:O	2.30	0.49
3:K:222:ASN:HD22	3:K:245[B]:SER:HA	1.78	0.49
1:A:5:ILE:CD1	1:A:135:PHE:CZ	2.93	0.49
1:A:7:ILE:HG21	1:A:153:LEU:CD2	2.43	0.49
1:A:15:GLN:O	1:A:18:ASN:HB2	2.13	0.49
1:A:26:LEU:HD11	1:A:361:THR:HG23	1.83	0.49
1:A:217:LEU:HD13	1:A:368:LEU:CD2	2.27	0.49
1:A:291:ILE:HD13	1:A:373:ARG:C	2.33	0.49
1:A:420:GLU:OE1	1:A:420:GLU:HA	2.13	0.49
2:B:44:LEU:C	2:B:47:GLU:CG	2.56	0.49
2:B:79:ARG:HB2	2:B:86:ILE:HD11	1.95	0.49
2:B:139:HIS:ND1	2:B:139:HIS:C	2.67	0.49
2:B:183:GLU:OE1	2:B:183:GLU:HA	2.13	0.49
2:B:213:CYS:CB	2:B:219:LEU:CD1	2.86	0.49
3:K:234:THR:HB	3:K:236:ILE:HD13	1.93	0.49
1:A:42:ILE:HD13	1:A:61:HIS:O	2.13	0.49
1:A:204:VAL:CG1	1:A:209:ILE:CG1	2.86	0.49
1:A:209:ILE:HD13	1:A:231:ILE:HG12	1.94	0.49
1:A:233:GLN:O	1:A:234:ILE:C	2.49	0.49
2:B:103:TRP:CD1	2:B:147:SER:C	2.85	0.49
2:B:426:ASN:C	2:B:428:LEU:H	2.17	0.49
3:K:215:SER:C	3:K:216:ARG:HD2	2.34	0.49
1:A:3:GLU:HB3	1:A:64:ARG:NH1	2.28	0.48
1:A:34:GLY:O	1:A:35:GLN:HG3	2.13	0.48
1:A:107:HIS:ND1	1:A:108:TYR:CD2	2.80	0.48
1:A:282:TYR:CD2	1:A:285:GLN:CA	2.81	0.48
1:A:312:TYR:CE1	1:A:341:ILE:HD12	2.47	0.48
2:B:13:GLY:CA	2:B:138:THR:CB	2.85	0.48
2:B:39:ASP:O	2:B:40:SER:HB3	2.08	0.48
2:B:47:GLU:OE2	2:B:85:GLN:OE1	2.30	0.48
2:B:61:TYR:O	2:B:61:TYR:CD1	2.66	0.48
2:B:101:ASN:HD22	2:B:101:ASN:HA	1.47	0.48
2:B:230:LEU:HD21	2:B:302:MET:HB2	1.94	0.48
3:K:215:SER:OG	3:K:216:ARG:HD2	2.13	0.48
1:A:180:ALA:CB	1:A:398:MET:HE3	2.41	0.48
1:A:241:SER:HB2	1:A:356:ASN:CG	2.32	0.48
1:A:361:THR:C	1:A:362:VAL:CG2	2.81	0.48
1:A:390:ARG:O	1:A:394:LYS:HG3	2.12	0.48
2:B:30:ILE:HG21	2:B:136:GLN:NE2	2.23	0.48
2:B:143:GLY:O	2:B:185:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG11	1:A:146:GLY:HA2	1.95	0.48
1:A:14:VAL:HB	1:A:74:VAL:CG1	2.43	0.48
1:A:16:ILE:HG23	1:A:138:PHE:CD1	2.47	0.48
1:A:171:ILE:N	1:A:203:MET:HE3	2.19	0.48
1:A:242:LEU:HD13	1:A:250:VAL:HB	1.94	0.48
1:A:248:LEU:CD2	5:B:501:GDP:C8	2.96	0.48
1:A:250:VAL:CB	1:A:254:GLU:HG2	2.43	0.48
1:A:311:LYS:O	1:A:312:TYR:C	2.51	0.48
2:B:2:ARG:NH2	2:B:243:ARG:O	2.46	0.48
2:B:102:ASN:CB	2:B:105:LYS:HG3	2.43	0.48
2:B:239:THR:O	2:B:243:ARG:CG	2.51	0.48
1:A:180:ALA:CB	1:A:398:MET:CE	2.92	0.48
1:A:228:ASN:O	1:A:232:GLY:N	2.39	0.48
2:B:12:CYS:O	2:B:16:ILE:HG13	1.98	0.48
2:B:70:LEU:HA	2:B:94:PHE:HB2	1.94	0.48
2:B:140:SER:HG	2:B:143:GLY:HA3	1.79	0.48
2:B:144:GLY:N	2:B:185:TYR:HE1	2.08	0.48
2:B:183:GLU:HB3	2:B:184:PRO:HD3	1.81	0.48
2:B:238:VAL:HG13	2:B:255:LEU:HD11	1.94	0.48
1:A:70:LEU:HD12	1:A:145:THR:CA	2.40	0.48
1:A:115:ILE:CB	1:A:152:LEU:HD21	2.43	0.48
2:B:52:TYR:N	2:B:52:TYR:CD1	2.81	0.48
2:B:192:HIS:O	2:B:196:GLU:HG2	2.05	0.48
2:B:273:ALA:HB1	2:B:294:GLN:CD	2.32	0.48
1:A:155:GLU:CG	1:A:196:GLU:HG3	2.34	0.48
2:B:64:ARG:NH2	2:B:125:GLU:C	2.67	0.48
2:B:385:GLN:O	2:B:389:LYS:CG	2.62	0.48
1:A:109:THR:HG21	1:A:411:GLU:CB	2.44	0.48
1:A:291:ILE:O	1:A:375:VAL:HG21	2.13	0.48
1:A:296:PHE:O	1:A:298:PRO:N	2.47	0.48
2:B:64:ARG:HH22	2:B:132:LEU:HD21	1.79	0.48
2:B:71:GLU:O	2:B:72:PRO:C	2.38	0.48
2:B:151:THR:C	2:B:192:HIS:HD2	2.12	0.48
2:B:272:PHE:O	2:B:275:LEU:HD21	2.13	0.48
2:B:347:ILE:N	2:B:348:PRO:HD3	2.27	0.48
1:A:212:ILE:HB	1:A:216:ASN:HD22	1.79	0.48
1:A:292:THR:N	1:A:375:VAL:HG21	2.28	0.48
2:B:23:VAL:O	2:B:23:VAL:HG12	2.14	0.48
1:A:174:ALA:CB	1:A:390:ARG:NH2	2.52	0.48
1:A:224:TYR:HD1	4:A:500:GTP:C2	2.31	0.48
1:A:252:LEU:HD23	1:A:255:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:GLU:O	1:A:433:GLU:CG	2.51	0.48
2:B:23:VAL:HG21	2:B:232:SER:HB2	1.95	0.48
2:B:191:VAL:CG2	2:B:421:ALA:CB	2.90	0.48
2:B:394:GLN:O	2:B:398:MET:HB2	2.14	0.48
1:A:35:GLN:O	1:A:36:MET:HG2	2.13	0.48
1:A:158:SER:N	1:A:166:LYS:CE	2.76	0.48
2:B:50:ASN:HD22	2:B:61:TYR:HB2	1.78	0.48
2:B:241:CYS:O	2:B:242:LEU:HG	2.14	0.48
2:B:311:ARG:O	2:B:381:SER:CA	2.62	0.48
2:B:328:VAL:HG12	2:B:353:THR:HG21	1.96	0.48
1:A:6:SER:O	1:A:66:VAL:N	2.46	0.47
1:A:20:CYS:SG	1:A:138:PHE:CE1	3.07	0.47
1:A:287:SER:O	1:A:291:ILE:HG13	2.13	0.47
2:B:4:ILE:HG21	2:B:30:ILE:HG21	1.93	0.47
2:B:102:ASN:CB	2:B:105:LYS:CD	2.79	0.47
2:B:192:HIS:CE1	2:B:193:GLN:HG2	2.48	0.47
2:B:211:ASP:O	2:B:215:ARG:HB2	2.14	0.47
2:B:435:TYR:O	2:B:436:GLN:OE1	2.29	0.47
1:A:137:VAL:HB	1:A:168:GLU:CG	2.40	0.47
1:A:346:TRP:CD1	1:A:346:TRP:N	2.82	0.47
2:B:114:LEU:HA	2:B:117:SER:OG	2.14	0.47
2:B:142:GLY:HA2	2:B:185:TYR:CE1	2.37	0.47
3:K:234:THR:CB	3:K:236:ILE:CD1	2.88	0.47
2:B:35:SER:CB	2:B:60:LYS:HE3	2.44	0.47
2:B:87:PHE:CD1	2:B:88:ARG:N	2.82	0.47
2:B:109:THR:CG2	2:B:411:GLU:O	2.61	0.47
2:B:180:THR:C	2:B:398:MET:HE1	2.29	0.47
2:B:270:PRO:HA	2:B:377:PHE:O	2.14	0.47
3:K:222:ASN:HD22	3:K:245[A]:SER:HA	1.78	0.47
1:A:40:LYS:C	1:A:42:ILE:N	2.65	0.47
1:A:48:SER:O	1:A:49:PHE:HB2	2.14	0.47
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.13	0.47
1:A:264:ARG:CZ	3:K:307:ARG:HB3	2.31	0.47
2:B:31:ASP:N	2:B:32:PRO:HD3	2.26	0.47
2:B:94:PHE:CZ	2:B:110:GLU:O	2.68	0.47
1:A:3:GLU:OE1	1:A:132:LEU:CD2	2.62	0.47
1:A:122:ILE:HG23	1:A:123:ARG:N	2.29	0.47
1:A:152:LEU:HD11	1:A:156:ARG:HH21	1.78	0.47
1:A:275:VAL:O	1:A:275:VAL:CG1	2.62	0.47
2:B:181:VAL:C	2:B:399:PHE:CE2	2.85	0.47
2:B:209:LEU:HB3	2:B:227:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:GLN:HG2	2:B:294:GLN:O	2.14	0.47
2:B:435:TYR:O	2:B:436:GLN:CB	2.56	0.47
1:A:66:VAL:HG22	1:A:125:LEU:HD13	1.92	0.47
2:B:24:ILE:CA	2:B:26:ASP:H	2.25	0.47
2:B:62:VAL:HG12	2:B:63:PRO:O	2.14	0.47
2:B:74:THR:O	2:B:75:MET:O	2.33	0.47
2:B:103:TRP:HE1	2:B:148:GLY:HA2	1.72	0.47
2:B:151:THR:HG21	2:B:189:LEU:HA	1.96	0.47
2:B:311:ARG:H	2:B:382:THR:HB	1.79	0.47
2:B:434:GLN:C	2:B:435:TYR:HD1	2.14	0.47
1:A:3:GLU:OE1	1:A:132:LEU:HD23	2.14	0.47
1:A:31:GLN:NE2	1:A:243:ARG:HB3	2.30	0.47
1:A:103:TYR:N	1:A:185:TYR:CE2	2.82	0.47
1:A:153:LEU:O	1:A:153:LEU:HG	2.14	0.47
1:A:169:PHE:CZ	1:A:235:VAL:CG2	2.78	0.47
1:A:175:PRO:HG3	1:A:304:LYS:NZ	2.29	0.47
1:A:209:ILE:CD1	1:A:231:ILE:CG1	2.90	0.47
1:A:256:GLN:O	1:A:260:VAL:HB	2.14	0.47
1:A:276:ILE:HB	1:A:369:ALA:HB2	1.95	0.47
1:A:340:THR:O	1:A:341:ILE:CD1	2.63	0.47
1:A:400:ALA:O	1:A:401:LYS:C	2.52	0.47
2:B:14:ASN:HB3	2:B:74:THR:CB	2.43	0.47
2:B:33:THR:CG2	2:B:34:GLY:H	2.28	0.47
2:B:75:MET:CE	2:B:79:ARG:CB	2.90	0.47
2:B:119:LEU:HD21	2:B:156:LYS:HD3	1.96	0.47
2:B:174:SER:CB	2:B:175:PRO:CD	2.89	0.47
2:B:179:ASP:O	2:B:180:THR:HG23	2.15	0.47
2:B:248:LEU:HD23	2:B:353:THR:O	2.15	0.47
2:B:414:ASP:C	2:B:416:MET:N	2.68	0.47
1:A:1:MET:CA	2:B:96:GLN:OE1	2.53	0.47
1:A:104:ALA:O	1:A:108:TYR:HD2	1.96	0.47
2:B:183:GLU:CD	2:B:394:GLN:HG3	2.35	0.47
2:B:196:GLU:HA	2:B:196:GLU:OE1	2.15	0.47
2:B:250:ALA:HB1	2:B:352:LYS:HZ3	1.80	0.47
1:A:23:LEU:CD2	1:A:233:GLN:HA	2.45	0.47
1:A:23:LEU:HD22	1:A:233:GLN:HA	1.96	0.47
1:A:196:GLU:HB3	1:A:197:HIS:CE1	2.50	0.47
1:A:209:ILE:CD1	1:A:231:ILE:HG12	2.45	0.47
1:A:282:TYR:O	1:A:284:GLU:C	2.53	0.47
1:A:305:CYS:O	1:A:307:PRO:CD	2.56	0.47
1:A:349:THR:O	1:A:351:PHE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLU:CB	2:B:36:TYR:HB3	2.44	0.47
2:B:98:GLY:C	2:B:99:ALA:O	2.52	0.47
2:B:140:SER:O	2:B:147:SER:OG	2.25	0.47
1:A:3:GLU:HB2	1:A:64:ARG:NH2	2.30	0.47
1:A:87:PHE:HZ	1:A:92:LEU:HD21	1.80	0.47
1:A:205:ASP:HB2	1:A:303:VAL:CA	2.31	0.47
1:A:259:LEU:CB	1:A:380:ASN:HD21	2.27	0.47
2:B:141:LEU:CB	2:B:186:ASN:ND2	2.67	0.47
2:B:143:GLY:CA	2:B:185:TYR:CE1	2.87	0.47
2:B:346:TRP:O	2:B:347:ILE:HG13	2.14	0.47
3:K:44:LYS:HE2	3:K:44:LYS:HB2	1.61	0.47
1:A:132:LEU:O	1:A:133:GLN:C	2.54	0.46
1:A:166:LYS:CE	1:A:197:HIS:CD2	2.63	0.46
1:A:277:SER:CB	1:A:279:GLU:H	2.23	0.46
1:A:389:ALA:O	1:A:393:HIS:ND1	2.47	0.46
2:B:23:VAL:HG22	6:B:502:TXL:C33	2.30	0.46
2:B:192:HIS:O	2:B:196:GLU:HG3	1.87	0.46
2:B:261:PRO:HG3	2:B:314:THR:HG23	1.97	0.46
1:A:312:TYR:CZ	1:A:377:MET:HE3	2.49	0.46
1:A:341:ILE:O	1:A:342:GLN:C	2.52	0.46
2:B:112:ALA:HA	2:B:115:VAL:HB	1.96	0.46
2:B:313:LEU:CD1	2:B:435:TYR:HD2	2.27	0.46
3:K:216:ARG:CG	3:K:216:ARG:NH1	2.67	0.46
1:A:3:GLU:CA	1:A:31:GLN:CB	2.61	0.46
1:A:3:GLU:CB	1:A:64:ARG:NH1	2.78	0.46
1:A:14:VAL:CB	1:A:74:VAL:CG1	2.94	0.46
1:A:31:GLN:OE1	1:A:243:ARG:HD3	2.01	0.46
1:A:261:PRO:HB2	1:A:346:TRP:CH2	2.50	0.46
1:A:289:ALA:CB	1:A:331:ALA:HB2	2.44	0.46
1:A:387:ALA:O	1:A:390:ARG:HB2	2.15	0.46
2:B:103:TRP:CD1	2:B:147:SER:O	2.59	0.46
2:B:313:LEU:H	2:B:381:SER:HA	1.81	0.46
1:A:81:GLY:C	1:A:83:TYR:N	2.68	0.46
1:A:192:HIS:O	1:A:193:THR:C	2.53	0.46
1:A:267:PHE:CD1	1:A:388:TRP:HZ2	2.34	0.46
1:A:430:LYS:O	1:A:434:GLU:HG3	2.15	0.46
2:B:50:ASN:HB2	2:B:61:TYR:CB	2.45	0.46
2:B:56:ALA:HB1	2:B:62:VAL:N	2.31	0.46
2:B:103:TRP:CD1	2:B:148:GLY:N	2.83	0.46
2:B:208:ALA:CB	2:B:303:ALA:C	2.81	0.46
2:B:249:ASN:O	2:B:249:ASN:OD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:ALA:CB	2:B:294:GLN:OE1	2.60	0.46
2:B:427:ASP:O	2:B:431:GLU:HG3	2.16	0.46
2:B:243:ARG:CZ	2:B:252:LEU:HD21	2.45	0.46
3:K:230:HIS:CG	3:K:231:ASP:N	2.83	0.46
1:A:8:HIS:HB2	1:A:67:PHE:HA	1.98	0.46
1:A:267:PHE:CE1	1:A:388:TRP:CH2	3.03	0.46
1:A:312:TYR:HE1	1:A:341:ILE:HD12	1.81	0.46
2:B:102:ASN:CB	2:B:105:LYS:HE3	2.46	0.46
2:B:194:LEU:HD21	2:B:267:PHE:CZ	2.48	0.46
2:B:312:TYR:C	2:B:381:SER:HA	2.36	0.46
2:B:319:PHE:CE1	2:B:328:VAL:HG13	2.32	0.46
6:B:502:TXL:H13	6:B:502:TXL:C17	2.31	0.46
1:A:30:ILE:HB	1:A:64:ARG:HB3	1.90	0.46
1:A:187:SER:OG	1:A:188:ILE:N	2.49	0.46
2:B:287:THR:C	2:B:290:GLU:HB3	2.36	0.46
1:A:16:ILE:O	1:A:19:ALA:HB3	2.16	0.46
1:A:271:THR:OG1	1:A:377:MET:N	2.48	0.46
1:A:293:ASN:O	1:A:297:GLU:HG3	2.16	0.46
2:B:166:MET:HG2	2:B:197:ASN:O	2.16	0.46
2:B:273:ALA:HB1	2:B:294:GLN:HB3	1.97	0.46
1:A:104:ALA:CA	1:A:108:TYR:CD2	2.83	0.46
1:A:272:TYR:HD1	1:A:275:VAL:CG2	2.28	0.46
2:B:35:SER:CB	2:B:60:LYS:CE	2.94	0.46
2:B:86:ILE:HB	2:B:87:PHE:H	1.29	0.46
2:B:212:ILE:HD12	2:B:302:MET:HB2	1.98	0.46
1:A:35:GLN:N	1:A:60:LYS:HD3	2.31	0.46
1:A:141:PHE:CE1	1:A:170:SER:HB2	2.51	0.46
1:A:170:SER:OG	1:A:202:PHE:O	2.34	0.46
1:A:275:VAL:O	1:A:368:LEU:CD1	2.64	0.46
1:A:306:ASP:OD2	1:A:308:ARG:HB2	2.16	0.46
1:A:334:THR:HA	1:A:337:THR:HG21	1.98	0.46
1:A:440:VAL:HB	2:B:402:LYS:NZ	2.27	0.46
2:B:273:ALA:CB	2:B:294:GLN:HB3	2.46	0.46
2:B:301:MET:CE	2:B:377:PHE:CD1	2.99	0.46
2:B:319:PHE:O	2:B:355:VAL:HG13	2.16	0.46
1:A:116:ASP:C	1:A:118:VAL:N	2.68	0.45
1:A:291:ILE:HD11	1:A:373:ARG:HB2	1.95	0.45
1:A:328:VAL:O	1:A:332:ILE:CG1	2.63	0.45
2:B:48:ARG:HD2	2:B:60:LYS:CA	2.38	0.45
2:B:275:LEU:CD1	2:B:300:ASN:ND2	2.67	0.45
2:B:417:GLU:OE1	2:B:417:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:GLN:C	2:B:435:TYR:N	2.67	0.45
1:A:3:GLU:OE2	1:A:129:CYS:CB	2.59	0.45
1:A:123:ARG:O	1:A:127:ASP:OD1	2.34	0.45
1:A:177:VAL:CG1	1:A:178:SER:N	2.49	0.45
1:A:344:VAL:HG12	1:A:345:ASP:H	1.81	0.45
2:B:30:ILE:CG2	2:B:243:ARG:HH11	2.23	0.45
2:B:141:LEU:CD1	2:B:173:PRO:CD	2.91	0.45
2:B:180:THR:C	2:B:398:MET:CE	2.73	0.45
2:B:184:PRO:CA	2:B:395:PHE:CD1	2.98	0.45
2:B:318:VAL:HG22	2:B:354:ALA:HB3	1.98	0.45
3:K:203:ARG:CZ	3:K:219:ALA:HB2	2.47	0.45
3:K:216:ARG:HG3	3:K:216:ARG:NH1	2.15	0.45
1:A:152:LEU:CD1	1:A:156:ARG:NE	2.75	0.45
1:A:267:PHE:CE2	1:A:388:TRP:HZ2	2.35	0.45
1:A:312:TYR:HE2	1:A:377:MET:CE	1.80	0.45
1:A:372:GLN:C	1:A:373:ARG:HG3	2.33	0.45
2:B:275:LEU:CB	2:B:294:GLN:HE22	2.28	0.45
2:B:286:LEU:HD12	2:B:372:LYS:CB	2.29	0.45
1:A:190:THR:O	1:A:191:THR:C	2.52	0.45
1:A:197:HIS:O	1:A:198:SER:OG	2.34	0.45
1:A:384:ILE:O	1:A:386:GLU:N	2.49	0.45
1:A:437:VAL:O	1:A:437:VAL:CG1	2.64	0.45
2:B:3:GLU:HA	2:B:31:ASP:HB2	1.85	0.45
1:A:20:CYS:SG	1:A:138:PHE:CZ	3.06	0.45
1:A:175:PRO:HD3	1:A:390:ARG:CZ	2.44	0.45
1:A:278:ALA:N	1:A:368:LEU:HD22	2.32	0.45
2:B:68:VAL:HA	2:B:92:PHE:HB2	1.98	0.45
2:B:213:CYS:HB3	2:B:219:LEU:HD13	1.93	0.45
2:B:280:SER:O	2:B:281:GLN:C	2.55	0.45
2:B:342:TYR:C	2:B:343:PHE:CG	2.90	0.45
1:A:175:PRO:HD2	1:A:207:GLU:HG2	1.98	0.45
1:A:183:GLU:HB3	1:A:394:LYS:HB2	1.87	0.45
1:A:267:PHE:HA	1:A:268:PRO:HD2	1.57	0.45
1:A:409:VAL:O	1:A:412:GLY:N	2.40	0.45
2:B:346:TRP:C	2:B:347:ILE:HG13	2.37	0.45
3:K:216:ARG:NH1	3:K:272:ASN:OD1	2.49	0.45
1:A:3:GLU:HG3	1:A:131:GLY:O	2.16	0.45
1:A:33:ASP:O	1:A:33:ASP:CG	2.49	0.45
1:A:248:LEU:HD21	5:B:501:GDP:C8	2.52	0.45
2:B:94:PHE:CD2	2:B:114:LEU:CD2	3.00	0.45
2:B:142:GLY:N	2:B:186:ASN:CG	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HH21	2:B:99:ALA:CB	2.24	0.45
1:A:26:LEU:HD13	1:A:361:THR:OG1	2.12	0.45
1:A:217:LEU:O	1:A:218:ASP:OD1	2.33	0.45
1:A:220:GLU:CB	1:A:220:GLU:CD	2.74	0.45
1:A:297:GLU:O	1:A:298:PRO:C	2.52	0.45
2:B:104:ALA:HA	2:B:413:MET:HE1	1.98	0.45
2:B:313:LEU:HD22	2:B:346:TRP:CH2	2.51	0.45
2:B:344:VAL:HB	2:B:347:ILE:HD12	1.99	0.45
2:B:389:LYS:HG2	2:B:429:VAL:HG11	1.75	0.45
1:A:97:GLU:OE2	1:A:114:ILE:HD11	2.16	0.45
1:A:103:TYR:CD2	1:A:148:GLY:N	2.85	0.45
2:B:241:CYS:O	2:B:242:LEU:CG	2.64	0.45
3:K:38:VAL:HG22	3:K:47:PRO:HG3	1.99	0.45
1:A:155:GLU:HG2	1:A:196:GLU:CB	2.46	0.45
1:A:157:LEU:HB2	1:A:166:LYS:HE2	1.98	0.45
1:A:217:LEU:C	1:A:218:ASP:OD1	2.55	0.45
1:A:409:VAL:O	1:A:412:GLY:O	2.35	0.45
2:B:312:TYR:N	2:B:381:SER:CB	2.80	0.45
1:A:5:ILE:HG13	1:A:64:ARG:NH2	2.31	0.44
1:A:172:TYR:CD1	1:A:173:PRO:O	2.64	0.44
1:A:182:VAL:O	1:A:183:GLU:O	2.34	0.44
1:A:276:ILE:CD1	1:A:371:VAL:CG2	2.87	0.44
1:A:312:TYR:CG	1:A:381:THR:CG2	2.90	0.44
2:B:183:GLU:OE1	2:B:394:GLN:HB2	2.14	0.44
2:B:227:LEU:HD12	2:B:227:LEU:HA	1.74	0.44
2:B:289:PRO:CD	2:B:290:GLU:H	2.29	0.44
1:A:152:LEU:O	1:A:156:ARG:HG3	2.17	0.44
1:A:312:TYR:CD1	1:A:341:ILE:HG23	2.51	0.44
2:B:4:ILE:CD1	2:B:30:ILE:C	2.40	0.44
2:B:15:GLN:C	2:B:17:GLY:N	2.70	0.44
2:B:34:GLY:C	2:B:35:SER:HG	2.13	0.44
2:B:184:PRO:CB	2:B:395:PHE:CD1	3.00	0.44
2:B:230:LEU:HD21	2:B:302:MET:HG3	1.99	0.44
2:B:250:ALA:HB2	2:B:352:LYS:HZ1	1.81	0.44
2:B:295:MET:HE1	2:B:375:ALA:HA	1.95	0.44
2:B:333:LEU:HG	2:B:337:ASN:HD21	1.81	0.44
3:K:189:TYR:O	3:K:192:ILE:HG22	2.16	0.44
1:A:103:TYR:CD2	1:A:188:ILE:HG22	2.50	0.44
1:A:147:SER:OG	1:A:148:GLY:N	2.50	0.44
1:A:184:PRO:HD2	1:A:398:MET:HB3	1.99	0.44
1:A:272:TYR:CE1	1:A:274:PRO:C	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:VAL:CG1	1:A:304:LYS:N	2.80	0.44
2:B:22:GLU:HB3	2:B:83:PHE:CE1	2.46	0.44
2:B:265:LEU:HD21	2:B:267:PHE:CE1	2.52	0.44
2:B:411:GLU:OE1	2:B:411:GLU:HA	2.17	0.44
3:K:112:GLU:O	3:K:114:ASP:N	2.50	0.44
1:A:328:VAL:CG1	1:A:332:ILE:HD11	2.16	0.44
1:A:328:VAL:O	1:A:332:ILE:HB	2.17	0.44
2:B:56:ALA:C	2:B:62:VAL:HB	2.38	0.44
2:B:75:MET:SD	2:B:93:VAL:HG21	2.57	0.44
2:B:166:MET:HG3	2:B:197:ASN:O	2.18	0.44
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.51	0.44
3:K:216:ARG:HA	3:K:250:ALA:HB1	2.00	0.44
1:A:31:GLN:NE2	1:A:243:ARG:CB	2.57	0.44
1:A:53:PHE:CA	1:A:88:HIS:HE1	1.94	0.44
1:A:204:VAL:HG13	1:A:209:ILE:CD1	2.30	0.44
1:A:312:TYR:HD1	1:A:341:ILE:O	2.01	0.44
2:B:104:ALA:C	2:B:108:TYR:HD2	2.20	0.44
2:B:259:MET:HB3	2:B:268:PHE:CD1	2.30	0.44
2:B:385:GLN:OE1	2:B:433:GLN:HB2	2.17	0.44
1:A:146:GLY:O	1:A:150:THR:OG1	2.25	0.44
1:A:309:HIS:CB	1:A:386:GLU:OE2	2.65	0.44
2:B:56:ALA:CB	2:B:62:VAL:N	2.80	0.44
2:B:114:LEU:C	2:B:116:ASP:N	2.71	0.44
2:B:146:GLY:O	2:B:150:GLY:N	2.48	0.44
2:B:157:ILE:O	2:B:161:TYR:HB2	2.18	0.44
2:B:250:ALA:HB1	2:B:352:LYS:NZ	2.32	0.44
1:A:122:ILE:HD13	1:A:122:ILE:HG21	1.83	0.44
1:A:170:SER:OG	1:A:203:MET:CA	2.66	0.44
1:A:184:PRO:HG2	1:A:399:TYR:CD2	2.51	0.44
1:A:211:ASP:OD1	1:A:214:ARG:NH1	2.51	0.44
2:B:94:PHE:CE2	2:B:114:LEU:CB	3.01	0.44
2:B:115:VAL:HG11	2:B:152:LEU:HB3	2.00	0.44
2:B:143:GLY:H	2:B:147:SER:HG	1.54	0.44
2:B:217:LEU:CD2	2:B:275:LEU:O	2.65	0.44
1:A:7:ILE:HB	1:A:136:SER:O	2.18	0.44
1:A:184:PRO:HB3	1:A:187:SER:OG	2.18	0.44
1:A:224:TYR:C	1:A:226:ASN:H	2.21	0.44
1:A:224:TYR:C	1:A:226:ASN:N	2.71	0.44
1:A:432:TYR:O	1:A:435:VAL:HB	2.17	0.44
2:B:3:GLU:CD	2:B:64:ARG:NH1	2.71	0.44
2:B:29:GLY:O	2:B:58:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PRO:HB2	2:B:59:ASN:HD22	0.60	0.44
2:B:191:VAL:HG23	2:B:421:ALA:HB1	2.00	0.44
1:A:38:SER:HB3	1:A:45:GLY:HA3	2.00	0.44
1:A:137:VAL:CG2	1:A:168:GLU:HG2	2.48	0.44
1:A:209:ILE:HG12	1:A:302:MET:CE	2.42	0.44
1:A:256:GLN:HB2	2:B:407:TRP:HZ3	1.81	0.44
1:A:298:PRO:O	1:A:301:GLN:HB2	2.18	0.44
1:A:312:TYR:C	1:A:313:MET:HG2	2.37	0.44
2:B:12:CYS:C	2:B:16:ILE:HG12	2.21	0.44
2:B:66:ILE:HG23	2:B:66:ILE:O	2.16	0.44
2:B:97:SER:CB	2:B:110:GLU:CD	2.60	0.44
2:B:274:PRO:C	2:B:276:THR:CG2	2.85	0.44
1:A:79:ARG:HG3	1:A:79:ARG:O	2.18	0.43
1:A:83:TYR:C	1:A:84:ARG:CG	2.73	0.43
1:A:181:VAL:O	1:A:185:TYR:HB2	2.18	0.43
1:A:205:ASP:CB	1:A:303:VAL:CA	2.78	0.43
1:A:241:SER:OG	1:A:242:LEU:N	2.51	0.43
2:B:64:ARG:HH12	2:B:132:LEU:HD21	1.83	0.43
2:B:133:GLN:NE2	2:B:253:ARG:HB2	2.33	0.43
1:A:238:ILE:CG2	1:A:255:PHE:CZ	2.99	0.43
1:A:397:LEU:CA	1:A:401:LYS:CB	2.84	0.43
2:B:118:VAL:O	2:B:118:VAL:CG1	2.62	0.43
2:B:212:ILE:O	2:B:216:THR:OG1	2.35	0.43
2:B:236:SER:O	2:B:240:THR:HB	2.18	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CE1	2.53	0.43
3:K:10:VAL:HG12	3:K:329:ALA:HB3	2.00	0.43
1:A:345:ASP:OD2	1:A:439:SER:HA	2.17	0.43
1:A:362:VAL:HG13	1:A:367:ASP:CB	2.48	0.43
1:A:363:VAL:HG12	1:A:364:PRO:HG3	1.99	0.43
3:K:100:GLY:N	8:K:503:ACP:H3B1	2.32	0.43
1:A:108:TYR:OH	1:A:417:GLU:CD	2.56	0.43
2:B:313:LEU:HA	2:B:344:VAL:CG2	2.30	0.43
2:B:386:GLU:O	2:B:387:LEU:C	2.57	0.43
1:A:5:ILE:CB	1:A:135:PHE:CE1	3.01	0.43
1:A:325:PRO:HG3	2:B:223:THR:HA	1.98	0.43
2:B:21:TRP:CE3	2:B:24:ILE:HD12	2.53	0.43
2:B:32:PRO:CG	2:B:33:THR:H	2.19	0.43
2:B:186:ASN:HA	2:B:189:LEU:HD12	2.00	0.43
2:B:259:MET:SD	2:B:378:ILE:CG2	3.05	0.43
3:K:233:GLU:CG	3:K:234:THR:N	2.50	0.43
1:A:14:VAL:CG2	1:A:74:VAL:CG1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:O	1:A:27:GLU:CB	2.66	0.43
1:A:126:ALA:C	1:A:132:LEU:HD11	2.32	0.43
1:A:172:TYR:HB3	1:A:203:MET:HE2	2.01	0.43
2:B:4:ILE:HG21	2:B:30:ILE:HG22	1.99	0.43
2:B:70:LEU:C	2:B:71:GLU:HG3	2.38	0.43
1:A:71:GLU:HG2	1:A:99:ALA:HB2	1.01	0.43
1:A:154:MET:HB2	1:A:192:HIS:HE1	1.75	0.43
1:A:312:TYR:HA	1:A:381:THR:CB	2.48	0.43
2:B:44:LEU:HG	2:B:85:GLN:CG	2.46	0.43
2:B:176:LYS:CD	2:B:207:GLU:OE2	2.67	0.43
2:B:431:GLU:O	2:B:434:GLN:HB2	2.18	0.43
1:A:157:LEU:HB2	1:A:166:LYS:CE	2.49	0.43
1:A:341:ILE:H	1:A:342:GLN:HG3	1.84	0.43
1:A:346:TRP:O	1:A:346:TRP:HE3	2.01	0.43
1:A:362:VAL:C	1:A:363:VAL:HG23	2.38	0.43
2:B:56:ALA:CB	2:B:62:VAL:CB	2.70	0.43
2:B:96:GLN:OE1	2:B:96:GLN:HA	2.19	0.43
2:B:398:MET:SD	2:B:399:PHE:CD2	3.12	0.43
3:K:304:ILE:HA	3:K:305:PRO:HD3	1.90	0.43
1:A:105:ARG:HG2	1:A:109:THR:HG1	1.84	0.43
1:A:119:LEU:HA	1:A:122:ILE:CG2	2.48	0.43
1:A:230:LEU:CD2	1:A:302:MET:HE3	2.47	0.43
1:A:335:ILE:C	1:A:337:THR:N	2.71	0.43
1:A:343:PHE:CE2	1:A:351:PHE:CE1	3.01	0.43
1:A:440:VAL:N	2:B:402:LYS:HZ1	1.98	0.43
2:B:196:GLU:O	2:B:197:ASN:HB3	2.19	0.43
2:B:319:PHE:CE1	2:B:353:THR:HG21	2.44	0.43
2:B:344:VAL:H	2:B:350:ASN:HD21	1.67	0.43
1:A:137:VAL:HB	1:A:168:GLU:CB	2.49	0.43
1:A:147:SER:N	1:A:189:LEU:HD13	2.33	0.43
1:A:362:VAL:O	1:A:363:VAL:HG23	2.19	0.43
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.19	0.43
2:B:6:HIS:CD2	2:B:21:TRP:CZ2	3.03	0.43
2:B:94:PHE:CD1	2:B:94:PHE:C	2.68	0.43
2:B:260:VAL:HG13	2:B:262:PHE:O	2.13	0.43
2:B:292:THR:O	2:B:293:GLN:C	2.54	0.43
2:B:301:MET:HG3	2:B:307:PRO:HG3	2.00	0.43
1:A:192:HIS:O	1:A:196:GLU:CB	2.67	0.42
1:A:259:LEU:CA	1:A:380:ASN:HD21	2.31	0.42
1:A:289:ALA:C	1:A:291:ILE:N	2.69	0.42
1:A:404:PHE:O	1:A:404:PHE:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLU:O	1:A:415:GLU:HB2	2.19	0.42
2:B:48:ARG:O	2:B:61:TYR:CE2	2.72	0.42
2:B:205:ASP:CG	2:B:304:ALA:N	2.72	0.42
1:A:76:ASP:O	1:A:76:ASP:OD1	2.37	0.42
1:A:114:ILE:HD13	1:A:114:ILE:HG21	1.84	0.42
1:A:424:ASP:CG	3:K:307:ARG:HH22	2.14	0.42
1:A:437:VAL:HG12	1:A:438:ASP:OD1	2.19	0.42
2:B:57:ALA:C	2:B:64:ARG:N	2.69	0.42
2:B:68:VAL:HG13	2:B:149:MET:CE	2.42	0.42
2:B:102:ASN:HB2	2:B:105:LYS:HG3	1.98	0.42
2:B:102:ASN:O	2:B:105:LYS:HB2	2.19	0.42
2:B:292:THR:HG22	2:B:332:MET:SD	2.58	0.42
1:A:307:PRO:C	1:A:309:HIS:N	2.68	0.42
3:K:18[A]:ARG:HE	3:K:22[A]:ARG:HH22	1.66	0.42
1:A:12:ALA:HB1	1:A:171:ILE:HD12	2.00	0.42
1:A:206:ASN:HD22	1:A:206:ASN:HA	1.46	0.42
1:A:229:ARG:HH11	1:A:229:ARG:HD2	1.40	0.42
2:B:114:LEU:O	2:B:118:VAL:HG23	2.20	0.42
2:B:234:THR:HG23	2:B:270:PRO:HB2	2.00	0.42
2:B:244:PHE:HE2	2:B:358:ILE:HD13	1.67	0.42
2:B:370:GLY:O	6:B:502:TXL:C18	2.38	0.42
2:B:385:GLN:NE2	2:B:433:GLN:HB2	2.34	0.42
1:A:273:ALA:HB2	1:A:294:ALA:HB3	1.98	0.42
2:B:27:GLU:HB2	2:B:36:TYR:CB	2.49	0.42
2:B:258:ASN:O	2:B:314:THR:HG21	2.19	0.42
2:B:346:TRP:CZ2	2:B:435:TYR:CD2	3.05	0.42
1:A:179:THR:HG21	1:A:181:VAL:CA	2.46	0.42
2:B:50:ASN:HB3	2:B:51:VAL:H	1.30	0.42
2:B:92:PHE:CD1	2:B:92:PHE:N	2.87	0.42
1:A:170:SER:OG	1:A:203:MET:CB	2.42	0.42
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.86	0.42
1:A:312:TYR:HD2	1:A:381:THR:HG23	1.84	0.42
2:B:48:ARG:CZ	2:B:60:LYS:HA	2.46	0.42
2:B:253:ARG:HH11	2:B:253:ARG:CB	2.29	0.42
2:B:313:LEU:HD22	2:B:346:TRP:CZ2	2.55	0.42
2:B:340:SER:OG	2:B:341:SER:N	2.38	0.42
3:K:83[A]:GLN:NE2	3:K:87:GLU:CD	2.73	0.42
1:A:31:GLN:NE2	1:A:243:ARG:NE	2.59	0.42
1:A:66:VAL:CG2	1:A:125:LEU:HD12	2.44	0.42
1:A:115:ILE:HD12	1:A:152:LEU:HD23	1.87	0.42
1:A:122:ILE:HD11	1:A:157:LEU:HD22	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:HD23	1:A:255:PHE:CD2	2.54	0.42
1:A:256:GLN:CB	2:B:407:TRP:HZ3	2.27	0.42
1:A:409:VAL:HG22	1:A:414:GLU:CG	2.43	0.42
2:B:69:ASP:OD2	2:B:74:THR:HG22	2.15	0.42
2:B:212:ILE:C	2:B:214:PHE:H	2.23	0.42
2:B:280:SER:O	2:B:283:TYR:HD1	2.02	0.42
1:A:67:PHE:CB	1:A:92:LEU:CD2	2.97	0.42
1:A:101:ASN:HD22	4:A:500:GTP:PG	2.42	0.42
2:B:151:THR:O	2:B:192:HIS:HD2	2.02	0.42
2:B:296:PHE:CD1	2:B:335:VAL:CG1	3.02	0.42
2:B:324:SER:O	2:B:328:VAL:HG23	2.19	0.42
3:K:161:LYS:H	3:K:161:LYS:HG2	1.25	0.42
1:A:130:THR:O	1:A:131:GLY:O	2.38	0.42
1:A:228:ASN:ND2	4:A:500:GTP:C6	2.72	0.42
1:A:292:THR:CG2	1:A:319:TYR:CE2	2.98	0.42
2:B:27:GLU:HG2	2:B:48:ARG:HH21	1.85	0.42
2:B:27:GLU:OE2	2:B:40:SER:O	2.37	0.42
2:B:157:ILE:HG21	2:B:166:MET:CE	2.49	0.42
2:B:183:GLU:HG3	2:B:398:MET:SD	2.59	0.42
2:B:431:GLU:CA	2:B:434:GLN:HG3	2.50	0.42
1:A:31:GLN:NE2	1:A:239:THR:HG23	2.35	0.41
1:A:34:GLY:O	1:A:35:GLN:CB	2.64	0.41
1:A:146:GLY:C	1:A:189:LEU:HD13	2.41	0.41
1:A:147:SER:HB3	1:A:189:LEU:HD11	0.97	0.41
1:A:434:GLU:HB2	3:K:303:PHE:CD1	2.55	0.41
2:B:102:ASN:HB2	2:B:105:LYS:CE	2.50	0.41
2:B:172:VAL:CG2	2:B:205:ASP:OD1	2.67	0.41
2:B:216:THR:HG21	2:B:275:LEU:HD13	2.00	0.41
2:B:320:ARG:CG	2:B:320:ARG:O	2.64	0.41
2:B:405:LEU:O	2:B:409:THR:CB	2.68	0.41
6:B:502:TXL:H162	6:B:502:TXL:O6	2.19	0.41
1:A:181:VAL:O	1:A:399:TYR:CE2	2.71	0.41
1:A:266:HIS:HD2	1:A:432:TYR:CZ	2.37	0.41
1:A:416:GLY:O	1:A:417:GLU:HB2	2.19	0.41
2:B:142:GLY:O	2:B:185:TYR:OH	2.34	0.41
2:B:259:MET:HG3	2:B:378:ILE:CG2	2.50	0.41
2:B:260:VAL:HG12	2:B:262:PHE:H	1.85	0.41
2:B:320:ARG:NH2	6:B:502:TXL:C27	2.78	0.41
2:B:388:PHE:O	2:B:391:ILE:N	2.54	0.41
1:A:9:VAL:HG13	1:A:150:THR:HG22	1.95	0.41
1:A:157:LEU:CB	1:A:166:LYS:HE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG12	1:A:185:TYR:HB2	2.01	0.41
1:A:276:ILE:HG22	1:A:277:SER:N	2.35	0.41
2:B:14:ASN:ND2	2:B:69:ASP:HA	2.35	0.41
3:K:347:TYR:CE2	3:K:350:ARG:NH1	2.89	0.41
1:A:77:GLU:CA	1:A:80:THR:CB	2.84	0.41
1:A:219:ILE:CG2	1:A:219:ILE:O	2.68	0.41
1:A:276:ILE:CD1	1:A:371:VAL:HG22	2.30	0.41
2:B:111:GLY:O	2:B:115:VAL:CA	2.66	0.41
2:B:301:MET:CE	2:B:377:PHE:CE1	3.03	0.41
2:B:339:ASN:CA	2:B:342:TYR:HD1	2.32	0.41
1:A:64:ARG:NH2	1:A:132:LEU:CB	2.83	0.41
1:A:107:HIS:HD1	1:A:108:TYR:N	2.18	0.41
1:A:191:THR:OG1	1:A:192:HIS:N	2.53	0.41
1:A:246:GLY:O	1:A:249:ASN:ND2	2.48	0.41
1:A:277:SER:C	1:A:368:LEU:HD22	2.40	0.41
1:A:344:VAL:HG12	1:A:345:ASP:N	2.34	0.41
1:A:35:GLN:C	1:A:36:MET:CG	2.89	0.41
1:A:110:ILE:HG21	1:A:110:ILE:HD13	1.85	0.41
1:A:262:TYR:CB	1:A:263:PRO:HD3	2.24	0.41
2:B:263:PRO:O	2:B:264:ARG:C	2.57	0.41
2:B:414:ASP:CG	3:K:253:GLU:CD	2.72	0.41
1:A:9:VAL:HG12	1:A:146:GLY:HA2	2.01	0.41
1:A:10:GLY:O	1:A:11:GLN:C	2.59	0.41
1:A:271:THR:CB	1:A:377:MET:HB3	2.50	0.41
1:A:282:TYR:CD2	1:A:284:GLU:O	2.74	0.41
2:B:6:HIS:CE1	2:B:30:ILE:CG1	3.00	0.41
2:B:174:SER:HB2	2:B:207:GLU:CG	2.51	0.41
2:B:191:VAL:HG23	2:B:421:ALA:HA	1.87	0.41
2:B:308:ARG:O	2:B:342:TYR:CE2	2.72	0.41
2:B:393:GLU:OE1	2:B:393:GLU:HA	2.20	0.41
3:K:98:GLN:HG2	3:K:99:THR:N	2.35	0.41
1:A:3:GLU:HB2	1:A:64:ARG:CZ	2.51	0.41
1:A:14:VAL:HG22	1:A:69:ASP:OD1	2.20	0.41
1:A:72:PRO:HA	1:A:94:THR:HG23	2.02	0.41
1:A:75:ILE:HG23	1:A:76:ASP:N	2.36	0.41
1:A:296:PHE:HD2	1:A:312:TYR:OH	2.03	0.41
1:A:397:LEU:HA	1:A:401:LYS:HD2	2.00	0.41
2:B:71:GLU:HG2	2:B:99:ALA:H	1.65	0.41
2:B:94:PHE:CE1	2:B:97:SER:HB3	2.52	0.41
2:B:115:VAL:HG12	2:B:156:LYS:HZ2	1.86	0.41
2:B:238:VAL:CG1	2:B:255:LEU:CD1	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:TYR:CB	2:B:436:GLN:HG3	2.51	0.41
3:K:168:VAL:HG21	3:K:310:VAL:CG1	2.48	0.41
1:A:4:CYS:CB	1:A:30:ILE:HG21	2.44	0.41
1:A:5:ILE:HB	1:A:135:PHE:CE1	2.55	0.41
1:A:173:PRO:HG3	1:A:186:ASN:ND2	2.35	0.41
1:A:212:ILE:HD12	1:A:230:LEU:HD21	1.75	0.41
1:A:287:SER:O	1:A:288:VAL:C	2.57	0.41
1:A:313:MET:HB2	1:A:380:ASN:HB2	2.03	0.41
1:A:397:LEU:CA	1:A:401:LYS:HB3	2.49	0.41
2:B:25:SER:O	2:B:27:GLU:CG	2.55	0.41
2:B:48:ARG:NH1	2:B:60:LYS:HG3	2.30	0.41
2:B:49:ILE:HG21	2:B:49:ILE:HD13	1.75	0.41
2:B:165:ILE:HD12	2:B:256:ALA:CB	2.51	0.41
2:B:172:VAL:HG12	2:B:173:PRO:O	2.20	0.41
2:B:210:TYR:O	2:B:211:ASP:C	2.59	0.41
2:B:212:ILE:CD1	2:B:302:MET:HA	2.51	0.41
2:B:296:PHE:CE2	2:B:335:VAL:CG1	2.98	0.41
1:A:197:HIS:C	1:A:198:SER:OG	2.56	0.41
1:A:242:LEU:HD11	1:A:318:LEU:CD1	2.51	0.41
2:B:44:LEU:HD21	2:B:85:GLN:HB2	1.07	0.41
2:B:239:THR:O	2:B:243:ARG:NE	2.42	0.41
2:B:312:TYR:N	2:B:381:SER:HB2	2.36	0.41
6:B:502:TXL:C21	6:B:502:TXL:C18	2.91	0.41
1:A:14:VAL:CG2	1:A:74:VAL:HG11	2.51	0.40
1:A:102:ASN:HA	1:A:408:TYR:CE1	2.56	0.40
1:A:154:MET:HB2	1:A:192:HIS:HE2	1.82	0.40
1:A:434:GLU:CB	3:K:303:PHE:HB3	2.43	0.40
2:B:70:LEU:O	2:B:70:LEU:HG	2.20	0.40
2:B:223:THR:HG1	2:B:226:ASP:HB2	1.86	0.40
2:B:242:LEU:HD13	2:B:250:ALA:O	2.20	0.40
1:A:12:ALA:O	1:A:16:ILE:HB	2.21	0.40
1:A:150:THR:O	1:A:192:HIS:NE2	2.53	0.40
1:A:242:LEU:HD22	1:A:250:VAL:HB	2.03	0.40
2:B:158:ARG:HB2	2:B:197:ASN:ND2	2.01	0.40
2:B:305:CYS:HG	2:B:387:LEU:HB2	1.85	0.40
2:B:335:VAL:C	2:B:339:ASN:ND2	2.59	0.40
3:K:159:ASN:C	3:K:161:LYS:N	2.74	0.40
1:A:116:ASP:O	1:A:119:LEU:HB2	2.22	0.40
1:A:306:ASP:C	1:A:308:ARG:N	2.72	0.40
1:A:311:LYS:O	1:A:382:THR:HG23	2.21	0.40
1:A:329:ASN:ND2	2:B:210:TYR:OH	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:GLN:HA	2:B:282:GLN:OE1	2.21	0.40
1:A:103:TYR:CZ	1:A:148:GLY:HA2	2.56	0.40
1:A:210:TYR:CE2	1:A:227:LEU:HD23	2.40	0.40
1:A:248:LEU:HD21	5:B:501:GDP:H2'	2.03	0.40
2:B:35:SER:HB3	2:B:60:LYS:HE3	2.02	0.40
2:B:142:GLY:N	2:B:186:ASN:ND2	2.69	0.40
2:B:152:LEU:O	2:B:155:SER:OG	2.34	0.40
2:B:194:LEU:HD11	2:B:428:LEU:HD22	2.03	0.40
2:B:274:PRO:HB2	2:B:371:LEU:CD2	2.51	0.40
3:K:340[B]:GLU:OE1	3:K:340[B]:GLU:HA	2.21	0.40
1:A:21:TRP:HA	1:A:24:TYR:HD2	1.87	0.40
1:A:31:GLN:CD	1:A:243:ARG:NE	2.70	0.40
1:A:107:HIS:ND1	1:A:107:HIS:C	2.74	0.40
1:A:116:ASP:OD1	1:A:156:ARG:NH1	2.54	0.40
2:B:236:SER:OG	6:B:502:TXL:H27	2.21	0.40
2:B:238:VAL:CG1	2:B:255:LEU:HD13	2.52	0.40
2:B:287:THR:O	2:B:290:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (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	438/451 (97%)	322 (74%)	63 (14%)	53 (12%)	0 6
2	B	425/445 (96%)	298 (70%)	48 (11%)	79 (19%)	0 2
3	K	332/394 (84%)	319 (96%)	11 (3%)	2 (1%)	25 66
All	All	1195/1290 (93%)	939 (79%)	122 (10%)	134 (11%)	1 7

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	33	ASP
1	A	35	GLN
1	A	39	ASP
1	A	42	ILE
1	A	46	ASP
1	A	50	ASN
1	A	51	THR
1	A	73	THR
1	A	83	TYR
1	A	129	CYS
1	A	133	GLN
1	A	174	ALA
1	A	177	VAL
1	A	183	GLU
1	A	185	TYR
1	A	193	THR
1	A	197	HIS
1	A	198	SER
1	A	219	ILE
1	A	248	LEU
1	A	265	ALA
1	A	268	PRO
1	A	275	VAL
1	A	281	ALA
1	A	283	HIS
1	A	284	GLU
1	A	312	TYR
1	A	341	ILE
1	A	344	VAL
1	A	348	PRO
1	A	359	PRO
1	A	364	PRO
1	A	368	LEU
1	A	369	ALA
2	B	2	ARG
2	B	25	SER
2	B	33	THR
2	B	36	TYR
2	B	39	ASP
2	B	40	SER
2	B	41	ASP
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
3	K	233	GLU
1	A	25	CYS
1	A	81	GLY
1	A	102	ASN
1	A	131	GLY
1	A	350	GLY
1	A	384	ILE
1	A	417	GLU
1	A	427	ALA
2	B	30	ILE
2	B	32	PRO

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Mol	Chain	Res	Type
2	B	50	ASN
2	B	72	PRO
2	B	75	MET
2	B	129	CYS
2	B	176	LYS
2	B	276	THR
2	B	285	ALA
2	B	341	SER
2	B	387	LEU
2	B	427	ASP
3	K	113	LYS
1	A	66	VAL
1	A	82	THR
1	A	194	THR
2	B	27	GLU
2	B	28	HIS
2	B	57	ALA
2	B	144	GLY
2	B	173	PRO
2	B	248	LEU
2	B	262	PHE
2	B	281	GLN
2	B	339	ASN
2	B	347	ILE
2	B	348	PRO
2	B	412	GLY
1	A	65	ALA
1	A	175	PRO
1	A	261	PRO
2	B	29	GLY
2	B	31	ASP
2	B	48	ARG
2	B	53	TYR
2	B	87	PHE
2	B	183	GLU
2	B	242	LEU
2	B	340	SER
1	A	98	ASP
1	A	410	GLY
2	B	222	PRO
2	B	360	PRO
2	B	389	LYS

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	369/377 (98%)	351 (95%)	18 (5%)	25 50
2	B	368/381 (97%)	348 (95%)	20 (5%)	22 47
3	K	300/345 (87%)	273 (91%)	27 (9%)	9 30
All	All	1037/1103 (94%)	972 (94%)	65 (6%)	23 43

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	101	ASN
1	A	172	TYR
1	A	184	PRO
1	A	192	HIS
1	A	206	ASN
1	A	212	ILE
1	A	214	ARG
1	A	219	ILE
1	A	229	ARG
1	A	264	ARG
1	A	293	ASN
1	A	320	ARG
1	A	390	ARG
1	A	396	ASP

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Mol	Chain	Res	Type
1	A	405	VAL
1	A	422	ARG
1	A	432	TYR
2	B	2	ARG
2	B	30	ILE
2	B	94	PHE
2	B	101	ASN
2	B	139	HIS
2	B	185	TYR
2	B	192	HIS
2	B	227	LEU
2	B	253	ARG
2	B	278	ARG
2	B	300	ASN
2	B	302	MET
2	B	308	ARG
2	B	319	PHE
2	B	390	ARG
2	B	416	MET
2	B	424	ASN
2	B	426	ASN
2	B	432	TYR
2	B	436	GLN
3	K	22[A]	ARG
3	K	22[B]	ARG
3	K	44	LYS
3	K	46	THR
3	K	83[A]	GLN
3	K	83[B]	GLN
3	K	111	GLN
3	K	112	GLU
3	K	115	GLN
3	K	132	ASP
3	K	141	SER
3	K	145[A]	SER
3	K	145[B]	SER
3	K	161	LYS
3	K	162	ASN
3	K	209	ASN
3	K	216	ARG
3	K	231	ASP
3	K	235	ASN

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Mol	Chain	Res	Type
3	K	236	ILE
3	K	242[A]	SER
3	K	242[B]	SER
3	K	271	ILE
3	K	275	LEU
3	K	303	PHE
3	K	304	ILE
3	K	323	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

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

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Mol	Chain	Res	Type
3	K	111	GLN
3	K	159	ASN
3	K	171	HIS
3	K	222	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GTP	A	500	1	26,34,34	1.92	8 (30%)	32,54,54	1.43	6 (18%)
5	GDP	B	501	2	24,30,30	1.73	5 (20%)	30,47,47	1.08	3 (10%)
6	TXL	B	502	2	63,63,63	4.24	46 (73%)	100,100,100	3.30	53 (53%)
8	ACP	K	503	7	27,33,33	1.46	5 (18%)	32,52,52	1.49	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	500	1	-	0/18/38/38	0/3/3/3
5	GDP	B	501	2	-	4/12/32/32	0/3/3/3
6	TXL	B	502	2	-	0/38/124/124	0/6/6/6
8	ACP	K	503	7	-	0/15/38/38	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TXL	O3-C4	-9.61	1.26	1.46
6	B	502	TXL	C41-C36	8.37	1.53	1.39
6	B	502	TXL	C8-C3	-7.73	1.38	1.57
6	B	502	TXL	C37-C36	-7.64	1.26	1.39
6	B	502	TXL	O6-C9	-7.57	1.08	1.21
6	B	502	TXL	C25-C24	-7.35	1.27	1.39
6	B	502	TXL	C14-C13	6.99	1.66	1.52
6	B	502	TXL	C13-C12	-6.87	1.37	1.51
6	B	502	TXL	O5-C7	-6.83	1.32	1.43
6	B	502	TXL	C16-C15	-6.57	1.41	1.53
6	B	502	TXL	C6-C7	5.79	1.63	1.53
6	B	502	TXL	C12-C11	-5.65	1.26	1.34
6	B	502	TXL	C43-C42	-5.65	1.30	1.49
6	B	502	TXL	C10-C11	-5.40	1.34	1.50
6	B	502	TXL	O8-C13	-5.15	1.36	1.45
6	B	502	TXL	C14-C1	-5.10	1.43	1.54
6	B	502	TXL	C20-C4	5.06	1.67	1.53
6	B	502	TXL	O4-C5	5.04	1.56	1.46
6	B	502	TXL	C17-C15	4.50	1.62	1.53
4	A	500	GTP	O4'-C1'	-4.34	1.35	1.41
6	B	502	TXL	C4-C3	4.33	1.64	1.54
6	B	502	TXL	C8-C9	4.07	1.67	1.55
6	B	502	TXL	C24-C23	-4.04	1.46	1.52
6	B	502	TXL	O11-C30	4.04	1.29	1.21
5	B	501	GDP	C2'-C1'	-3.97	1.47	1.53
6	B	502	TXL	O12-C30	-3.94	1.26	1.34
6	B	502	TXL	C30-N1	3.92	1.44	1.34
4	A	500	GTP	C5-C6	-3.86	1.39	1.47
6	B	502	TXL	O10-C22	3.77	1.49	1.42
6	B	502	TXL	C40-C39	-3.71	1.28	1.38
8	K	503	ACP	O4'-C1'	3.63	1.46	1.41
6	B	502	TXL	C28-C27	-3.61	1.28	1.38
6	B	502	TXL	C22-C21	-3.51	1.43	1.52
6	B	502	TXL	C40-C41	3.48	1.46	1.38
6	B	502	TXL	C23-N1	-3.46	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TXL	O12-C31	3.36	1.54	1.48
4	A	500	GTP	O2'-C2'	-3.27	1.35	1.43
4	A	500	GTP	C2'-C1'	-3.24	1.48	1.53
6	B	502	TXL	C36-C35	-3.13	1.42	1.50
6	B	502	TXL	O2-C35	3.07	1.40	1.34
8	K	503	ACP	C4-N3	2.83	1.39	1.35
6	B	502	TXL	C34-C31	-2.78	1.43	1.51
6	B	502	TXL	O4-C20	-2.77	1.38	1.45
6	B	502	TXL	O8-C21	2.74	1.40	1.34
6	B	502	TXL	O13-C35	-2.72	1.15	1.22
8	K	503	ACP	PG-O3G	-2.55	1.49	1.54
5	B	501	GDP	C5-C6	-2.51	1.42	1.47
8	K	503	ACP	PG-O2G	2.51	1.60	1.54
6	B	502	TXL	C10-C9	2.49	1.60	1.53
5	B	501	GDP	C8-N7	-2.46	1.30	1.35
5	B	501	GDP	PB-O2B	-2.46	1.45	1.54
6	B	502	TXL	C4-C5	-2.42	1.50	1.55
5	B	501	GDP	PB-O1B	-2.41	1.42	1.50
6	B	502	TXL	C6-C5	-2.40	1.47	1.52
6	B	502	TXL	O1-C1	-2.33	1.40	1.44
4	A	500	GTP	C3'-C4'	-2.30	1.47	1.53
6	B	502	TXL	C28-C29	-2.28	1.34	1.38
6	B	502	TXL	O3-C42	2.28	1.40	1.35
6	B	502	TXL	C39-C38	-2.20	1.32	1.38
6	B	502	TXL	C32-C31	-2.17	1.45	1.51
4	A	500	GTP	C8-N7	-2.14	1.31	1.35
4	A	500	GTP	C4-N3	-2.13	1.32	1.37
4	A	500	GTP	C5'-C4'	-2.09	1.45	1.51
8	K	503	ACP	C2-N1	2.00	1.37	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	502	TXL	C15-C1-C2	10.95	123.90	111.91
6	B	502	TXL	C39-C38-C37	9.00	133.89	120.19
6	B	502	TXL	C38-C37-C36	-8.09	110.78	120.34
6	B	502	TXL	O7-C10-C9	7.22	121.55	109.51
6	B	502	TXL	C8-C9-C10	6.23	131.97	122.69
8	K	503	ACP	N3-C2-N1	-6.02	119.27	128.68
6	B	502	TXL	C13-C12-C11	-6.00	108.09	117.72
6	B	502	TXL	O11-C30-N1	5.78	134.31	124.85
6	B	502	TXL	C11-C10-C9	-5.62	107.58	114.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	502	TXL	O2-C2-C1	5.30	115.99	104.76
6	B	502	TXL	C6-C5-C4	-5.11	112.42	119.61
6	B	502	TXL	C39-C40-C41	-5.02	112.54	120.19
6	B	502	TXL	C17-C15-C1	4.97	122.23	111.11
6	B	502	TXL	O4-C5-C6	4.67	122.10	113.21
6	B	502	TXL	C18-C12-C11	4.66	130.95	125.30
6	B	502	TXL	C10-C11-C12	-4.41	113.97	120.65
6	B	502	TXL	O12-C30-N1	-4.39	102.64	110.02
6	B	502	TXL	C16-C15-C1	-4.36	101.36	111.11
6	B	502	TXL	O10-C22-C23	4.36	122.21	109.80
6	B	502	TXL	C33-C31-C32	4.28	122.38	111.16
6	B	502	TXL	C14-C1-C15	-4.20	103.75	111.50
6	B	502	TXL	O12-C31-C32	-4.05	91.19	107.20
6	B	502	TXL	C2-O2-C35	4.01	125.37	117.79
6	B	502	TXL	O6-C9-C10	-3.97	112.83	117.37
6	B	502	TXL	C31-O12-C30	-3.82	115.11	120.99
6	B	502	TXL	O7-C10-C11	-3.75	105.42	111.48
6	B	502	TXL	C20-C4-C3	3.70	126.20	120.30
6	B	502	TXL	O3-C42-O14	3.70	130.40	123.61
6	B	502	TXL	O2-C35-C36	3.69	117.88	111.92
6	B	502	TXL	C19-C8-C9	3.68	116.55	106.55
6	B	502	TXL	C24-C23-N1	3.56	119.08	112.11
6	B	502	TXL	C15-C11-C12	3.39	124.30	119.61
8	K	503	ACP	C4-C5-N7	-3.30	105.96	109.40
4	A	500	GTP	O3G-PG-O3B	3.11	115.08	104.64
6	B	502	TXL	C13-O8-C21	-3.11	110.76	116.67
6	B	502	TXL	O5-C7-C6	3.01	115.26	109.12
6	B	502	TXL	C1-C2-C3	-2.91	113.73	118.18
6	B	502	TXL	C24-C23-C22	-2.90	103.89	111.36
4	A	500	GTP	PB-O3B-PG	-2.90	122.87	132.83
6	B	502	TXL	C34-C31-C33	-2.79	103.85	111.16
6	B	502	TXL	C20-C4-C5	-2.78	82.45	85.40
6	B	502	TXL	C37-C36-C35	-2.69	114.33	120.40
6	B	502	TXL	C23-N1-C30	-2.68	116.22	121.72
6	B	502	TXL	C18-C12-C13	2.66	120.88	116.13
4	A	500	GTP	PA-O3A-PB	-2.57	124.00	132.83
6	B	502	TXL	O12-C31-C34	2.51	117.12	107.20
6	B	502	TXL	O4-C5-C4	2.49	93.38	90.58
6	B	502	TXL	O8-C13-C12	-2.48	103.78	109.78
6	B	502	TXL	O3-C42-C43	-2.47	106.17	110.68
6	B	502	TXL	O8-C21-O9	2.46	128.53	123.94
6	B	502	TXL	C41-C36-C35	2.42	125.87	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	501	GDP	C3'-C2'-C1'	2.42	104.62	100.98
6	B	502	TXL	C19-C8-C3	-2.41	105.64	113.15
4	A	500	GTP	O6-C6-C5	2.41	129.09	124.37
4	A	500	GTP	C3'-C2'-C1'	2.37	104.55	100.98
6	B	502	TXL	C14-C1-C2	-2.35	107.46	111.70
6	B	502	TXL	O10-C22-C21	-2.32	103.76	110.17
5	B	501	GDP	O2B-PB-O1B	2.29	119.64	110.68
6	B	502	TXL	C3-C4-C5	2.23	123.69	119.52
6	B	502	TXL	O1-C1-C2	-2.23	100.59	105.49
6	B	502	TXL	O3-C4-C5	-2.19	107.07	112.28
4	A	500	GTP	O2G-PG-O3B	2.15	111.86	104.64
6	B	502	TXL	O2-C2-C3	-2.06	104.35	108.17
5	B	501	GDP	O6-C6-C5	2.01	128.29	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

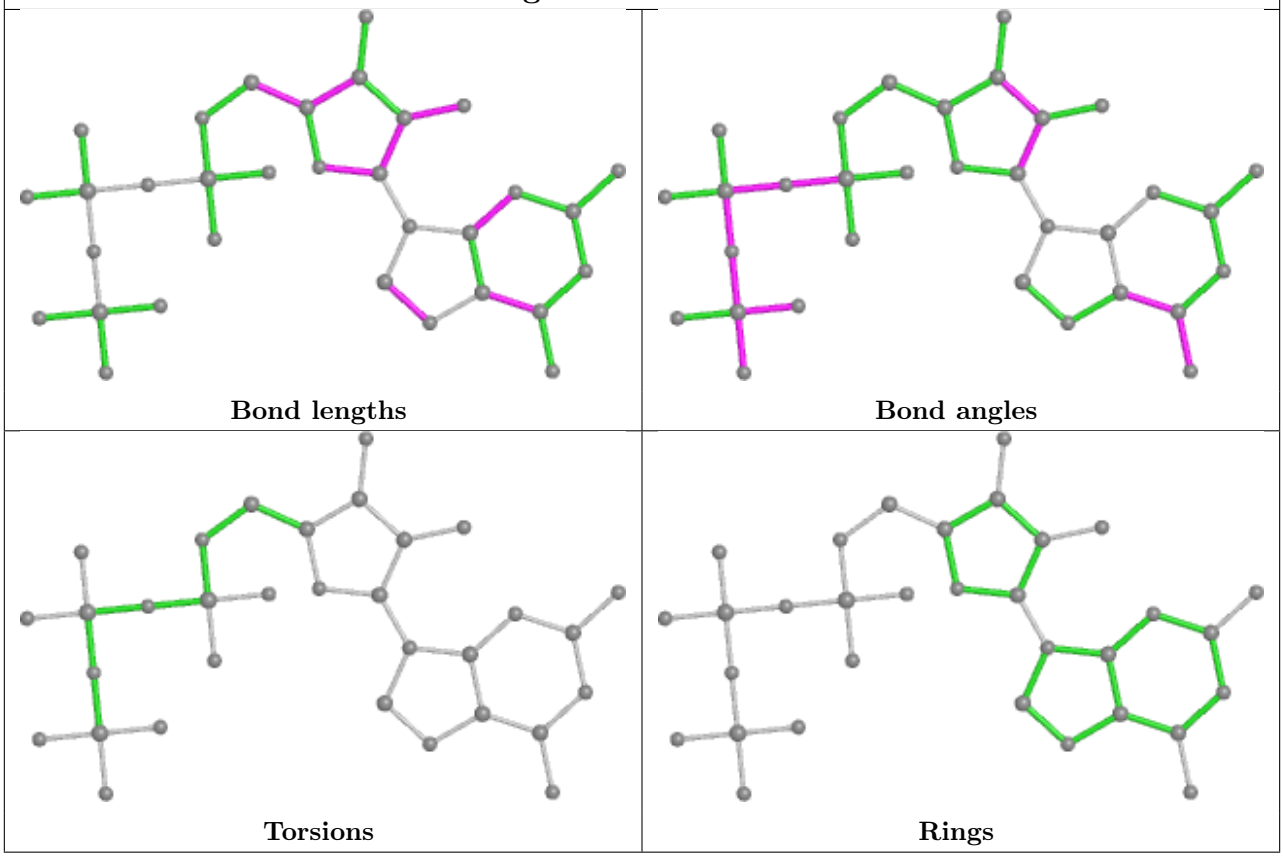
4 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	GTP	21	0
5	B	501	GDP	17	0
6	B	502	TXL	57	0
8	K	503	ACP	2	0

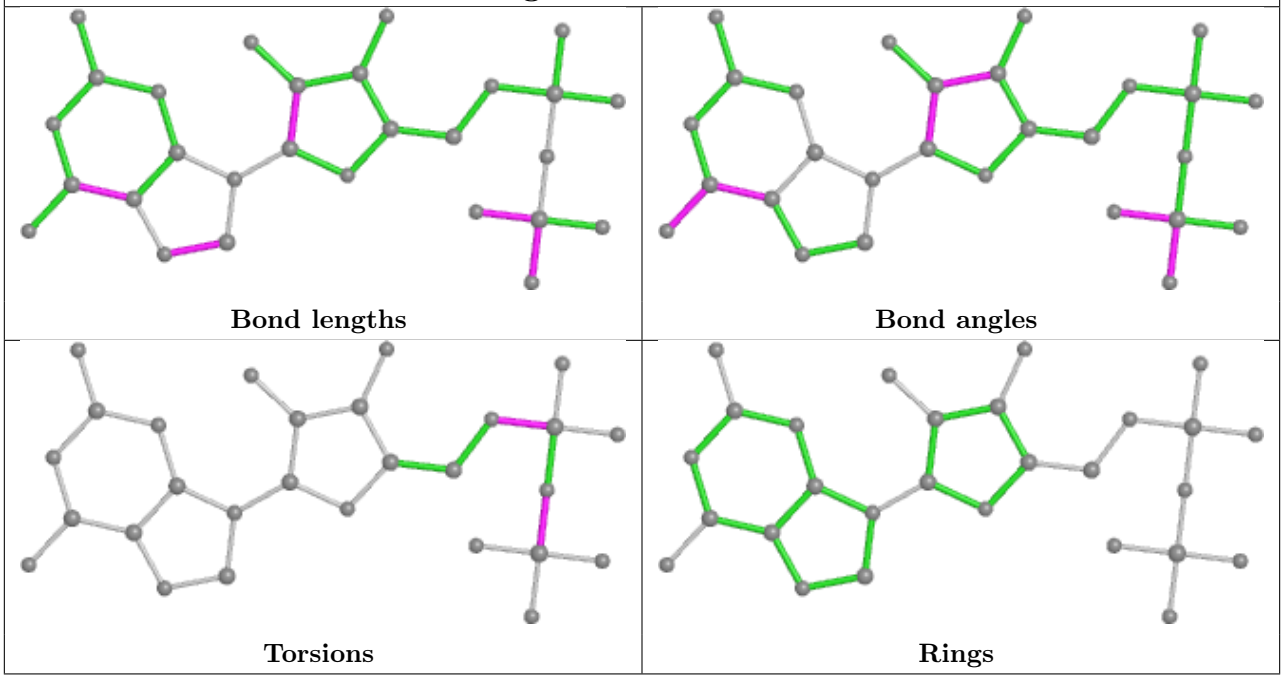
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

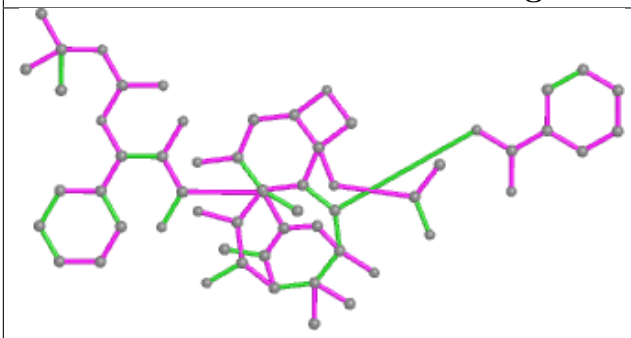
Ligand GTP A 500



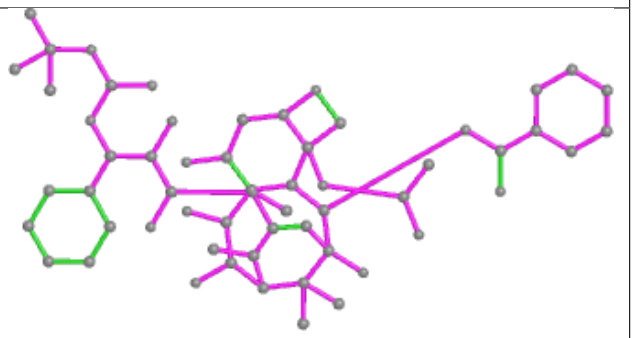
Ligand GDP B 501



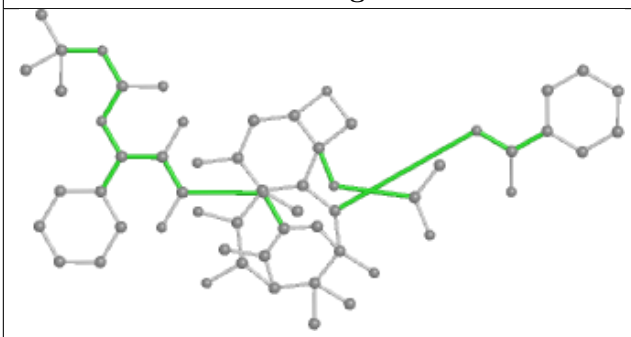
Ligand TXL B 502



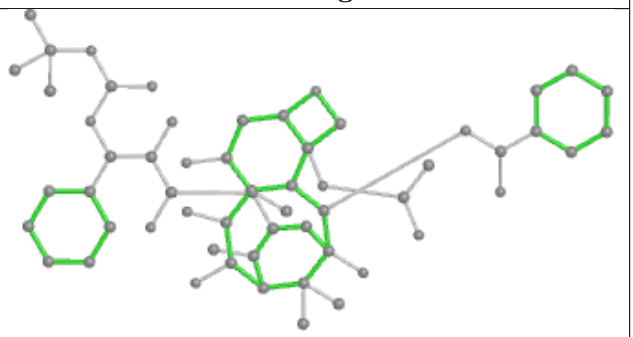
Bond lengths



Bond angles

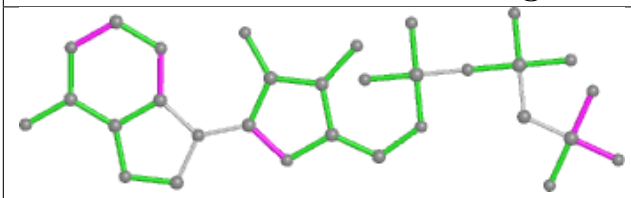


Torsions

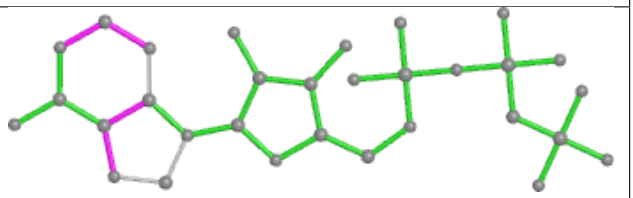


Rings

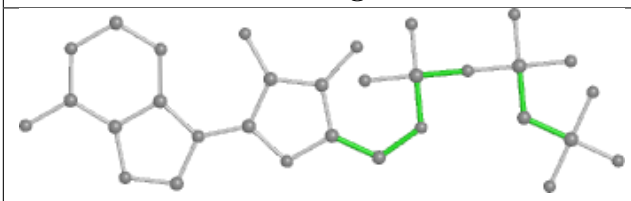
Ligand ACP K 503



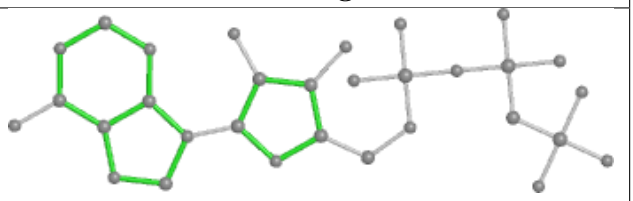
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	52
1	A	41

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	387:LEU	C	388:PHE	N	1.63
1	A	283:HIS	C	284:GLU	N	1.20
1	A	380:ASN	C	381:THR	N	1.20
1	A	437:VAL	C	438:ASP	N	1.20
1	B	52:TYR	C	53:TYR	N	1.20
1	A	111:GLY	C	112:LYS	N	1.19
1	A	137:VAL	C	138:PHE	N	1.19
1	A	140:SER	C	141:PHE	N	1.19
1	A	146:GLY	C	147:SER	N	1.19
1	A	149:PHE	C	150:THR	N	1.19
1	A	377:MET	C	378:LEU	N	1.19
1	A	383:ALA	C	384:ILE	N	1.19
1	B	72:PRO	C	73:GLY	N	1.19
1	B	111:GLY	C	112:ALA	N	1.19
1	B	178:SER	C	179:ASP	N	1.19
1	B	193:GLN	C	194:LEU	N	1.19
1	B	194:LEU	C	195:VAL	N	1.19
1	B	234:THR	C	235:MET	N	1.19
1	B	244:PHE	C	245:PRO	N	1.19
1	B	259:MET	C	260:VAL	N	1.19
1	B	347:ILE	C	348:PRO	N	1.19
1	B	348:PRO	C	349:ASN	N	1.19
1	A	34:GLY	C	35:GLN	N	1.18
1	A	433:GLU	C	434:GLU	N	1.18
1	B	130:ASP	C	131:CYS	N	1.18
1	A	259:LEU	C	260:VAL	N	1.17
1	A	346:TRP	C	347:CYS	N	1.17
1	A	367:ASP	C	368:LEU	N	1.17
1	B	53:TYR	C	54:ASN	N	1.17
1	B	299:LYS	C	300:ASN	N	1.17
1	A	204:VAL	C	205:ASP	N	1.16
1	A	233:GLN	C	234:ILE	N	1.16
1	A	274:PRO	C	275:VAL	N	1.16
1	B	70:LEU	C	71:GLU	N	1.16
1	B	89:PRO	C	90:ASP	N	1.16
1	B	171:VAL	C	172:VAL	N	1.16
1	B	243:ARG	C	244:PHE	N	1.16
1	A	24:TYR	C	25:CYS	N	1.15

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	379:SER	C	380:ASN	N	1.15
1	B	154:ILE	C	155:SER	N	1.15
1	B	173:PRO	C	174:SER	N	1.15
1	B	337:ASN	C	338:LYS	N	1.15
1	B	151:THR	C	152:LEU	N	1.14
1	B	436:GLN	C	437:ASP	N	1.14
1	A	90:GLU	C	91:GLN	N	1.13
1	B	292:THR	C	293:GLN	N	1.13
1	A	33:ASP	C	34:GLY	N	1.12
1	A	280:LYS	C	281:ALA	N	1.12
1	B	273:ALA	C	274:PRO	N	1.12
1	A	87:PHE	C	88:HIS	N	1.11
1	B	64:ARG	C	65:ALA	N	1.11
1	B	334:ASN	C	335:VAL	N	1.11
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	350:GLY	C	351:PHE	N	0.95
1	A	416:GLY	C	417:GLU	N	0.95
1	B	340:SER	C	341:SER	N	0.92
1	A	53:PHE	C	54:SER	N	0.90
1	B	182:VAL	C	183:GLU	N	0.90
1	B	197:ASN	C	198:THR	N	0.90
1	B	200:GLU	C	201:THR	N	0.90
1	A	347:CYS	C	348:PRO	N	0.89
1	B	321:GLY	C	322:ARG	N	0.88
1	A	218:ASP	C	219:ILE	N	0.84
1	B	105:LYS	C	106:GLY	N	0.80
1	A	38:SER	C	39:ASP	N	0.70
1	B	73:GLY	C	74:THR	N	0.69